High Oxidation State N-Heterocyclic Carbene Molybdenum Alkylidene Complexes: Functional-Group Tolerant Olefin Metathesis Catalysts

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vorgelegt von

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This work was carried out from December 2012 to April 2016 at the Institute of Polymer Chemistry, University of Stuttgart, under the supervision of Prof. Dr. Michael R. Buchmeiser.

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Publications

- Molybdenum imido alkylidene N-heterocyclic carbene complexes: structure-activity correlations and mechanistic Insights
  S. Sen, C. Lienert, L. Widmann, R. Schowner, K. Herz, P. Hauser, W. Frey, M. R. Buchmeiser, mansucript in preparation (2016).

- An anionic molybdenum amidato bisalkyl alkylidyne complex
  S. Sen, W. Frey, J. Meisner, J. Kästner, M. R. Buchmeiser, *J. Organomet. Chem.*, 799-800, 223-225 (2015).

- Neutral and cationic molybdenum imido alkylidene N-heterocyclic complexes: reactivity in selected olefin metathesis reaction and immmobilization on silica
  S. Sen, R. Schowner, D. A. Imbrich, W. Frey, M. R. Buchmeiser, *Chem. Eur. J*., 21, 13778-13787 (2015).

- On the mechanism of the regio- and stereo selective cyclopolymerization of 1,6-Hepta- and 1,7-Octadiynes by high oxidation state Mo-imido alkylidene N-heterocyclic carbene initiators
  K. Herz, J. Unold, J. Haenle, R. Schowner, **S. Sen**, W. Frey, M. R. Buchmeiser, *Macromolecules*, 2015, 48, 4768-4778.

- Molybdenum imido alkylidene and tungsten oxo alkylidene *N* -heterocyclic carbene complexes for olefin metathesis
  S. Sen, R. Schowner, M. R. Buchmeiser, invited paper, *Chem. Monthly*, 146 (7), 1037-1042 (2015).

- N-heterocyclic carbene, high oxidation state molybdenum alkylidene complexes: functional-group tolerant cationic metathesis catalysts
  S. Sen, J. Unold, W. Frey, M. R. Buchmeiser, *Angew. Chem.* 2014, *126*, 9538-9542*; Angew. Chem. Int. Ed.* 2014, *53*, 9384-9388.

- A catalytic and DFT study of selective ethylene oligomerization by nickel (II) oxime-based complexes
  K. N. Tayade, M.V. Mane, **S. Sen**, C. N. Murthy, G. L. Tembe, S. M. Pillai, K. Vanka, S. Mukherjee, *J. Mol. Catal. A: Chem*. 2013, 366, 238-246.

Patents

- N-heterocyclic carbene complexes of metalimidoalkylidene and metaloxoalkylidene

M. R. Buchmeiser, **S. Sen**, R. Schowner, WO2015/162245 A2, DE 10 2014 105 885 A1.

Posters

- N-heterocyclic carbene molybdenum alkylidene complexes: functional-group tolerant metathesis catalysts
  S. Sen, M. R. Buchmeiser, *The 21st International Symposium on Olefin Metathesis and Related Chemistry* (ISOM XXI), July 12-16, 2015, Graz, Austria, ***Best Poster Award**

- Cationic imido alkylidene-NHCs complexes: staggering catalysts for the homo-metathesis of 1-alkenes
  S. Sen, M. R. Buchmeiser, *The 21st International Symposium on Olefin Metathesis and Related Chemistry* (ISOM XXI), July 12-16, 2015, Graz, Austria

- Reactivity of Mo(N-2,6-Me_2-C_6H_3)(CHCMe_3)(OTf)(IMesH2)(OR): controlling metathesis activity through the choice of different fluorinated alkoxides
  S. Sen, M. R. Buchmeiser, *The 21st International Symposium on Olefin Metathesis and Related Chemistry* (ISOM XXI), July 12-16, 2015, Graz, Austria

- N-heterocyclic carbene molybdenum alkylidene complexes: functional-group tolerant metathesis catalysts
  S. Sen, M. R. Buchmeiser, *Covestro Doktorandenworkshop*, Sept 23rd, 2015, Bayreuth, Germany

Oral Presentations

- N-heterocyclic carbene molybdenum alkylidene complexes: functional-group tolerant metathesis catalysts
  19. *Tag der Organischen Chemie-TOCUS*, October 09, 2015, Stuttgart, Germany

Dedicated to my mom . . . Mrs. Nandita Sen

Contents

Abbreviations and Symbols

Å	Ångström
ATR	Attenuated total reflection
CM	Cross metathesis
COE	*Cis*-cyclooctene
d	Doublet
DAFA	*N,N*-diallyl trifluoroacetamide
DCM	Dichloromethane
DEDAM	Diethyl diallyl malonate
DEDPM	Dipropargyl diethyl malonate
DME	1,2-Dimethoxyethane
DMF	*N,N*-Dimethylformamide
DMSO	Dimethylsulfoxide
equiv.	Equivalents
EI	Electron ionization
ESI	Electrospray ionization
Et	Ethyl
Et_2O / DEE	Diethyl ether
Et_3N	Triethylamine
EtOAc	Ethyl acetate
EVE	Ethyl vinyl ether
FT-IR	Fourier transform infrared spectroscopy
g	Gram
GC-MS	Gas chromatography-mass spectrometry
GH	*Grubbs-Hoveyda* catalyst
GPC	Gel permeation chromatography
h	Hours
Hz	Hertz
ICP-OES	Inductively-coupled plasma optical emission spectroscopy
IL	Ionic liquid

$IMesH_2$	1,3-Dimesitylimidazolin-2-ylidene
ISEC	Inverse size exclusion chromatography
J	Coupling constant
KHMDS	Potassium bis(trimethylsilyl)amide
ki	Rate constant of initiation
kp	Rate constant of propagation
M	Molar
m	Multiplet
m/z	Mass/charge
M+	Molecular ion
MALDI-TOF	Matrix-assisted laser desorption ionization time-of-flight
Me	Methyl
MeOH	Methanol
mg	Milligram
MHz	Megahertz
min	Minute
mL	Milliliter
mmol	Millimol
*M*n	Number-average molecular weight
mol-%	Molar percentage
MS	Mass spectroscopy
*M*w	Weight-average molecular weight
NBE	Norborn-2-ene
NHC	*N*-Heterocyclic carbene
NMR	Nuclear magnetic resonance
OTf	Trifluoromethanesulfonate
PCy_3	Tricyclohexylphosphine
PDI	Polydispersity index
Ph	Phenyl
ppm	Parts per million
Pr	Propyl
PrOH	Propanol

Py^+	Pyridinium
q	Quartet
RCM	Ring-closing metathesis
ROMP	Ring-opening metathesis polymerization
rt	Room temperature
s	Singlet
SEC	Size exclusion chromatography
SILP	Supported ionic-liquid phase
SM	Self-metathesis
SPS	Solvent purification system
t	Triplet
Tf2N	Bis(trifluoromethanesulfonyl)imide
THF	Tetrahydrofuran
TMS	Tetramethylsilane
TON	Turn-over number
UV-Vis	Ultra violet-visible
wt.-%	Weight percentage

Zusammenfassung

Sowohl in der organischen Synthese als auch in der Polymerchemie gehört die Olefinmetathese zu den wichtigsten Werkzeugen zur Bildung von Kohlenstoff-Kohlenstoffbindungen. Seit der Entdeckung der ersten metatheseaktiven Systeme wurden bereits große Fortschritte in der Aktivität, Selektivität und in der Toleranz gegenüber funktionellen Gruppen erzielt. Dennoch liegen die Wechselzahlen (TON) mit wenigen Ausnahmen immer noch weit unter der 100,000, meist unter 5000. Die modernen, strukturell aufgeklärten Olefinmetathesekatalysatoren finden ihre Nutzung momentan vor allem in Highend- Anwendungen in der Pharmaindustrie. Hier werden sowohl Schrock als auch Grubbs Katalysatoren eingesetzt. Die Synthese strukturell aufgeklärter Katalysatoren, die die Unzulänglichkeiten der existierenden Systeme in Angriff nehmen, ist daher unerlässlich.

Kapitel 1

Das erste Kapitel dieser Arbeit befasst sich mit der Geschichte der Olefinmetathese und gibt einen kurzen Überblick über die Synthese und Anwendungen von Schrock Katalysatoren. Es enthält zudem eine kurze Beschreibung der verschiedenen Olefinmetathesereaktionen sowie einen Abschnitt über N- Heterozyklische Carbene.

Kapitel 2

Die Synthese eines Metathese-Katalysators mit hoher katalytischer Aktivität (TON) und hoher Wechselzahl (TOF), der zudem unempfindlich gegenüber Wasser und Luft, sowie tolerant gegenüber funktionellen Gruppen und stereo-und regioselektiv ist, stellt auch zehn Jahre nach der Vergabe des Nobelpreises für die Metathese noch eine große Herausforderung dar. Auf der Suche nach einem aktiven Metathesekatalysator auf der Basis eines günstigen Metalls, der die oben genannten Kriterien erfüllt, wurden die ersten NHC Komplexe der Schrock Bistriflat Molybdän Imido Alkyliden Präkursoren synthetisiert. Im Gegensatz zu den existierenden Bistriflat- Komplexen enthalten die neuen fünffach koordinierten 16-Elektronenkomplexe sowohl ein Schrock Carben als auch ein N-Heterozyklisches Carben. Einzelkristall-Röntgenstrukturanalyse der Komplexe zeigte, dass die Komplexe eine verzerrte quadratisch planare Geometrie einnehmen, wobei einer der Triflat Liganden *trans* zum

NHC angeordnet ist. Während der Metathesereaktion dissoziiert dieser Triflatligand und bildet den aktiven trigonal bipyramidalen 14-elektronenkomplex (vgl. ^{19}F NMR Studien). Besonders interessant ist hierbei die hohe Aktivität der Katalysatoren in der Ringschlussmetathese (RCM), Kreuzmetathese (CM), der Ringöffnenden Metathesepolymerisation (ROMP), sowie in der Zyklopolymerisation von *α,ω*- Diinen. Herausragend ist auch die hohe Toleranz gegenüber funktionellen Gruppen wie sekundären Aminen sowie Hydroxyl- und Carbonsäure- Funktionalitäten, welche von den bisher bekannten Variationen der Schrock-Katalysatoren nicht toleriert werden. Die neuen Katalysatoren zeigen zudem auch bei hohen Temperaturen (140 °C) eine hohe Aktivität in der Ringschlussmetathese. Anhand der Beobachtung, dass die beiden Triflatliganden in den Komplexen eine Koaleszenztemperatur aufweisen, wurde ein Mechanismus für die Bildung der aktiven Spezies basierend auf einer Berry-Pseudorotation postuliert. Hierbei gehen zwei trigonal bipyramidale Komplexe über ein quadratisch planares Intermediat ineinander über. Die Aktivierung der Komplexe durch Dissoziation eines Triflatliganden in der SP-Konfiguration ist in Übereinstimmung mit der Reaktivität der isolierten neutralen und kationischen Komplexe, sowie mit den ^{19}F- NMR Experimenten. Die Umsetzung der Bistriflat NHC Komplexe mit einem Äquivalent eines fluorierten Alkoxids (z.B. $-OCH(CF_3)_2$, $-OC_6F_5$, $-OCCH_3(CF_3)_2$) oder mit $AgB(Ar^F)_4$ in Dichlorethan führte zur Isolation der Monoalkoxid- Komplexe, bzw. der kationischen Komplexe. Hierbei stabilisiert der NHC- Ligand das kationische Molybdänzentrum indem er die positive Ladung delokalisiert. Die Festkörperstrukturen aller Komplexe wurden durch Einkristall-Röntgenstrukturanalyse verifiziert und die Reaktivität in verschiedenen Metathesereaktionen untersucht. Hierbei wurden in ausgesuchten Reaktionen TON´s bis zu 545.000 erreicht. Vorallem Molybdän Imido Alkyliden Komplexe mit einem elektronenziehenden fluorierten Alkoxid, sowie die korrespondierenden kationischen Komplexe, in denen ein Triflat durch $AgB(Ar^F)_4$ substituiert wurde, zeigten eine hohe Aktivität und eine große Toleranz gegenüber funktionellen Gruppen. Der Einsatz anderer Carbene wie Triazol-2-yliden, Benzimidazol-yliden und CAAC (Zyklisches Alkyl Amino Carben) ermöglichte die Isolation neuer Molybdän Carben Alkyliden Komplexe. Tatsächlich zeigten diese Molybdän Imido NHC Komplexe eine bisher nicht dagewesene Toleranz gegenüber funktionellen Gruppen. Diese Katalysatoren besitzen ein großes Potenzial für die Anwendung in der organischen Chemie und in der Polymerchemie, da sie den Einsatz protischer Monomere erlauben.

Kapitel 3

In diesem Kapitel wird die Synthese des ersten anionischen Molybdän(VI) Imido Bisalkyl Alkyliden Komplexes [(Mo(N-2,6-Me_2-C_6H_3)(CH_2CMe_3)$_2$($CCMe_2Ph$)($Mg{\cdot}Et_2O$-μ-Cl)$_2$](**29**) beschrieben. Komplex **29** entsteht bei der Reaktion von [Mo(N-2,6-Me_2)C_6H_3)(CH_2CMe_2Ph)$_2$(O_3SCF_3)$_2$(DME)], (DME = 1,2-Dimethoxyethan) mit einem Überschuss an Neopentylmagnesiumchlorid. [Mo(N-2,6-(2-Pr)$_2$-C_6H_3)($CCMe_2Ph$)(2,5-Me_2-Pyrrolid)$_2$(1,3-Dimesityl-4,5-Dihydro-1H-Imidazol-3-ium)] (**30**) kann durch Umsetzung von [Mo(N-2,6-(2-Pr)$_2$-C_6H_3)($CCMe_2Ph$)(2,5-Me_2-Pyrrolid)$_2$(1,3-Dimesityl-4,5-Dihydro-1H-Imidazol-3-ium)] (**30**) mit 1,3-Dimesitylimidazoliniumchlorid in Benzol erhalten werden. Die Einkristall-Röntgenstrukturen beider Komplexe wurden bestimmt. Während **29** keine Aktivität in der Alkinmetathese und RCM (Ringschlussmetathese) zeigt, konnte sowohl in der ROMP (Ringöffnende Metathesepolymerisation) von (substituierten) Norborn-2-enen als auch in der 1- Alkinpolymerisation von 2-Ethynyl-Trimethylsilylbenzol Aktivität beobachtet werden. Die über ROMP erhaltenen Polymere zeigen einen hohen *cis*-Gehalt von bis zu ≥ 96%. Sowohl die vorgeschlagene Mesomerie über d_π-p_π-Wechselwirkungen mit Mo(IV) zwischen einem Molybdän Amidatoalkyliden und einem Molybdän Amidoalkylidenat, als auch die [1,3-H]-Umlagerung im Falle einer Polymerisation, welche für die einzigartige Reaktivität von **29** verantwortlich gemacht wird, werden durch Dichtefunktionaltheorie- Rechnungen unterstützt.

Abstract

Olefin metathesis reactions belong to the most powerful tools for the formation of carbon-carbon double bonds both in organic synthesis and polymer chemistry. Enormous progress has been made both in terms of activity, selectivity and functional-group tolerance of the catalysts. Nonetheless, turn-over numbers (TONs) are still, with very few exceptions, far below 100,000 in most cases below 5,000. The use of modern, molecularly well-defined olefin metathesis catalysts are mostly restricted to high-end pharmaceutical applications. There, both *Schrock* and *Grubbs* catalysts find ample use. Therefore, the synthesis of well-defined catalysts which conquered the weakness of the existing systems has received great attention.

Chapter 1

The first chapter of this thesis deals with a history of olefin metathesis as well as a short overview on the synthesis and applications of *Schrock* catalysts. The context also offers a short description about different olefin metathesis reactions and N-heterocyclic carbenes (NHC).

Chapter 2

A single-site catalyst, which is highly active both in terms of turn-over numbers (TONs) and turn-over frequency (TOF), which is tolerant toward water, air and functional-groups with high stereo- and regioselectivity remains a challenge in olefin metathesis. In search for olefin active metathesis catalysts based on cheap metals (Mo/W) and fulfill all the above mentioned criteria, the first N-heterocyclic carbene (NHC) complexes of molybdenum imido alkylidene bis(triflate) complexes have been synthesized. Unlike existing bis(triflate) complexes, the novel 5-fold coordinated 16-electron Mo-complexes contain two carbenes, i.e. a *Schrock* carbene and an NHC. Single crystal X-ray analysis revealed that the above mentioned complexes are distorted square pyramidal with one triflate (OTf) ligand *trans* to the NHC. In course of a metathesis reaction, this triflate leaves the complex and generates a trigonal bipyramidal cationic 16-electron Mo-NHC complex (^{19}F-NMR studies). The most important observation is this type of catalysts is active in ring-closing metathesis (RCM), cross-metathesis (CM), the cyclopolymerisation of *α*,*ω*-diynes and ring-

opening metathesis polymerisation (ROMP). Monomers containing functional-groups, *e.g., sec*-amine, hydroxy, and carboxylic acid moieties, which are not tolerated by the existing variations of *Schrock* catalysts, can be used. This novel class of catalysts displays substantial activity even at high temperatures (140 °C), *e.g.,* in RCM. Based on the observation that bis(triflate) complexes show a coalescence temperature for the two triflate groups, an activation mechanism based on a Berry-type pseudorotation, i.e. interconversion between trigonal biyramidal (TBP) configurations through a square pyramidal (SP), is proposed. Activation of the catalysts through the release of one triflate in the SP configuration is in full accordance with the observed reactivity of both neutral and cationic Mo-imido alkylidene NHC complexes and with ^{19}F-NMR. Furthermore, reactions of the Mo-NHC bis(triflate) complexes with one equivalent of a fluorinated alkoxide (*e.g.,* -OCH$(CF_3)_2$, -OC_6F_5, -$OCCH_3(CF_3)_2$) or with $AgB(Ar^F)_4$ in dichloroethane afforded the corresponding monoalkoxide and the cationic Mo-imido alkylidene NHC complexes. This particular feature is the presence of the NHC ligand, which delocalizes the cationic charge and stabilizes the molybdenum center. The structures of all compounds have been determined by single-crystal X-ray diffraction and their reactivities in various olefin metathesis reactions have been explored. In selected metathesis reactions, TONs up to 545,000 have been reached. Nonetheless, Mo-imido alkylidene NHC complexes with one electron-withdrawing fluorinated alkoxide and the corresponding cationic complexes in which the remaining triflate replaced by $AgB(Ar^F)_4$ afforded remarkably active and functional-group tolerant metathesis catalysts. Employing different NHCs such as triazole-2-ylidene, benzimidazolylidene and CAAC (Cyclic Alkyl Amino Carbene) provides access to another novel class of Mo-NHC alkylidene complexes. In fact, Mo-imido alkylidene NHC complexes prepared recently display unprecedented functional-group tolerance. Therefore, these catalysts hold great promise in both organic and polymer chemistry.

Chapter 3

In this chapter, the first anionic high oxidation state molybdenum (VI) imido bisalkyl alkylidyne complex [(Mo(N-2,6-Me_2-C_6H_3)$(CH_2CMe_3)_2$($CCMe_2Ph$)$(Mg{\cdot}Et_2O$-μ-$Cl)_2$] (**29**) is reported. It forms via reaction of [Mo(N-2,6-Me_2-C_6H_3)$(CH_2CMe_2Ph)_2(O_3SCF_3)_2$(DME)], (DME = 1,2-dimethoxyethane) with an excess of neopentylmagnesium chloride. [Mo(N-2,6-(2-*i*Pr)$_2$-C_6H_3)($CCMe_2Ph$)(2,5-Me_2-pyrrolide)$_2$(1,3-dimesityl-4,5-dihydro-1H-imidazol-3-ium)] (**30**) is accessible via

reaction of Mo(N-2,6-(2-*i*Pr)$_2$-C$_6$H$_3$)(IMesH$_2$)(CHCMe$_2$Ph)(2,6-Me$_2$-pyrrolide)$_2$ with 1,3-dimesitylimidazolidinium chloride in benzene. X-ray studies of both complexes are also presented. While **29** is inactive in alkyne metathesis and in ring-closing metathesis (RCM), it is active in the ring-opening metathesis polymerization (ROMP) of (substituted) norborn-2-ene(s) and in the 1-alkyne polymerization of 2-ethynyl-trimethylsilylbenzene. The ROMP derived polymers display a high *cis*-content up to ≥ 96%. Both the proposed mesomerism via d_π-p_π interactions through Mo(IV) between a molybdenum amidatoalkylidyne and a molybdenum amidoalkylidenate and a [1,3-H] shift in course of polymerization that accounts for the unique reactivity of **29** are supported by density functional calculations (DFT).

Aim

Olefin metathesis has had a great impact on organic chemistry and polymer synthesis. Enormous developments were made in terms of catalysts synthesis and applications in different olefin metathesis reactions. In this view, group 6 and 8 metal based alkylidenes are commonly used. However, the pronounced oxophilic character of group 6 metal alkylidenes is challenging and in fact, Ru-alkylidenes, known as *Grubbs* catalysts have turned out to be stable towards a large number of protic groups, air and moisture. Moreover, *Grubbs* catalysts play a crucial role in several industrial applications due to their flexibility. However, stereo- and regio-selectivity with *Grubbs* catalysts is limited. Looking at the structural features of highly active *Grubbs* 2nd-generation catalysts, that comprise the electron-donating N-heterocyclic carbene ligand, the question was, why not use N-heterocyclic carbenes as a ligand for group 6 metal alkylidene complexes?

In this PhD work, in fact, the first novel high oxidation state Mo(VI) imido alkylidene NHC complexes were successfully prepared and isolated. In principle, the concept disclosed here combined the advantages of both group 6 and 8 metal alkylidenes to develop one single-site catalyst. Unlike existing bis(triflate) complexes, the novel 5-fold coordinated 16-electron molybdenum complexes contain two carbenes, *i.e.* a *Schrock* carbene and an NHC. Single crystal X-ray analysis revealed distorted square pyramidal complexes with one triflate (OTf) ligand relatively *trans* to NHC.

The main objective was to explore the activity of these complexes in different olefin metathesis reactions. Interestingly, all the complexes are active in ROMP, cyclopolymerization and different olefin metathesis reactions of monomers containing functional-groups, which are not tolerated by the existing variations of *Schrock* catalysts, e.g., *sec*-amines, hydroxy, and carboxylic acid moieties.

Subsequently, the focus was put on replacement of one triflate group by different electron-withdrawing alkoxides and non-coordinating anions to make it more reactive and more functional-groups tolerant. By using mono-alkoxide complexes, the

feasibility of functional-group tolerance with small molecule synthesis was to be investigated.

A further aim was to investigate the reactive propagating species by ^{19}F-NMR and to establish a possible mechanism for *trans* selectivity during ROMP. In this regards, the performance of novel molybdenum imido alkylidene NHC complexes are painted on chapter two.

Also different NHCs were investigated and variations in catalyst structure again comprised of different anionic ligands such as alkoxides, phenoxides, carboxylates and isocyanates as well as of different imido ligands. Structure-activity relationships at different temperatures have to be investigate. The chosen approach will allow elucidating the activating effect of the NHC on the metal alkylidene in terms of ligand dissociation and concomitant formation of cationic alkylidene species.

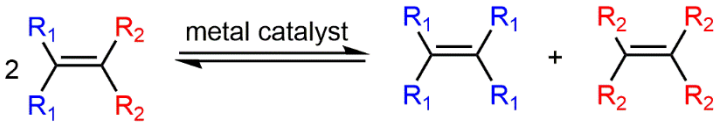
Chapter 3 comprises the synthesis of first dinuclear anionic high oxidation state molybdenum(VI) amidato bisalkyl alkylidyne complexes. The anionic alkylidyne complexes are proposed to convert into the corresponding imido alkylidento complexes in the presence of monomer. In this regard, a high quality quantum mechanical calculation *i.e.* DFT should give more accurate scenario about the electron density in the complex.

Chapter 1

Introduction

1.1 A condensed history of olefin metathesis

Metathesis comes from the Greek word *μεταθεσιζ* and means transposition.[1] An olefin metathesis reaction between two olefin molecules is defined by the exchange of substituents on carbon-carbon double bonds in the presence of a metal catalyst (**Scheme 1**).[2] Olefin metathesis was the focus of the 2005 Nobel Prize in Chemistry, which was awarded to *Yves Chauvin*, *Robert H. Grubbs* and *Richard R. Schrock*. Olefin metathesis originated from polymer research in a way reminiscent of other great inventions. It was by chance that *Ziegler's* group discovered the exclusive formation of 1-butene from a reaction of triethylaluminum with ethylene under high pressure in the presence of a nickel catalyst in 1955.[3] *R. L. Banks* and *G. C. Bailey* reported that propene reacts to form ethylene and 2-butenes when treated with a mixture of triisobutyl aluminium and molybdenum oxide on alumina at high temperature.[4] *N. Calderon* and co-workers at Goodyear Tire and Rubber Company, USA, recognized that the polymerization of cycloolefins[5] and the disproportionation of acyclic alkenes are the same type of reaction and named it "olefin metathesis" in 1967.[6] The above mentioned classical heterogeneous systems have an important place in commercial application of olefin metathesis but the efficiency of these catalysts was limited because of incompatibility with functional groups, difficulties with initiation and reaction control, in summary rendering this process a 'black box'.



Scheme 1. Olefin metathesis reaction.

Olefin metathesis can be classified according to the substrates and products that are involved in this reaction.[7-10] The most common types of olefin metathesis are ring-closing/ring-opening metathesis (RCM/ROM), cross-metathesis (CM), acyclic diene metathesis (ADMET) polymerization, ring-opening metathesis polymerization (ROMP), the cyclopolymerization of diynes, 1-alkyne polymerization and ring-opening cross metathesis (ROCM) (**Figure 1**).[11-12] *Y. Chauvin* and his student *Hérisson* first

proposed an olefin metathesis mechanism in 1971, which was finally universally recognized and accepted. The *Chauvin* mechanism involves an active species or catalyst. The catalyst possesses a metal-carbon double bond (a metal-alkylidene). The metathesis reaction proceeds through the coordination of the olefin to the metal center followed by forming a metallacyclobutane intermediate ([2+2] cycloaddition). The metallacyclobutane produced can then undergo a retro-[2+2] cycloreversion to generate the original active species and a new olefin (**Scheme 2**).[13-14]

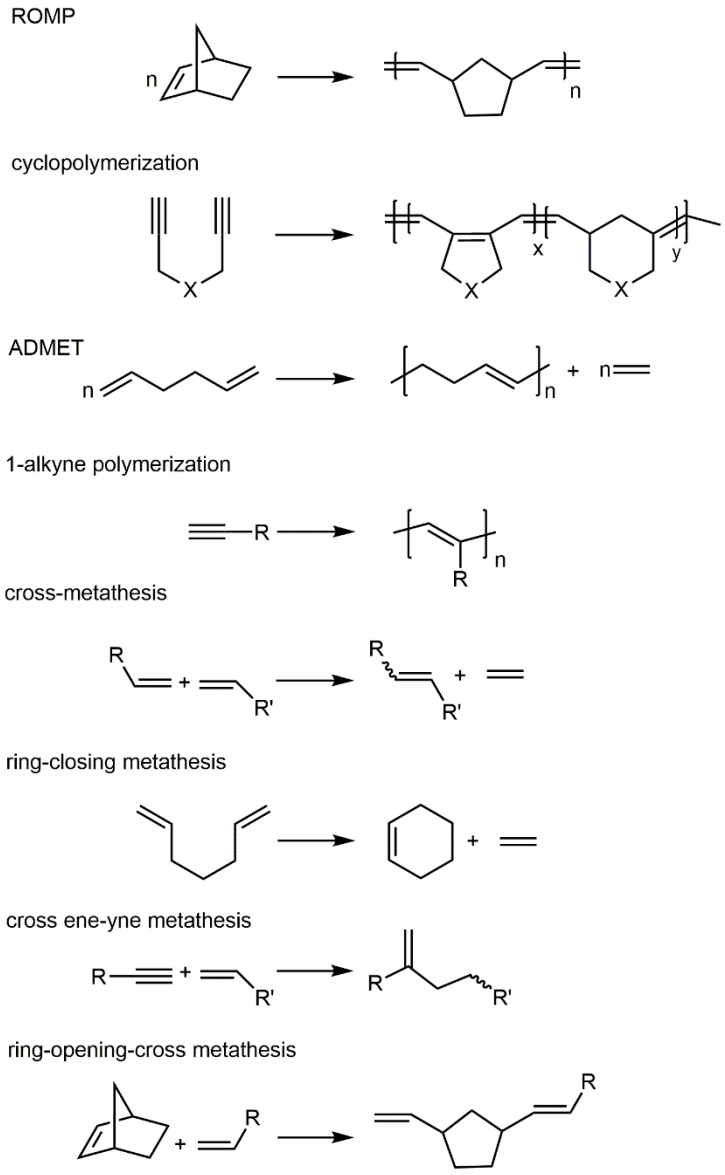
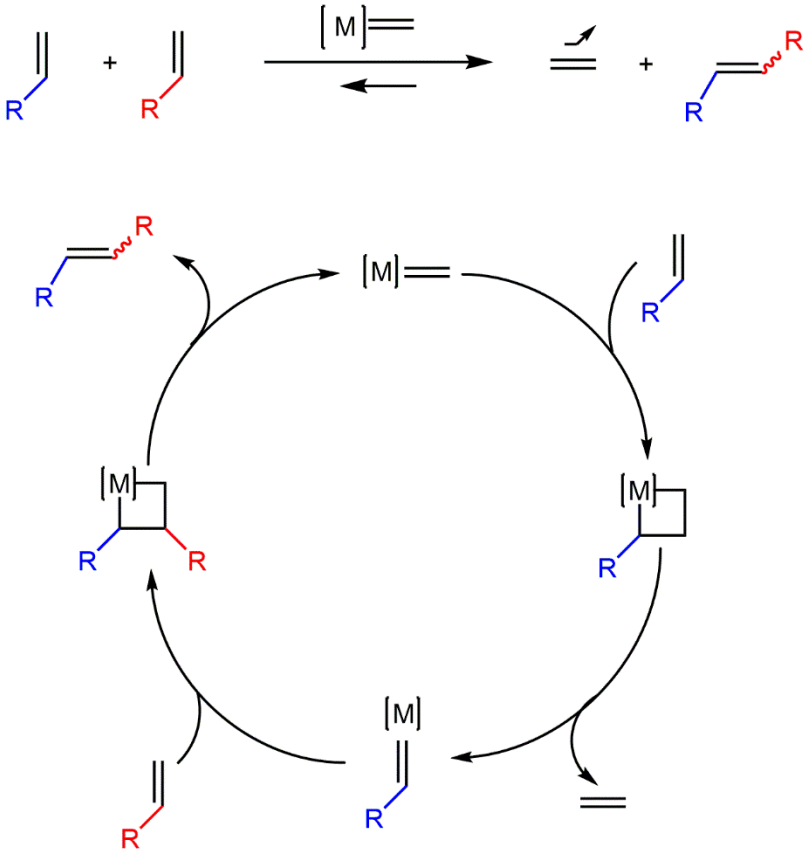


Figure 1. The most common types of olefin metathesis reactions.



Scheme 2. Representation of the *Chauvin* metathesis mechanism.

The first metal-carbon double bond (carbene) was established in 1964 by *E. O. Fischer*[15] who later won the Nobel Prize in Chemistry with *Sir G. Wilkinson*[16-17] for the pioneering work on the chemistry of organometallic compounds. The *Fischer* carbene contains a late-transition metal having a low oxidation state. The carbene carbon in a *Fischer* carbene usually has *π*–donor substituents such as alkoxy and alkylated amino groups, as in $(CO)_5W{=}C(OMe)(Ph)$, which makes it a singlet carbene as well as electrophilic.[18] The *Chauvin* mechanism inspired organometallic chemists to develop a stable and highly efficient metal-carbon double bond complexes. *Tebbe*[19] and *Grubbs*[20] successfully prepared such compounds of titanium, but this type of compound followed Wittig-type chemistry and showed no catalytic activity. When the scientific grandson of *Sir G. Wilkinson*, *R. R. Schrock* went to Du Pont in 1972, transition metal organometallic chemistry and homogeneous catalysis were of great importance in academia as well as in industry. He synthesized $[TaMe_5]$, $[Ta(CH_2Ph)_5]$[21] and attempted to synthesize $[Ta(CH_2CMe_3)_5]$ by treatment of $[Ta(CH_2CMe_3)_3Cl_2]$ with two equivalents of $LiCH_2CMe_3$. He recognized that the

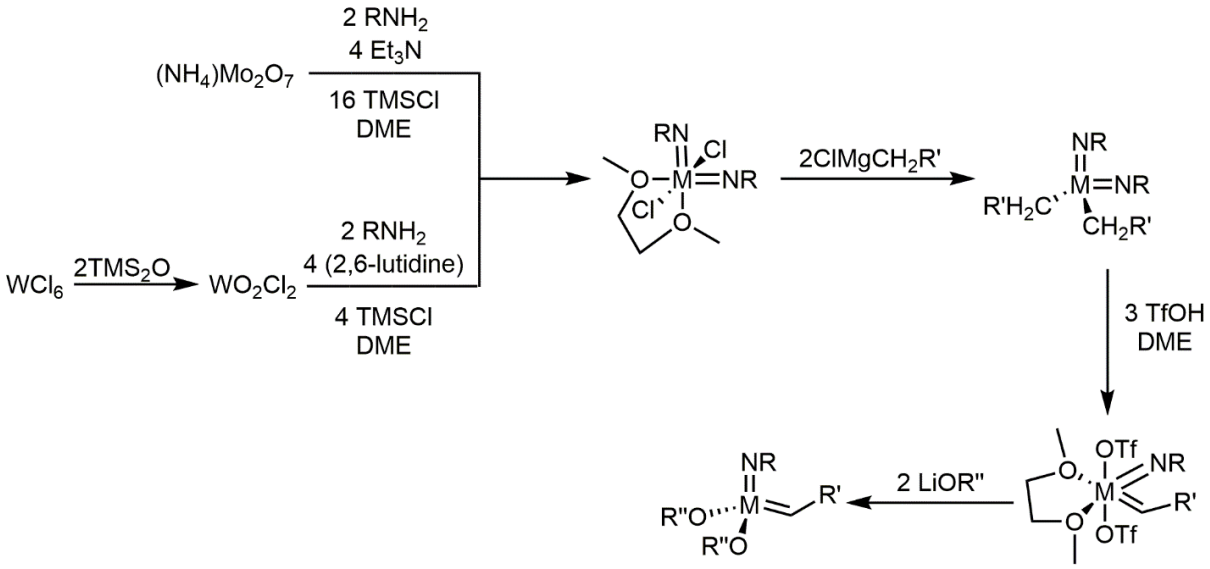
isolated complex was the first thermally stable, 10-electron containing high oxidation state tantalum alkylidene complex, *i.e.* [Ta(CHCMe$_3$)(CH$_2$CMe$_3$)$_3$].[22-23] Alkylidenes differ from *Fischer* carbenes in that the carbenic carbon has a triplet and nucleophilic character.

1.2 Development of well-defined *Schrock* catalysts

In 1980, *Schrock's* group at MIT reported the first unimolecular well-defined high oxidation state tantalum alkylidene complex, [Ta(=CH-*t*Bu)(Cl)(PMe$_3$)(O-*t*Bu)$_2$] (along with Nb and W complexes), that promoted the metathesis of *cis*-2-penetene.[24-25] The reason behind the metathetical activity of these complexes was the presence of ancillary alkoxide ligands in the catalyst but the expectancy for tantalum based alkylidene complexes as effective olefin metathesis catalysts for use in organic synthesis did not appear promising because the above complexes were not functional-group tolerant. At the same time, titanium alkylidene complexes were prepared but they were only active for ring-opening metathesis polymerization (ROMP).[26] From the somewhat less effective tantalum and niobium alkylidene complexes, *Schrock* moved forward to the preparation of group 6 (Mo, W) and group 7 (Re) metal alkylidene complexes. The first tungsten alkylidene oxo complexes like WO(CH-*t*-Bu)Cl$_2$(PEt$_3$)$_2$ were prepared by treating WO(O-*t*Bu)$_4$ with one equivalent Ta(CH-*t*Bu)Cl$_3$(PEt$_3$)$_2$.[27] The new complex was an 18-electron complex and therefore it did not seem that it could react with an olefin unless a phosphane or a chloride ligand dissociated to yield an 16-electron complex. At the same time, *Ösborn* and coworkers prepared a different type of tungsten oxo alkylidene complex in the presence of various Lewis acids.[28-29] However, metathesis activity of these catalysts were limited since alkylidene complexes other than the neopentylidene complexes were unstable towards bimolecular decomposition, ligand scrambling (*e.g.,* chloride transfer) or alkylidene coupling to give an olefin.

The most significant molecular olefin metathesis catalysts reported by *Schrock* and coworkers in the late 1980s can be described by the general formula M(NR)(CHR')(OR'')$_2$, where M = Mo, W; R = alkyl or phenyl; R' = *tert*-butyl, CMe$_2$Ph, SiMe$_3$; R'' = alkyl, phenyl, fluorinated alkyl, diolate. These complexes are relatively stable towards bimolecular decomposition[30] because of the bulky imdio ligand and

ancillary ligands and also showed the highest metathesis activity so far. The metal centers in these catalysts have a high oxidation state, which makes the metal relatively Lewis acidic. The most accessible route to make this catalyst involves a four step synthesis when M = Mo and a five step synthesis when M = W. The overall reaction scheme is shown in **Scheme 3**.[31-35]

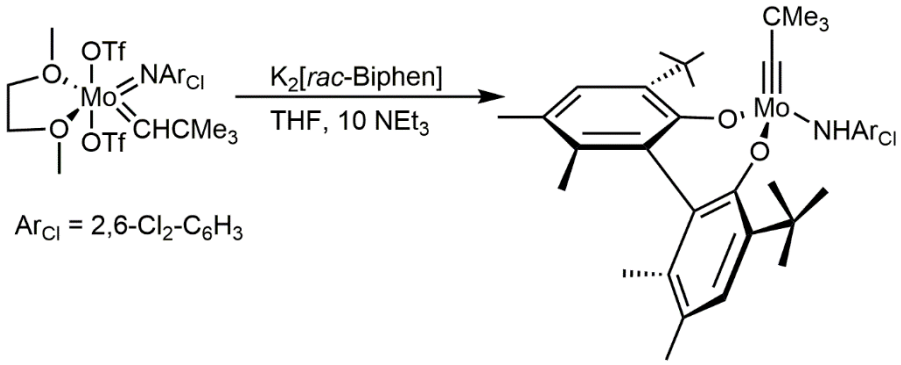


Scheme 3. General route to $M(NR)(CHR')(OR'')_2$ complexes.

It was proposed that $[M(NAr)_2(DME)Cl_2]$ can be synthesized in large quantities from $(NH_4)_2Mo_2O_7$ or WO_2Cl_2 with two equivalents of $ArNH_2$, four equivalents of trimethylamine and sixteen equivalents of Me_3SiCl in dimethoxyethane. In case of M = W, the first step involves preparation of WO_2Cl_2 from WCl_6 by treatment with hexamethyldisiloxane. Alkylation of $[M(NAr)_2(DME)Cl_2]$ with neopentyl or neophyl Grignard reagents to form $[M(NAr)_2(CH_2R')_2]$, gives the "universal precursors" of the general formula $[M(NAr)(CHR')(OTf)_2(DME)]$ after treatment with three equivalents of triflic acid in presence of dimethoxyethane. The *α*-hydrogen abstraction is more efficient when the alkyl group is CH_2CMe_3 or CH_2CMe_2Ph. When universal precursors are treated with two equivalent of various LiOR'' or diolate, molybdenum or tungsten based bis(alkoxy) imido alkylidene complexes result.

The main problem for the synthesis of $M(NR)(CHR')(OR'')_2$ with diolate was the conversion of an imido/alkylidene species to the amido/alkylidyne species during substitution of the triflates by alkoxides. The amido/alkylidyne species was formed due

to the abstraction of the alkylidene *α*-proton instead of attack on the metal center; consequently, the imido nitrogen is protonated (**Scheme 4**).[36-37]



Scheme 4. Synthesis of amido/alkylidyne species.

The biggest advantage of this synthetic route (**Scheme 3**) is that a wide variety of imido and alkoxide ligands can be used and a large number of Mo/W catalysts therefore become accessible. The bond between the metal center and the nitrogen atom of the imido ligand in M(NR)(CHR')(OR'')$_2$ can be considered a pseudo triple bond, since the free electron pair of the imido nitrogen pushes the electron density to the metal center into an empty *d*-orbital. Therefore, the angle of the Mo-N-C bond is close to 180°. Here the metal center is four-coordinated and the *d*-orbitals of the metal involved in the formation of the M=C bond must lie perpendicular to the N-M-C$_{ipso}$ plane. Thus, the metal complex can exist as in two stereoisomeric forms. In one, the R' group of the alkylidene points towards the imido ligand (*syn*) and in the other it points away from the imido ligand (*anti*)[38], **Figure 2**. In general, the *syn* and *anti*-isomer can be converted into each other by simple rotation around the M-C double bond. The degree of conversion of these two isomers depends on the ligand environment. The *syn* isomer is more stable because of an *α*-agostic interaction between empty metal orbital with the C-H *σ*-bond of the alkylidene. In the *anti*-configuration, there is no agostic interaction, because the C-H bond points away from the metal center.[39-41] The above mentioned two isomers can be differentiated by using ^{1}H-NMR spectra and the alkylidene J_{CH} (^{13}C-NMR) coupling constant. The J_{CH} coupling constant in the *syn* species typically ranges between 110-130 Hz (due to the *α*-agostic interaction), while the J_{CH} coupling in the *anti*-species is > 140 Hz. Additionally, from single crystal X-ray diffraction studies one can get information about

the metal carbon bond length and bond angle of the *syn*/*anti* species, which suggest the presence of an agostic interaction in *syn* complexes.[42-43]

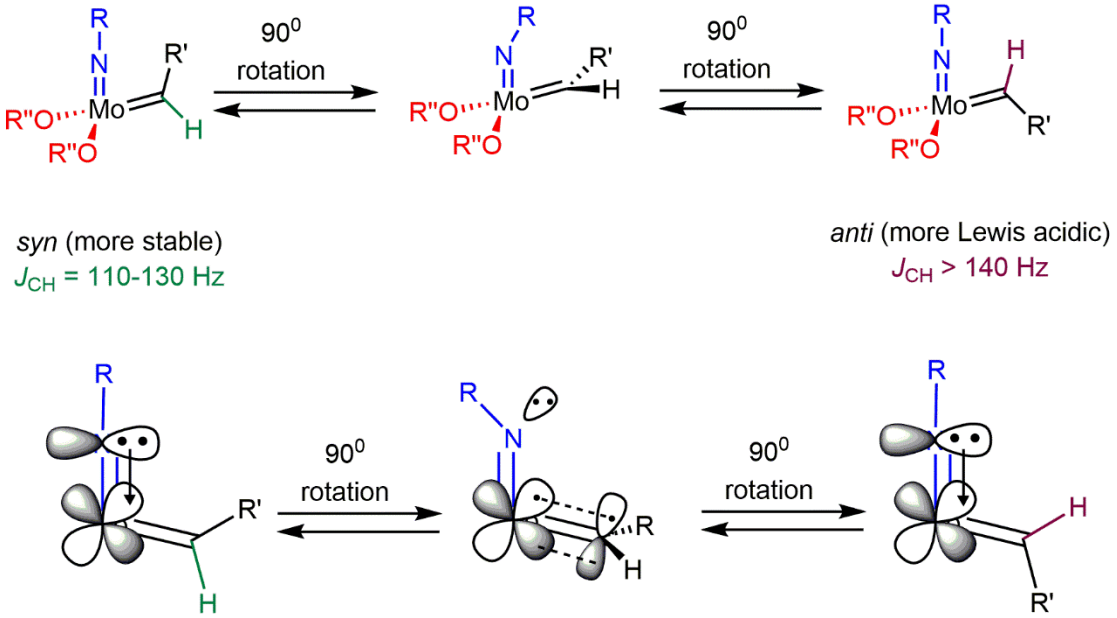


Figure 2. Conversion of *syn* and *anti* isomers via rotation of the alkylidene group in Mo(NR)(CHR')(OR'')$_2$. An orbital diagram is shown at the bottom for simplicity.

Schrock and co-workers reported that bisalkoxide Mo-complexes exist as a *syn* isomer at 22 °C, and can be transformed into an equilibrium 1:2 mixture of *anti* and *syn* alkylidene complex upon UV/Vis photolysis of the corresponding solution of the complex at 360 nm at -78 °C.[44] The alkoxides ligands also has a great influence on the *syn* and *anti* interconversion. Progress in olefin metathesis was also made after preparation of Mo and W based bisalkoxide complexes. In 1997, the first enantiomerically enriched chiral biphen Mo-complex was synthesized by *Schrock* and co-workers (**Figure 3**). These C_2-symmetric ligands shield one face of the Mo-C double bond and the resulting complex serves as an efficient catalyst for enantioselective metathesis reactions. The biphen Mo-complex is able to achieve asymmetric ring-closing metathesis with *ee* up to 90%.[45-46] Additionally, ROMP of substituted norbornenes and norbornadienes with the catalyst in **Figure 3** afforded a *cis*, *isotactic* polymer microstructure.[47-48] In both cases, the selectivity is governed by the enantiomorphic site control due to the chiral ligand.

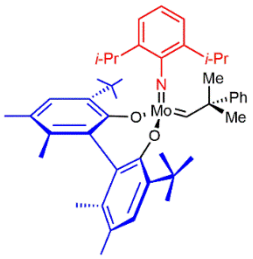
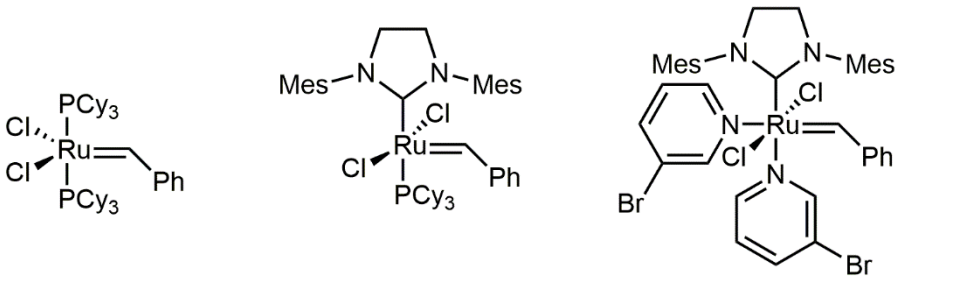


Figure 3. First enantioselective olefin metathesis catalyst.

Active olefin metathesis catalysts are not limited to Mo and W. A remarkable finding was made by *Grubbs* and co-workers in 1993.[7,49] The development was based on Ru-alkylidene complexes, generally known as *Grubbs* catalysts.

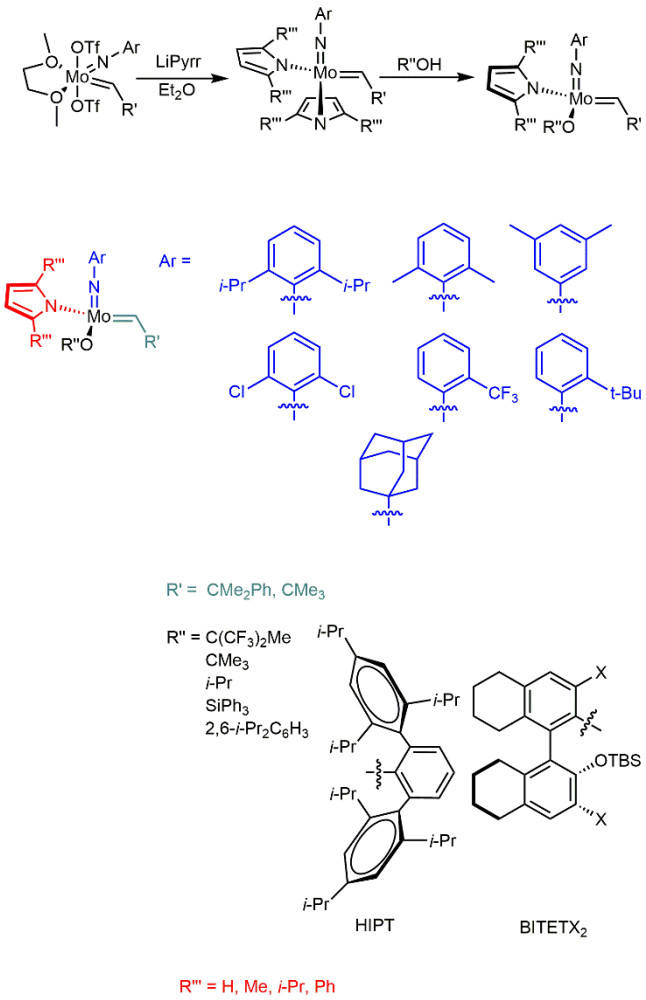


Grubbs 1st generation Grubbs 2nd generation Grubbs 3rd generation

Figure 4. Common Ru-based olefin metathesis catalysts.

Since that time many Ru-complexes with different ligand variations have been prepared [50-51] and thoroughly explored.[49-71] The most common ruthenium based olefin metathesis catalysts are depicted in **Figure 4**. The above Ru-alkylidene complexes can be used in air as well as with protic functional-group containing substrates for various olefin metathesis reactions. These complexes are 16-electron species and during metathesis reactions one of the phosphine ligand leaves the Ru-metal center to generate an 14-electron complex, which is metathesis active. The black box of Mo/W-based metathesis catalysts in the past decade was the exploration of monoalkoxide pyrolide (MAP) imido alkylidene complexes.[72] The MAP catalyst can be prepared in two steps from the “universal precursors” (**Scheme 5**). Exchange of triflate by addition of different lithium pyrrolides yields imido alkylidene bispyrrolide

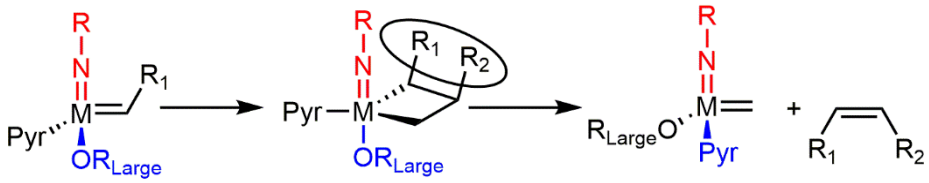
complexes[73], which upon treatment with one equivalent of alcohol offer access to the corresponding MAP-type catalysts.[72]



Scheme 5. Synthetic route to MAP-type catalysts (top) and ligand variations in MAP catalysts (bottom).[43,74-79]

The pyrolide is bound to the metal center in an η^1-fashion, which leaves the metal with a 14-electron count. Binding of the pyrrolide in an η^5-fashion is probably disfavored for steric reason. The activity of MAP catalysts is promising compared to bisalkoxide compounds. MAP catalysts are active in ring-closing metathesis reactions that were not possible previously with bisalkoxide complexes, including examples of ene-yne metathesis.[80] Another great discovery in olefin metathesis was the enantioselective ring-closing metathesis using MAP catalysts containing monofuntional chiral alkoxide ligands.[81-82] The remarkable applicability of MAP-type catalysts were not limited to

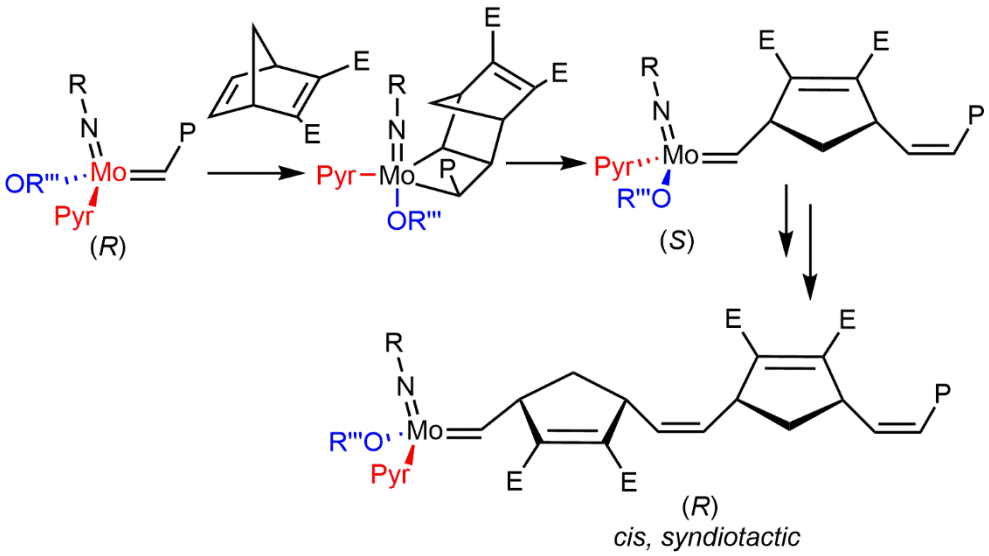
enantioselective synthesis. MAP catalysts also proved highly *Z*-selective for double bond formation when containing small imido groups and sterically hindered alkoxide ligands, *i.e.* OHIPT (HIPT = 2,6-bis-(2,4,6–triisopropylphenyl)phenyl).



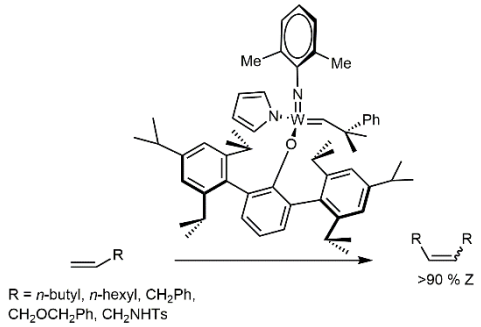
Scheme 6. Mechanism for *Z*-selectivity using MAP-type catalysts.

The metathesis intermediate in MAP catalyst systems is a trigonal bipyramidal structure where imido and alkoxide ligand adopt axial positions. An olefin approaches to the pyrrolide (CNO face) and leaves *trans* to the pyrrolide. Each substituent on the trigonal bipyramidal metallacycle intermediate orients itself either towards the small imido group or towards the big alkoxides. When R_{Large} = OHIPT, which is sterically demanding, the substituent on the metallacyclobutane preferentially points toward the smaller imido group (**Scheme 6**). The corresponding metathesis product comes out as *Z*-isomer of the double bond. There are many recent example of *Z*-selective metathesis catalysts, especially MAP-type catalysts are available. The other significant use of MAP catalysts is for stereoregular ROMP of substituted norbornadienes, which yields stereo-regular poly(norbornene) with high *cis*/*trans* configuration, depending on the catalysts. For example polymerization of substituted norbornadienes with Mo(NAd)(CH_2CMe_2Ph)(pyr)(OHIPT) (Ad = 1-admantyl, pyr = pyrrolide or 2,5-Me_2-pyrrolide, HIPT = 2,6-bis-(2,4,6–triisopropylphenyl)phenyl) allow for access to *cis*, *syndiotactic* polymer dyads (**Scheme 7**).[83-84] In contrast, the *trans*, *isotactic* polymer is formed when (+)-5,6-dicarbomethoxynorbornene is used as a monomer.[85] At the same time W-based well-defined oxo alkylidene complexes[86-87] were prepared for *Z*-selective olefin metathesis reactions and used for the polymerization of DCMNNBD (DCMNBD = 2,3-dicarbomethoxynorbornadiene), (+)-5,6-dicarbomethoxynorbornene to yield a high *cis*,*syndiotactic* polymer. The ROMP based polymer preparation is obviously not only limited to homopolymerization; alternating *trans* AB block copolymers were prepared from cyclooctene (A) and 2,3-dicarbomethoxy-7-isopropylidenenorbornadiene (B), or from cycloheptene (A') and

dimethylspiro[bicyclo[2.2.1]hepta2,5-diene-2,3-dicarboxylate-7,1′-cyclopropane (B') using first-generation *Schrock* catalysts.[88]



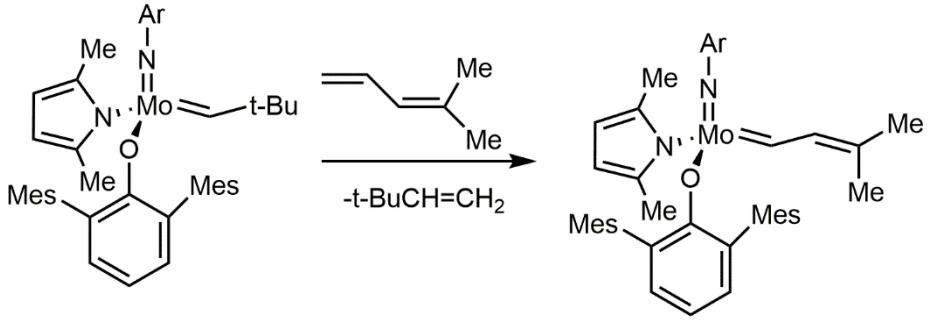
Scheme 7. Synthesis of *cis*,*syndiotactic* poly(norbornadienes) using Mo(NAd)(CH_2CMe_2Ph)(Pyr)(OHIPT).



Scheme 8. Example of W-based MAP catalyzed *Z*-selective metathesis reactions.

For the homometathesis of terminal olefins, W-based MAP catalysts showed exceptional *Z*-selectivity[86,89-90] as shown in **Scheme 8**. The complexes of the type M(NAr)(CH_2CMe_2Ph)(Pyr)(OHIPT) (M = Mo or W, Ar = 2,6-*i*Pr_2-C_6H_3, 2,6-Me_2-C_6H_3) were employed for *Z*-selective homocoupling of simple (*E*)-1,3-diene and gave a (*E*,*Z*,*E*)-triene in high yield.[91] A vinylalkylidene complex *i.e.* Mo(NAr)($CHCHCMe_2$)(Me_2Pyr)(OHMT) (Ar = 2,6-*i*Pr_2-C_6H_3; Me_2Pyr = 2,5-dimethylpyrrolide, OHMT = 2,6-dimesitylphenoxide) was isolated in pure form by

reaction of Mo(NAr)(CHCMe$_3$)(Me$_2$Pyr)(OHMT) with an excess of 4-methyl-1,3-pentadiene, which is shown in **Scheme 9**.



Scheme 9. Synthesis of a vinylalkylidene Mo-complex.

A macrocyclic tri-substituted alkene with high *Z*-selectivity can be prepared by using Mo-bisaryloxide complexes containing an electron-withdrawing pentafluoro imido ligand.[92] Recently, the *Schrock* and *Hoveyda* group reported the synthesis of 1,2-disubstituted *Z*-alkenyl halides by application of a chiral MAP catalyst with electron-withdrawing imido groups. [93] So far, all high oxidation state Mo or W-based olefin metathesis catalyst have been neutral. In 2006, *Schrock* and coworkers reported the first cationic alkylidene complexes which contain a non-coordinating anion. The cationic alkylidene compounds were prepared by reaction of universal precursors with Li{Ar^x-Nacnac = [2,6-X$_2$-C6H3NC(Me)$_2$]CH; X = Me, Cl} to give mono-triflate complex, which further reacted with NaB(Ar^F)$_4$ (Ar^F = 3,5-(CF$_3$)$_2$C$_6$H$_3$) in CH$_2$Cl$_2$ to afford the cationic {Mo(NAr)(CHCMe$_2$Ph)(Ar^{Cl}-Nacnac)}[B(Ar^F)$_4$] complex.[94] The other type of cationic molybdenum imido alkylidene complexes was prepared by addition of [HNMe$_2$Ph]B(Ar^F)$_4$ (Ar^F = 3,5-(CF$_3$)$_2$C$_6$H$_3$) to Mo(NAr)(CHCMe$_2$Ph)(Pyrrolide)$_2$.[95] Unfortunately both cationic complexes were not stable enough and not active in olefin metathesis.

The success of olefin metathesis in organic chemistry can be credited to well-defined homogeneous olefin metathesis catalysts (both *Schrock* and *Grubbs* catalysts), but purification techniques, re-use and easy workup are still a challenging task. Therefore, the immobilization and support systems of these catalysts could be a decisive alternative to the above mentioned problems. The first polymer-supported chiral *Schrock* catalyst was reported by *Schrock* and *Hoveyda* containing the BINOL ligand

for enantioselective olefin metathesis reactions (**Figure 5**).[96] Soon after, *Buchmeiser* group reported a chiral *Schrock* catalyst supported by ROMP-derived polymer for enantioselective ring-closing metathesis with good enantioselectivity.[97-99]

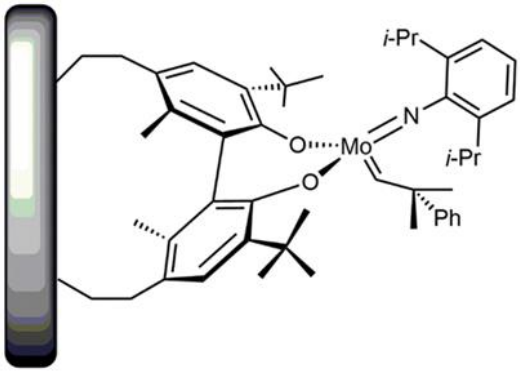


Figure 5. Supported chiral Mo imido alkylidene catalysts.

In a very similar fashion, a *Schrock*-type metal alkylidene with polymer-bound binaphtholate ligand was prepared by *Schrock*, *Hoveyda et al*.[100] On the other hand, the first inorganic solid (silica) supported well-defined Mo-imido alkylidene catalyst (**Figure 6**) was reported and its activity explored in terms of self-metathesis of ethyl oleate (EO).[101] In the meantime, also different Mo and W imido alkylidene surface species were reported by *Schrock* and *Copéret*.[102-107]

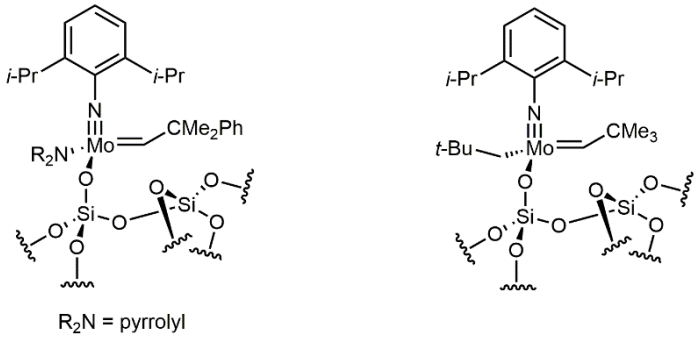


Figure 6. Structure of silica supported Mo-imido alkylidene catalysts.

1.3 Different types of olefin metathesis reactions

1.3.1 Ring-Opening Metathesis Polymerization (ROMP)

The ring-opening metathesis polymerization is an important tool in polymer chemistry, which affords polymers retaining double bonds in backbone.[108] Cyclic olefins containing considerable ring strain are therefore used for ROMP, *i.e.* cyclobutene (CBE), cyclopentene (CPE), *cis*-cyclooctene (COE), norborn-2-ene and norborn-2-ene derivatives (**Figure 7**).[109]

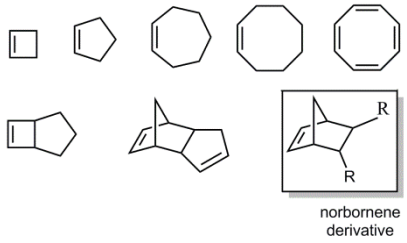
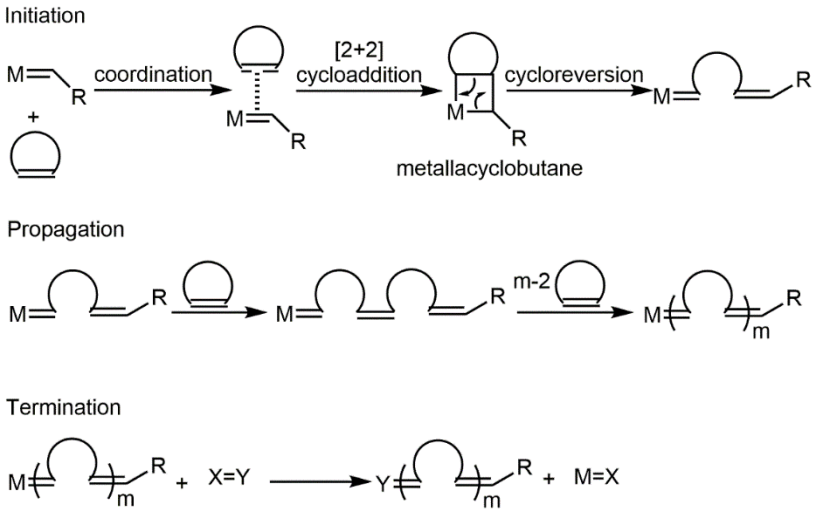


Figure 7. Representative ROMP monomers.[109-111]

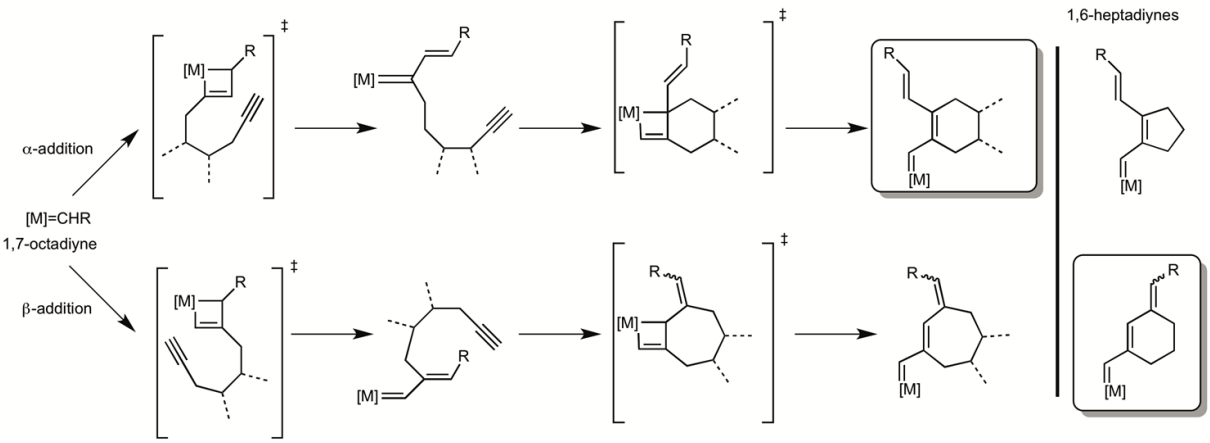
The basic mechanism of ROMP is well-known thanks to research efforts during the last few decades. The main mechanism consists of initiation, propagation and termination (**Scheme 10**).[112] The initiation step involves first coordination of a cyclic olefin on to the metal alkylidene double bond followed by [2+2] cycloaddition to form the corresponding metallacyclobutane intermediate, which then undergoes cycloreversion to generate a new linear metal alkylidene. The chain propagation proceeds in analogy to initiation. In the termination step, a suitable chain terminator is added to react with the active metal alkylidene and remove the metal alkylidene from the growing polymer chain. For *Schrock* catalyst initiated ROMP, the reactions are often terminated by the addition of an aldehyde which reacts with the metal alkylidene in the fashion of a *Wittig*-type reaction.[113] Alternatively, vinyl ether is a common reagent to achieve this chain termination for *Grubbs* catalysts triggered ROMP.[113]



Scheme 10. General mechanism of ROMP.

1.3.2 Cyclopolymerization

Cyclopolymerization with metal alkylidenes is one of the most important polymerization techniques to preapare conjugated polymer backbones.[114-115] Cyclopolymerization of *α*,*ω*-diynes usually produce soluble polymers with conjugated *π*-systems, which can be used as smart materials for electronics applications.[116-117] In the polymerization of *α*,*ω*-heptadiynes both five-membered and six-membered rings can occur in the polymer chain. The mechanism is shown in **Scheme 11** and is applicable to all metal alkylidene triggered cyclopolymerizations. According to **Scheme 11**, a diyne monomer can add to a metal alkylidene double bond in two different ways.[118] One, referred to as *α*-addition, consists of an approach to the metal-carbon double bond in a way that [2+2] cycyloaddition leads to a transition state in which the *α*-carbon to the metal in the metallacyclobutene is trisubstituted. An alternative way, referred to as *β*-addition, entails the approach of the first alkyne group in the diyne to the metal alkylidene in a way that the intermediary metallacyclobuten contains a *β*-carbon that is trisubstituted. Consecutively, productive [2+2] cycloreversion and incorporation of the second alkyne moiety via intramolecular reaction leads in the case of 1,6-heptadiynes to repeat units either consisting of five- or six-membered rings in the repeat units.[115] Accordingly, the use of 1,7-octadiynes leads to six- (*α*-addition) and seven-membered rings (*β*-addition) in the repeat units.[119-120]



Scheme 11. Mechanism of cyclopolymerization by metal alkylidenes.

The most common monomer used for cyclopolymerization is DEDPM (diethyldipropargylmalonate); DEDPM-derived polymer that exclusively contains six-membered rings has a λ_{max} value of 480 nm, compared to a DEDPM-derived polymer containing predominately five-membered rings, which has a λ_{max} value at 530 nm and 590 nm. *Buchmeiser* group reported that first-generation *Schrock* catalysts, *i.e.* $Mo(NAr)(CHCMe_2Ph)(OCMe_3)_2$ in the presence of quinuclidiene, gave poly(DEDPM) that contain > 95% five-membered rings.[121-122]

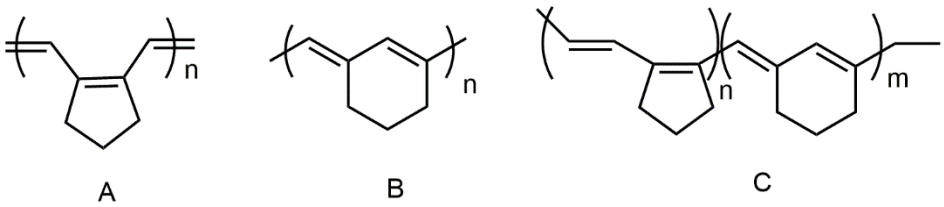
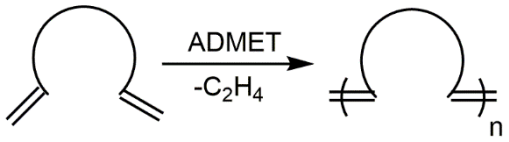


Figure 8. Possible ring structure of poly(1,6-heptadiyenes) prepared by cyclopolymerisation. Poly(cyclopent-1-enylene-1-vinylene)s (A), poly(cyclohex-1-ene-3-methylidene)s (B); and mixed structures (C).

1.3.3 Acyclic Diene Metathesis (ADMET)

In addition to ROMP, the acyclic diene metathesis (ADMET) is considered to be a step-growth/polycondensation type polymerization technique in olefin metathesis. The first successful ADMET polymerization was reported by the *Wagner* group in 1991.[123-

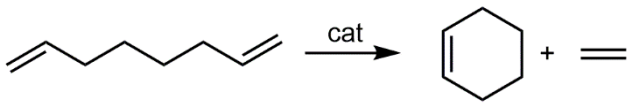
[125] However, while there are no by-products in the case of ROMP, in the ADMET polymerization one molecule of ethylene (CH_2=CH_2) is formed per molecule of monomer. The driving force of the reaction is the loss of small molecules in course of the reaction. The polymer isolated from ADMET-type polymerizations is a strictly linear, unconjugated poly(ene). The equation for ADMET polymerization can be seen in **Scheme 12**. [126-127]



Scheme 12. ADMET polymerization.

1.3.4 Ring-Closing Metathesis (RCM)

Ring-closing metathesis is widely used in organic chemistry for making unsaturated rings and heterocycles. In RCM, terminal dienes are cyclized under release of ethylene. The first RCM reaction was reported in parallel by D. *Villemin*[128] and J. *Tsuri*[129] for the cyclization of diene esters. RCM usually proceeds through [2+2] cyclo-addition/cyclo-reversion steps via metallacyclobutane intermediates.[13] The driving force for RCM reaction is the release of ethylene or other volatile side-products. Dilution governs whether RCM or ADMET is conducted. High dilution favours the ADMET reaction.

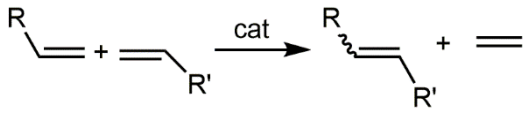


Scheme 13. RCM reaction.

In general, the product formation during RCM depends on the size of the ring and the conformation of the double bond.[130] RCM reaction is currently widely used in natural product synthesis,[131] preparation of different range of heterocycles[132-133] and in enantioselective synthesis.[82,134-137]

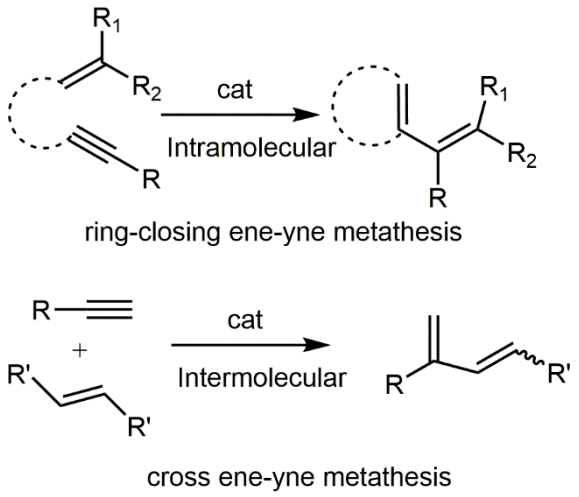
1.3.5 Cross-Metathesis (CM)

The cross metathesis (CM) is the homocoupling between two different olefins to produce more substituted internal olefinic products.[138] The conformation of double bond produced by CM is a mixture of *E*/*Z* isomers. The ratio of *E*/*Z* isomers depends on the starting material, the nature of initiator, and steric effect during reactions.[139]



Scheme 14. Cross-metathesis (CM) reaction.

1.3.6 Ene-Yne Metathesis



Scheme 15. Different types of ene-yne metathesis reactions.

In 1985, *Katz* and coworkers[140] first discovered ene-yne metathesis reaction by using a *Fischer* tungsten carbene complex. Ene-yne metathesis is interesting as well as unique in olefin metathesis reactions. The reaction proceeds by cleavage of double and triple bonds, which afforded a cyclic 1,3-diene. The selectivity (*exo* or *endo*) of the product during ene-yne metathesis depends upon whether the alkene or the alkyne first coordinate to the metal alkylidene.[141] The *endo* selective ring-closing ene-yne

metathesis reaction was reported by *Schrock* and *Hoveyda* using stereogenic molybdenum catalysts.[142]

1.4 N-Heterocyclic Carbenes (NHC)

N-Heterocyclic Carbene (NHC) have emerged as useful and versatile ligands in organometallic chemistry.[143-144] The first use of NHCs as ligand for transition metal complexes was reported almost 40 years ago by *Öfele*[145] and *Wanzlick*.[146] NHCs are cyclic singlet carbenes, which have at least one nitrogen atom in *α*-position to the carbene carbon. NHCs have been widely used because of their nucleophilic character as ligands in metal complexes. A free N-heterocyclic carbene was isolated by *Arduengo et.al.* in 1991[147].

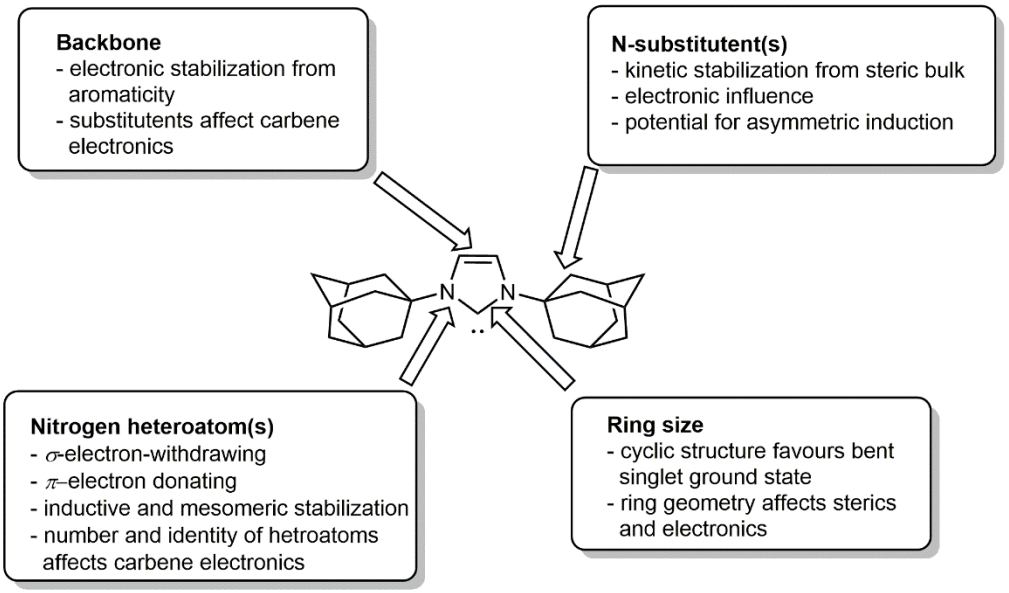


Figure 9. General structural features of a free NHC.

The large adamantly group provides the carbene with kinetic stability. However, NHCs with less bulky substituents on the nitrogen atoms can be isolated, too. The thermodynamic stability is mainly due to the +M effect of the nitrogen atoms, which compensates for the octet gap at the carbene carbon. NHCs are considered strong *σ*-donors with a *π*-back bonding character of up to 45%.[148] For unsaturated NHCs a further stabilization is associated with the 4n+2 *Hückel* aromaticity.[149] The bulky

substituent on nitrogen may enhance the stability of free carbene but it is not a thumb rule because some free NHCs carbene also isolated without sterically demanding substituent on N-atom.[150] The initial hypothesis for the stability of free NHCs was based on steric factors, which prevent dimerization of free carbene. Such a type of stable free carbenes are the imidazolin-2-ylidenes, 1,2,4-triazol-5-ylidene and benzimidazolylidines.[147,151-158]

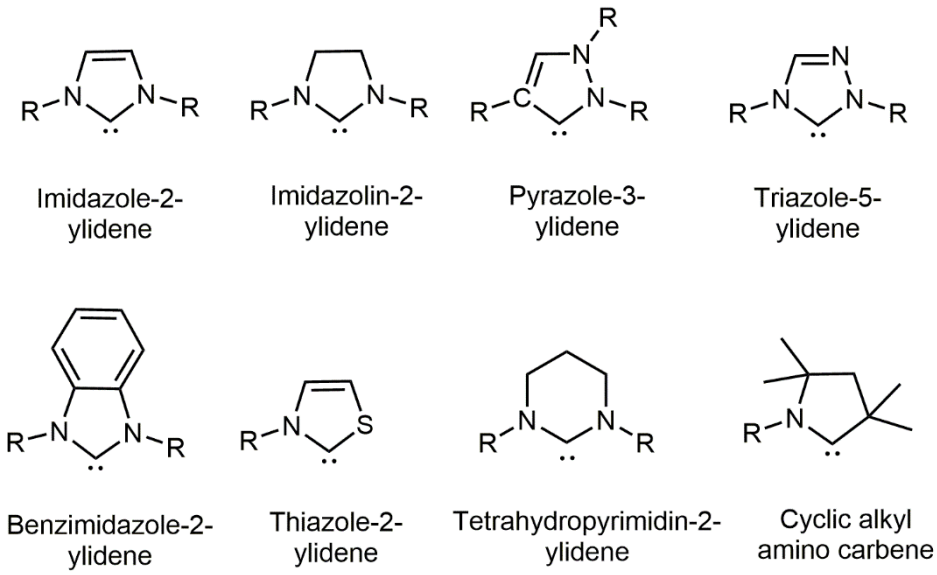


Figure 10. Different carbene frameworks.

Later, the saturated version of IMes was isolated and considered as more *σ*-donating than its unsaturated analogous.[159-160] However, recent studies show that the basicity of free NHCs has a little influence on their saturated and unsaturated analogous. The steric demand of the N-substituent on saturated carbenes determines whether they exist as free NHCs or as entetramine dimers (*Wanzlick equilibrium*). After that, a large variety of free NHCs have been reported with different ring sizes, substitution on the N-atom and on their backbones, but the NHCs with five-membered ring structure are most commonly used. Later, also four-[161-162] and six-membered [163-170] NHCs have been reported. Seven-membered NHC ligands were prepared *in situ* without isolation of the free carbene.[171-172] In the last few years, several novel NHC frameworks have been reported by *Alder*[173-174], *Warkentin*[175], and *Bertrand et.al*.[176-178] In the last few years, *Bertrand* group has developed stable cyclic alkyl amino carbenes (CAAC).[177,179] These stable carbene ligands replaced phosphine in many catalytic

systems, for example with Ru-CAAC alkylidene complexes.[54] These carbene ligands comprise five-member rings similar to NHCs, but one of the *σ*-withdrawing and *π*-donating nitrogen heteroatoms is replaced by a strongly *σ*-donating alkyl group which makes CAAC ligands more nucleophilic. The presence of a quaternary carbon in the *α*-position to the carbene center provides variable steric environments for the CAAC ligand.[180-181]

1.5 References

[1] V. César, G. Lavigne, *Angew. Chem. Int. Ed.*, **2015**, *54*, 3856-3857.

[2] N. Calderon, *Acc. Chem. Res.*, **1972**, *5*, 127-132.

[3] K. Ziegler, E. Holzkamp, H. Breil, H. Martin, *Angew. Chem.*, **1955**, *67*, 426-426.

[4] R. L. Banks, G. C. Bailey, *Ind. Eng. Chem. Prod. Res. Dev.*, **1964**, *3*, 170-173.

[5] G. Natta, G. Dall'Asta, I. W. Bassi, G. Carella, *Macromol. Chem. Phys.*, **1966**, *91*, 87-106.

[6] N. Calderon, H. Y. Chen, K. W. Scott, *Tetrahedron Lett.*, **1967**, *8*, 3327-3329.

[7] T. M. Trnka, R. H. Grubbs, *Acc. Chem. Res.*, **2001**, *34*, 18-29.

[8] R. H. Grubbs, *Tetrahedron*, **2004**, *60*, 7117-7140.

[9] R. H. Grubbs, *Progress in Inorganic Chemistry*, John Wiley & Sons, Inc., **2007**, p 1-50.

[10] A. Fürstner, *Angew. Chem. Int. Ed.*, **2000**, *39*, 3012-3043.

[11] M. R. Buchmeiser, *Chem. Rev.*, **2000**, *100*, 1565-1604.

[12] A. H. Hoveyda, A. R. Zhugralin, *Nature*, **2007**, *450*, 243-251.

[13] P. Jean-Louis Hérisson, Y. Chauvin, *Macromol. Chem. Phys.*, **1971**, *141*, 161-176.

[14] Y. Chauvin, *Angew. Chem. Int. Ed.*, **2006**, *45*, 3740-3747.

[15] E. O. Fischer, A. Maasböl, *Angew. Chem. Int. Ed.*, **1964**, *3*, 580-581.

[16] G. Wilkinson, *Angew. Chem.*, **1974**, *86*, 664-667.

[17] E. O. Fischer, *Angew. Chem.*, **1974**, *86*, 651-663.

[18] E. O. Fischer, G. Kreis, C. G. Kreiter, J. Müller, G. Huttner, H. Lorenz, *Angew. Chem. Int. Ed.*, **1973**, *12*, 564-565.

[19] F. N. Tebbe, G. W. Parshall, G. S. Reddy, *J. Am. Chem. Soc.*, **1978**, *100*, 3611-3613.

[20] T. R. Howard, J. B. Lee, R. H. Grubbs, *J. Am. Chem. Soc.*, **1980**, *102*, 6876-6878.

[21] R. R. Schrock, G. W. Parshall, *Chem. Rev.*, **1976**, *76*, 243-268.

[22] R. R. Schrock, *J. Am. Chem. Soc.*, **1974**, *96*, 6796-6797.

[23] R. R. Schrock, J. D. Fellmann, *J. Am. Chem. Soc.*, **1978**, *100*, 3359-3370.

[24] S. M. Rocklage, J. D. Fellmann, G. A. Rupprecht, L. W. Messerle, R. R. Schrock, *J. Am. Chem. Soc.*, **1981**, *103*, 1440-1447.

[25] R. Schrock, S. Rocklage, J. Wengrovius, G. Rupprecht, J. Fellmann, *J. Mol. Catal.*, **1980**, *8*, 73-83.

[26] R. R. Schrock, *Acc. Chem. Res.*, **1979**, *12*, 98-104.

[27] J. H. Wengrovius, R. R. Schrock, M. R. Churchill, J. R. Missert, W. J. Youngs, *J. Am. Chem. Soc.*, **1980**, *102*, 4515-4516.

[28] J. R. M. Kress, M. J. M. Russell, M. G. Wesolek, J. A. Osborn, *J. Chem. Soc., Chem. Commun.*, **1980**, 431-432.

[29] J. Kress, M. Wesolek, J.-P. Le Ny, J. A. Osborn, *J. Chem. Soc., Chem. Commun.*, **1981**, 1039-1040.

[30] H. H. Fox, M. H. Schofield, R. R. Schrock, *Organometallics*, **1994**, *13*, 2804-2815.

[31] R. R. Schrock, R. T. DePue, J. Feldman, C. J. Schaverien, J. C. Dewan, A. H. Liu, *J. Am. Chem. Soc.*, **1988**, *110*, 1423-1435.

[32] R. R. Schrock, J. S. Murdzek, G. C. Bazan, J. Robbins, M. DiMare, M. O'Regan, *J. Am. Chem. Soc.*, **1990**, *112*, 3875-3886.

[33] R. R. Schrock, R. T. DePue, J. Feldman, K. B. Yap, D. C. Yang, W. M. Davis, L. Park, M. DiMare, M. Schofield, *Organometallics*, **1990**, *9*, 2262-2275.

[34] J. H. Oskam, H. H. Fox, K. B. Yap, D. H. McConville, R. O`Dell, B. J. Lichtenstein, R. R. Schrock, *J. Organomet. Chem.*, **1993**, *459*, 185-198.

[35] H. H. Fox, K. B. Yap, J. Robbins, S. Cai, R. R. Schrock, *Inorg. Chem.*, **1992**, *31*, 2287-2289.

[36] R. R. Schrock, J. Y. Jamieson, J. P. Araujo, P. J. Bonitatebus Jr, A. Sinha, L. P. H. Lopez, *J. Organomet. Chem.*, **2003**, *684*, 56-67.

[37] Z. J. Tonzetich, R. R. Schrock, P. Müller, *Organometallics*, **2006**, *25*, 4301-4306.

[38] J. H. Oskam, R. R. Schrock, *J. Am. Chem. Soc.*, **1993**, *115*, 11831-11845.

[39] M. Brookhart, M. L. H. Green, L.-L. Wong, *Progress in Inorganic Chemistry*, John Wiley & Sons, Inc., **2007**, p 1-124.

[40] T. R. Cundari, M. S. Gordon, *J. Am. Chem. Soc.*, **1991**, *113*, 5231-5243.

[41] T. R. Cundari, M. S. Gordon, *Organometallics*, **1992**, *11*, 55-63.

[42] R. R. Schrock, A. H. Hoveyda, *Angew. Chem. Int. Ed.*, **2003**, *42*, 4592-4633.

[43] L. C. H. Gerber, R. R. Schrock, P. Müller, M. K. Takase, *J. Am. Chem. Soc.*, **2011**, *133*, 18142-18144.

[44] J. H. Oskam, R. R. Schrock, *J. Am. Chem. Soc.*, **1992**, *114*, 7588-7590.

[45] J. B. Alexander, D. S. La, D. R. Cefalo, A. H. Hoveyda, R. R. Schrock, *J. Am. Chem. Soc.*, **1998**, *120*, 4041-4042.

[46] D. S. La, J. B. Alexander, D. R. Cefalo, D. D. Graf, A. H. Hoveyda, R. R. Schrock, *J. Am. Chem. Soc.*, **1998**, *120*, 9720-9721.

[47] D. H. McConville, J. R. Wolf, R. R. Schrock, *J. Am. Chem. Soc.*, **1993**, *115*, 4413-4414.

[48] R. O'Dell, D. H. McConville, G. E. Hofmeister, R. R. Schrock, *J. Am. Chem. Soc.*, **1994**, *116*, 3414-3423.

[49] S. T. Nguyen, L. K. Johnson, R. H. Grubbs, J. W. Ziller, *J. Am. Chem. Soc.*, **1992**, *114*, 3974-3975.

[50] R. H. Grubbs, *Angew. Chem. Int. Ed.*, **2006**, *45*, 3760-3765.

[51] G. C. Vougioukalakis, R. H. Grubbs, *Chem. Rev.*, **2010**, *110*, 1746-1787.

[52] H. Clavier, K. Grela, A. Kirschning, M. Mauduit, S. P. Nolan, *Angew. Chem. Int. Ed.*, **2007**, *46*, 6786-6801.

[53] R. H. Grubbs, A. G. Wenzel, *Handbook of Metathesis, Volume 1: Catalyst Development and Mechanism*, 2nd ed., Wiley, **2015**.

[54] V. M. Marx, A. H. Sullivan, M. Melaimi, S. C. Virgil, B. K. Keitz, D. S. Weinberger, G. Bertrand, R. H. Grubbs, *Angew. Chem. Int. Ed.*, **2015**, *54*, 1919-1923.

[55] J. S. Kingsbury, J. P. A. Harrity, P. J. Bonitatebus, A. H. Hoveyda, *J. Am. Chem. Soc.*, **1999**, *121*, 791-799.

[56] Z. Wu, S. T. Nguyen, R. H. Grubbs, J. W. Ziller, *J. Am. Chem. Soc.*, **1995**, *117*, 5503-5511.

[57] C. Samojłowicz, M. Bieniek, K. Grela, *Chem. Rev.*, **2009**, *109*, 3708-3742.

[58] M. S. Sanford, J. A. Love, R. H. Grubbs, *Organometallics*, **2001**, *20*, 5314-5318.

[59] B. K. Keitz, J. Bouffard, G. Bertrand, R. H. Grubbs, *J. Am. Chem. Soc.*, **2011**, *133*, 8498-8501.

[60] T. Ung, A. Hejl, R. H. Grubbs, Y. Schrodi, *Organometallics*, **2004**, *23*, 5399-5401.

[61] M. B. Herbert, R. H. Grubbs, *Angew. Chem. Int. Ed.*, **2015**, *54*, 5018-5024.

[62] S. Gessler, S. Randl, S. Blechert, *Tetrahedron Lett.*, **2000**, *41*, 9973-9976.

[63] A. Michrowska, R. Bujok, S. Harutyunyan, V. Sashuk, G. Dolgonos, K. Grela, *J. Am. Chem. Soc.*, **2004**, *126*, 9318-9325.

[64] R. K. M. Khan, S. Torker, A. H. Hoveyda, *J. Am. Chem. Soc.*, **2013**, *135*, 10258-10261.

[65] M. J. Koh, R. K. M. Khan, S. Torker, M. Yu, M. S. Mikus, A. H. Hoveyda, *Nature*, **2015**, *517*, 181-186.

[66] M. J. Koh, R. K. M. Khan, S. Torker, A. H. Hoveyda, *Angew. Chem. Int. Ed.*, **2014**, *53*, 1968-1972.

[67] M. R. Buchmeiser, I. Ahmad, V. Gurram, P. S. Kumar, *Macromolecules*, **2011**, *44*, 4098-4106.

[68] P. S. Kumar, K. Wurst, M. R. Buchmeiser, *J. Am. Chem. Soc.*, **2009**, *131*, 387-395.

[69] T. S. Halbach, S. Mix, D. Fischer, S. Maechling, J. O. Krause, C. Sievers, S. Blechert, O. Nuyken, M. R. Buchmeiser, *J. Org. Chem.*, **2005**, *70*, 4687-4694.

[70] C. P. Ferraz, B. Autenrieth, W. Frey, M. R. Buchmeiser, *ChemCatChem*, **2014**, *6*, 191-198.

[71] B. Autenrieth, W. Frey, M. R. Buchmeiser, *Chem. Eur. J.*, **2012**, *18*, 14069-14078.

[72] S. C. Marinescu, R. Singh, A. S. Hock, K. M. Wampler, R. R. Schrock, P. Müller, *Organometallics*, **2008**, *27*, 6570-6578.

[73] A. S. Hock, R. R. Schrock, A. H. Hoveyda, *J. Am. Chem. Soc.*, **2006**, *128*, 16373-16375.

[74] S. C. Marinescu, R. R. Schrock, B. Li, A. H. Hoveyda, *J. Am. Chem. Soc.*, **2009**, *131*, 58-59.

[75] R. R. Schrock, *Chem. Rev.*, **2009**, *109*, 3211-3226.

[76] A. J. Jiang, J. H. Simpson, P. Müller, R. R. Schrock, *J. Am. Chem. Soc.*, **2009**, *131*, 7770-7780.

[77] R. R. Schrock, A. J. Jiang, S. C. Marinescu, J. H. Simpson, P. Müller, *Organometallics*, **2010**, *29*, 5241-5251.

[78] A. G. Lichtscheidl, V. W. L. Ng, P. Müller, M. K. Takase, R. R. Schrock, *Organometallics*, **2012**, *31*, 2388-2394.

[79] L. C. H. Gerber, R. R. Schrock, P. Müller, *Organometallics*, **2013**, *32*, 2373-2378.

[80] R. Singh, R. R. Schrock, P. Müller, A. H. Hoveyda, *J. Am. Chem. Soc.*, **2007**, *129*, 12654-12655.

[81] S. J. Malcolmson, S. J. Meek, E. S. Sattely, R. R. Schrock, A. H. Hoveyda, *Nature*, **2008**, *456*, 933-937.

[82] E. S. Sattely, S. J. Meek, S. J. Malcolmson, R. R. Schrock, A. H. Hoveyda, *J. Am. Chem. Soc.*, **2009**, *131*, 943-953.

[83] M. M. Flook, A. J. Jiang, R. R. Schrock, P. Müller, A. H. Hoveyda, *J. Am. Chem. Soc.*, **2009**, *131*, 7962-7963.

[84] M. M. Flook, L. C. H. Gerber, G. T. Debelouchina, R. R. Schrock, *Macromolecules*, **2010**, *43*, 7515-7522.

[85] M. M. Flook, J. Börner, S. M. Kilyanek, L. C. H. Gerber, R. R. Schrock, *Organometallics*, **2012**, *31*, 6231-6243.

[86] D. V. Peryshkov, R. R. Schrock, M. K. Takase, P. Müller, A. H. Hoveyda, *J. Am. Chem. Soc.*, **2011**, *133*, 20754-20757.

[87] D. V. Peryshkov, R. R. Schrock, *Organometallics*, **2012**, *31*, 7278-7286.

[88] H. Jeong, J. M. John, R. R. Schrock, A. H. Hoveyda, *J. Am. Chem. Soc.*, **2015**, *137*, 2239-2242.

[89] A. J. Jiang, Y. Zhao, R. R. Schrock, A. H. Hoveyda, *J. Am. Chem. Soc.*, **2009**, *131*, 16630-16631.

[90] S. C. Marinescu, R. R. Schrock, P. Müller, M. K. Takase, A. H. Hoveyda, *Organometallics*, **2011**, *30*, 1780-1782.

[91] E. M. Townsend, R. R. Schrock, A. H. Hoveyda, *J. Am. Chem. Soc.*, **2012**, *134*, 11334-11337.

[92] C. Wang, F. Haeffner, R. R. Schrock, A. H. Hoveyda, *Angew. Chem. Int. Ed.*, **2013**, *52*, 1939-1943.

[93] M. J. Koh, T. T. Nguyen, H. Zhang, R. R. Schrock, A. H. Hoveyda, *Nature*, **2016**, *531*, 459-465.

[94] Z. J. Tonzetich, A. J. Jiang, R. R. Schrock, P. Müller, *Organometallics*, **2006**, *25*, 4725-4727.

[95] A. J. Jiang, R. R. Schrock, P. Müller, *Organometallics*, **2008**, *27*, 4428-4438.

[96] K. C. Hultzsch, J. A. Jernelius, A. H. Hoveyda, R. R. Schrock, *Angew. Chem. Int. Ed.*, **2002**, *41*, 589-593.

[97] R. M. Kroll, N. Schuler, S. Lubbad, M. R. Buchmeiser, *Chem. Commun.*, **2003**, 2742-2743.

[98] D. Wang, R. Kröll, M. Mayr, K. Wurst, M. R. Buchmeiser, *Adv. Synth. Catal.*, **2006**, *348*, 1567-1579.

[99] M. R. Buchmeiser, *Olefin Metathesis*, John Wiley & Sons, Inc., **2014**, p 495-514.

[100] S. J. Dolman, K. C. Hultzsch, F. Pezet, X. Teng, A. H. Hoveyda, R. R. Schrock, *J. Am. Chem. Soc.*, **2004**, *126*, 10945-10953.

[101] F. Blanc, J. Thivolle-Cazat, J.-M. Basset, C. Copéret, A. S. Hock, Z. J. Tonzetich, R. R. Schrock, *J. Am. Chem. Soc.*, **2007**, *129*, 1044-1045.

[102] C. Coperet, *Dalton Trans.*, **2007**, 5498-5504.

[103] V. Mougel, C. B. Santiago, P. A. Zhizhko, E. N. Bess, J. Varga, G. Frater, M. S. Sigman, C. Copéret, *J. Am. Chem. Soc.*, **2015**, *137*, 6699-6704.

[104] M. P. Conley, W. P. Forrest, V. Mougel, C. Copéret, R. R. Schrock, *Angew. Chem. Int. Ed.*, **2014**, *53*, 14221-14224.

[105] M. P. Conley, V. Mougel, D. V. Peryshkov, W. P. Forrest, D. Gajan, A. Lesage, L. Emsley, C. Copéret, R. R. Schrock, *J. Am. Chem. Soc.*, **2013**, *135*, 19068-19070.

[106] N. Rendón, R. Berthoud, F. Blanc, D. Gajan, T. Maishal, J.-M. Basset, C. Copéret, A. Lesage, L. Emsley, S. C. Marinescu, R. Singh, R. R. Schrock, *Chem. Eur. J.*, **2009**, *15*, 5083-5089.

[107] F. Blanc, R. Berthoud, C. Copéret, A. Lesage, L. Emsley, R. Singh, T. Kreickmann, R. R. Schrock, *Proc. Natl. Acad. Sci.*, **2008**, *105*, 12123-12127.

[108] R. H. Grubbs, E. Khosravi, *Handbook of Metathesis, Volume 3: Polymer Synthesis*, Wiley, **2015**.

[109] C. W. Bielawski, R. H. Grubbs, *Prog. Polym. Sci.*, **2007**, *32*, 1-29.

[110] R. Walker, R. M. Conrad, R. H. Grubbs, *Macromolecules*, **2009**, *42*, 599-605.

[111] R. H. Grubbs, *Handbook of metathesis: Applications in polymer synthesis*, Wiley-VCH, **2003**.

[112] S. Sutthasupa, M. Shiotsuki, F. Sanda, *Polym. J.*, **2010**, *42*, 905-915.

[113] S. Hilf, A. F. M. Kilbinger, *Nat. Chem.*, **2009**, *1*, 537-546.

[114] H. H. Fox, R. R. Schrock, *Organometallics*, **1992**, *11*, 2763-2765.

[115] H. H. Fox, M. O. Wolf, R. O'Dell, B. L. Lin, R. R. Schrock, M. S. Wrighton, *J. Am. Chem. Soc.*, **1994**, *116*, 2827-2843.

[116] S.-K. Choi, Y.-S. Gal, S.-H. Jin, H. K. Kim, *Chem. Rev.*, **2000**, *100*, 1645-1682.

[117] A. Hagfeldt, M. Grätzel, *Acc. Chem. Res.*, **2000**, *33*, 269-277.

[118] M. R. Buchmeiser, *Polym. Rev.*, **2016**, 00-00.

[119] S. Naumann, J. Unold, W. Frey, M. R. Buchmeiser, *Macromolecules*, **2011**, *44*, 8380-8387.

[120] J. Unold, D. Wang, W. Frey, M. R. Buchmeiser, *Polym. Chem.*, **2013**, *4*, 4219-4233.

[121] U. Anders, O. Nuyken, M. R. Buchmeiser, K. Wurst, *Angew. Chem. Int. Ed.*, **2002**, *41*, 4044-4047.

[122] U. Anders, M. Wagner, O. Nuyken, M. R. Buchmeiser, *Macromolecules*, **2003**, *36*, 2668-2673.

[123] K. B. Wagener, J. M. Boncella, J. G. Nel, *Macromolecules*, **1991**, *24*, 2649-2657.

[124] D. W. Smith, K. B. Wagener, *Macromolecules*, **1993**, *26*, 1633-1642.

[125] M. D. Schulz, K. B. Wagener, *Macromol. Chem. Phys*, **2014**, *215*, 1936-1945.

[126] T. Haque, K. Nomura, *Catalysts*, **2015**, *5*, 500.

[127] H. Mutlu, L. M. de Espinosa, M. A. R. Meier, *Chem. Soc. Rev.*, **2011**, *40*, 1404-1445.

[128] D. Villemin, *Tetrahedron Lett.*, **1980**, *21*, 1715-1718.

[129] J. Tsuji, S. Hashiguchi, *Tetrahedron Lett.*, **1980**, *21*, 2955-2958.

[130] M. Schuster, S. Blechert, *Angew. Chem. Int. Ed.*, **1997**, *36*, 2036-2056.

[131] S. Hölder, S. Blechert, *Synlett*, **1996**, *1996*, 505-506.

[132] G. C. Fu, R. H. Grubbs, *J. Am. Chem. Soc.*, **1992**, *114*, 5426-5427.

[133] S. E. Denmark, S.-M. Yang, *Tetrahedron*, **2004**, *60*, 9695-9708.

[134] J. A. Jernelius, R. R. Schrock, A. H. Hoveyda, *Tetrahedron*, **2004**, *60*, 7345-7351.

[135] M. Murakami, S. Kadowaki, T. Matsuda, *Org. Lett.*, **2005**, *7*, 3953-3956.

[136] A.-L. Lee, S. J. Malcolmson, A. Puglisi, R. R. Schrock, A. H. Hoveyda, *J. Am. Chem. Soc.*, **2006**, *128*, 5153-5157.

[137] S. J. Dolman, R. R. Schrock, A. H. Hoveyda, *Org. Lett.*, **2003**, *5*, 4899-4902.

[138] S. J. Connon, S. Blechert, *Angew. Chem. Int. Ed.*, **2003**, *42*, 1900-1923.

[139] A. K. Chatterjee, T.-L. Choi, D. P. Sanders, R. H. Grubbs, *J. Am. Chem. Soc.*, **2003**, *125*, 11360-11370.

[140] T. J. Katz, T. M. Sivavec, *J. Am. Chem. Soc.*, **1985**, *107*, 737-738.

[141] E. C. Hansen, D. Lee, *J. Am. Chem. Soc.*, **2004**, *126*, 15074-15080.

[142] Y.-J. Lee, R. R. Schrock, A. H. Hoveyda, *J. Am. Chem. Soc.*, **2009**, *131*, 10652-10661.

[143] W. A. Herrmann, *Angew. Chem. Int. Ed.*, **2002**, *41*, 1290-1309.

[144] M. N. Hopkinson, C. Richter, M. Schedler, F. Glorius, *Nature*, **2014**, *510*, 485-496.

[145] K. Öfele, *J. Organomet. Chem.*, **1968**, *12*, P42-P43.

[146] H. W. Wanzlick, H. J. Schönherr, *Angew. Chem. Int. Ed.*, **1968**, *7*, 141-142.

[147] A. J. Arduengo, R. L. Harlow, M. Kline, *J. Am. Chem. Soc.*, **1991**, *113*, 361-363.

[148] H. Jacobsen, A. Correa, A. Poater, C. Costabile, L. Cavallo, *Coord. Chem. Rev.*, **2009**, *253*, 687-703.

[149] M. K. Denk, J. M. Rodezno, S. Gupta, A. J. Lough, *J. Organomet. Chem.*, **2001**, *617–618*, 242-253.

[150] A. J. Arduengo, H. V. R. Dias, R. L. Harlow, M. Kline, *J. Am. Chem. Soc.*, **1992**, *114*, 5530-5534.

[151] D. Enders, K. Breuer, G. Raabe, J. Runsink, J. H. Teles, J.-P. Melder, K. Ebel, S. Brode, *Angew. Chem. Int. Ed.*, **1995**, *34*, 1021-1023.

[152] D. Enders, H. Gielen, *J. Organomet. Chem.*, **2001**, *617–618*, 70-80.

[153] G. Altenhoff, R. Goddard, C. W. Lehmann, F. Glorius, *J. Am. Chem. Soc.*, **2004**, *126*, 15195-15201.

[154] M. Alcarazo, S. J. Roseblade, A. R. Cowley, R. Fernández, J. M. Brown, J. M. Lassaletta, *J. Am. Chem. Soc.*, **2005**, *127*, 3290-3291.

[155] W. A. Herrmann, L. J. Goossen, G. R. J. Artus, C. Köcher, *Organometallics*, **1997**, *16*, 2472-2477.

[156] W. A. Herrmann, L. J. Goossen, M. Spiegler, *Organometallics*, **1998**, *17*, 2162-2168.

[157] A. Furstner, M. Alcarazo, V. Cesar, C. W. Lehmann, *Chem. Commun.*, **2006**, 2176-2178.

[158] G. Altenhoff, R. Goddard, C. W. Lehmann, F. Glorius, *Angew. Chem. Int. Ed.*, **2003**, *42*, 3690-3693.

[159] A. M. Magill, K. J. Cavell, B. F. Yates, *J. Am. Chem. Soc.*, **2004**, *126*, 8717-8724.

[160] R. Dorta, E. D. Stevens, N. M. Scott, C. Costabile, L. Cavallo, C. D. Hoff, S. P. Nolan, *J. Am. Chem. Soc.*, **2005**, *127*, 2485-2495.

[161] E. Despagnet-Ayoub, R. H. Grubbs, *J. Am. Chem. Soc.*, **2004**, *126*, 10198-10199.

[162] E. Despagnet-Ayoub, R. H. Grubbs, *Organometallics*, **2005**, *24*, 338-340.

[163] Y. Zhang, D. Wang, K. Wurst, M. R. Buchmeiser, *J. Organomet. Chem.*, **2005**, *690*, 5728-5735.

[164] P. Bazinet, G. P. A. Yap, D. S. Richeson, *J. Am. Chem. Soc.*, **2003**, *125*, 13314-13315.

[165] R. W. Alder, M. E. Blake, C. Bortolotti, S. Bufali, C. P. Butts, E. Linehan, J. M. Oliva, A. Guy Orpen, M. J. Quayle, *Chem. Commun.*, **1999**, 241-242.

[166] J. Yun, E. R. Marinez, R. H. Grubbs, *Organometallics*, **2004**, *23*, 4172-4173.

[167] I. Özdemir, S. Demir, B. Çetinkaya, E. Çetinkaya, *J. Organomet. Chem.*, **2005**, *690*, 5849-5855.

[168] M. Mayr, K. Wurst, K.-H. Ongania, M. R. Buchmeiser, *Chem. Eur. J.*, **2004**, *10*, 1256-1266.

[169] W. A. Herrmann, S. K. Schneider, K. Öfele, M. Sakamoto, E. Herdtweck, *J. Organomet. Chem.*, **2004**, *689*, 2441-2449.

[170] S. K. Schneider, W. A. Herrmann, E. Herdtweck, *J. Mol. Catal. A: Chem.*, **2006**, *245*, 248-254.

[171] C. C. Scarborough, M. J. W. Grady, I. A. Guzei, B. A. Gandhi, E. E. Bunel, S. S. Stahl, *Angew. Chem. Int. Ed.*, **2005**, *44*, 5269-5272.

[172] C. C. Scarborough, B. V. Popp, I. A. Guzei, S. S. Stahl, *J. Organomet. Chem.*, **2005**, *690*, 6143-6155.

[173] R. W. Alder, C. P. Butts, A. G. Orpen, *J. Am. Chem. Soc.*, **1998**, *120*, 11526-11527.

[174] R. W. Alder, P. R. Allen, M. Murray, A. G. Orpen, *Angew. Chem. Int. Ed.*, **1996**, *35*, 1121-1123.

[175] P. Couture, J. K. Terlouw, J. Warkentin, *J. Am. Chem. Soc.*, **1996**, *118*, 4214-4215.

[176] V. Lavallo, J. Mafhouz, Y. Canac, B. Donnadieu, W. W. Schoeller, G. Bertrand, *J. Am. Chem. Soc.*, **2004**, *126*, 8670-8671.

[177] V. Lavallo, Y. Canac, C. Präsang, B. Donnadieu, G. Bertrand, *Angew. Chem. Int. Ed.*, **2005**, *44*, 5705-5709.

[178] X. Cattoën, H. Gornitzka, D. Bourissou, G. Bertrand, *J. Am. Chem. Soc.*, **2004**, *126*, 1342-1343.

[179] V. Lavallo, Y. Canac, A. DeHope, B. Donnadieu, G. Bertrand, *Angew. Chem. Int. Ed.*, **2005**, *44*, 7236-7239.

[180] M. Soleilhavoup, G. Bertrand, *Acc. Chem. Res.*, **2015**, *48*, 256-266.

[181] B. Rao, H. Tang, X. Zeng, L. Liu, M. Melaimi, G. Bertrand, *Angew. Chem. Int. Ed.*, **2015**, *54*, 14915-14919.

Chapter 2

High Oxidation State Mo-NHC Alkylidene Complexes: Functional-Group Tolerant Cationic Olefin Metathesis Catalysts

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2.1 Introduction

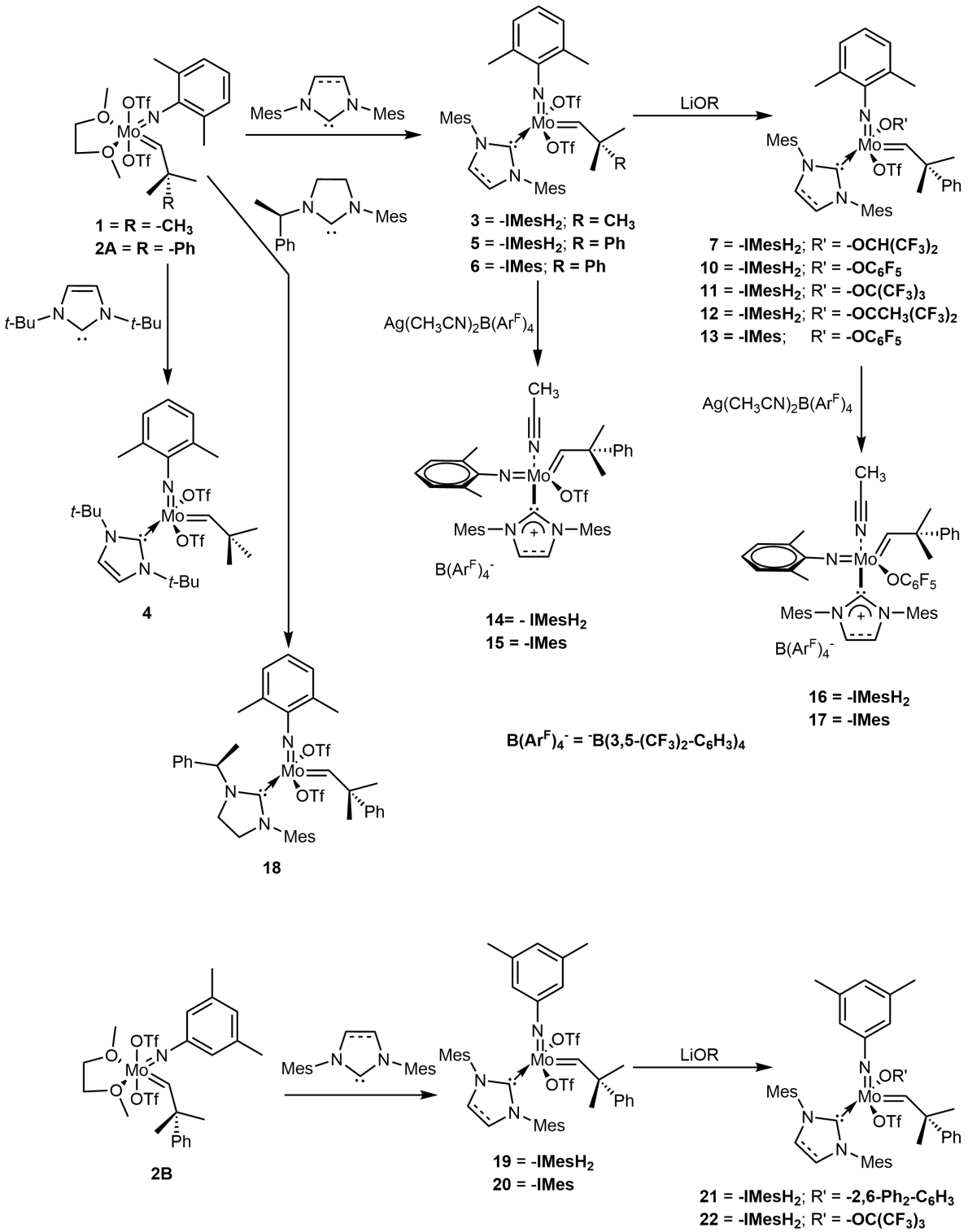
Olefin metathesis has become one of the most important tools for both organic and polymer chemistry.[1-9] It is now over 40 years since the first well-defined *Schrock* catalyst was isolated and fully characterized. In fact, there exist many variations of *Schrock* catalysts, whether for use in polymer chemistry or organic synthesis.[8] Still, today the most challenging task in olefin metathesis is a single-site catalyst, which is highly active, tolerant *vs.* a large number of functional groups, water and air. Also, it should be highly stereo- and regio-selective. Concomitantly, high oxidation state group 6 metal imido alkylidene and oxo alkylidene catalysts clearly fulfill the requirements of stereo-selectivity and regio-selectivity but the functional-group tolerance of group 6 metal alkylidenes is a challenging aspect.[10-16] However, so far they are not competitive to group 8 metal alkylidenes (Ru-alkylidene complexes), which proved to be stable towards a large number of protic groups, water and air.[17] In search for olefin metathesis active catalysts based on cheap metals, this work aims on combining the advantages of group 6 and 8 metal alkylidene catalytic systems. In doing that, the first high oxidation state N-heterocyclic carbene (NHC) complexes of *Schrock* molybdenum imido alkylidene bis(triflate) complexes were prepared. The novel Mo-imido alkylidene NHC complexes are tolerant to functional-groups and have reactivities that can in some cases even reveal though of ruthenium catalysts. Particularly Mo-imido alkylidene bis(triflate) NHC catalysts display functional-group tolerance for hydroxyls, aldehydes, carboxylic acids and *sec*-amines, at least in ring-opening metathesis polymerization (ROMP) and in the cyclopolymerization of *α*,*ω*-diynes, exceeding in this regard high oxidation state molybdenum-based *Schrock* catalysts. In view of these interesting and attracting properties of these novel catalysts, the first cationic 14-electron Mo-imido alkylidene NHC complexes have been prepared and used in various olefin metathesis reactions. Also, tailored structural variations in the imido and in the NHC-ligand, both to get access to defined catalyst structures and to determine any structural limits in this novel class of olefin metathesis catalysts have been carried out. Finally, using a chiral NHC, the first enantiomerically pure Mo-imido alkylidene NHC complex has been prepared. Selected results in ring-closing metathesis (RCM), cross-metathesis (CM) and homometathesis (HM) reactions are presented. Finally, it is demonstrated that this novel class of catalysts displays

substantial activity even at high temperature (140 °C), *e.g.,* in RCM. Based on the observation that the Mo-imido alkylidene bis(triflate) NHC complexes show a coalescence temperature (T_c) for two triflate groups, activation mechanisms, *e.g.,* based on a Berry-type pseudorotation, *i.e.* interconversion between trigonal bipyramidal (TBP) configurations through a square pyramidal (SP) one, are proposed. Activation of the catalysts through release of a triflate in the SP configuration is in full accordance with the observed reactivity of the neutral Mo-imido alkylidene bis(triflate) NHC complexes and with ^{19}F-NMR. In this chapter, a comprehensive overview over the synthesis as well as the applications of these novel catalysts with reference to different olefin metathesis reactions are given.

2.2 Results and Discussion

2.2.1 Synthesis of molybdenum imido alkylidene NHC complexes

The Mo-imido alkylidene bis(triflate) complexes of the general formula Mo(NR')(CHCMe$_2$Ph)(OTf)$_2$DME[18] (R' = 2,6-Me$_2$-C$_6$H$_3$; 3,5-Me$_2$-C$_6$H$_3$; OTf = CF$_3$SO$_3$; DME = 1,2-dimethoxyethane) were used as starting materials. Mo-imido alkylidene NHC complexes **3-22** have been prepared as outlined in **Scheme 16**. Reactions of the corresponding Mo-imido alkylidene bis(triflate) progenitors, for example, [Mo(N-2,6-Me$_2$-C$_6$H$_3$)(CH-*t*Bu)(OTf)$_2$DME] (**1**) and [Mo(N-2,6-Me$_2$-C$_6$H$_3$)(CHCMe$_2$Ph)(OTf)$_2$DME] (**2A**) (switching from [Mo(N-2,6-Me$_2$-C$_6$H$_3$)(CH-*t*Bu)(OTf)$_2$DME] (**1**) to [Mo(N-2,6-Me$_2$-C$_6$H$_3$)(CHCMe$_2$Ph)(OTf)$_2$(DME)] (**2A**), because of synthetic difficulties with neopentylidene compared to neophylidene progenitors) with 1,3-dimesitylimidazolin-2-ylidene (IMesH$_2$), 1,3-dimesitylimidazol-2-ylidene (IMes) and 1,3-ditertbutylimidazol-2-ylidene (I-*t*Bu) yielded the corresponding target complexes **3**, **4**, **5** and **6** in quantitative yield.[19] The two triflate anions in the Mo-imido alkylidene bis(triflate) NHC complexes can generally be addressed independently (**3**-**6**, **18** and **25**) or cooperatively (**19** and **20**). Thus, their reactions with one equivalent of LiOR [R = -CH(CF$_3$)$_2$, -C$_6$F$_5$, -C(CF$_3$)$_3$ and -C(CH$_3$)(CF$_3$)$_2$] offer access to compounds **7**, **10**-**13**, respectively. Compounds **5** and **6** were converted to the cationic complexes **14** and **15** via reactions with Ag(CH$_3$CN)$_2$B(Ar^F)$_4$.



Scheme 16. Synthesis of compounds **3**-**22**.

The monoalkoxide cationic complexes **16** and **17** were accessible via reaction of the corresponding monoalkoxide complexes (**10** and **13**) with $Ag(CH_3CN)_2B(Ar^F)_4$. Compound **18** was only accessible via reaction of (1-*R*-phenethyl)-3-

mesitylimidazolidin-2-ylidene), which was prepared via *in-situ* deprotonation with KHMDS. Compound **3** (**Figure 11**) is a five-fold coordinated 16-electron complex and crystallizes in the orthorhombic system *Pbca*, a = 1824.13(6), b = 2117.49(6), c = 2216.35(5) pm, $\alpha = \beta = \gamma = 90°$, Z = 8. In the solid state, complex **3** exists in its neutral form. The ligands adopt a square pyramidal (SP) (τ = 0.013)[20] geometry with the Mo-alkylidene unit in the apical position. The distance Mo(1)-C(30) is 187.3(3) pm and thus somewhat shorter than that in the Mo-alkylidene in [Mo(NAr')(CH-*t*Bu)(OTf)$_2$DME](190.0/193.0 pm).[21] The distance Mo(1)-O(1) with the triflate being *trans* to the NHC (δ_F = -76.7 ppm) is somewhat longer than for the one that is *trans* to the imido (δ_F = -74.6 ppm) ligand [Mo(1)-O(4) 211.45(18) *vs.* 213.52 (18) pm].

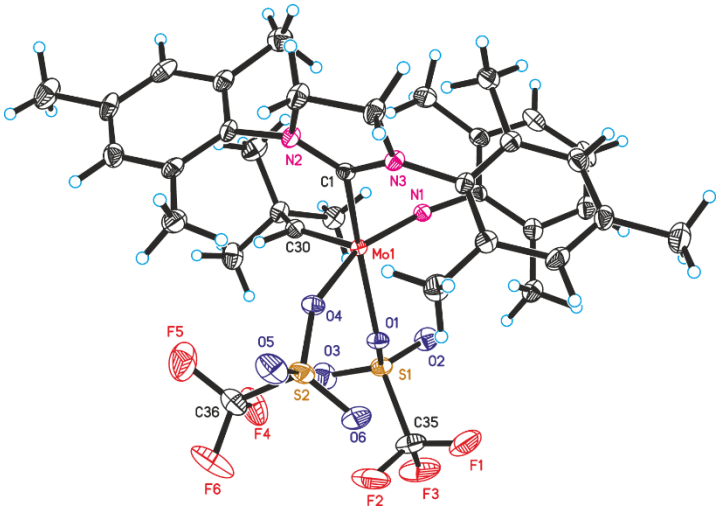


Figure 11. Single-crystal X-ray structure of **3**. Selected bond lengths [pm] and angles [°]: Mo(1)–N(1) 172.9(2), Mo(1)–C(30) 187.3(3), Mo(1)–O(4) 211.45(18), Mo(1)–O(1) 213.52(18), Mo(1)–C(1) 223.5(3); N(1)-Mo(1)-C(30) 101.61(11), N(1)-Mo(1)-O(4) 153.17(9), C(30)-Mo(1)-O(4) 105.17(10), N(1)-Mo(1)-O1 96.08(9), C(30)-Mo(1)-O(1) 97.82(10), O(4)-Mo(1)-O(1) 78.86(7), N(1)-Mo(1)-C(1) 96.84(10), C(30)-Mo(1)-C(1) 103.36(11), O(4)-Mo(1)-C(1) 78.59(9), O(1)-Mo(1)-C(1) 152.35(9).

Clearly, the mesityl containing NHC (IMesH$_2$) in **3** has an unpronounced *trans* effect on the triflate ligand, which is a direct consequence of the distorted geometry of the complex with a C(1)-Mo(1)-O(1) angle of only 152.35(9)°. In the solid state, the alkylidene adopts a *syn*-configuration, which also predominates in solution as evidenced by J_{CH} = 118 Hz. Apart from the signal for the *syn*-alkylidene, **3** shows

approximately 0.1% of the *anti*-isomer at δ_H = 14.52 ppm (**Figure 12**). Compound **4** (**Figure 13**) crystallizes in the tetragonal system $P42_1c$, a = 2449.86(11), b = 2449.86(11), c = 1093.68(7) pm, $\alpha = \beta = \gamma = 90°$, Z = 8. As in **3**, the complex **4** is neutral; the ligands adopt a distorted SP geometry (τ = 0.32) with the Mo-alkylidene unit in the apical position. Unlike **3** and despite an unfavorable small angle for O(1)-Mo(1)-C(9) of 147.93(5)°, the triflate group is located *trans* to the N-aryl imido ligand (δ_F = -78.075 ppm) experiences the most pronounced *trans* effect, resulting in a weaker binding of this anionic ligand as suggested by the different bond lengths [Mo(1)-O(1) = 211.07(11) and Mo(1)-O(2) = 217.98(12) pm].

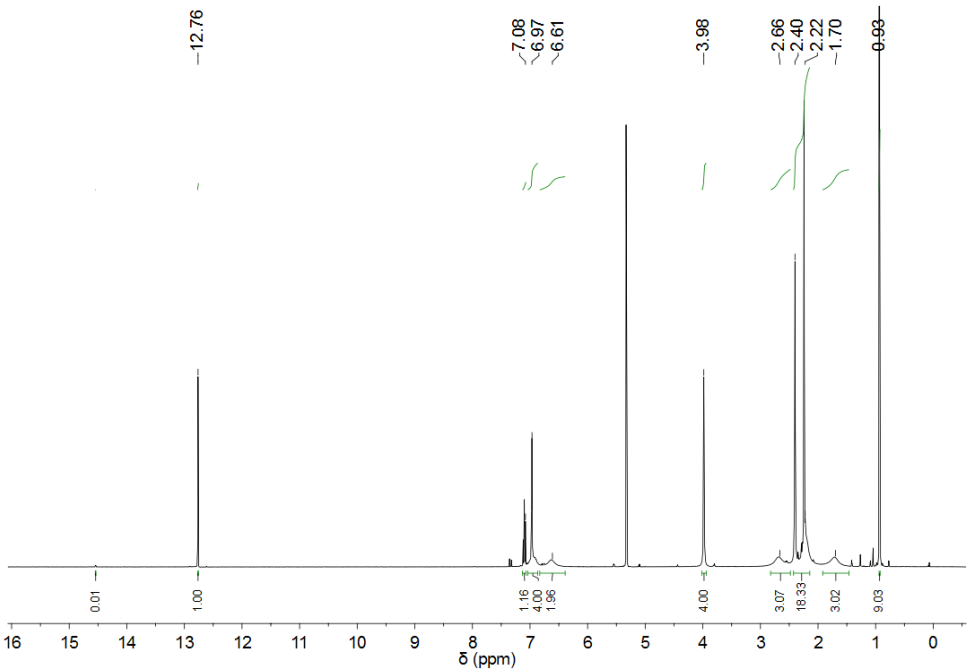


Figure 12. ^{1}H-NMR spectrum (400 MHz, CD_2Cl_2) of **3**.

Particularly the Mo(1)-O(2) distance is significantly larger than the distances in the "universal precursors" of the general formula [Mo(NAr')(CH-*t*Bu)(OTf)$_2$DME] [208.5 < Mo-O < 210.5 pm].[21] Notably, neither IMesH$_2$ nor I-*t*Bu, though strong bases, caused any (permanent) deprotonation of the *α*-hydrogen at the alkylidene ligand, a reaction that would result in the formation of Mo-alkylidyne complexes.[22-23] This is because the NHCs used are more nucleophilic than basic[24] with I-*t*Bu being more nucleophilic than IMesH$_2$ and IMes[25-27] which can be explained by the *Hückel's* aromaticity of [I-*t*Bu]$^+$. In case of IMesH$_2$ and IMes, due to the absence of *π*-system in IMesH$_2$, the

carbene is not resonance stabilized. This makes the carbene more nucleophilic than its unsaturated analogous, *i.e.* IMes.

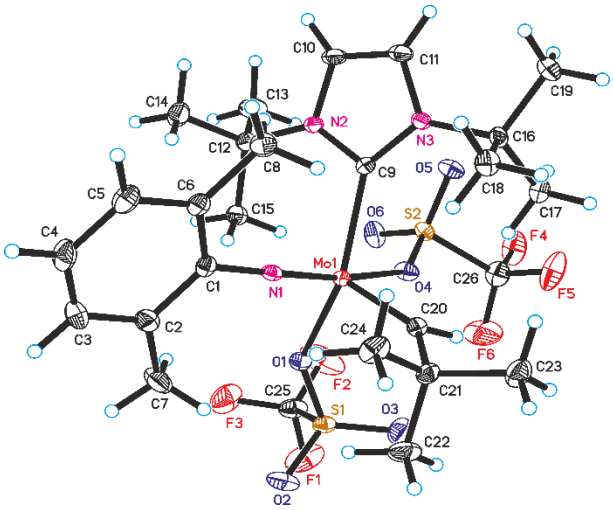


Figure 13. Single-crystal X-ray structure of **4**. Selected bond lengths [pm] and angles [°]: Mo(1)-C(20) 188.69(18), N(1)-Mo(1)-C(20) 97.03(8), N(1)-Mo(1)-O(1) 99.04(6), C(20)-Mo(1)-O(1) 98.13(6), N(1)-Mo(1)-O(4) 167.42(6), C(20)-Mo(1)-O(4) 95.48(7), O(1)-Mo(1)-O(4) 80.44(5), N(1)-Mo(1)-C(9) 93.43(6), C(20)-Mo(1)-C(9) 109.57(7), O(1)-Mo(1)-C(9) 147.93(5), O(4)-Mo(1)-C(9) 81.11(5).

This order in nucleophilicity is also reflected by the chemical shifts of the corresponding alkylidenes. Thus, the chemical shift of the alkylidene in **4** (δ_H = 14.64 ppm) strongly suggests that the partial positive charge at Mo is larger in **4** than in **3** (δ_H = 12.76 ppm). These data are also in line with the single-crystal X-ray data, which clearly show a more pronounced *trans* effect on one triflate and thus charge separation in **4**. Compound **5** (**Figure 14**) crystallizes in the monoclinic space group, $P2_1/n$, a = 1084.19(8), b = 1814.47(14), c = 2147.66(16) pm, $\alpha = \beta$ = 90°, γ = 96.689(4)°, Z = 4. The ligands are arranged in a distorted square pyramidal (SP) (τ = 0.27) configuration around the molybdenum. One triflate is arranged fairly *trans* to the NHC [O(1)-Mo(1)-C(1) = 155.85(4)°]. The effect of neophylidene ligands is clearly seen in the alkylidene signal of compound **5** (δ_H = 13.11 ppm compared to δ_H = 12.76 ppm in **3**). Compound **6** (**Figure 15**) crystallizes in the monoclinic space group $P2_1/n$, a = 1074.22(12), b = 1816.58(16), c = 2149.5(2) pm, $\alpha = \gamma$ = 90°. β = 96.218(7)°, Z = 4. As in **5**, one triflate is *trans* to the NHC [O(1)-Mo(1)-C(1) = 157.5(2)°].

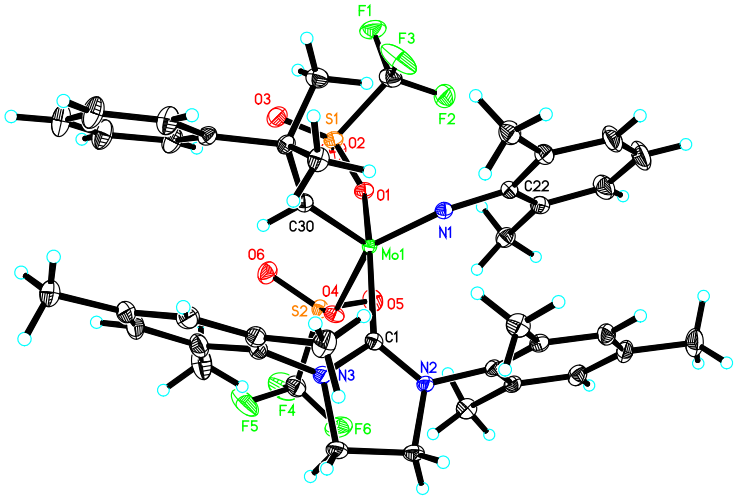


Figure 14. Single crystal X-ray structure of **5**. Relevant bond lengths [pm] and angles [°]: Mo(1)-N(1) 173.18(12), Mo(1)-C(30) 187.04(14), Mo(1)-O(4) 213.60(10), Mo(1)-O(1) 214.79(10), Mo(1)-C(1) 222.66(14); N(1)-Mo(1)-C(30) 104.75(6), N(1)-Mo(1)-O(4) 139.94(5), C(30)-Mo(1)-O(4) 115.25(5), N(1)-Mo(1)-O(1) 92.85(5), C(30)-Mo(1)-O(1) 99.65(5), O(4)-Mo(1)-O(1) 78.95(4), N(1)-Mo(1)-C(1) 99.72(5), C(30)-Mo(1)-C(1) 96.98(6), O(4)-Mo(1)-C(1) 78.16(5), O(1)-Mo(1)-C(1) 155.85(4).

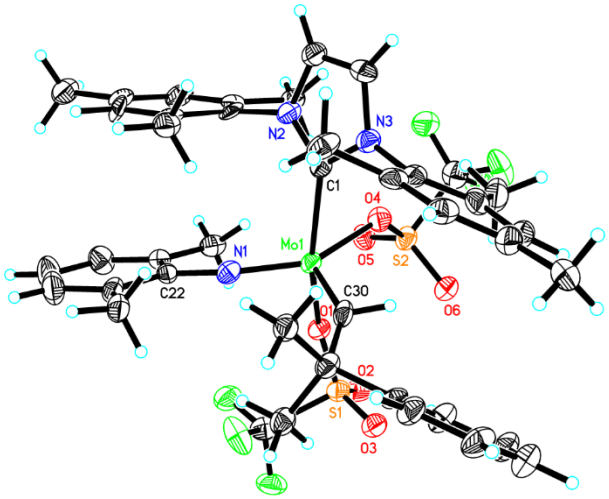


Figure 15. Single crystal X-ray structure of **6**. Relevant bond lengths [pm] and angles [°]: Mo(1)-N(1) 173.2(6), Mo(1)-C(30) 187.3(7), Mo(1)-O(4) 213.5(5), Mo(1)-O(1) 215.3(5), Mo(1)-C(1) 221.7(7); N(1)-Mo(1)-C(30) 104.0(3), N(1)-Mo(1)-O(4) 139.6(2), C(30)-Mo(1)-O(4) 116.2(3), N(1)-Mo(1)-O(1), 92.1(2), C(30)-Mo(1)-O(1) 99.7(2), O(4)-

Mo(1)-O(1) 78.80(18), N(1)-Mo(1)-C(1) 99.9(3), C(30)-Mo(1)-C(1) 95.8(3), O(4)-Mo(1)-C(1) 79.7(2), O(1)-Mo(1)-C(1) 157.5(2).

Compound **7** (**Figure 16**) crystallizes in the triclinic space group *P*-1, *a* = 1080.28(6), *b* = 1119.26(7), *c* = 2157.61(13) pm, *α* = 85.488(3)°, *β* = 88.695(3)°, *γ* = 61.342(3)°, Z = 2. The ligands are arranged in an intermediate between SP/TBP (τ = 0.43) configuration around Mo. One triflate is in first approximation arranged *trans* to the NHC [O(2)-Mo(1)-C(1) = 162.76(6)°]. Unlike all other complexes, where the angle Mo(1)-N(3)-C_{aryl} is close to 180°, this angle is 155.44(13)° in **7**, which suggests a weak interaction between the nitrogen and the molybdenum.

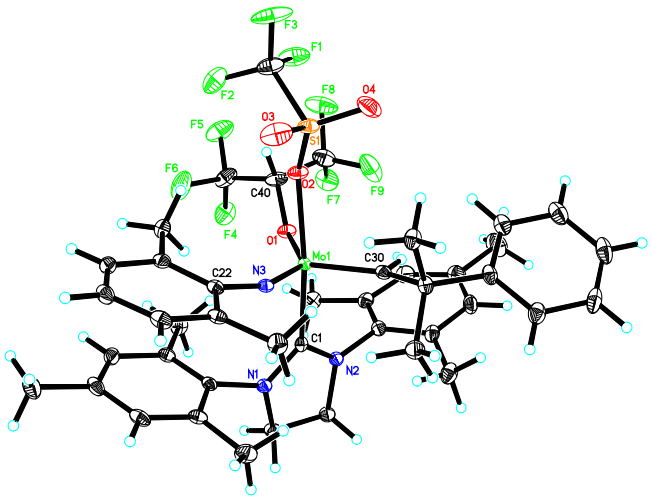


Figure 16. Single crystal X-ray structure of **7**. Relevant bond lengths [pm] and angles [°]: Mo(1)-N(3) 174.69(15), Mo(1)-C(30) 189.95(19), Mo(1)-O(1) 200.88(13), Mo(1)-O(2) 218.50(13), Mo(1)-C(1) 224.25(18); N(3)-Mo(1)-C(30) 104.04(8), N(3)-Mo(1)-O(1) 137.24(6), C(30)-Mo(1)-O(1) 118.40(7), N(3)-Mo(1)-O(2) 91.87(6), C(30)-Mo(1)-O(2) 95.73(6), O(1)-Mo(1)-O(2) 79.59(5), N(3)-Mo(1)-C(1) 99.16(6), C(30)-Mo(1)-C(1) 94.40(7), O(1)-Mo(1)-C(1) 83.33(6), O(2)-Mo(1)-C(1) 162.76(6).

In solution, complex **7** exists in a cationic form, as can be judged from the chemical shift of the triflate group (δ_F = - 78.07 ppm). The release of the triflate in solution can be anticipated from the long distance of the Mo-O_{OTf} bond in the solid state [218.50(13) pm], which is a consequence of the comparable large O_{OTf}-Mo-C_{NHC} angle of 162.76(6)° (**Table 1**) and the more pronounced *trans* effect of the NHC on the triflate.

Table 1 shows that all the molybdenum imido alkylidene bis(triflate) NHC compounds (**3**-**6**, **19**, **20** and **25**) are distorted square pyramidal (SP) geometries while compounds **7**, **10**, **18** and **22** adopt an intermediate SP/TBP geometry. The space groups that are found in compounds **5**, **6**, **7**, **10**, **14**, **18**, **21** and **22** ($P2_1/n$, P-1) are indicative for the fact that all these complexes form and crystallize as true racemates, *i.e.* 50:50 mixtures of the corresponding two enantiomers. This is not surprising, clearly the NHC can approach the progenitors **2A** or **2B** from either enantiomorphic face and form the corresponding enantiomeric adducts. The same accounts for **7**, **10**, **14**, **21** and **22**, they are formed through selective removal of one triflate group, however, starting from a racemate, again leading to a racemic compound. Reaction of **3** with one equivalent of lithium *tert*-butoxide and sodium ethoxide afforded corresponding complexes [Mo(N-2,6-Me_2-C_6H_3)($IMesH_2$)(CH-*t*Bu)(OTf)(O-*t*Bu)] (**8**) and [Mo(N-2,6-Me_2-C_6H_3)($IMesH_2$)(CH-*t*Bu)(OTf)(OEt)] (**9**), but both **8** and **9** are not stable in the solid state and thus could not be used further. The plausible explanations behind the instability of complexes **8** and **9** are the electron-donating alkoxide groups as well as the small alkoxides in the case of complex **9**. Compound **10** (**Figure 17**) crystallizes in the chiral orthorhombic space group $P2_12_12_1$ with a = 1049.91(6), b = 1986.61(11), c = 2129.05(12) pm, $\alpha = \beta = \gamma = 90°$, Z = 4. The unit cell contains only one of the two possible enantiomers; nonetheless, the existence of both enantiomers in the entire sample cannot be ruled out, in fact it must be anticipated. The ligands adopt a distorted SP/TBP (τ = 0.51) configuration with [O(2)-Mo(1)-C(1) = 161.6(2)°]. Relevant bond lengths and angles are inconspicuous and are summarized in **Figure 17**. Compound **14** (**Figure 18**) crystallizes in the triclinic space group P-1, a = 1284.25(13), b = 18.420(2), c = 18.727(2) pm, α = 64.388(3)°, β = 71.487(4)°, γ = 72.459(4)°, Z = 2. The complex adopts a slightly distorted SP (τ = 0.02, CH_3CN consider as a ligand) configuration with the alkylidene in the apices. The Mo-NHC, Mo=C and Mo=N distances were inconspicuous and comparable to those found in other complexes. Reaction of complex **5** with two equivalents of $PhMe_2CH_2MgCl$ replaced both triflate groups in **5**, resulting in the bis(alkyl) complex, however, at the same time de-coordination of NHC occurred.

Table 1. Summary of relevant bond lengths [pm] and bond angles [°] in complexes **3-22**.

Complex	Geometry index (τ)	Geometry	Mo=N (pm)	Mo-NHC (pm)	Mo=C (pm)	Mo-triflate (longest) [°]	OTf-Mo-NHC [°]	OTf-Mo-NAr' [°]
3	0.01	SP	172.9	223.5	187.3	213.52	152.35	153.17
4	0.33	SP	172.98	222.12	188.69	217.98	147.93	167.42
5	0.27	SP	173.18	222.66	187.04	214.79	155.85	139.94
6	0.30	SP	173.2	221.7	187.3	215.3	157.5	139.6
7	0.43	SP/TBP	174.69	224.25	189.95	218.50	162.76	91.87
10	0.51	SP/TBP	175.1	223.2	190.5	216.1	161.6	93.8
14	0.02	SP	173.0	223.3	187.6	213.6	82.62	156.83
18	0.50	SP/TBP	172.64	220.15	188.69	219.08	139.81	169.77
19	0.22	SP	173.2	220.4	187.9	214.0	147.62	160.57
20	0.23	SP	171.7	218.8	187.2	214.7	149.14	162.87
21	0.16	SP	174.43	222.5	189.88	220.69	159.88	88.42
22	0.51	SP/TBP	172.0	223.2	187.6	224.9	80.14	167.76

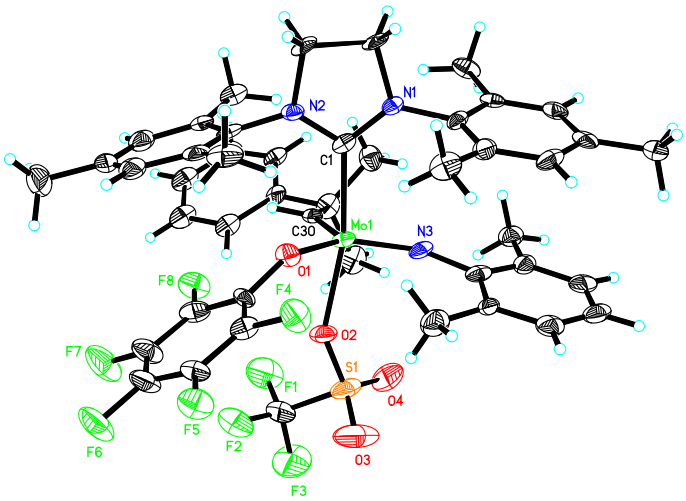


Figure 17. Single crystal X-ray structure of **10**. Selected bond lengths [pm] and angles [°]: Mo(1)-N(3) 175.1(5), Mo(1)-C(30) 190.5(6), Mo(1)-O(1) 197.1(4), Mo(1)-O(2) 216.1(4), Mo(1)-C(1) 223.2(5); N(3)-Mo(1)-C(30) 108.0(3), N(3)-Mo(1)-O(1) 131.2(2), C(30)-Mo(1)-O(1) 120.6(2), N(3)-Mo(1)-O(2) 93.8(2), C(30)-Mo(1)-O(2) 96.1(2), O(1)-

Mo(1)-O(2) 78.25(18), N(3)-Mo(1)-C(1) 99.1(3), C(30)-Mo(1)-C(1) 92.4(2), O(1)-Mo(1)-C(1) 83.4(2), O(2)-Mo(1)-C(1) 161.6(2).

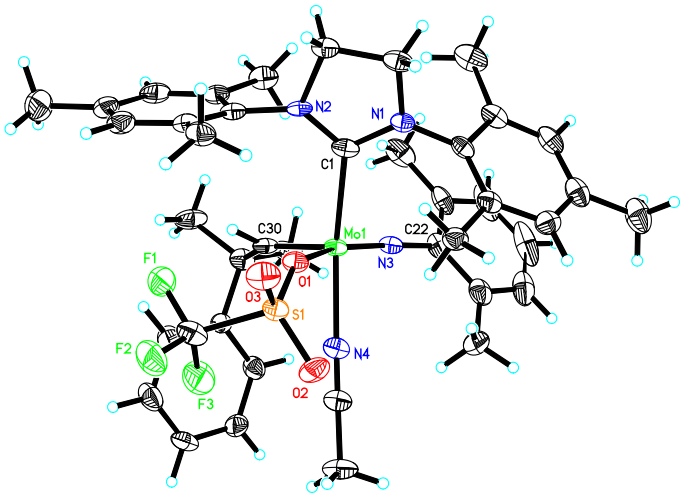


Figure 18. Single crystal X-ray structure of **14**. Relevant bond lengths [pm] and angles [°]: Mo(1)-N(3) 173.0(3), Mo(1)-C(30) 187.6(4), Mo(1)-O(1) 213.6(3), Mo(1)-N(4) 217.0(4), Mo(1)-C(1) 223.3(4); N(3)-Mo(1)-C(30) 101.25(18), N(3)-Mo(1)-O(1) 156.83(14), C(30)-Mo(1)-O(1) 101.16(16), N(3)-Mo(1)-N(4) 93.16(15), C(30)-Mo(1)-N(4) 92.64(16), O(1)-Mo(1)-N(4) 80.00(12), N(3)-Mo(1)-C(1) 97.64(16), C(30)-Mo(1)-C(1) 103.84(17), O(1)-Mo(1)-C(1) 82.62(13), N(4)-Mo(1)-C(1) 158.04(14). Anion $B(Ar^F)_4$ omitted for clarity.

Compound **18** (**Figure 19**) crystallizes in the chiral monoclinic space group $P2_1$ with a = 1094.44(5), b = 1803.72(9), c = 1196.49(6) pm, α = 90°, β = 111.600(2)°, γ = 90°, Z = 2. The ligands are arranged in a distorted SP/TBP manner (τ = 0.50) [N(3)-Mo(1)-O(1) = 169.77(5)°] with the alkylidene ligand forming the apexes. One triflate is only barely *trans* to the NHC [O(4)-Mo(1)-C(1) = 139.81(4)°], which results in a weak *trans*-effect of the NHC on the triflate in the solid state [Mo(1)-O(4) = 208.95(10) pm]. In contrast, in view of the angle [N(3)-Mo(1)-O(1) = 169.77(5)°], the triflate *trans* to the imido-ligand must experience a quite strong *trans*-effect as reflected by the bond length [Mo(1)-O(1) = 219.08(10) pm]. Still, in solution (CD_2Cl_2) compound **18** exists in its neutral, non-ionic state. Notably, the chiral NHC induces chirality at Mo. As evidenced by the chiral space group and by NMR, only the one configuration at Mo (**Figure 19**) is found; the corresponding diastereomer is absent. This is, to the best of

our knowledge, the first example of steric induction of a chiral NHC ligand to a group 6 metal imido alkylidene, resulting in one selective formation out of two possible diastereomers.

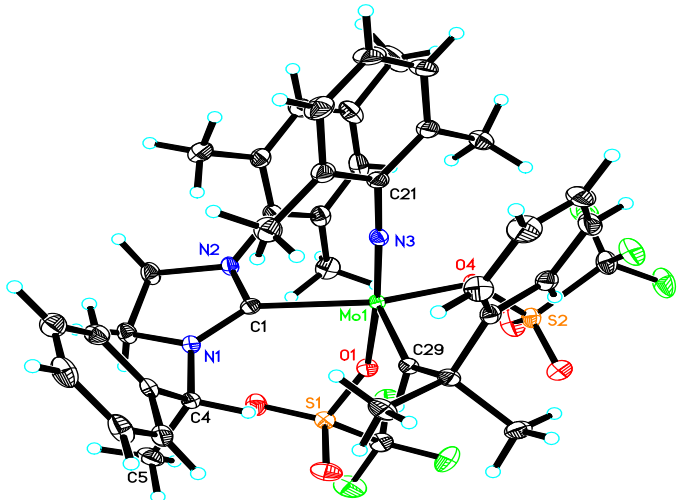


Figure 19. Single crystal X-ray structure of **18**. Relevant bond lengths [pm] and angles[°]: Mo(1)-N(3) 172.64(12), Mo(1)-C(29) 188.69(14), Mo(1)-O(4) 208.95(10), Mo(1)-O(1) 219.08(10), Mo(1)-C(1) 220.15(14); N(3)-Mo(1)-C(29) 97.92(6), N(3)-Mo(1)-O(4) 99.66(5), C(29)-Mo(1)-O(4) 105.36(5), N(3)-Mo(1)-O(1) 169.77(5), C(29)-Mo(1)-O(1) 92.28(5), O(4)-Mo(1)-O(1) 78.20(4), N(3)-Mo(1)-C(1) 96.54(5), C(29)-Mo(1)-C(1) 108.49(5), O(4)-Mo(1)-C(1) 139.81(4), O(1)-Mo(1)-C(1) 79.42(4).

As one can see from MAP-type catalysts,[28-29] *Z*-selectivity in different metathesis reactions is governed by a small imido group (*e.g.,* an Ad imido ligand, Ad = adamantly). In view of that, the 3,5-dimethyl imido ligand was introduced. Complexes **19** and **20** were accessible via reaction of [Mo(N-3,5-Me_2-C_6H_3)(CHCMe_2Ph)(OTf)$_2$DME] with 1,3-dimesitylimidazolin-2-ylidene ($IMesH_2$) and 1,3-dimesitylimidazol-2-ylidene (IMes), respectively. Reaction of **19** with one equivalent of LiO-2,6-Ph_2-C_6H_3 or $LiOC(CF_3)_3$ yielded compounds **21** and **22**, respectively. Compound **19** (**Figure 20**) crystallizes in the monoclinic space group *Pc* with *a* = 1057.10(6), *b* = 2098.82(13), *c* = 1908.12(10) pm, $\alpha = \gamma = 90°$, $\beta = 96.356(3)°$, *Z* = 4. The configuration at the metal is described best as distorted SP ($\tau = 0.22$) with the alkylidene forming the apex. For selected bond lengths and angles refer to **Figure 20**. Compound **20** (**Figure 21**) also crystallizes in the monoclinic space group $P2_1/c$

with *a* = 1118.60 (5), *b* = 2095.70 (10), *c* = 1996.31 (10) pm, *α* = *γ* = 90°, *β* = 106.25(2)°, *Z* = 4. As in **19**, the configuration at the metal is best described as distorted SP (τ = 0.23) with the alkylidene forming the apex.

Compound **21** (**Figure 22**) crystallizes in the monoclinic space group $P2_1/c$ with *a* = 1208.34(5), *b* = 1814.59(8), *c* = 2662.95(12) pm, *α* = 90°, *β* = 97.644(2)°, *γ* = 90°, *Z* = 4. In **21**, the ligands adopt a distorted SP (τ = 0.16) ligand sphere with the alkylidene forming the apex. The triflate is *trans* to the NHC [O(2)-Mo(1)-C(1) = 159.88(6)°] while the terphenoxide is *trans* to the imido-ligand [N(3)-Mo(1)-O(1) = 150.26(7)°].

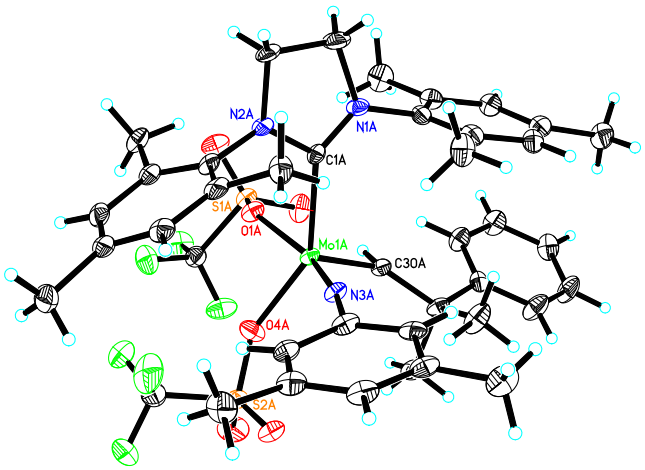


Figure 20. Single crystal X-ray structure of **19**. Relevant bond lengths [pm] and angles [°]: Mo(1A)-N(3A) 173.2(4), Mo(1A)-C(30A) 187.9(5), Mo(1A)-O(4A) 210.5(3), Mo(1A)-O(1A) 214.0(3), Mo(1A)-C(1A) 220.4(5); N(3A)-Mo(1A)-C(30A) 101.6(2), N(3A)-Mo(1A)-O(4A) 98.16(16), C(30A)-Mo(1A)-O(4A) 101.04(17), N(3A)-Mo(1A)-O(1A) 160.57(15), C(30A)-Mo(1A)-O(1A) 97.81(17), O(4A)-Mo(1A)-O(1A) 77.56(13), N(3A)-Mo(1A)-C(1A) 96.44(18), C(30A)-Mo(1A)-C(1A) 104.09(18), O(4A)-Mo(1A)-C(1A) 147.62(15), O(1A)-Mo(1A)-C(1A) 79.08(15).

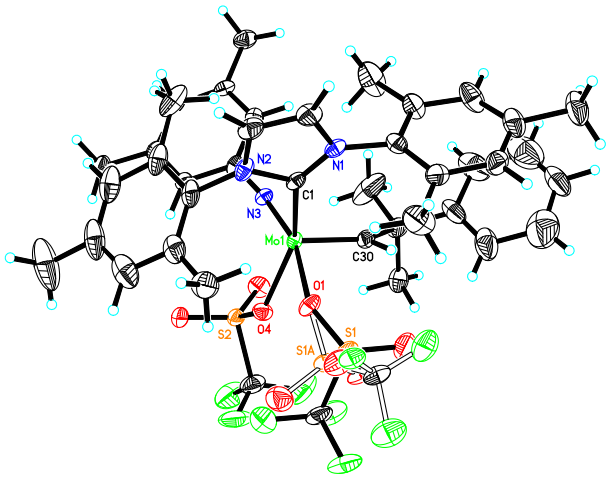


Figure 21. Single crystal X-ray structure of **20**. Relevant bond lengths [pm] and angles [°]: Mo(1)-N(3) 171.7(4), Mo(1)-C(30) 187.2(5), Mo(1)-O(4) 213.9(4), Mo(1)-O(1) 214.7(4), Mo(1)-C(1) 218.8(5); N(3)-Mo(1)-C(30) 101.0(2), N(3)-Mo(1)-O(4) 95.31(17), C(30)-Mo(1)-O(4) 102.85(19), N(3)-Mo(1)-O(1) 162.87(18), C(30)-Mo(1)-O(1) 95.7(2), O(4)-Mo(1)-O(1) 77.03(15), N(3)-Mo(1)-C(1) 94.78(19), C(30)-Mo(1)-C(1) 103.7(2).

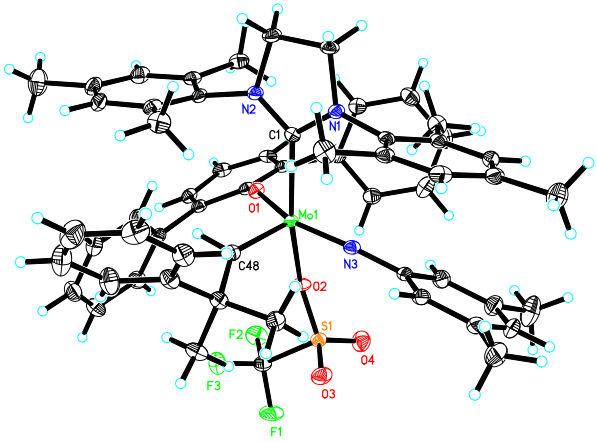


Figure 22. Single crystal X-ray structure of **21**. Relevant bond lengths [pm] and angles [°]: Mo(1)-N(3) 174.43(17), Mo(1)-C(48) 189.88(19), Mo(1)-O(1) 195.16(13), Mo(1)-O(2) 220.69(14), Mo(1)-C(1) 222.5(2); N(3)-Mo(1)-C(48) 101.25(8), N(3)-Mo(1)-O(1) 150.26(7), C(48)-Mo(1)-O(1) 106.69(7), N(3)-Mo(1)-O(2) 88.42(7), C(48)-Mo(1)-O(2) 100.77(7), O(1)-Mo(1)-O(2) 76.68(6), N(3)-Mo(1)-C(1) 96.85(7), C(48)-Mo(1)-C(1) 97.24(8), O(1)-Mo(1)-C(1) 89.63(6), O(2)-Mo(1)-C(1) 159.88(6).

Compound **22** (**Figure 23**) crystallizes in the triclinic space group *P*-1 with *a* = 1085.67(6), *b* = 1102.51(5), *c* = 2118.63(12) pm, *α* = 103.491(3)°, *β* = 92.687(4)°, *γ* = 110.454(3)°, *Z* = 2. Its geometry is an intermediate between SP/TBP (τ = 0.51).

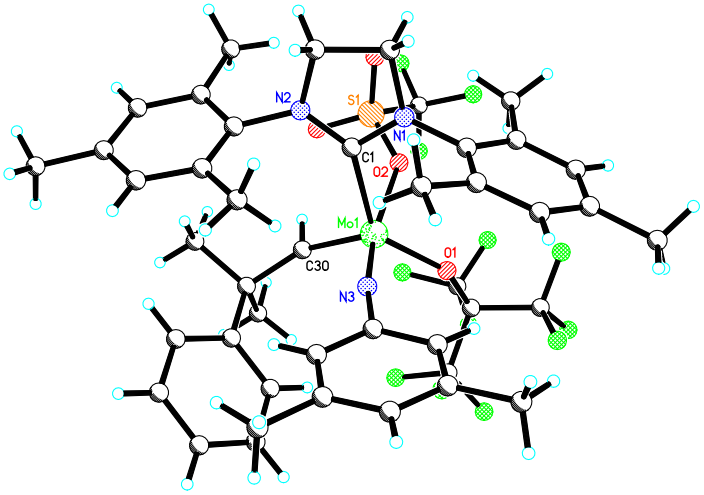
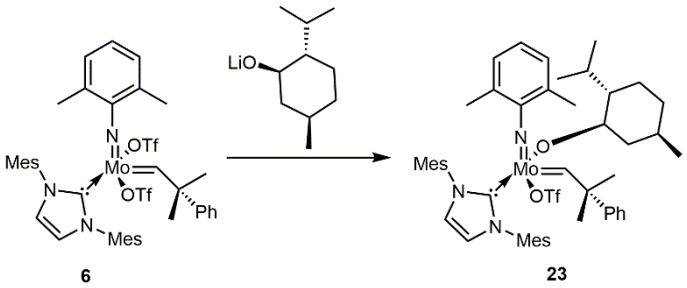


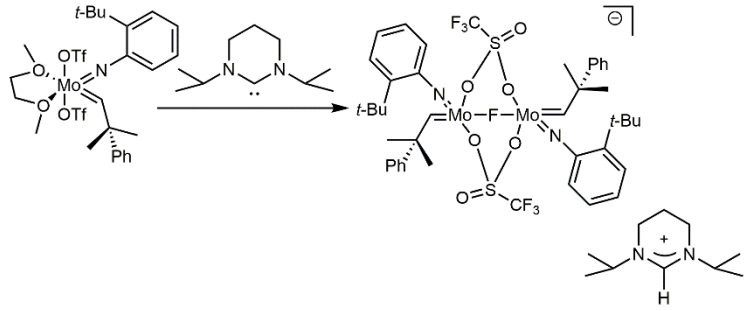
Figure 23. Single-crystal X-ray structure of **22**. Selected bond lengths [pm] and angles [°]: Mo(1)-N(3) 172.0(4), Mo(1)-C(30) 187.6(5), Mo(1)-O(1) 200.2(4), Mo(1)-C(1) 223.2(5), Mo(1)-O(2) 224.9(4); N(3)-Mo(1)-C(30)101.3(2), N(3)-Mo(1)-O(1) 98.33(18), C(30)-Mo(1)-O(1) 112.84(19), N(3)-Mo(1)-C(1) 94.87(18), C(30)-Mo(1)-C(1) 104.1(2), O(1)-Mo(1)-C(1)137.21(17), N(3)-Mo(1)-O(2)167.76(16).

Complex **18** was prepared for implementation in enantioselective synthesis. Unfortunately, **18** was not promising for any enantioselective olefin metathesis reactions. One reason is that the chiral group at NHC is located far away from Mo-center and not has any influence on the metal center. In view of this, replacement of one of the triflate in complex **5** by lithium (1R,2S,5R)-2-isopropyl-5-methylcyclohexan-1-olate offered access to compound **23** (**Scheme 17**).

Surprisingly, reaction of Mo(N-2-*t*Bu-C_6H_4)(CHCMe$_2$Ph)(OTf)$_2$DME with 1,3-(2-*i*Pr)$_2$-tetrahydropyrimidin-2-ylene does not result in the formation of the desired Mo-imido alkylidene NHC complex but in the formation of a dinuclear anionic complex [(1,3-(2-*i*Pr)$_2$-tetrahydropyrimidin-2-ium)$^+$(Mo(N-2-*t*Bu-C_6H_4)(CHCMe$_2$Ph)(OTf)(μ^2-(CF_3-SO_3)$_2$(μ^2-F)$^-$] (**24**, **Scheme 18**). The mechanism for the formation of compound **24** is still speculative.



Scheme 17. Synthesis of **23**.



Scheme 18. Synthesis of **24**.

Compound **24** crystallizes in the monoclinic space group *C*2/*c*, *a* = 2663.57(18), *b* = 1370.56(8), *c* = 2465.39(15) pm, $\alpha = \gamma = 90°$, $\beta = 122.487(5)°$, *Z* = 4. The complex shows C_2-symmetry. The ligands at both Mo atoms adopt a distorted octahedral configuration [O(2)-Mo(1)-C(11) = 168.37(8)°] with the alkylidene and the triflate forming the apexes. Relevant bond lengths and angles are summarized in **Figure 24**.

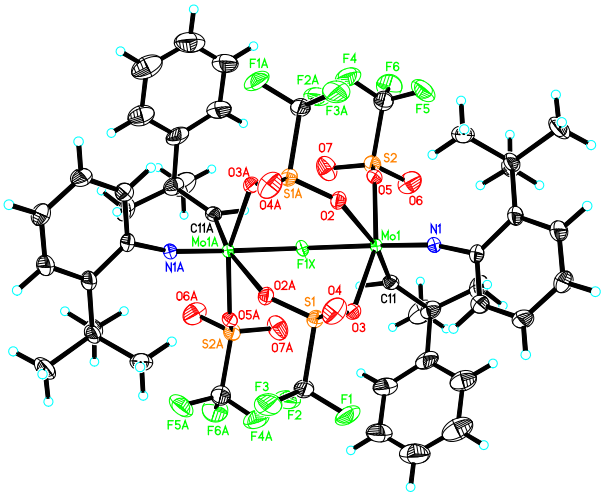
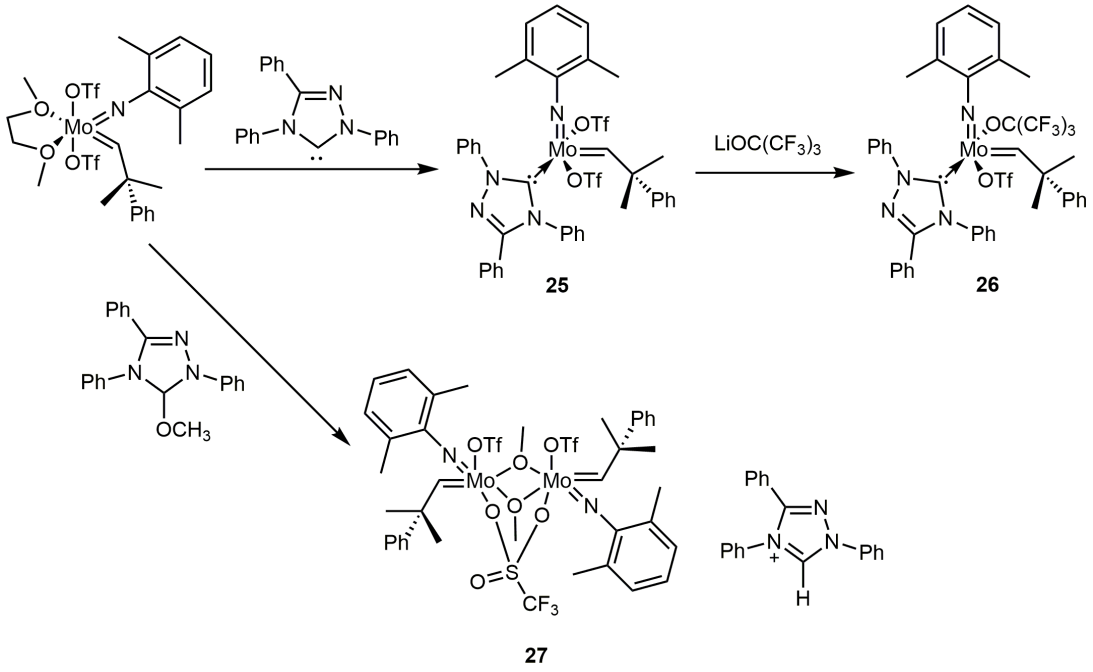


Figure 24. Single crystal X-ray structure of **24**. Selected bond lengths [pm] and angles [°]: Mo(1)-N(1) 171.86(19), Mo(1)-C(11) 189.6(2), Mo(1)-O(5) 208.00(15), Mo(1)-F(1X) 208.44(5), Mo(1)-O(3) 215.35(15), Mo(1)-O(2) 238.68(16); N(1)-Mo(1)-C(11) 99.70(10), N(1)-Mo(1)-O(5) 100.96(8), C(11)-Mo(1)-O(5) 99.75(8), N(1)-Mo(1)-F(1X) 167.08(8), C(11)-Mo(1)-F(1X) 90.27(8), O(5)-Mo(1)-F(1X) 85.27(5), N(1)-Mo(1)-O(3) 91.83(8), C(11)-Mo(1)-O(3) 92.42(8), O(5)-Mo(1)-O(3) 160.51(6), F(1X)-Mo(1)-O(3) 79.47(5), N(1)-Mo(1)-O(2) 91.24(7), C(11)-Mo(1)-O(2) 168.37(8), O(5)-Mo(1)-O(2) 81.88(6), F(1X)-Mo(1)-O(2) 78.35(5), O(3)-Mo(1)-O(2) 83.21(6). The (1,3-(2-*i*Pr)$_2$-tetrahydropyrimidin-2-ium) cation is disordered and was omitted for clarity.

Finally, a novel class of 1,2,4-triazole NHC based Mo-imido alkylidene complexes was prepared. Complex **25** was accessible via reaction of the corresponding Mo-imido alkylidene bis(triflate) progenitor (**2A**) with 1,3,4-triphenyl-4,5-dihydro-1H-1,2,4-triazole-5-ylidene (**Scheme 19**). Reaction of **25** with LiOC(CF$_3$)$_3$ resulted in the formation of catalyst **26**.



Scheme 19. Synthesis of **25**-**27**.

Compound **25** crystallizes in the monoclinic space group *C*2/c, *a* = 2810.45(14), *b* = 1413.61(7), *c* = 2447.93(11) pm, *α* = 90°, *β* = 111.926(2)°, *γ* = 90°, *Z* = 8. In the solid

state, the complex exists in its neutral form. The ligands adopt a distorted SP (τ = 0.24) geometry with the Mo-alkylidene unit in the apical position. The distance Mo(1)–C(29) is 187.8(3) pm and thus somewhat shorter than that in [Mo(NAr')(CH-*t*Bu)$(OTf)_2$(DME)](190.0/193.0 pm).[21] The triflate group located *trans* to the N-aryl imido ligand experiences the most pronounced *trans* effect, resulting in a weaker binding of this anionic ligand as suggested by different bond lengths [Mo(1)-O(4) = 210.85 (17) pm] and [(Mo(1)-O(1) = 215.84 (16) pm]. Complex **25** is a mixture of two conformational isomers, due to the in-plane rotation of the phenyl group in the NHC. In the ^{1}H-NMR, only the two signals for *syn*-alkylidenes were observed (δ_H = 14.37 ppm and δ_H = 14.08 ppm, ratio 64:36). The phenyl group were not resolved. Compound **26** crystallizes in the monoclinic space group $P2_1/c$, a = 1453.45(7), b = 15.8850(7), c = 21.3143(10) pm, α = 90°, β= 97.229(2)°, γ = 90°, Z = 4. In the solid state, **26** exists in its neutral form. The ligands adopt a distorted SP (τ = 0.28) geometry with the Mo-alkylidene unit in the apical position. Relevant bond lengths and angles are summarized in **Figure 26**.

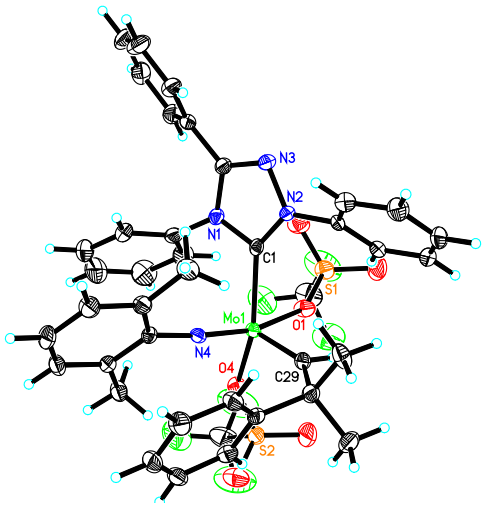


Figure 25. Single crystal X-ray structure of **25**. Relevant bond lengths [pm] and angles [°]: Mo(1)-N(4) 171.83(19), Mo(1)-C(29) 187.8(3), Mo(1)-O(4) 210.85(17), Mo(1)-O(1) 215.84(16), Mo(1)-C(1) 218.6(2); N(4)-Mo(1)-C(29) 97.76(10),N(4)-Mo(1)-O(4) 99.96(8), C(29)-Mo(1)-O(4) 105.60(9), N(4)-Mo(1)-O(1) 163.32(8), C(29)-Mo(1)-O(1) 98.29(9), O(4)-Mo(1)-O(1) 80.01(7), N(4)-Mo(1)-C(1) 88.06(8), C(29)-Mo(1)-C(1) 102.63(10), O(4)-Mo(1)-C(1) 149.21(8).

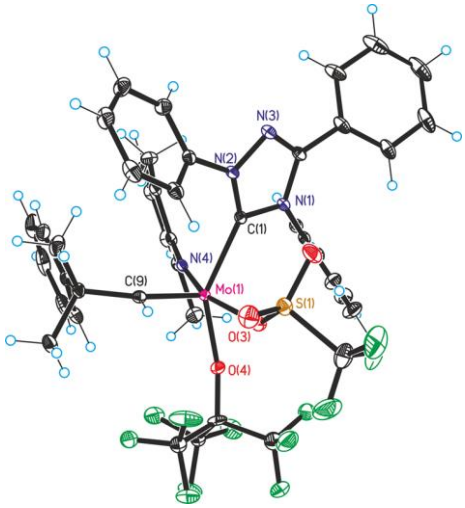


Figure 26. Single crystal X-ray structure of **26**. Relevant bond lengths [pm] and angles [°]: Mo(1)-N(4) 173.1(3), Mo(1)-C(9) 188.5(3), Mo(1)-O(4) 201.8(2), Mo(1)-C(1) 221.8(3), Mo(1)-O(1) 221.9(2); N(4)-Mo(1)-C(9) 98.39(13), N(4)-Mo(1)-O(4) 101.37(10), C(9)-Mo(1)-O(4) 107.35(11), N(4)-Mo(1)-C(1) 86.87(11), C(9)-Mo(1)-C(1) 103.91(12), O(4)-Mo(1)-C(1) 145.98(10), N(4)-Mo(1)-O(1) 162.55(10), C(9)-Mo(1)-O(1) 97.13(12), O(4)-Mo(1)-O(1) 81.46(9), C(1)-Mo(1)-O(1) 81.70(10).

The methanol adduct of triazole, i.e. Ph_3tri(H)OMe, has been isolated by *Ender* and coworkers.[30] This methanol-triazole adduct reacted with a Mo-imido alkylidene bis(triflate) progenitor (**2A**) and surprisingly provided an anionic dinuclear complex **27** [(1,3,4-Triphenyl-1H-1,2,4-triazol-4-ium)$^+$(Mo(N-2,6-Me_2-C_6H_3)(CHCMe_2Ph)(OTf)(μ^2-(CF_3-SO_3)(μ^2-$(OMe)_2$)$^-$] in quantitative yield. Compound **27** crystallizes in the orthorhombic space group *Pna*2_1, *a* = 2045.4(3), *b* = 2116.9(2), *c* = 1651.5(2) pm, α = β = γ = 90°, Z = 4. In the solid state, the complex exists in its anionic form. The complex shows C_2-symmetry. The ligands at both Mo atoms adopt a distorted octahedral bipyramidal configuration [N(1)-Mo(1)-O(3) = 175.0(2)°] with the imido and the bridging triflate forming the apexes. Relevant bond lengths and angles are summarized in **Figure 27**. Surprisingly, reaction of Mo(N-3,5-Me_2-C_6H_3)(CHCMe_2Ph)$(OTf)_2$(DME) (**2B**) with 1,3,4-triphenyl-4,5-dihydro-1H-1,2,4-triazole-5-ylidene did not result in the formation of the desired Mo-imido alkylidene NHC complex; instead a complex formed, which comprised of a mixture of two octahedral complexes, *i.e.* [Mo(N-3,5-Me_2-C_6H_3)(1,3,4-triphenyl-4,5-dihydro-1H-1,2,4-triazole-5-ylidene)(CHCMe_2Ph)(OTf)-(DME)] (**28A**) and [Mo(N-3,5-Me_2-C_6H_3(CHCMe_2Ph)$(OTf)_3(Et_2O)$] (**28B**). Compound

28A and **28B** crystallizes in the triclinic space group *P*-1, *a* = 1571.15(9), *b* = 1708.59(10), *c* = 1952.75(2) pm, *α* = 98.805(3), *β* = 110.138 (2), *γ* = 107.805°, *Z* = 2. In the solid state, the complex exists in its neutral form. For clarity, compound **28B** is omitted for the discussion. The ligands at both Mo atoms adopt a distorted octahedral configuration. In Complex **28A**, the distance Mo(1)–C(29) is 191.9(3) pm and thus somewhat compares to [Mo(NAr')(CH-*t*Bu)(OTf)$_2$DME](190.0/193.0 pm).[21] Relevant bond lengths and angles are summarized in **Figure 28**.

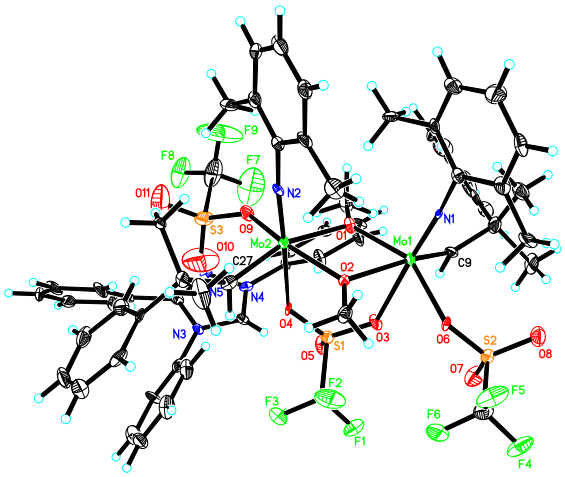


Figure 27. Single-crystal X-ray structure of **27**. Relevant bond lengths [pm] and angles [°]: Mo(1)-N(1) 171.6(5), Mo(1)-C(9) 192.0(7), Mo(1)-O(1) 202.4(5), Mo(1)-O(6) 211.4(5), Mo(1)-O(2) 225.6(5), Mo(1)-O(3) 231.7(4), Mo(2)-N(2) 172.5(5), Mo(2)-C(27) 192.0(7); N(1)-Mo(1)-C(9) 98.4(3), N(1)-Mo(1)-O(1) 103.1(2), C(9)-Mo(1)-O(1) 99.2(3), N(1)-Mo(1)-O(6) 97.6(2), C(9)-Mo(1)-O(6) 98.4(3), O(1)-Mo(1)-O(6) 150.36(18), N(1)-Mo(1)-O(2) 98.9(2), C(9)-Mo(1)-O(2) 161.9(2), N(1)-Mo(1)-O(3) 175.0(2),

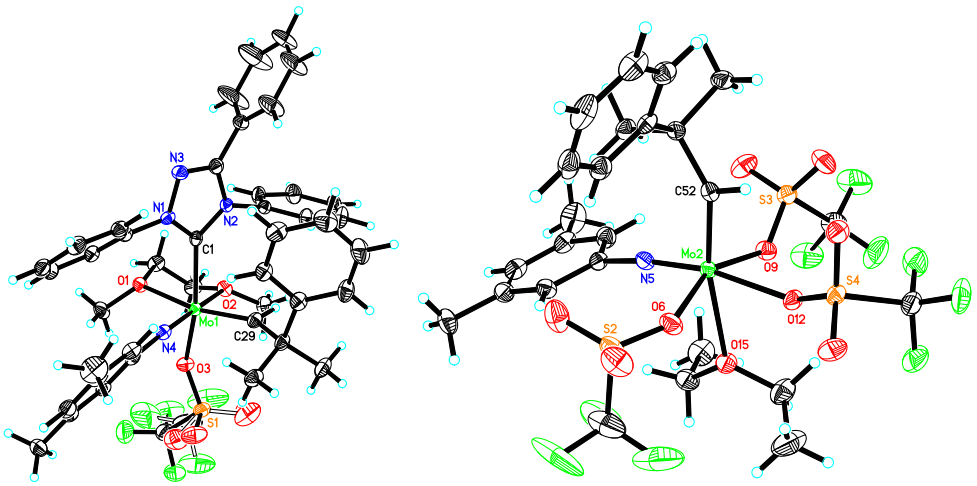
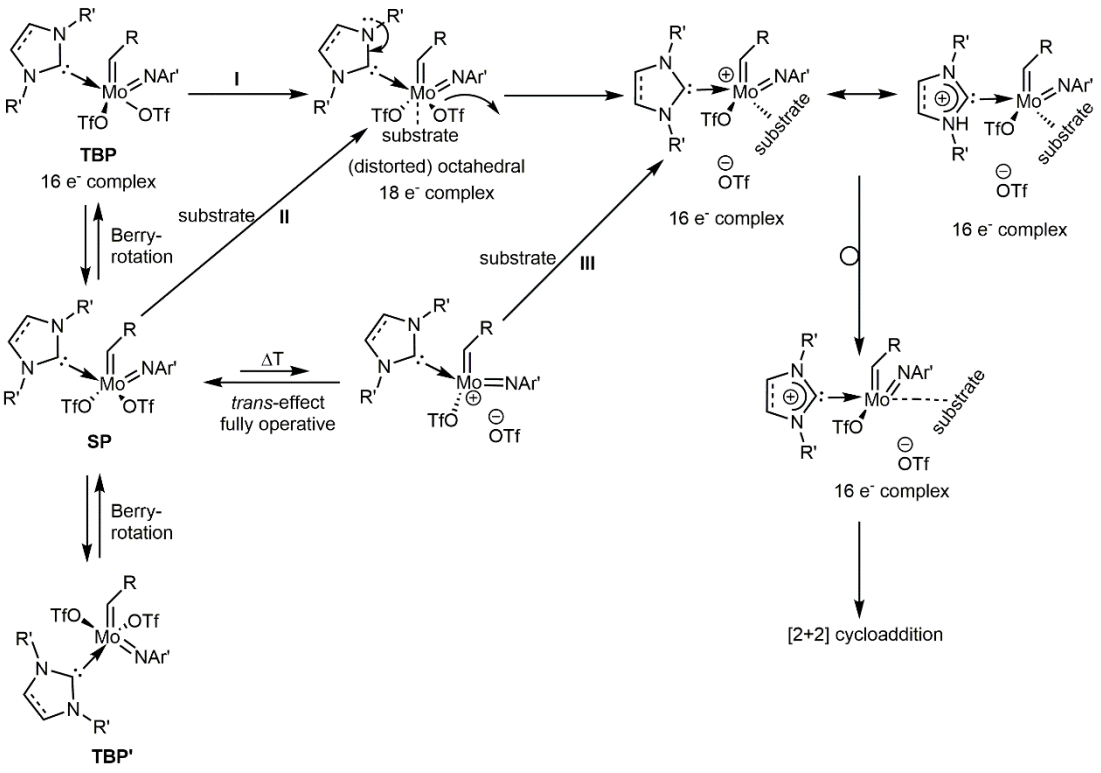


Figure 28. Single-crystal X-ray structure of **28A**. Relevant bond lengths [pm] and angles [°]: Mo(1)-N(4) 171.9(2), Mo(1)-C(29) 191.9(3), Mo(1)-O(3) 215.15(19), Mo(1)-C(1) 221.9(3), Mo(1)-O(1) 230.92(18) Mo(1)-O(2) 231.07(19); N(4)-Mo(1)-C(29) 98.59(11), N(4)-Mo(1)-O(3) 93.77(9), C(29)-Mo(1)-O(3) 102.64(10), N(4)-Mo(1)-C(1) 96.75(10), C(29)-Mo(1)-C(1) 91.43(11), O(3)-Mo(1)-C(1) 160.98(9), N(4)-Mo(1)-O(1) 100.05(9), C(29)-Mo(1)-O(1) 161.25(10), O(3)-Mo(1)-O(1) 78.14(7).

In general, both the Mo-imido and the Mo-NHC distances are within a narrow range (171.7-175.1 and 218.8-224.25 pm, respectively, **Table 1**). The same accounts for the Mo-alkylidene bond length, which is in the range of 187.04-190.5 pm (**Table 1**). As previously outlined in **Table 1**, the bonding of the triflates allows very rough predictions about the reactivity of the novel catalysts. Thus, the stronger the *trans* effect of the NHC ligand is, *i.e.* the closer the angle NHC-Mo-triflate is to 180°, the more labile the triflate becomes, ultimately resulting in the formation of cationic complexes. The latter has unambiguously been identified in the presence of an olefin. Now, there are in principle two ways to render the *trans* effect fully operative. One entails coordination of a substrate to form an octahedral 18-electron complex in which one triflate is in plane with the substrate and thus *trans* to the NHC (**Scheme 20**, paths I and II). Alternatively, one can imagine a Berry-type pseudorotation of TBP five-coordinate species. In course of such a rearrangement, the intermediate has a SP configuration with one triflate in the same plane and again *trans* to the NHC (**Scheme 20**, path III). In this case, one can consider alkylidene ligands as a pivot ligand and its position does not change during Berry-type pseudorotation. With such an SP configuration at least

small fractions of the 16-electron complex can release one triflate and form a cationic complex. In the absence of a substrate, the neutral complexes reform, while in the presence of a substrate (path III in **Scheme 20**), *i.e.* coordination of an olefin to the cationic species followed by [2+2]cycloaddition, becomes operative. Despite the fact that most Mo-imido alkylidene NHC complexes reported here adopt a strongly distorted SP configuration in the solid state, it seems prudent to check for any Berry-type rotations in the Mo-imido alkylidene bis(triflate) NHC complexes. In case there is an interconversion between two TBP configurations, which is known to proceed through an SP intermediate and is fast with respect on the NMR time scale, the two triflates must become magnetically equivalent. In fact, different coalescence temperatures (T_c) for the two triflates can be identified for compounds **5**, **6**, **18**, **19**, **20** and **25**.



Scheme 20. Possible reaction pathways for the formation of cationic species in Mo-imido alkylidene NHC complexes.

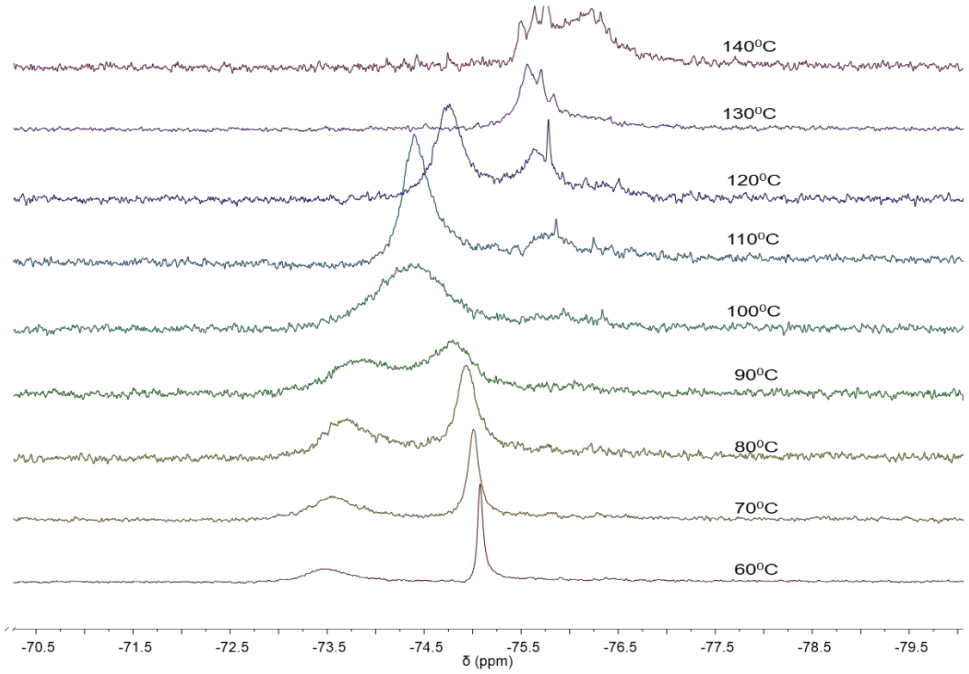


Figure 29. VT ^{19}F-NMR spectra (376 MHz, 1,2-dichlorobenzene-d$_4$) of **5**.

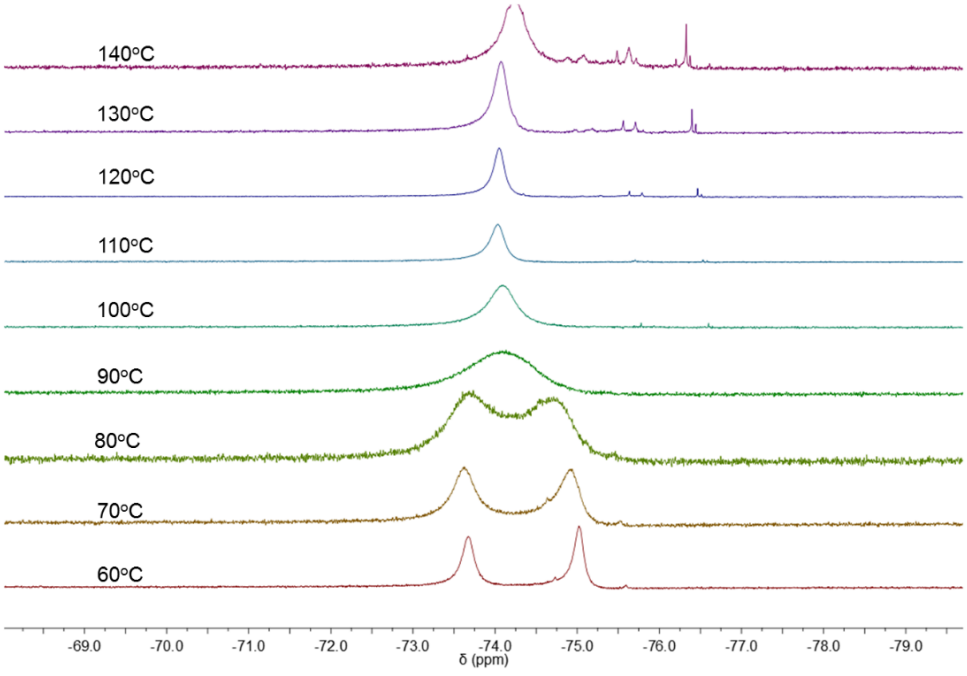


Figure 30. VT ^{19}F-NMR spectra (376 MHz, 1,2-dichlorobenzene-d$_4$) of **6**.

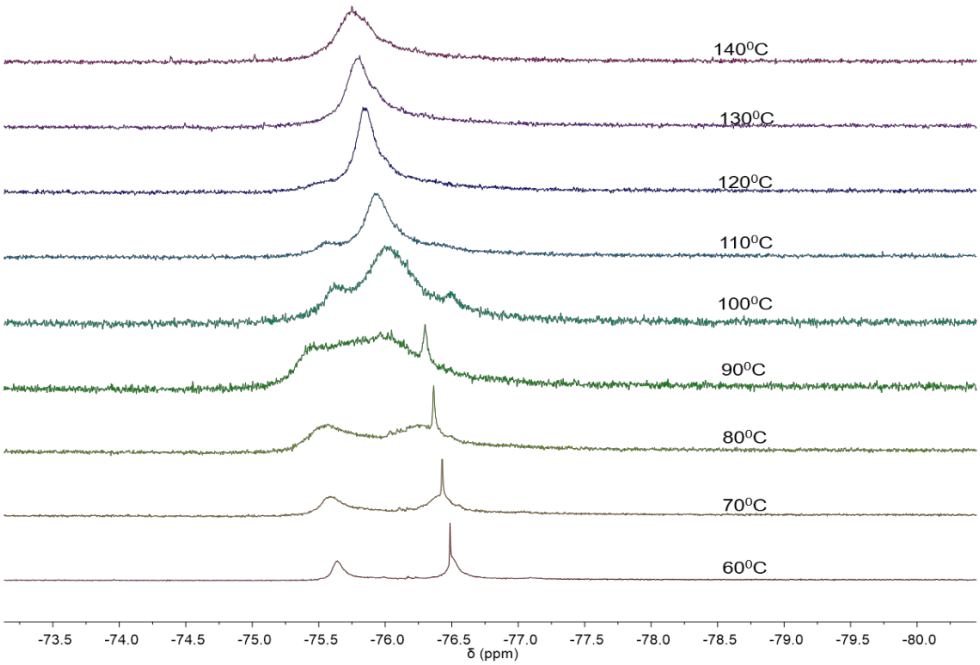


Figure 31. VT ^{19}F-NMR spectra (376 MHz, 1,2-dichlorobenzene-d_4) of **18**.

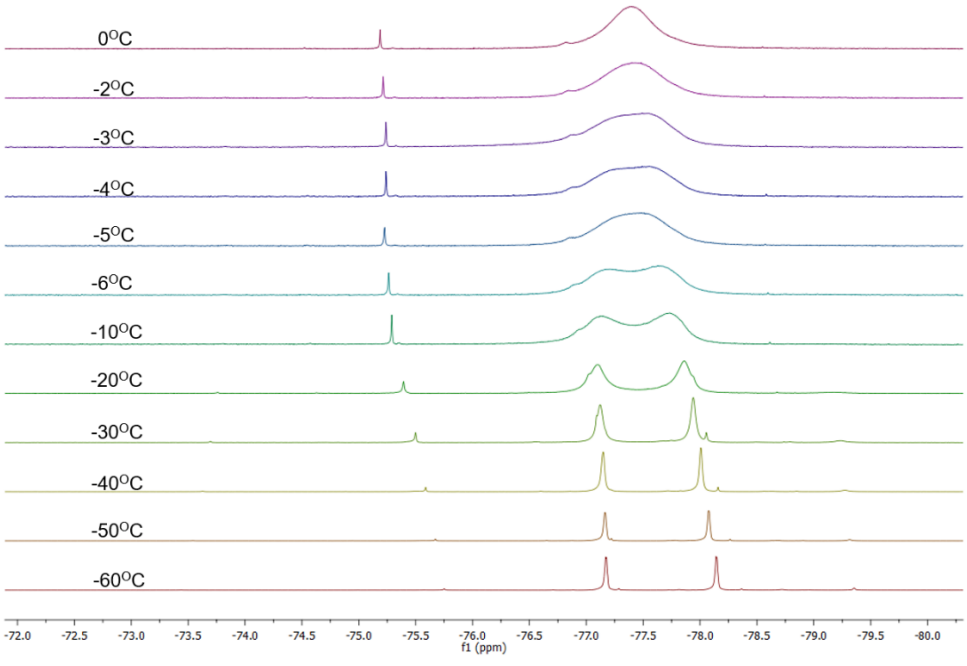


Figure 32. VT ^{19}F-NMR spectra (376 MHz, 1,2-dichlorobenzene-d_4) of **19**.

Table 2 summarizes the results. It is worth pointing out that a switch from IMesH_2 to IMes in compounds **19** and **20**, respectively, results in a significant increase in T_c (-3

→ 60 °C). This is in line with the general observation[31] that electron-withdrawing substituents or here those with a reduced *σ*-donor propensity such IMes compared to $IMesH_2$ increase the barriers of rotation in pentacoordinated complexes.

Table 2. Summary of coalescence temperatures (T_c) for the Mo-imido alkylidene NHC bis(triflate) complexes **5**, **6**, **18**, **19**, and **20**.

Compound	**5**	**6**	**18**	**19**	**20**
T_c **(°C)**	100	85	130	-3	60

As outlined in **Table 1**, there is no direct correlation between the length of the Mo-triflate bond in the solid state and the chemical shift in ^{19}F-NMR of the triflate(s) in solution. This is not really surprising in view of the low energy barriers for Berry-type rotation in five-coordinated transition metal complexes. However, there is a correlation between T_c and reactivity (*vide infra*). The reactivities of novel Mo-imido alkylidene NHC complexes in various olefin metathesis reactions are outlined in the following.

2.2.2 Reactivity of molybdenum imido alkylidene NHC complexes during ROMP and cyclopolymerization

In contrast to the progenitors **1** and **2A**, the corresponding Mo-imido alkylidene bis(triflate) NHC (**3**-**6**) and monoalkoxide (**7**) complexes are active in various metathesis polymerization reactions. In the following, illustrative examples for the reactivity and performance of the novel catalysts in ROMP and cyclopolymerization are given. Thus, with **3**, **5** and **6**, poly(**M1**) could be prepared in 28-90% yield with low PDI, the polymers contained ≥ 90% *trans* double bonds (**Table 3**). With catalyst **4** and **7**, the corresponding polymer had a lower *trans* content of 50% and 64%, respectively (**Table 3**). The k_p/k_i value obtained for **M1** with **3** was 35. The high values for k_p/k_i showed that polymerization is fast in case of **M1** and matches the observed almost complete monomer conversion for polymerization. The polymerization kinetics of **M1** with **3** showed 1st-order kinetics (**Figure S108**, **Appendix I**), with full monomer conversion after 45 min at room temperature. Similar results were found for poly(**M2**), which was obtained in 65-90% yield by the action of **3, 5** and **6** and also displayed a high *trans* content of 75-85% (**Table 3**). With catalysts **4** and **7**, the *trans* content of

this polymer was 33% and 50%. To our knowledge, these are the first high yield metathesis reactions reported for any Mo-imido alkylidene bis(triflate) complex.

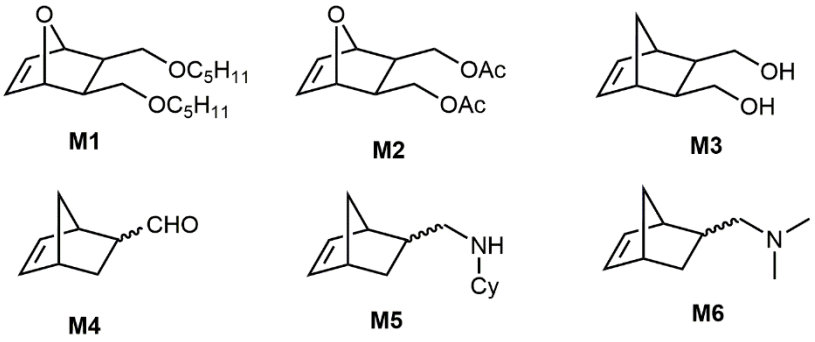


Figure 33. Monomers in ROMP.

The most striking features of these novel catalysts are related to the ring-opening metathesis polymerization of norborn-5-ene-2,3-dimethanol (**M3**) with **3**; the corresponding polymer was isolated in 80% yield (M_n = 2,800 g/mol, PDI = 1.12, M_n (theor.) = 1,540 g/mol, σ_{trans} = 43%). Similar results were obtained with 2-(*N*-cyclohexylaminomethyl)norborn-2-ene (**M5**) and 2-(*N*,*N*-dimethylaminomethyl)norborn-2-ene (**M6**) giving the corresponding polymers poly[2-(*N*-cyclohexylaminomethyl)norborn-2-ene] M_n = 13,100 g/mol, PDI = 1.10, σ_{trans} = 35%, poly[2-(*N*,*N*-dimethylaminomethyl)-norborn-2-ene], M_n = 10,500 g/mol, PDI = 1.21 and poly[2-(N-cyclohexylaminomethyl)norborn-2-ene], isolated in 90% and 80% yield. With catalyst **3**, poly(NBE)-*co*-poly(CPE) was obtained in 80% yield with 48% alternating units (**Figure S124**, **Appendix I**).

Another remarkable application of these catalysts were the cyclopolymerization of 4,4-bis(hydroxymethyl)-1,6-heptadiyne (**M9**) (**Figure 34**), a monomer with two unprotected hydroxy groups. Unlike classic *Schrock* catalysts, which are very sensitive towards protic functionalities, this monomer was quantitatively polymerized with **3** within less than 5 min to yield the corresponding purple conjugated polymer (M_n(theor.) = 7,700 g/mol, M_n = 6,500 g/mol, PDI = 1.3, λ_{max} = 554, 593 nm). Unfortunately, no high-quality ^{13}C-NMR spectra of this polyene could be obtained, probably as a result of severe aggregation of the highly polar and protic polymer. Similar results were found with poly(**M9**), which were obtained in 70-54% yield by the action of **5**-**7** (**Table 4**)**.** Furthermore, a dinitrile compound, that is, dipropargylmalodinitrile (**M10**) (**Figure 34**)

was cyclopolymerized by the action of **3** and isolated in 60% yield (M_n = 1,100 g/mol, PDI = 1.15, M_n (theor.) = 1,420 g/mol).

Table 3. Summary of ROMP results with catalysts **3**-**7**.

Monomer	Catalyst	M/C ratio	T [°C]	t [h]	Yield [%][a]	M_n [g/mol]	PDI	*trans/cis*
M1	**3**	50/1	rt	4	90	9,000	1.2	90/10
M1	**4**	50/1	rt	4	60	8,500	1.1	50/50
M1	**5**	50/1	rt	4	84	8,300	1.1	95/05
M1	**6**	50/1	rt	4	86	8,200	1.1	97/03
M1	**7**	50/1	rt	4	28	11,400	1.2	64/36
M2	**3**	50/1	rt	24	97	13,000	1.7	85/15
M2	**4**	50/1	rt	24	35	1,800	1.2	33/67
M2	**5**	50/1	70 °C	4	65	13,000	1.7	81/19
M2	**6**	50/1	70 °C	4	67	14,200	2.1	76/24
M2	**7**	50/1	70 °C	4	77	15,700	1.9	50/50
M3	**3**	10/1	55 °C	5	80	2,800	1.1	43/57
M4	**3**	50/1	rt	20	55	5,000	2.1	n.a
M5	**3**	50/1	70 °C	4	90	13,100	1.1	35/65
M5	**5**	50/1	70 °C	4	65	n.a	n.a	n.a
M5	**6**	50/1	70 °C	4	54	n.a	n.a	n.a
M5	**7**	50/1	70 °C	4	90	n.a	n.a	n.a
M6	**3**	50/1	70 °C	4	90	10,500	1.2	n.a

[a] Yields of isolated product; n.a = not analyzed; monomer:catalyst = 50:1 (mol/mol).

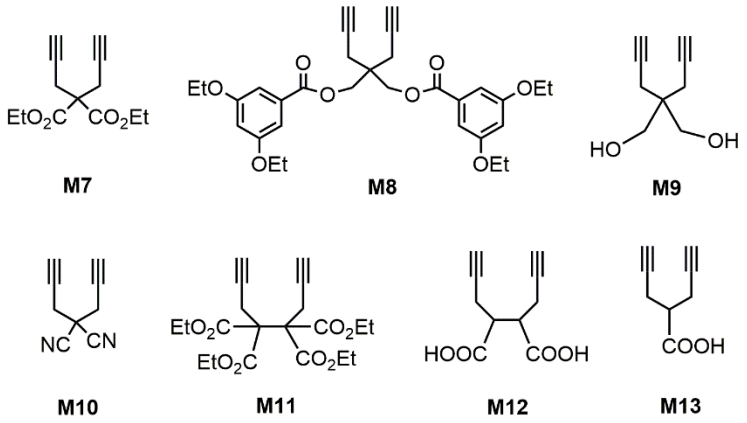


Figure 34. Monomers used in cyclopolymerizations.

In contrast, the high regioselectivity also holds for cyclopolymerisation by subjecting the less reactive 1,7-octadiyne, that is, 4,4,5,5-tetrakis(ethoxycarbonyl)-1,7-octadiyne (**M11**) (**Figure 34**) to polymerize by the action of **3**, **5**, **6** and **7**, the corresponding polymers were isolated in 81-75% yield and formed via 96% *α*-selectivity (**Table 4**). NMR and UV/Vis spectroscopy data fit those of independently prepared samples.[32] Similar results were obtained for the cyclopolymerization of 4,4-bis[(3,5-diethoxybenzoyloxy)methyl]-1,6-heptadiyne (**M8**). The corresponding polyene was isolated in 50-100% yield by the action of **3**, **4**, **5**, **6** and **7** with a maximum 96% *α*-selectivity upto (**Table 4**). With **4**, only 52% yield was obtained after 24 h. However, these catalysts were also found to be excellent promotors for the regioselective cyclopolymerization of diethyl dipropergylmalonate (**M7**), which can be polymerized with **3**, **5**-**7** with isolated yields ranging from 89-46% and ~100% *α*-selectivity. Kinetic investigations of cyclopolymerizations catalyzed by **3** showed different reactivities of the monomers, but in all cases an almost linear 1st-order plot. Using THF instead of CH_2Cl_2, the reaction rate was reduced, in case of **M8** by a factor of about two (**Figure 35**).

Table 4. Summary of cyclopolymerization results with catalysts **3**-**7**.

Monomer	Catalyst	Solvent/T (°C)/time	Yield [%][a]	α-Selectivity	M_n (g/mol)	PDI
M7	**3**	CH_2Cl_2, -30 to rt, 1 h	89	≥ 95 %	9,600	1.6
M7	**4**	CH_2Cl_2, -30 to rt, 24 h	46	n.a	1,600	2.7
M7	**5**	CH_2Cl_2, -30 to rt, 1 h	84	≥ 95 %	8,500	2.1
M7	**6**	CH_2Cl_2, -30 to rt, 1 h	86	≥ 99 %	84,000	2.3
M7	**7**	CH_2Cl_2, -30 to rt, 1h	54	≥ 96 %	67,400	2.7
M8	**3**	CH_2Cl_2, rt, 2 h	94	≥ 91 %	12,400	1.5
M8	**4**	CH_2Cl_2, rt, 24 h	52	n.a	20,000	2.3
M8	**5**	$CHCl_3$, -30 to 80, 1 h	100	≥ 93 %	11,600	1.8
M8	**6**	$CHCl_3$, -30 to 80, 1 h	60	≥ 93 %	14,900	2.7
M8	**7**	$CHCl_3$, -30 to 80, 1 h	50	≥ 96 %	20,300	1.6
M9	**3**	CH_2Cl_2, rt, 1 h	80	n.a	6,500	1.3
M9	**5**	CH_2Cl_2, rt, 1 h	70	n.a	5,000	2.1
M9	**6**	CH_2Cl_2, rt, 1 h	56	n.a	3,900	1.8
M9	**7**	CH_2Cl_2, rt, 1 h	54	n.a	3,000	1.3
M10*	**3**	CH_2Cl_2, rt, 2 h	60	n.a	1,100	1.2
M11	**3**	CH_2Cl_2, rt, 1 h	81	≥ 96%	13,200	1.9
M11	**5**	$CHCl_3$, -30 to 80, 1 h	81	≥ 96%	15,000	2.2
M11	**6**	$CHCl_3$, -30 to 80, 1 h	75	≥ 96%	17,100	1.8
M11	**7**	$CHCl_3$, -30 to 80, 1 h	75	n.a	20,000	2.2
M12**	**3**	CH_2Cl_2, rt, 2 h	90	n.a	2,600	1.3
M13	**5**	$CHCl_3$, -30 to 80, 4 h	65	n.a	6,200	1.5
M13	**6**	$CHCl_3$, -30 to 80, 4 h	55	n.a	5,600	1.3
M13	**7**	$CHCl_3$, -30 to 80, 4 h	55	n.a	2,800	2.0

[a] Yields of isolated product; n.a = not analyzed; monomer:catalyst = 50:1 (mol/mol); * monomer:catalyst = 10:1 (mol/mol); ** monomer:catalyst = 25:1 (mol/mol).

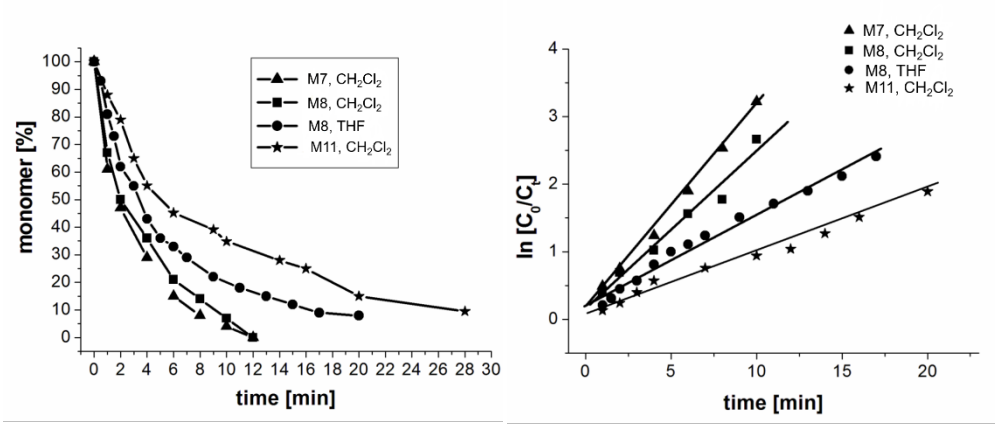


Figure 35. 1st-order plot ($\ln[c_0/c_t]$ *vs.* time) for **M7, M8** and **M11** cyclopolymerized by **3** at room temperature (right). Kinetic investigations for **M7, M8** and **M11** cyclopolymerized by **3** at room temperature (left).

The high functional-group tolerance of **3** is also reflected by the fact that polymerization reactions cannot be terminated by the addition of an aldehyde, for example, ferrocene-carboxaldehyde (**Figure 36**). In case of initiator **3** there was no *Wittig* type reaction observed and even **3** was stable in CD_2Cl_2 in the presence of an excess of ferrocene-carboxaldehyde (**Figure 36**). Termination and MALDI-TOF mass analysis of oligomeric **M11** with different protic compounds did not succeed. Furthermore, initiator **3** was stable for some hours in the presence of two equivalents of *iso*propanol (**Figure 37**). After some time (ca. 5 min), new alkylidene signals were observed. Maybe the NHC deprotonates the *iso*propanol and a mixture of mono- and bis-alkoholate cationic complexes forms. Instead, cross-metathesis with an olefin, for example, any *α*-olefin is required to terminate the living polymer chain. Alternatively, termination can be accomplished by the addition of a HCl-containing methanol solution or by using trifluoroacetic acid. This unreactivity towards aldehydes in turn allowed poly(norborn-5-ene-2-yl carbaldehyde) (**M4**) to be synthesized by the action of **3**, and to be isolated in 55% yield (M_n = 5,000 g/mol, PDI = 2.1, M_n (theor.) = 6,100 g/mol). Finally, and again absolutely unprecedented for molybdenum based metathesis catalysts, a diyne containing two free carboxylic acids, that is, 1,7-octadiyne-4,5-dicarboxylic acid could be cyclopolymerized and the product was isolated in 90% yield by the action of **3** (M_n = 2,600 g/mol, PDI = 1.3, M_n (theor.) = 5,000 g/mol).

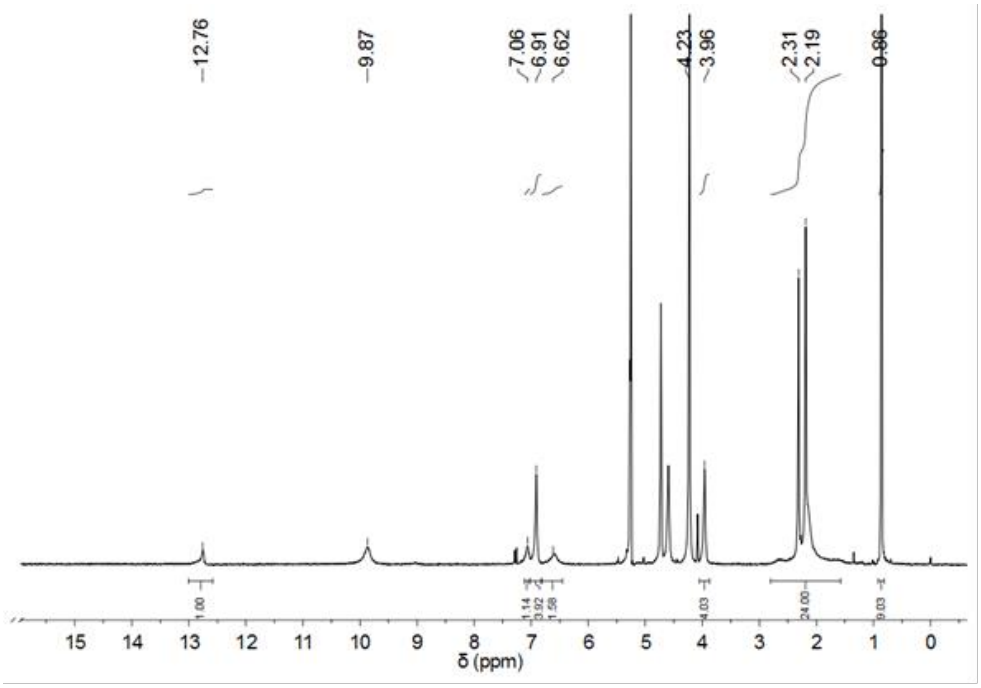


Figure 36. ^{1}H-NMR spectrum (400 MHz, CD_2Cl_2) of **3** in the presence of ferocenaldehyde.

The high solution stability of catalyst **3** is shown in **Figure 38**, no decomposition of **3** was observed up to 180 days in NMR tube. In view of this remarkable metathesis activity and functional-group tolerance of a high oxidation state Mo- alkylidene, the question about the nature of the propagating species. At first glance, the high reactivity in ROMP and cyclopolymerization is very surprising, since the "universal precursors" of the general formula [Mo(NR')(CHCMe$_2$R)(OTf)$_2$(DME)] (R = -CH$_3$, -C$_6$H$_5$) do not display any metathetical activity and so far solely served as progenitors for the metathetically active alkoxide, phenoxide, and carboxylate complexes.[18] However, "universal precursors" are 18-electron complexes in which decoordination of DME does not occur. Catalysts **3**-**7** are 16-electron complexes with one triflate located nearly *trans* to the NHC and the imido ligand. Unlike the bipyridyl and phenantroyl adducts of *Schrock* catalysts reported by *Fürstner*,[33] no dissociation of the NHC is required to activate the catalyst. Thus, NMR spectroscopy clearly shows that the NHC ligand remains bound to the metal center and that no free NHC or imidazol(in)ium salt is observed. However, polymerization commences with the dissociation of one triflate ligand, presumably the one that experiences the strongest *trans*-effect (**Scheme 21**) once substrate (monomer) has been added.

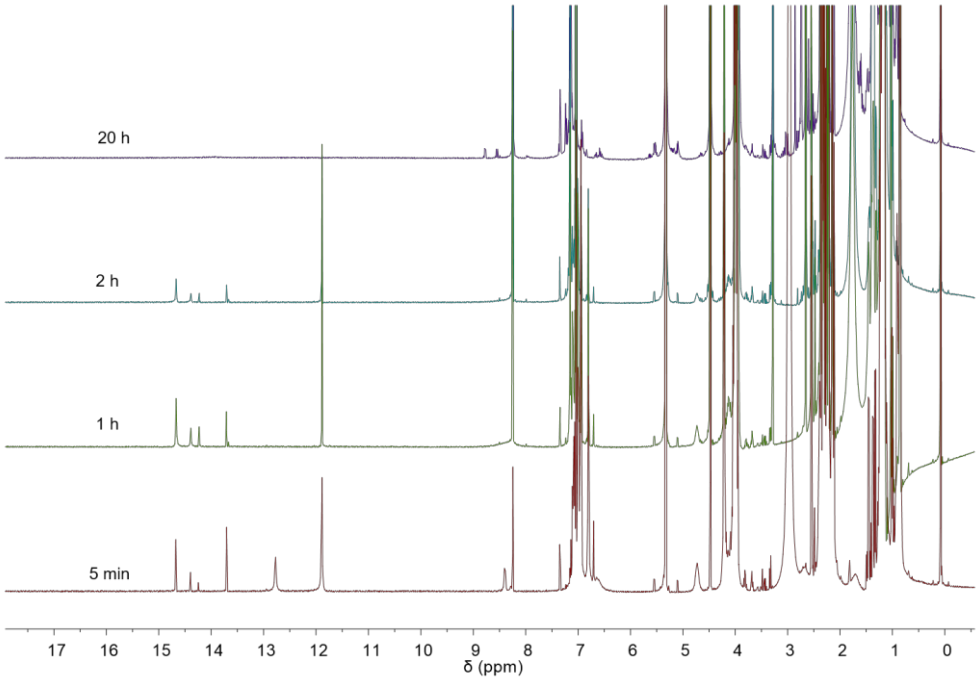


Figure 37. ^{1}H-NMR (400 MHz, CD_2Cl_2) of **3** in the presence of isopropanol.

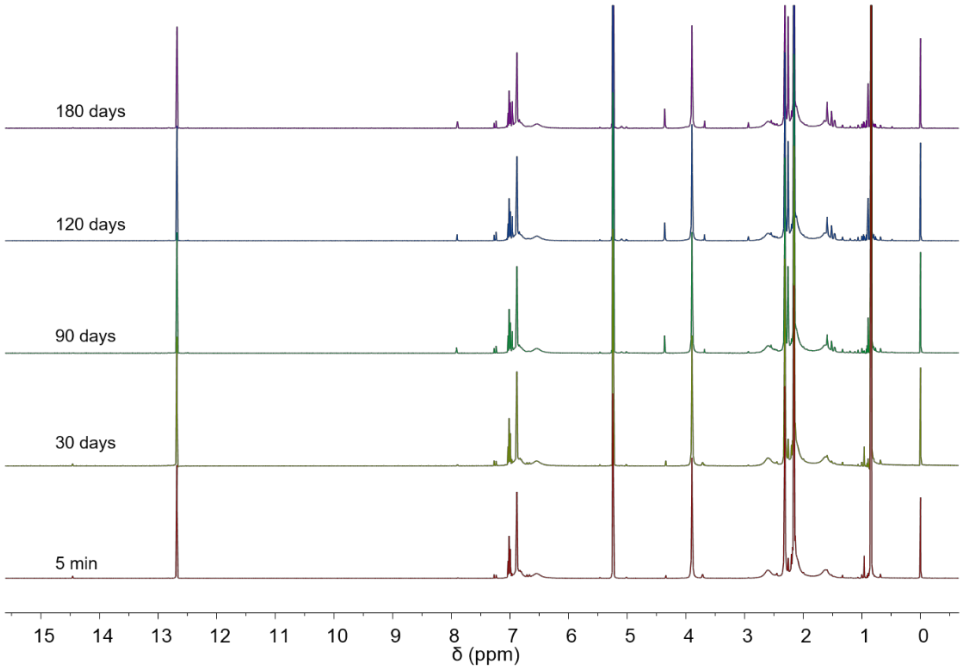
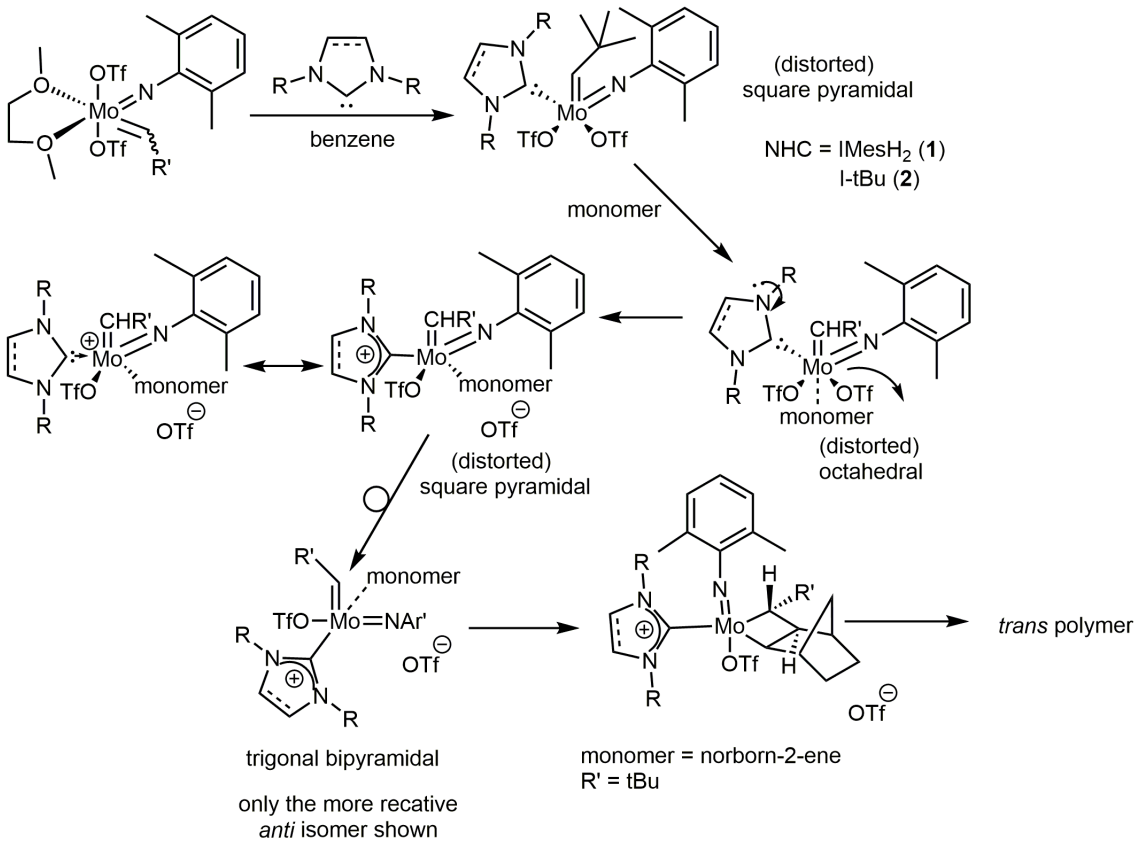


Figure 38. ^{1}H-NMR spectrum (400 MHz, CD_2Cl_2) of **3** in different time intervals.



Scheme 21. Formation of the cationic species in the presence of monomer, and *trans*-selectivity in ROMP.

The approach of the substrate (monomer) must be expected to occur *trans* to the Mo-alkylidene unit, thereby forming an octahedral 18-electron complex. This 18-electron complex is characterized by a more linear orientation of at least one triflate *trans* with respect to the Mo-NHC or Mo-arylimido bond. Consecutively, the *trans*-effect triggers the release of the corresponding triflate and a cationic, 16-electron complex forms (**Scheme 21**). This complex can either adopt a (distorted) SP or a TBP geometry. In view of the reactivity of Mo-monoalkoxy pyrrolide (MAP) complexes,[34-36] it is assumed that either directly or out of the SP geometry, a TBP metallacyclobutane forms through rearrangement. [2+2]cycloaddition of the monomer to the alkylidene then starts ROMP. Formation of a polymer with a high *trans* content should then start from the *anti*-isomer. Notably, this activation pathway has so far been confirmed for both ROMP and cyclopolymerization.[37] Clearly, the propensity to form a cationic complex strongly depends on both the nucleophilic character of the NHC and the ability to arrange at least one triflate *trans* to either the NHC or the aryl imido ligand. **Figure 39** shows the

^{19}F-NMR spectra of the polymerization of (norborn-5-ene-2-yl-carbaldehyde) (**M4**) measured in different time interval by the action of **3**.

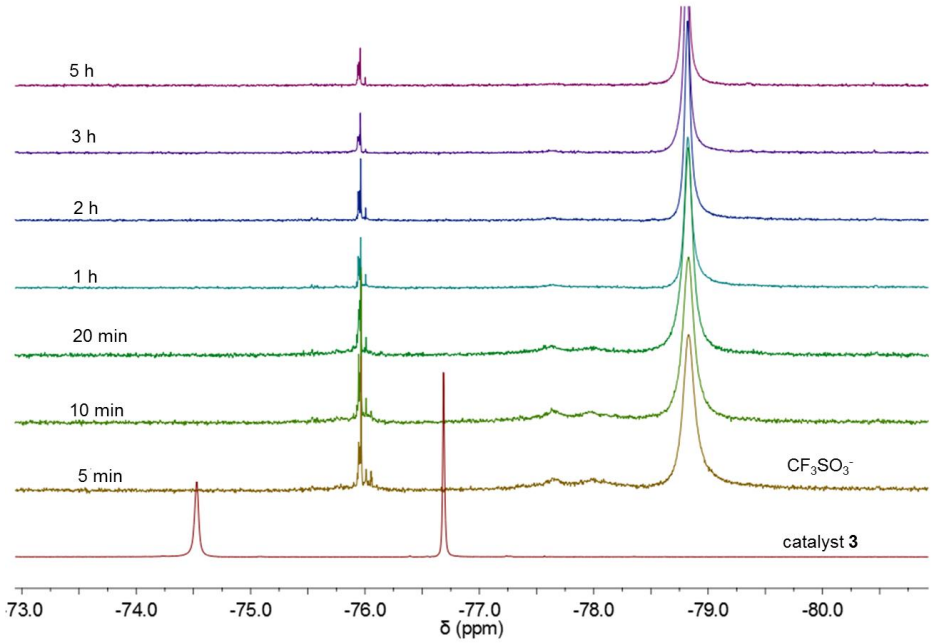


Figure 39. ^{19}F-NMR spectra (CD_2Cl_2) recorded at different time intervals for the polymerization of (norborn-5-ene-2-yl carbaldehyde) by the action of **3**.

As can be seen, the parent two signals for the two individual triflate ligands at δ_F = -74.65 and - 76.7 ppm (integral ratio 1:1) vanish within less than 5 min and new signals are observed at δ_F = -76.85 and -78.8 ppm. While the signal at δ_F = -76.85 ppm can be assigned to a triflate bound to Mo, the signal at δ_F = -78.8 ppm corresponds to free triflate. Since the polymer with the initiator attached to it precipitates in the course of the reaction, the signal of the triflate bound to molybdenum appears weaker than the one for the fully soluble free triflate anion.

An analogous release of one triflate is detected in the ^{19}F-NMR spectra recorded during the polymerization of 5,6-bis[(pentyloxy)methyl]bicyclo[2.2.1]hept-2-ene (**M1**)(**Figure 40**), and with diethyl dipropargylmalonate (**M7**) (**Figure 41**). Again, the signals for the parent catalyst vanish, while the one of free triflate and those for different Mo-triflates bound to the polymer (different initiation products) develop over time.

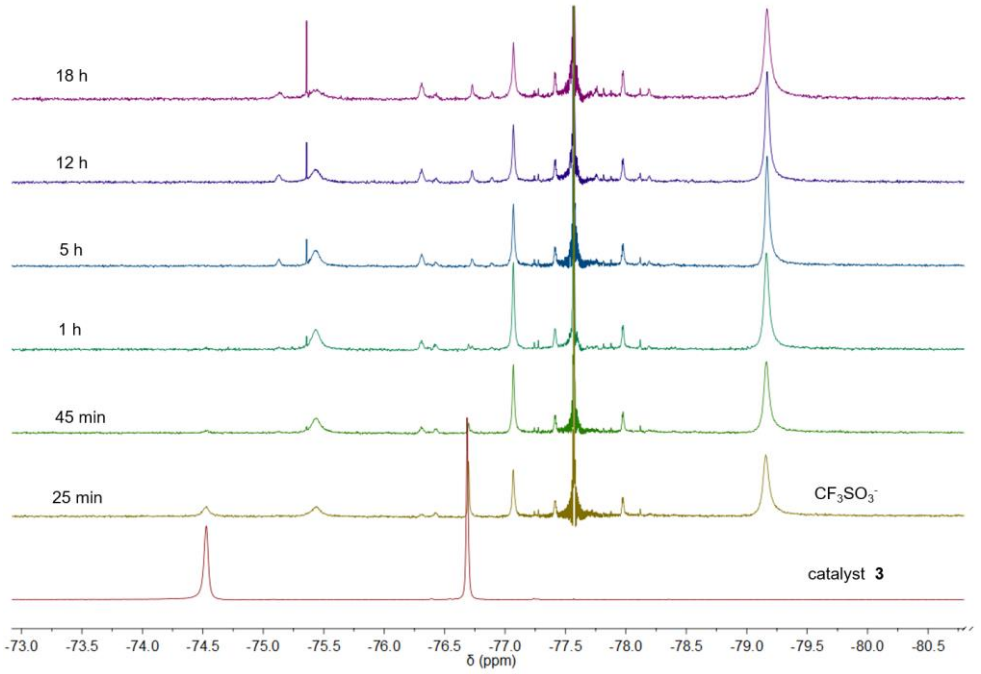


Figure 40. ^{19}F-NMR spectra (CD_2Cl_2) recorded at different time intervals for the polymerization of 5,6-bis[(pentyloxy)methyl]bicyclo[2.2.1]hept-2-ene by the action of **3**.

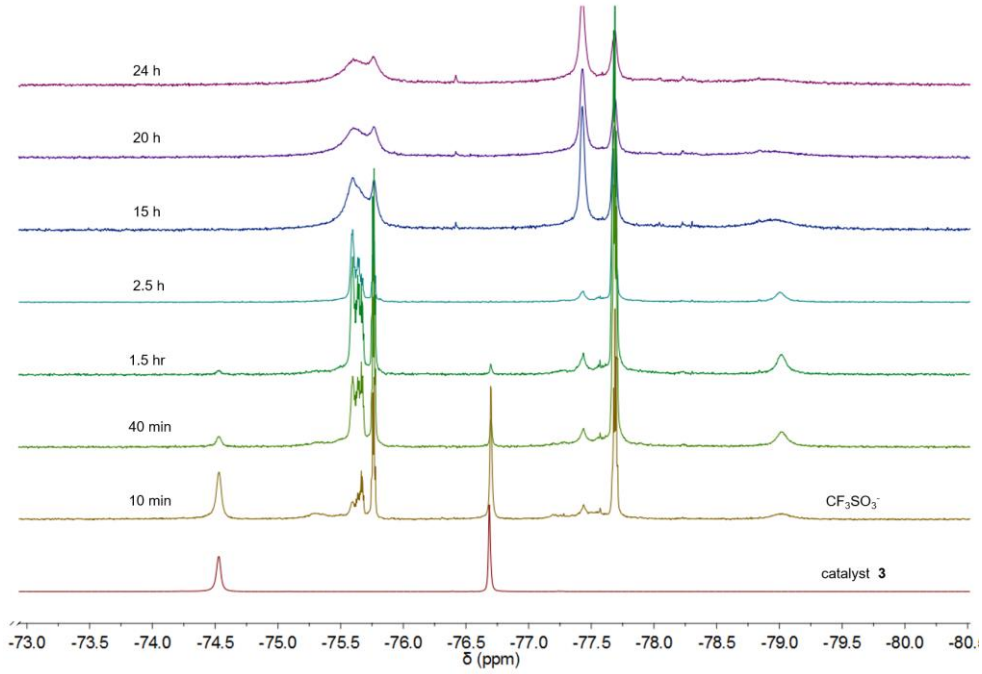


Figure 41. ^{19}F-NMR spectra (CD_2Cl_2) recorded at different time intervals for the polymerization of diethyl dipropargylmalonate by the action of **3**.

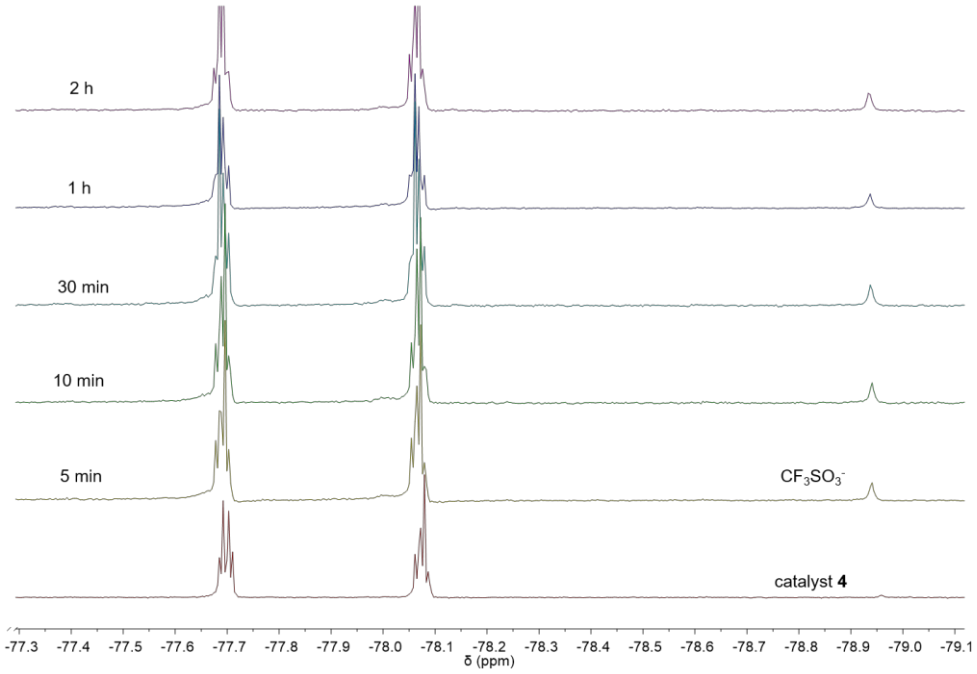


Figure 42. ^{19}F-NMR spectra (CD_2Cl_2) recorded at different time intervals for the polymerization of 5,6-bis[(pentyloxy)methyl]bicyclo[2.2.1]hept-2-ene by the action of **4**.

These data clearly show that in the presence of monomer, but notably not in its absence, **3** converts quickly into a cationic 16-electron species catalyst [Mo(NAr')(IMesH$_2$)(monomer)(CH-*t*Bu)(OTf)]$^+$[OTf]$^-$), which then initiates the corresponding metathesis reaction (**Scheme 21**). In contrast, catalyst **4** is much more reluctant to release a triflate (**Figure 42**), a finding that corroborates with its lower metathesis activity and with the proposition that a cationic14-electron species is the active catalyst.

Nonetheless, in view of the more pronounced nucleophilicity of I-*t*Bu, this is somewhat surprising, since the more nucleophilic NHC in **4** must stabilize the cationic charge better than the less nucleophilic one in **3**, **5** and **6**. On the other hand, the bulky character of I-*t*Bu might well impede the realization of a linear alignment of the NHC–Mo–OTf or arylimido–Mo–OTf bond that is a prerequisite for an effective release of the triflate. In case of catalyst **6**, due to presence of *π*-electrons in the NHC, the carbene is resonance stabilized. This makes the carbene less basic than its saturated analogue, however, this could not result in any significant impact on polymerization. The ^{19}F-NMR of complex **7** during cyclopolymerization (**Figure 43**) suggests the

presence of a small fraction of free triflate and some release of $^{-}OCH(CF_3)_2$ (**Scheme 22**).

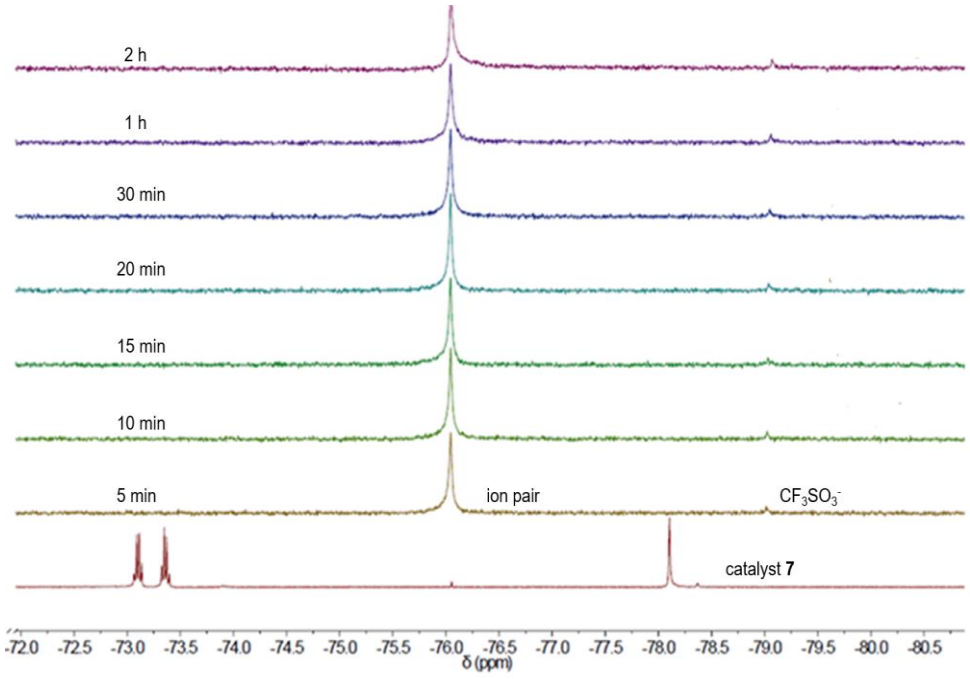
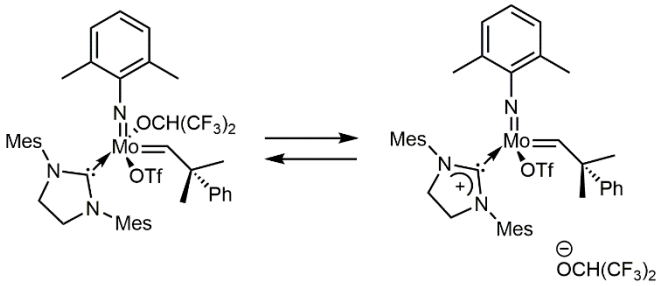


Figure 43. ^{19}F-NMR spectra (CD_2Cl_2) recorded at different time intervals for the polymerization of 4,4-bis(hydroxymethyl)-1,6-heptadiyne by the action of **7.**



Scheme 22. Formation of free-alkoxides during polymerization.

Clearly, the influence of the ring size and substituents at the NHC on the formation of the *syn*- and *anti*-isomers, their rates of interconversion and finally, on the propensity of the corresponding catalyst to form cationic metal alkylidene complexes, need to be investigated. It is only possible to speculate about the reasons for the higher *trans* content of polymers prepared by the action of **3**, **5** and **6**. One possible explanation is

that this catalyst, in contrast to **4** and **7**, contains a small fraction of the *anti*-alkylidene. If these systems behave like existing *Schrock* catalysts (**Scheme 21**), then an involvement of the *anti*-isomer in conjunction with a fast *syn–anti* interconversion should give rise to high *trans* contents.[38] As outlined by *Schrock et.al.*, a fast *syn–anti* interconversion requires the presence of electron-donating anionic ligands, for example, alkoxides. In fact, NHCs are strongly electron-donating and thus fulfill this requirement. However, at this point, this explanation is only a reasonable hypothesis and the rates of interconversion need to be measured by photolysis experiment. In due course, theoretical studies of these novel Mo-imido alkylidene NHC complexes during polymerization might provide a more accurate scenario of the active species in terms of energy profiles.

2.2.3 Reactivity of molybdenum imido alkylidene NHC complexes during different metathesis reactions

A set of reactions and substrates were chosen for determining the activity and functional-group tolerance of these novel catalysts. For these purposes, catalysts **3**-**27** were used in a series of olefin metathesis reactions including ring-closing metathesis (RCM), homometathesis (SM), ethenolysis and cross-metathesis (CM) reactions. Unless indicated otherwise, reactions were carried out at 80 °C in $C_2H_4Cl_2$ used as a solvent. Complementary catalysts were used in ROMP and cyclopolymerization of various 1,6-hepta- and 1,7-octadiynes. Notably, unlike catalysts **3**-**6**, **18**, **19** and **20** used herein, the parent Mo-arylimido alkylidene bis(triflates) complexes do not display any olefin metathesis activity themselves. Instead, they are widely used as progenitors for a vast variety of "1st-generation" *Schrock* catalysts. With these bis(triflates), anion metathesis with, *e.g.*, alkoxides, amides or phenolates is required for the synthesis of olefin metathesis-active complexes. With diallyl diphenylsilane, **3** allows for turnover numbers of 480 in 1,2-dichloroethane at T = 80 °C for 4 h and thus clearly rivals with other cationic Mo-complexes.[19] Catalyst **3** was also active in homometathesis of allyltrimethylsilane, 1-hexene and cross-metathesis of allyltrimethylsilane with 1-hexene. 49% Cross-metathesis product was observed in the CM of allyltrimethylsilane:1-hexene, (1:1).

Table 5. Homo- and cross-metathesis results with **3**.

Substrates	Solvent	T [°C]/t [h]	TON	*E/Z*
allyltrimethylsilane	CH_2Cl_2	rt, 4 h	0	-
allyltrimethylsilane	$C_2H_4Cl_2$	80 °C, 4 h	500	72/28
1-hexene	CH_2Cl_2	rt, 4 h	20	80/20
1-hexene	$C_2H_4Cl_2$	80 °C, 4 h	200	80/20
allyltrimethylsilane +1-hexene	$C_2H_4Cl_2$	80 °C, 4 h	500	85/15

Catalyst:substrate = 1:500 (mol/mol), internal standard for GC-MS = *n*-dodecane. rt = room temperature.

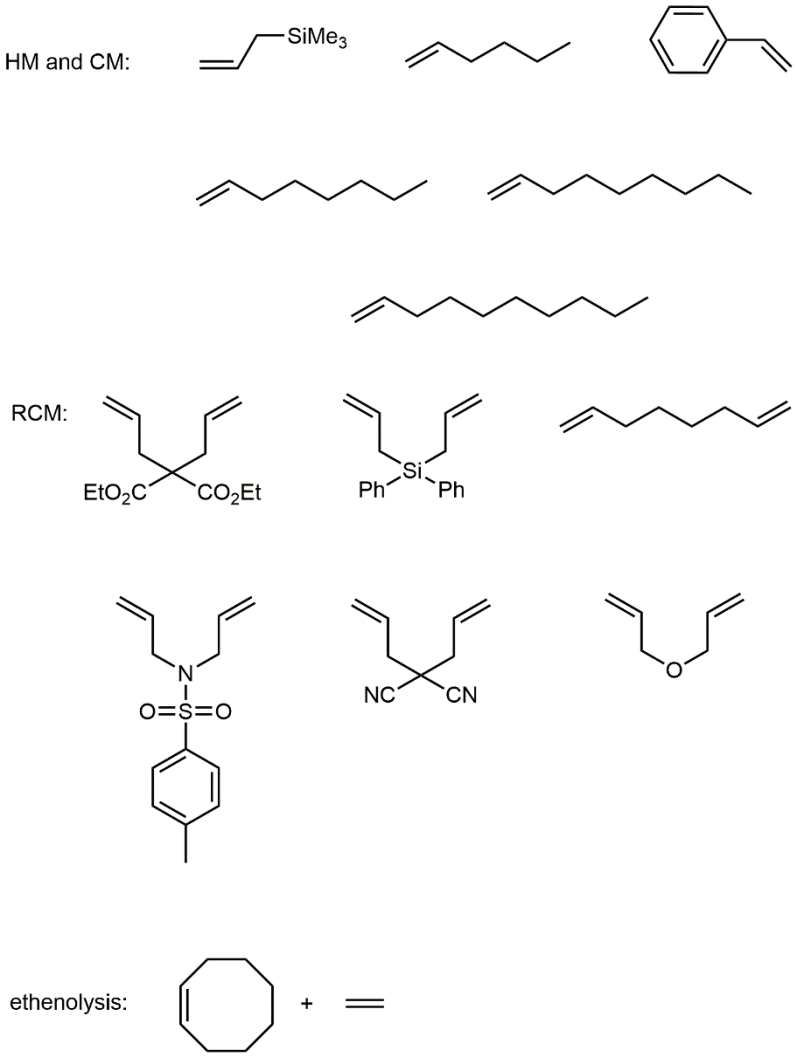


Figure 44. Substrates for RCM, HM, CM and ethenolysis.

Table 6. Productivity of catalysts **5**-**27** in RCM[a].

Cat.	diethyl diallylmalonate	diallyl diphenylsilane	1,7-octadiene	N,N-diallyl-*p*-tosylamide	diallylmalodinitrile	diallyl ether
5	175	620	140	180	190	220
6	90	490	920	160	70	245
7	3,200[b]	390	4,100[b]	420	360	690
10	500[b]	580	3,300[b]	365	100	850
11	65	210	350	110	65	85
14	0	0	80,000[c] 100,000[d]	-	-	-
16	700	960	1000 87,100[e]	700	390	600
18	80	530	230	0	0	250
19	130	440	130	80	0	160
20	50	240	120	60	85	70
21	0	130	160	0	0	55
22	0	770	790	160	70	860
24	0	231	213	159	-	177
25	-	450	85	-	-	-
26	-	70	150	-	-	-
27	155	170	40	-	-	200

[a] Condition unless otherwise stated: $ClCH_2CH_2Cl$, 80 °C, 4 h, catalyst:substrate = 1:1000 (mol/mol); [b] $ClCH_2CH_2Cl$, 80 °C, 4 h, catalyst:substrate = 1:5,000 (mol/mol); [c] $ClCH_2CH_2Cl$, room temperature, overnight, catalyst:substrate = 1:100,000 (mol/mol); [c] $ClCH_2CH_2Cl$, room temperature, 1 h, catalyst:substrate = 1:100,000 (mol/mol); [d] $ClCH_2CH_2Cl$, room temperature, 1 h, catalyst:substrate = 1:500,000(mol/mol); [e] $ClCH_2CH_2Cl$, 80 °C, 4 h, catalyst:substrate = 1:140,000 (mol/mol); internal standard for GC-MS = *n*-dodecane.

Among all catalysts investigated, complexes **7**, **10**, **14**, **15**, **16** and to some extent **22** stand out in productivity (TON). While **14**, **15**, **16** and **17** are cationic complexes, but **7**, **10**, **11**, **12**, **13**, **22** and **26** have one electron-withdrawing group and one triflate bound to molybdenum. Notably, as outlined in **Table 6** and **7**, all catalysts show distinct differences in HM and RCM of the chosen substrates, whereas the cationic catalysts

14, **15** and **16** exhibits outstanding activity for pure hydrocarbons. All together, this supports our proposed mechanism and finding that Mo-imido alkylidene NHC complexes must either be cationic to be highly active in olefin metathesis reactions or have one very good leaving group such as triflate. Only in this case, a cationic complex can form in the presence of substrate, i.e. of an olefin (*vide* **Scheme 20**).

TON in the HM of 1-hexene, styrene and 1-octene were in the range of 45,000-210,000. Similarly, the TON of **14** for the RCM of 1,7-octadiene was 100,000. The cationic complex **15** also deserves special attention. It allows for turnover numbers of 192,000 (95% *E*) in the homometathesis (HM) of 1-octene (room temperature, 1,2-dichlorethane) using a ratio of **15**:1-octene = 1:680,000. At 80 °C, a TON of 323,000 (93% *E*) is achieved even at a lower ratio of **15**:1-octene = 1:500,000. In the HM of 1-nonene, a TON of 352,000 (92% E) was achieved at room temperature (1,2-dichlorethane) using a ratio of **15**:1-nonene of 1:570,000. At 80°C, a TON of 545,000 (90 % E) was achieved using a ratio of **15**:1-nonene of 1:1,000,000. Also worth to be mentioned, the cationic complex **16** is also active in the RCM of ester-, silane-, amide-, nitrile- and ether-containing substrates (**Table 6**). In that regard, **16** strongly differs from **14** and **15** which do not tolerate any functional group and nicely demonstrates the impact of changing one triflate to pentafluorophenolate. Furthermore, the TON of **16** for the RCM of 1,7-octadiene was 87,100.

Table 7. Productivity for catalysts **5**, **6**, **7**, **14**-**16** during homo-metathesis (HM).

Complex	allyltrimethylsilane	1-hexene	styrene	1-octene	1-nonene
5	520(60)	340 (100)	60 (100)	680 (85)	-
6	435(55)	490 (100)	80 (100)	560 (85)	-
7	-	790 (100)	200 (100)	-	-
14	-	140,000[d] (100)	45,000[d,e] (100)	210,000[d] (86)	-
15	-	-	-	192,000[f] (95) 323,000[g] (93)	352,000[h] (92) 545,000[i] (92)
16	800 (88)	-	-	75,000[j] (92)	-

[a] Condition unless otherwise stated: $ClCH_2CH_2Cl$, 80 °C, 4 h, catalyst:substrate = 1:1000 (mol/mol); [c] $ClCH_2CH_2Cl$, room temperature, overnight, catalyst:substrate = 1:100,000 (mol/mol); [c] $ClCH_2CH_2Cl$, room temperature, 1 h, catalyst:substrate = 1:100,000 (mol/mol); [d] $ClCH_2CH_2Cl$, room temperature, 1 h, catalyst:substrate = 1:500,000(mol/mol); [e] along with approximately 10% 1,3-diphenylprop-1-ene; [f] $ClCH_2CH_2Cl$, room temperature, 4 h, catalyst:substrate = 1:680,000(mol/mol); [g] $ClCH_2CH_2Cl$, 80 °C, 4 h, catalyst:substrate = 1:500,000 (mol/mol); [h] $ClCH_2CH_2Cl$, room temperature, 4 h, catalyst:substrate = 1:570,000 (mol/mol); [i] $ClCH_2CH_2Cl$, 80 °C, 4 h, catalyst:substrate = 1:1,000,000 (mol/mol). [j] $ClCH_2CH_2Cl$, 80 °C, 4 h, catalyst:substrate = 1:140,000 (mol/mol). Values in parentheses refer to the *E* fraction; -: reaction was not carried out; internal standard for GC-MS = *n*-dodecane.

Interestingly, complexes **10** and **11** show different activities, despite comparable pK_a values of the conjugated acids of the anionic ligands ($pK_{a,\ water}$, C_6F_5OH = 5.5; pK_a, $(CF_3)_3COH$ = 5.2). Similar accounts for **11** and **22**, which both contain one nonafluoro-*tert*-butoxide and one triflate ligand but two different imido ligands (2,6-dimethylphenylimido *vs.* 3,5-dimethylphenylimido). The activities of catalysts **19** and **20**, both of them bear a small aryl-imido ligand, were found to be comparable to those of **5** and **6**. Surprisingly, catalysts **19** and **20** that contain 3,5-dimethylphenylimido ligand are more reactive than **5** and **6**, at least for the homometathesis of methyl oleate. With methyl oleate, **19** allows for turnover numbers of 240 in 1,2-

dichloroethane at T = 80 °C for 4 h. All that underlines the importance of subtle changes in catalyst structure on catalytic behavior. In the ethenolysis of *cis*-cyclooctene with catalyst **14** (COE, **Table 8)** TONs upto 30,000 were obtained at 30 bar using non-purified ethylene.

Table 8. Ethenolysis of *cis*-cyclooctene (COE) with catalyst **14**.

Pressure [bar]	T [°C]	Time [h]	Conversion [%]	TON	COE:14
5	rt	3	34	6,800	20,000:1
50	rt	6	15	15,000	100,000:1
30	80	6	30	30,000	100,000:1

Solvent = toluene (ca. 50 mL); internal standard for GC-MS = *n*-dodecane; catalyst was added in CH_2Cl_2; ethylene (99%) was used.

Another important finding is that the bis(triflate) complexes were found to be highly temperature resistant. Accordingly, elevated temperature can be used to promote dissociation of one triflate, thereby enhancing catalyst activity. And in fact, complex **19**, which is stable in solution at high temperature (**Figure 46**), shows impressive productivity in case reactions run at 140 °C in 1,2-dichlorobenzene using a catalyst:substrate ratio of 1:20,000 (t = 4 h). TONs for the RCM of diallyldiphenylsilane, diethyl diallylmalonate and N,N-diallyl-*p*-toluolsulfonamide increased from 440, 130 and 80 to 9600, 1600 and 4200, respectively. High productivity was also found in the self-metathesis (SM) of methyl oleate (TON = 2,500) (**Table 9**).

Next, correlated the coalescence temperature, T_c, with catalyst activity. If the proposal that the five-coordinate complexes undergo Berry-type pseudorotation is valid, this interconversion, which passes through an SP configuration or vice versa, must result in chemically and magnetically equivalent triflate groups. This results in the coalescence of the parent two signals for the triflates. Consequently, T_c should be indicative for the temperature at which a bistriflate complex becomes active. **Table 10** summarizes the results in selected RCM reactions obtained at room temperature for complexes **18**, **19** and **20**, covering T_c values between -3 and 130 °C. Clearly, **19** having the *lowest* T_c value shows the *highest* productivity while **18** with *highest* T_c value remains *inactive* in RCM or delivers much lower TONs than **19** and **20** do.

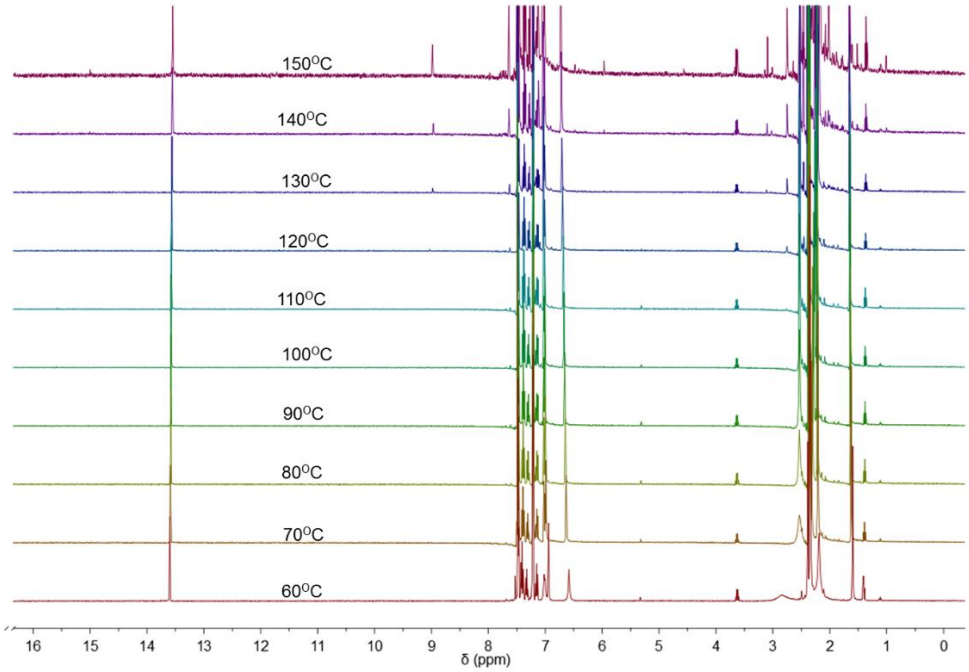


Figure 45. VT ^{1}H-NMR spectra (400 MHz, 1,2-dichlorobenzene-d$_4$) of **6**.

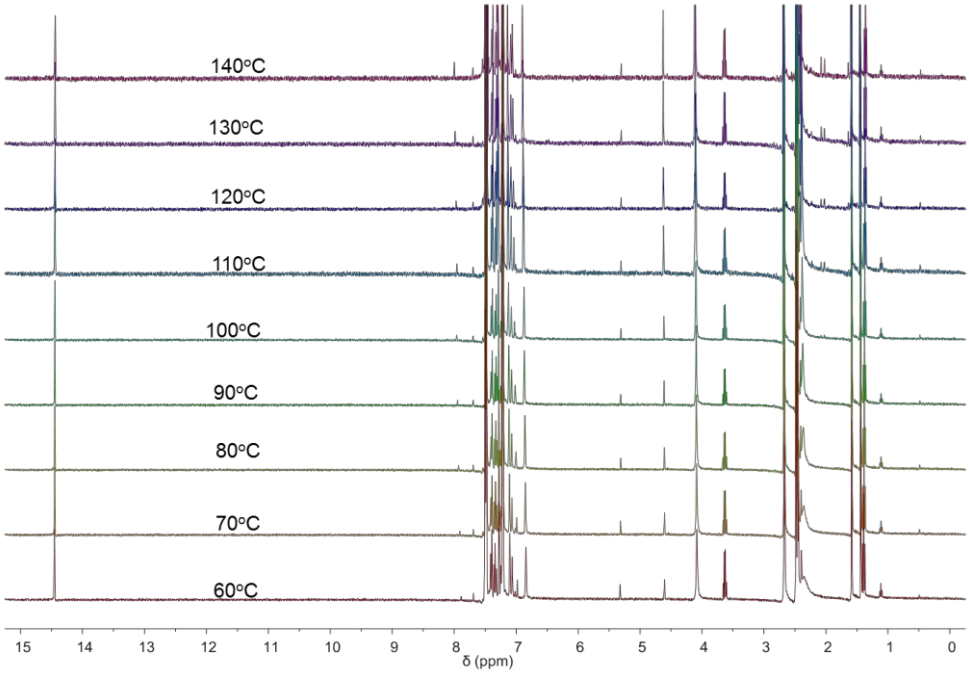


Figure 46. VT ^{1}H-NMR spectra (400 MHz, 1,2-dichlorobenzene-d$_4$) of **19**.

Table 9. Productivity of catalysts **5, 6** and **19** in RCM at high temperature[a].

substrate	catalysts	time [h]	TON
diallyl diphenylsilane	**5**	4	10,500
diallyl diphenylsilane	**6**	4	8,500
diallyl diphenylsilane	**19**	4	9,600
diethyl diallylmalonate	**5**	4	1,500
diethyl diallylmalonate	**6**	4	1,200
diethyl diallylmalonate	**19**	4	1,600
methyl oleate	**5**	4	0
methyl oleate	**6**	4	0
methyl oleate	**19**	4	2,500
diallylamine	**5**	4	0
diallylamine	**6**	4	0
diallylamine	**19**	4	0
N,N-diallyl-p-toluolsulfonamide	**5**	4	900
N,N-diallyl-p-toluolsulfonamide	**6**	4	1,230
N,N-diallyl-p-toluolsulfonamide	**19**	4	4,200
2-allylpent-4-enoic acid	**5**	4	0
2-allylpent-4-enoic acid	**6**	4	0
2-allylpent-4-enoic acid	**19**	4	0

[a]Condition unless otherwise stated: 1,2-dichlorobenzene, 140 °C, 4 h, catalyst:substrate = 1:20,000 (mol/mol); internal standard for GC-MS = *n*-dodecane.

From the catalytic data presented here, one can conclude that molybdenum imido alkylidene NHC complexes are indeed activated through release of one anionic ligand, thereby forming a cationic complex. Consequently, to achieve high productivity, they need to bear one good leaving group, *e.g.*, a triflate and one strongly electron-withdrawing anionic ligand, *e.g.*, $-OC_6F_5$. Alternatively, they can be prepared in their cationic form with one strongly electron-withdrawing anionic ligand at molybdenum as realized in **14-16**. This proposal fits the high productivities of complexes **7**, **10**, **11**, **14-16** and **22** but also the low productivities of complexes **3**, **4**, **5**, **6**, **18**, **19**, **25**. Although complexes **19** and **20** showed better activity than **5** and **6** in most cases. The reason might be combined electronic and steric effects of the 3,5-dimethylimido ligand, which is also reflected by the ^{19}F-NMR spectra of these complexes. At room temperature only one signal is observed.

Table 10. Productivity of catalysts **18**, **19** and **20** in RCM at room temperature[a].

#	18	19	20
T_c (°C)	130	-3	60
diethyl diallylmalonate	0	300	120
diallyl diphenylsilane	90	450	100
1,7-octadiene	90	80	75
N,N-diallyl-*p*-tosylamide	0	150	0
diallylmalodinitrile	0	60	0
diallyl ether	0	160	45

[a] 1,2-dichloroethane, room temperature, 4 h, catalyst:substrate = 1:1,000(mol/mol).

Finally, a comparison of the *Z*-selectivity of catalysts **5**, **11**, **19**-**22** provides an insight into the structure of the transition state. Clearly, catalysts **19** and **22** bearing the "small" 3,5-dimethylphenylimido-ligand displayed higher *Z*-selectivity in CM than catalysts **5**, **10, 11, 16** and **18** based on the 2,6-dimethylphenylimido-ligand (37 and 34 *vs*. 12-28% *Z*, respectively, **Table 11**). A comparable *Z*-selectivity is also obtained with catalyst **19** (32% *Z*) also bearing the 3,5-dimethylphenylimido-ligand. The highest *Z*-value (40%) obtained so far was realized with catalyst **21** bearing the 3,5-dimethylphenylimido and the large "terphenoxide" ligand.

Table 11. Productivity of catalysts in the CM of 1-hexene with 1-dodecene.

Catalyst	5	10	11	16	18	19	20	21	22
TON	150	1,060	820	1,200	430	320	260	1,100	820
Z/E	15/85	18/82	12/88	18/82	28/72	37/63	32/68	40/60	34/66

1,2-dichloroethane, T = 80 °C, t = 4 h, catalyst:substrate = 1:2,000.

This strongly points towards a TBP transition state in which the metallacyclobutane is *trans* to the NHC (**Figure 47**). Such proposal is also in line with calculations on Mo-imido alkylidenes, which suggest approach of the olefin and formation of the molybdacyclobutane *trans* to the strongest *σ*-donor,[39-41] which is here the NHC. In that regard, our novel Mo-imido alkylidene NHC complexes behave similar to the MAP

catalysts[15,35,42-45] published by the *Schrock* group. Clearly, further ligand tuning is required to push the *Z*-content up to > 90%.

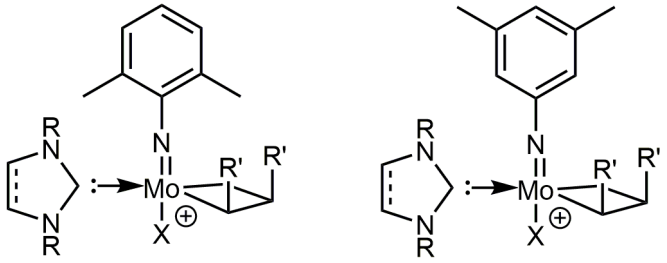


Figure 47. TBP molybdacyclobutanes with all substituents pointing towards the smaller imido groups. X = -OTf, -O-2,6-Ph_2-C_6H_3O, -$OC(CF_3)_3$; R = Mes.

2.3 Summary

A series of high oxidation state 16-electron Mo-imido alkylidene bis(triflate) NHC and monoalkoxide complexes were designed, which are active in ROMP, cyclopolymerization of both 1,6-hepta and 1,7-octadiynes, as well as in RCM, HM and CM. They are based on cheap metals and are accessible in high yields from standard progenitors and mostly inexpensive ligands. Unprecedented functional-group tolerance was observed during ROMP and cyclopolymerization. The cyclopolymerisation of a hydroxy based heptadiyene proceeded quickly (within 5 min) and in high yield. Even though, all molybdenum imido alkylidene bis(triflate) NHC complexes displayed high regio-selectivity (*α*-addition) during cyclopolymerisation. The formation of reactive species during polymerization reactions was followed by investigated by ^{19}F-NMR studies. Based on these results a possible mechanism was established for ROMP with high *trans* selectivity. However, replacement of one of the triflates in Mo-imido alkylidene bis(triflate) NHC complexes by different electron with-drawing alkoxides, chiral (bi-) phenoxide, amides, etc. offers access to a new family of *in-situ* cationic molybdenum alkylidenes that are chiral at the metal center. These monoalkoxide complexes represent a first compromise between high activity and functional-group tolerance. The four coordinate cationic systems evidently display very high catalytic activity, although no functional group tolerance. However, cationic Mo-imido alkylidene NHC complexes having one electron withdrawing alkoxide and

$B(Ar^F)_4^-$ as non-coordinating anion displayed high activity and functional group-tolerance. The selectivity and reactivity were tuned by replacement of the 2,6-dimethyl imido ligand by the 3,5-dimethyl imido ligand; up to 40% *Z*-selectivity was achieved. Also, most of the Mo-imido alkylidene bis(triflate) NHC complexes displayed stability at high temperature (no decomposition up to 140 °C for complexes **18**, **19** and **25**). Concomitantly, the first triazole-5-ylidene based Mo-imido alkylidene NHC complexes were isolated and its reactivity towards different olefin metathesis reactions were explored. A probable reaction pathway has been postulated and the first, very fundamental structure-reactivity relationships have been established. However, in view of the possibility of geometrical changes, *e.g.*, from TBP to SP, and in view of the very subtle differences in free energy between individual structures it becomes obvious that only high-level quantum chemical calculations will allow predictions on reactivity. In view of the possible variations in the imido-, NHC-, alkylidene- and anionic ligands, high-level quantum-chemical calculations will probably have to be carried out for every single catalyst-substrate combination and reaction types (RCM, CM, SM, ROMP, etc.) in order to come up with resilient data. The propensity of the novel catalysts to form cationic species can be tuned by using different NHCs such as CAAC, different five and six-member ring heterocycles, abnormal NHCs, etc. Selectivity towards ROMP and cross-metathesis can be tuned by combination of small imido, big alkoxides or vice versa. Immobilized version should be accessible by immobilization on silica through the NHCs, alkoxides or polymeric-supports which can be used as a heterogeneous version of these catalyst as well as different surface-organometallic chemistry studies. All in all, high oxidation state Mo-imido alkylidene NHC complexes are expected to become highly relevant catalysts for organic chemistry, polymer chemistry and also for many industrial olefin metathesis processes.

2.4 References

[1] G. C. Vougioukalakis, R. H. Grubbs, *Chem. Rev.*, **2010**, *110*, 1746-1787.

[2] M. R. Buchmeiser, *Chem. Rev.*, **2009**, *109*, 303-321.

[3] S. T. Diver, A. J. Giessert, *Chem. Rev.*, **2004**, *104*, 1317-1382.

[4] R. R. Schrock, *Chem. Rev.*, **2009**, *109*, 3211-3226.

[5] S. Fustero, A. Simón-Fuentes, P. Barrio, G. Haufe, *Chem. Rev.*, **2015**, *115*, 871-930.

[6] M. D. McReynolds, J. M. Dougherty, P. R. Hanson, *Chem. Rev.*, **2004**, *104*, 2239-2258.

[7] A. H. Hoveyda, A. R. Zhugralin, *Nature*, **2007**, *450*, 243-251.

[8] R. R. Schrock, A. H. Hoveyda, *Angew. Chem. Int. Ed.*, **2003**, *42*, 4592-4633.

[9] R. R. Schrock, *Chem. Rev.*, **2002**, *102*, 145-180.

[10] H. Zhang, E. C. Yu, S. Torker, R. R. Schrock, A. H. Hoveyda, *J. Am. Chem. Soc.*, **2014**, *136*, 16493-16496.

[11] E. T. Kiesewetter, R. V. O'Brien, E. C. Yu, S. J. Meek, R. R. Schrock, A. H. Hoveyda, *J. Am. Chem. Soc.*, **2013**, *135*, 6026-6029.

[12] A. W. H. Speed, T. J. Mann, R. V. O'Brien, R. R. Schrock, A. H. Hoveyda, *J. Am. Chem. Soc.*, **2014**, *136*, 16136-16139.

[13] B. Autenrieth, H. Jeong, W. P. Forrest, J. C. Axtell, A. Ota, T. Lehr, M. R. Buchmeiser, R. R. Schrock, *Macromolecules*, **2015**, *48*, 2480-2492.

[14] M. M. Flook, V. W. L. Ng, R. R. Schrock, *J. Am. Chem. Soc.*, **2011**, *133*, 1784-1786.

[15] M. M. Flook, L. C. H. Gerber, G. T. Debelouchina, R. R. Schrock, *Macromolecules*, **2010**, *43*, 7515-7522.

[16] R. R. Schrock, *Dalton Trans.*, **2011**, *40*, 7484-7495.

[17] T. M. Trnka, R. H. Grubbs, *Acc. Chem. Res.*, **2001**, *34*, 18-29.

[18] J. H. Oskam, H. H. Fox, K. B. Yap, D. H. McConville, R. O`Dell, B. J. Lichtenstein, R. R. Schrock, *J. Organomet. Chem.*, **1993**, *459*, 185-198.

[19] M. R. Buchmeiser, S. Sen, J. Unold, W. Frey, *Angew. Chem. Int. Ed.*, **2014**, *53*, 9384-9388.

[20] A. W. Addison, T. N. Rao, J. Reedijk, J. van Rijn, G. C. Verschoor, *J. Chem. Soc., Dalton Trans.*, **1984**, 1349-1356.

[21] R. R. Schrock, J. S. Murdzek, G. C. Bazan, J. Robbins, M. DiMare, M. O'Regan, *J. Am. Chem. Soc.*, **1990**, *112*, 3875-3886.

[22] Z. J. Tonzetich, R. R. Schrock, P. Müller, *Organometallics*, **2006**, *25*, 4301-4306.

[23] S. M. Rocklage, R. R. Schrock, M. R. Churchill, H. J. Wasserman, *Organometallics*, **1982**, *1*, 1332-1338.

[24] S. Naumann, F. G. Schmidt, R. Schowner, W. Frey, M. R. Buchmeiser, *Polym. Chem.*, **2013**, *4*, 2731-2740.

[25] E. M. Higgins, J. A. Sherwood, A. G. Lindsay, J. Armstrong, R. S. Massey, R. W. Alder, A. C. O'Donoghue, *Chem. Commun.*, **2011**, *47*, 1559-1561.

[26] S. P. Nolan, *N-Heterocyclic Carbenes in Synthesis*, Wiley, **2006**.

[27] S. Naumann, A. P. Dove, *Polym. Chem.*, **2015**, *6*, 3185-3200.

[28] I. Ibrahem, M. Yu, R. R. Schrock, A. H. Hoveyda, *J. Am. Chem. Soc.*, **2009**, *131*, 3844-3845.

[29] M. M. Flook, A. J. Jiang, R. R. Schrock, P. Müller, A. H. Hoveyda, *J. Am. Chem. Soc.*, **2009**, *131*, 7962-7963.

[30] D. Enders, K. Breuer, U. Kallfass, T. Balensiefer, *Synthesis*, **2003**, *2003*, 1292-1295.

[31] E. P. A. Couzijn, J. C. Slootweg, A. W. Ehlers, K. Lammertsma, *J. Am. Chem. Soc.*, **2010**, *132*, 18127-18140.

[32] J. Unold, D. Wang, W. Frey, M. R. Buchmeiser, *Polym. Chem.*, **2013**, *4*, 4219-4233.

[33] J. Heppekausen, A. Fürstner, *Angew. Chem. Int. Ed.*, **2011**, *50*, 7829-7832.

[34] A. J. Jiang, J. H. Simpson, P. Müller, R. R. Schrock, *J. Am. Chem. Soc.*, **2009**, *131*, 7770-7780.

[35] H. Jeong, D. J. Kozera, R. R. Schrock, S. J. Smith, J. Zhang, N. Ren, M. A. Hillmyer, *Organometallics*, **2013**, *32*, 4843-4850.

[36] S. C. Marinescu, R. Singh, A. S. Hock, K. M. Wampler, R. R. Schrock, P. Müller, *Organometallics*, **2008**, *27*, 6570-6578.

[37] K. Herz, J. Unold, J. Hänle, R. Schowner, S. Sen, W. Frey, M. R. Buchmeiser, *Macromolecules*, **2015**, *48*, 4768-4778.

[38] J. H. Oskam, R. R. Schrock, *J. Am. Chem. Soc.*, **1992**, *114*, 7588-7590.

[39] X. Solans-Monfort, C. Coperet, O. Eisenstein, *J. Am. Chem. Soc.*, **2010**, *132*, 7750-7757.

[40] A. Poater, X. Solans-Monfort, E. Clot, C. Copéret, O. Eisenstein, *J. Am. Chem. Soc.*, **2007**, *129*, 8207-8216.

[41] X. Solans-Monfort, E. Clot, C. Copéret, O. Eisenstein, *J. Am. Chem. Soc.*, **2005**, *127*, 14015-14025.

[42] C. Wang, M. Yu, A. F. Kyle, P. Jakubec, D. J. Dixon, R. R. Schrock, A. H. Hoveyda, *Chem. Eur. J.*, **2013**, *19*, 2726-2740.

[43] M. R. Reithofer, G. E. Dobereiner, R. R. Schrock, P. Müller, *Organometallics*, **2013**, *32*, 2489-2492.

[44] S. C. Marinescu, R. R. Schrock, P. Müller, A. H. Hoveyda, *J. Am. Chem. Soc.*, **2009**, *131*, 10840-10841.

[45] L. C. H. Gerber, R. R. Schrock, P. Müller, *Organometallics*, **2013**, *32*, 2373-2378.

Chapter 3

A Ring-Opening Metathesis Polymerization Active Anionic Molybdenum Amidato Bisalkyl Alkylidyne Complex with High *cis*-Selectivity

The material covered in this chapter has appeared in:

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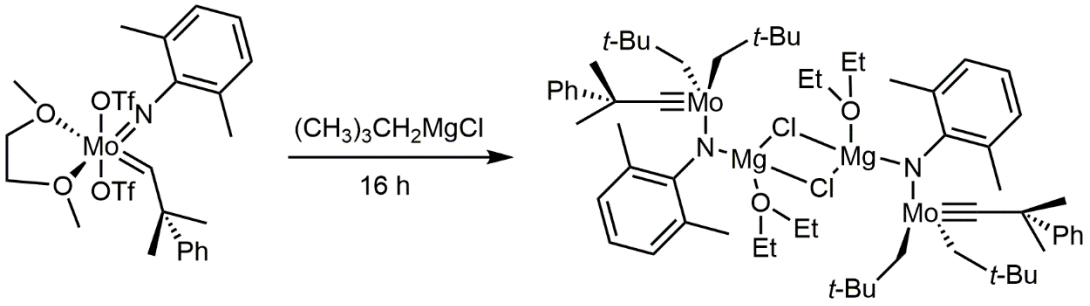
3.1 Introduction

Molybdenum and tungsten alkylidynes[1-4] have been known since the 1980s and are nowadays widely used in alkyne metathesis.[1,5-14] Notably, both well-defined metal alkylidynes as well as progenitors that are transformed into the corresponding metal alkylidynes in course of the reaction are used for alkyne metathesis. To the best of our knowledge, all molybdenum alkylidynes that have been reported exist in form of *neutral* complexes with one exception. In 2006, *Schrock et. al*. reported on an anionic Mo-alkylidyne that forms via the reaction of a Mo-imido bisalkoxy alkylidene with a *Wittig* reagent to form the corresponding anionic Mo-imido alkylidyne complex.[15] In view of early work on high oxidation state metal alkylidynes and in particular on synthetic routes that involve the deprotonation of metal alkylidynes by a base,[16-17] such reaction is not particularly surprising, the more since the two fluorinated alkoxides strongly polarize the Mo=C bond, which can be expected to facilitate *α*-H elimination. In a recent paper, *Schrock et. al*. reported on the reaction of, e.g., [Mo(N-2,6-Cl_2-C_6H_3)($CHCMe_3$)(CF_3SO_3)$_2$(DME)] (DME = dimethoxyethane) with the dipotassium salt of *S*-3,3'-di-t-butyl-5,5',6,6'-tetramethyl-1,1'-biphenyl-2,2'-diolate (*S*-BiPhen) to yield the corresponding Mo-amido-(*S*-Biphen) alkylidyne.[18] Such reactions strongly suggest deprotonation of the alkylidene by the base and re-addition of the proton to the Mo=N-bond. It is, however, quite surprising that a similar reaction also occurs with Mo-imido bisalkyl alkylidenes,[19-20] which contain a less polarized Mo-alkylidene, and the resulting anionic Mo-amidato bisalkyl alkylidyne represent stable species.

3.2 Results and Discussion

3.2.1 Synthesis of anionic molybdenum amidato bisalkyl alkylidyne complex and DFT calculation

Reaction of [Mo(N-2,6-Me_2-C_6H_3)($CHCMe_2Ph$)(CF_3SO_3)$_2$(DME)][21] with an excess of $(CH_3)_3CCH2MgCl$ (3 equiv.) results in the formation of [Mo(N-2,6-Me_2-C_6H_3)($CCMe_2Ph$) ($CH_2C(CH_3)_3$)$_2$($Mg{\cdot}Et_2O$-*μ*-Cl)$_2$], **29** (**Scheme 23**).[22] Complex **29** is to the best of our knowledge, the first anionic Mo-imido bisalkyl alkylidyne complex.



29

Scheme 23. Synthesis of **29**.

Compound **29** crystallizes in the monoclinic space group $P2_{1/n}$ with a = 1715.96(11), b = 1024.35(7), c = 2066.39(13) pm, $\alpha = \gamma = 90°$, β = 110.763(3)°, Z = 2. In the solid state, a dimer form with two anionic molybdenum arylimido bisalkyl alkylidyne moieties linked via a bridging dicationic $[Mg_2Cl_2{\cdot}Et_2O]^{2+}$ species. Molybdenum adopts a distorted tetrahedral geometry with [C(9)-Mo(1)-N(1) = 104.80(7)°], [C(9)-Mo(1)-C(24) = 105.98(7)°], [N(1)-Mo(1)-C(24) = 114.71(6)°], [C(9)-Mo(1)-C(19) = 107.34(7)°], [N(1)-Mo(1)-C(19) = 110.57(6)°], [C(24)-Mo(1)-C(19) = 112.74(7)°]. The same is true for Mg, the corresponding angles are [O(1X)-Mg(1)-N(1) = 112.85(6)°], [O(1X)-Mg(1)-Cl(1A) = 106.43(5)°], [N(1)-Mg(1)-Cl(1A) = 108.72(5)°], [O(1X)-Mg(1)-Cl(1) = 105.69(5)°]. The Mo-alkylidyne structure is supported by the chemical shift for C(9) in ^{13}C-NMR (δ_C = 307.2 ppm) (**Figure 49**), the large angle [Mo(1)-C(9)-C(10) = 174.3°] and the short Mo(1)-C(9) distance of 175.00(16) pm, which is comparable to the one found in $[(Ph_3PMe)^+(Mo(N\text{-}2,6\text{-}(2\text{-}i Pr_2)\text{-}C_6H_3)(C\text{-}t Bu)(OCMe(CF_3)_2)_2^-]$ [Mo(1)-C(1) = 175.4(2) pm].[15]

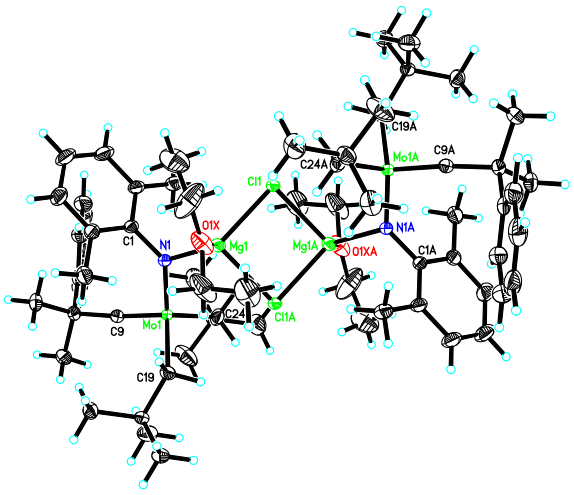


Figure 48. Single-crystal X-ray structure of **29**. Selected bond angles [°] and lengths [pm]: Mo(1)-C(9) 175.00(16), Mo(1)-N(1)189.30(13), Mo(1)-C(24) 214.55(16), Mo(1)-C(19) 215.92(16), Mo(1)-Mg(1) 332.28(6), Cl(1)-Mg(1A) 238.38(7), Cl(1)-Mg(1) 238.84(7), Mg(1)-O(1X) 198.19(15), Mg(1)-N(1) 199.07(14), Mg(1)-Cl(1A) 238.38(7) Mg(1)-C(1) 280.33(16), Mg(1)-Mg(1A) 330.64(12), C(9)-Mo(1)-N(1) 104.80(7)°, C(9)-Mo(1)-C(24) 105.98(7)°, N(1)-Mo(1)-C(24) 114.71(6)°, C(9)-Mo(1)-C(19) 107.34(7)°, N(1)-Mo(1)-C(19) 110.57(6)°, C(24)-Mo(1)-C(19) 112.74(7)°, O(1X)-Mg(1)-N(1) 112.85(6)°, O(1X)-Mg(1)-Cl(1A) 106.43(5)°, N(1)-Mg(1)-Cl(1A) 108.72(5)°, O(1X)-Mg(1)-Cl(1) 105.69(5)°.

The distance Mo(1)-N(1) is 189.30(13) pm, which is significantly larger than the one found in the corresponding anionic Mo-imido bis(alkoxy) complex [(Ph_3PMe)$^+$(Mo(N-2,6-(2-*i*Pr_2)-C_6H_3)(C-*t*Bu)(OCMe(CF_3)$_2$)$_2$)$^-$] [Mo(1)-N(1) = 181.3(2) pm],[15] but shorter than the Mo-N(Ar')R bond in Mo-amido complexes (Ar' = substituted aryl), which are typically in the range of 198-208 pm.[23] The Mo(1)-N(1) bond character in **29** is thus somewhere between an amido and an imido bond.[22] In solution, NMR data suggest the existence of a dissociated "monomeric" form with the anionic charge at the nitrogen (**Figure 50**).

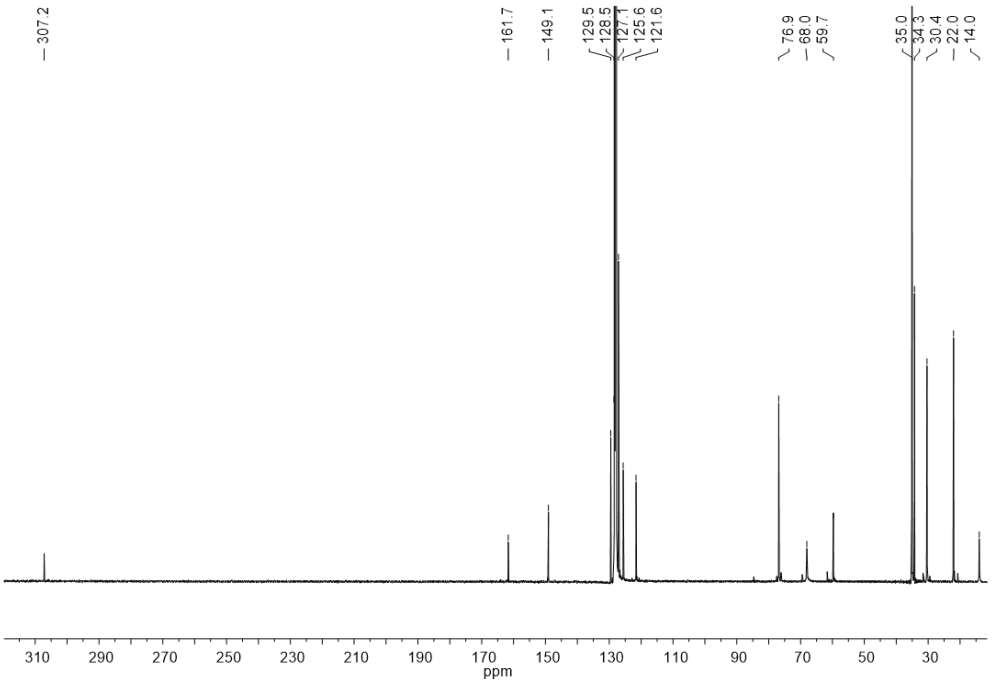


Figure 49. ^{13}C-NMR (C_6D_6, 101 MHz) of catalyst **29**.

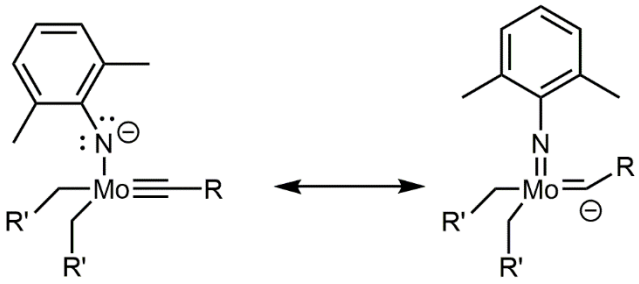
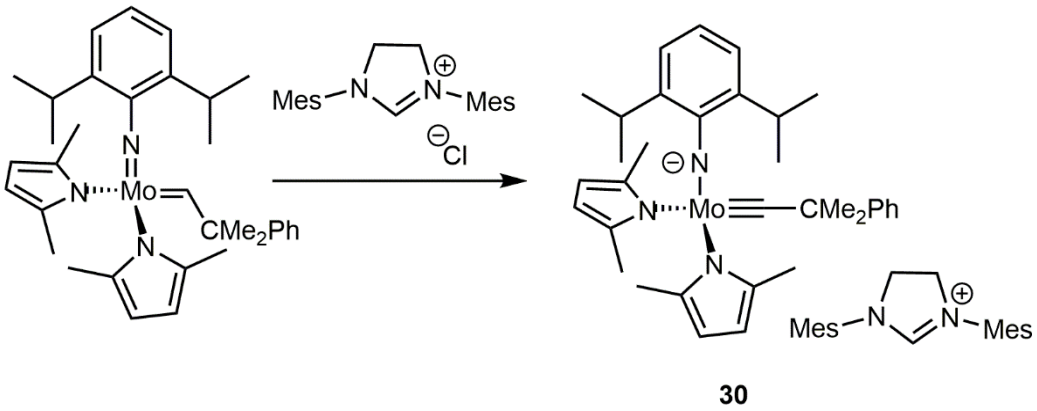


Figure 50. Mesomeric structures for the “monomeric” from of **29**.[22]

[(1,3-dimesityl-4,5-dihydro-1H-imidazol-3-ium)$^+$(Mo(N-2,6-(2-*i*Pr)$_2$-C_6H_3)(CCMe$_2$Ph)-(2,5-Me$_2$-pyrrolide)$_2^-$] (**30**) was accessible via reaction of Mo(N-2,6-(2-*i*Pr)$_2$-C_6H_3)(CHCMe$_2$Ph)(2,5-Me$_2$-pyrrolide)$_2$ with 1,3-dimesitylimidazolidinium chloride in benzene. Compound **30** crystallizes in the monoclinic space group *Pc* with *a* = 1993.97(13), *b* = 1232.06(8), *c* = 2113.94(12) pm, *α* = *γ* = 90°, *β* = 92.843(3)°, *Z* = 4. In the solid state, a tetragonal complex formed. The distance Mo(1A)-N(1A) is 179.5(5) pm, which is significantly smaller than in complex **29** but comparable to the one in complex [(Ph$_3$PMe)$^+$(Mo(N-2,6-(2-*i*Pr$_2$)-C_6H_3)(C-*t*Bu)(OCMe(CF$_3$)$_2$)$_2$)$^-$] (Mo(1)-N(1) = 181.3(2) pm). The reason might be that complex **29** exists as a dimer with two electron-

donating bis-alkyl group attached to the molybdenum center. Complex **30** could not be used further.



30

Scheme 24. Synthesis of **30**.

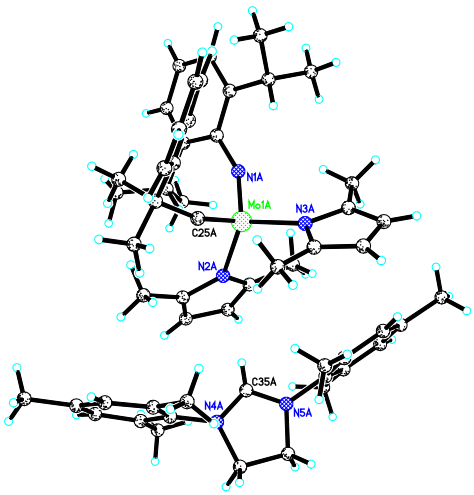


Figure 51. Single-crystal X-ray structure of **30**. Selected bond angles [°] and lengths [pm]: Mo(1A)-C(25A) 174.5(8), Mo(1A)-N(1A) 179.5(5), Mo(1A)-N(2A) 212.1(6), Mo(1A)-N(3A) 214.6(6), N(1A)-C(1A) 137.4(7); C(25A)-Mo(1A)-N(1A) 107.6(3), C(25A)-Mo(1A)-N(2A) 104.9(3), N(1A)-Mo(1A)-N(2A) 107.7(2), C(25A)-Mo(1A)-N(3A) 104.2(3), N(1A)-Mo(1A)-N(3A) 111.0(2), N(2A)-Mo(1A)-N(3A) 120.5(2), C(1A)-N(1A)-Mo(1A) 153.6(5), N(1A)-C(1A)-C(6A) 121.6(5), N(1A)-C(1A)-C(2A) 119.9(5).

While DFT calculations show that the equilibrium in the solid state is strongly on the left side, *i.e.* the carbyne structure of the dimeric, $[Mg_2Cl_2{\cdot}Et_2O]^{2+}$-bridged form (**29**), the same calculations reveal that for the free anionic molybdenum arylimido bisalkyl

alkylidyne moiety the equilibrium is shifted significantly to the right side with a Mo-imido bond. While the angle Mo(1)-C(9)-C(10) is predicted as 176.7° by DFT (which is very close to the experimental value of 174.3°) for the dimer (**29**), it drops to 166.82° for the "monomeric", anionic form shown in **Figure 50** (**Table 12**). This leads to an accumulation of negative charge at C(9), which is illustrated in **Figure 52**. The equilibrium is further shifted to the right side in the presence or absence of monomer (norborn-2-ene).

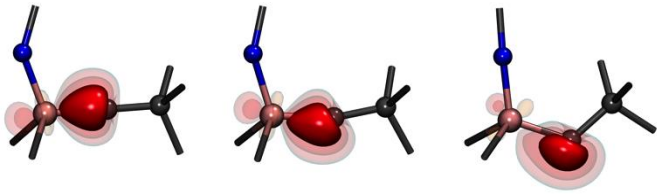


Figure 52. Response of the electronic structure to a bending of Mo(1)-C(9)-C(10) in complex **29**: 180° (left) shows an orbital best described as a sigma bond while 120° (right) corresponds to a lone pair at C(9). The energy minimum at 166.8° (middle) exhibits a significant accumulation of charge at C(9).

Figure 52 depicts orbitals, which are localized with the intrinsic bond orbital. Intrinsic bond orbitals (IBOs) span the *Kohn-Sham* wave function exactly, while often allowing for chemical interpretation. Individual IBOs can be followed along chemical reactions, as described by *Klein*.[24]

Table 12. Geometric data of the monomer anionic complex **29**. Bond angles [°] and lengths [pm].

Mo-C-C	Mo-C	Mo-N	Mo-N-C
180.0	177.3	184.4	143.2
170.0	177.6	183.9	147.5
166.823959	177.9	183.8	150.4
160	178.2	183.4	152.8
150	179.0	182.8	155.5
140	180.5	181.9	164.3
130	182.0	181.1	169.6
120	183.9	181.0	176.4

X-ray:

174.3	175.0	189.3	132.4

Calculated data for complex 29 (dimeric):

176.7	175.4	191.8	132.5

3.2.2 Activity of anionic molybdenum amidato bisalkyl alkylidyne complex during ROMP

So far, no metathetical reactions have been reported for the only existing anionic Molybdenum complex [$(Ph_3PMe)^+$(Mo(N-2,6-(2-*i*Pr_2)-C_6H_3)(C-*t*Bu)(OCMe$(CF_3)_2)_2)^-$].[15] In view of the bonding situation in the anionic complex **29**, it was used in various metathesis reactions. While **29** displays no activity in the RCM reaction of diethyldiallylmalonate and in the alkyne metathesis reaction with 1-benzyl-but-3-yne-1-yl ether, **29** does polymerize norborn-2-ene (NBE) to yield poly(NBE) with a *cis*-content ≥ 96% (M_n = 90,000 g/mol, PDI = 3.7, **Figure 53**). Though polymerization activity as such is certainly of limited practical value, the fact that a Mo-alkylidyne catalyzes the ROMP of a cyclic alkene with high *cis*-selectivity certainly deserves attention. In fact, the mesomeric structure of **29** in which the negative charge is located at the alkylidyne carbon results in a Mo-imido alkylidenate. Since Mo(VI) is electron-deficient and partially positively polarized as such, the Mo- alkylidenate in this mesomeric form must be polarized at least to some extent, which explains for its activity in ROMP.

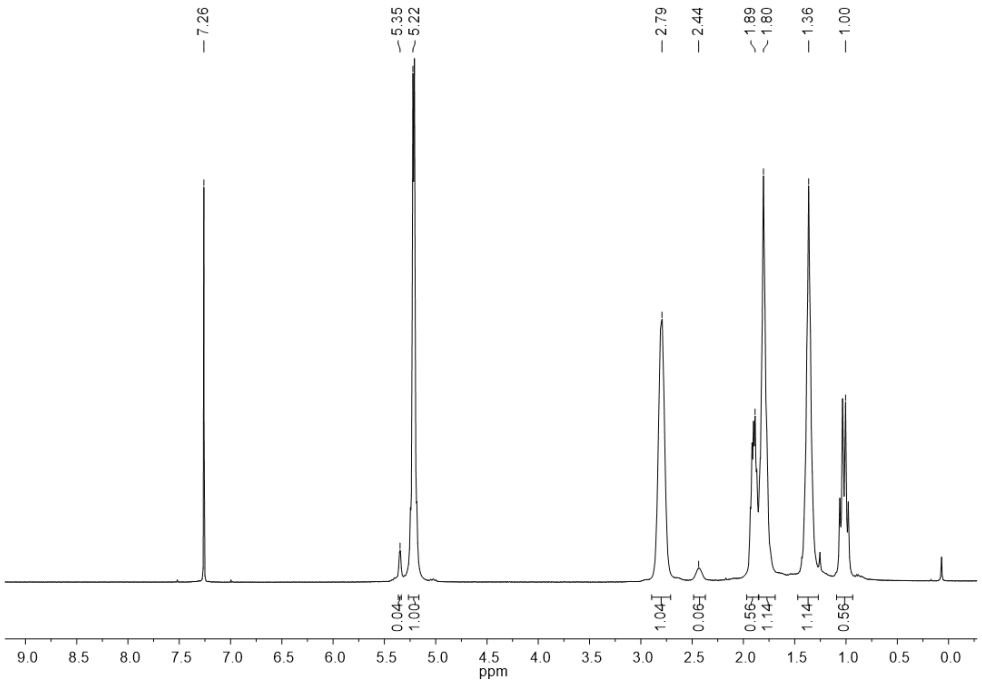


Figure 53. ^{1}H-NMR spectrum (400 MHz, $CDCl_3$) of poly(NBE) obtained by the action of **29**. σ_{cis} = 96%.

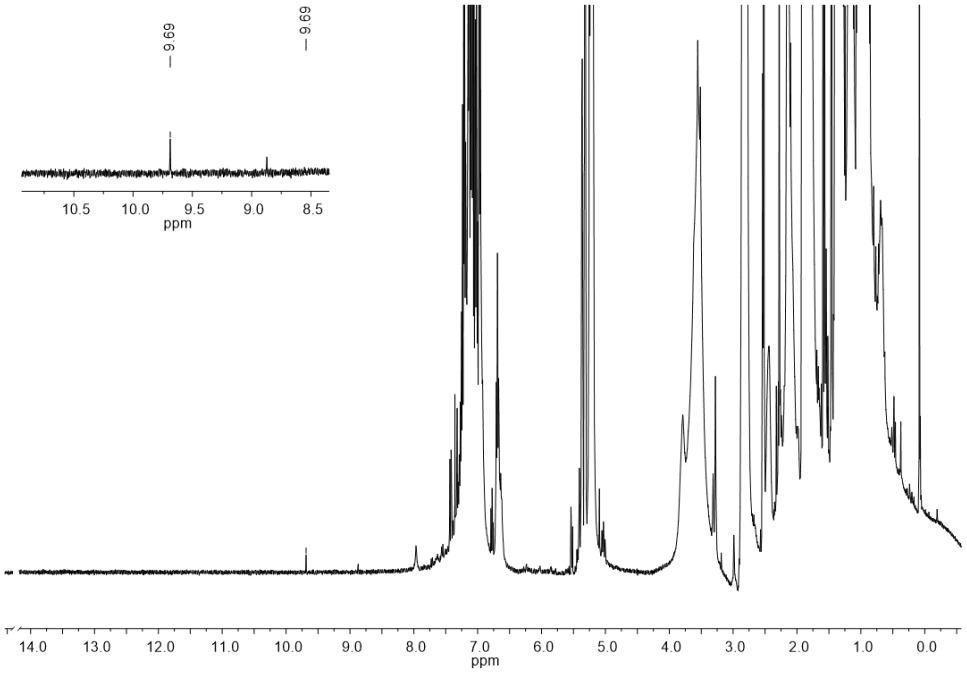
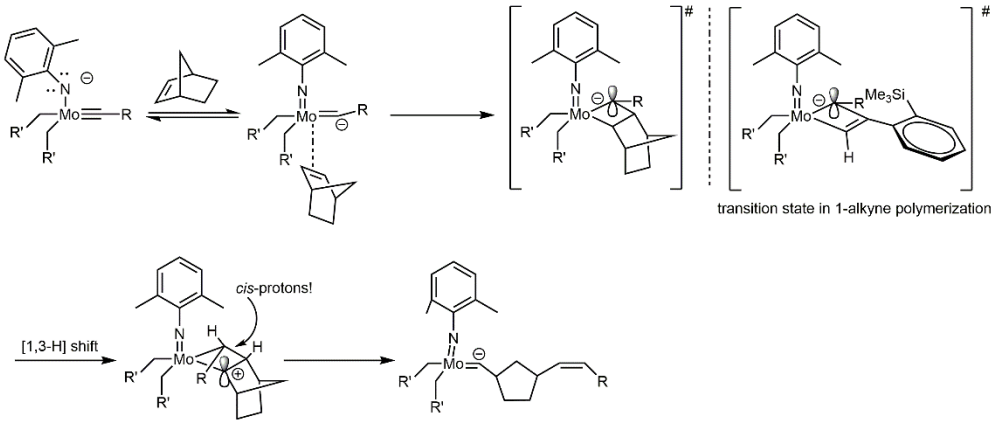


Figure 54. ^{1}H-NMR spectrum (400 MHz, CD_2Cl_2) of the reaction of norborn-2-ene with **29** after 5 h.

Addition of 5 equivalents of NBE to **29** in CD_2Cl_2 allowed for the observation of alkylidene signals evolving at δ_H = 8.87 and 9.69 ppm after several hours. Both the existence and chemical shift of these alkylidene signals clearly support the involvement of the above discussed anionic Mo-N-arylimido alkylidenate species. Formation of the neutral alkylidene presumably proceeded via reaction with solvent or substrate and occurred only after prolonged time and to a very minor extent (**Figure 54**). Notably, the involvement of traces of water, which would certainly react with **29** to yield $MgCl_2/Mg(OH)_2$ and $Mo(NHAr')(CCMe_2Ph)(CH_2C(CH_3)_3)_2$, which would then most probably rearrange into $Mo(NAr')(CHCMe_2Ph)(CH_2C(CH_3)_3)_2$ via intramolecular H-shift as described for $WCl(C_5H_5)$(CC-adamantyl)(NH-*t*Bu)[25] can be ruled out. $Mo(NHAr')$(C-*t*Bu)$(CH_2C(CH_3)_3)_2$ prepared independently turned out to be totally inactive both in the ROMP and 1-alkyne polymerization of the monomers used here, which is in line with literature reports.[19] Notably, two further monomers, *i.e*. 5,6-bis((pentyloxy)methyl)bicycle[2.2.1]hept-2-ene and 7-oxabicyclo[2.2.1]hept-5-ene-2,3-diyl bis(methylendiacetate) also undergo ROMP with **29**, the corresponding polymers also displayed a high *cis*-content of 85 and 86% (**Table 13**), respectively. Molecular weights differed from the theoretical ones by a factor of 6–50, which points towards low initiation efficiency, *i.e*. a low fraction of the Mo-amido alkylidenate. In line with its ROMP-activity but definitely surprising, **29** was also active in the 1-alkyne polymerization of 2-ethynyl-trimethylsilybenzene, yielding highly conjugated, high molecular weight poly(2-ethynyl-trimethylsilybenzene) (M_n = 11,300 g/mol, PDI = 2.5, λ_{max} = 527 nm) whose UV/Vis and NMR data exactly fitted with published ones.[26-27] In view of the proposed mechanism, which includes a [1,3-H] shift (*vide infra*), *β*-insertion of the monomer is anticipated (**Scheme 25**).[28] Finally, the high *cis*-content of the NBE-based polymers deserves attention. Assuming that addition of NBE to the catalyst proceeds through the CNC face defined by [C(9)-N(1)-C(24)-(C(19)], the molybdacyclobutenate shown in **Scheme 25** is formed. *Syn*-facial [1,3-H] shift and cycloreversion via productive metathesis forms the ROMP-derived polymer structure and re-establishes the anionic charge at the Mo-alkylidene. Since both the CMe_2Ph group in the Mo-imido alkylidenate as well as the growing polymer chain must be expected to interfere with the 2,6-dimethylphenylimido ligand, a transition state in which protonation of the *β*-position proceeds in a way that the R-group points *away* from the imido ligand with two *vicinal*-hydrogens in a *cis*-position can be postulated. This configuration of the transition state yields polymers with a high *cis*-content.

Table 13. Summary of polymerization results. Monomer:**29** = 50:1 in ROMP and 30:1 in 1-alkyne polymerization.

Polymer	M_n (g/mol)	PDI	Yield (%)
Poly(norborn-2-ene)	90,000	3.7	50
Poly(5,6-bis((pentyloxy)methyl)bicycle[2.2.1]hept-2-ene)	730,000	2.4	56
Poly(7-oxabicyclo[2.2.1]hept-5-ene-2,3-diylbis(methylene) diacetate)	75,000	1.2	44
Poly(2-ethynyl-trimethylsilylbenzene)	11,300	2.5	44



Scheme 25. Proposed ROMP-reactivity and origin of *cis*-selectivity.

DFT calculations support this pathway. Thus, the C=C_{NBE}-derived bond in the molybdacyclobutenate remains intact (150 pm) after [1,3-H] shift while the Mo-C(9)-bond is enlarged to 248 pm. In view of the length of a typical Mo-alkylidene, which is around 190 pm, such elongation to 248 pm of the Mo-C9 bond is strongly indicative for the concomitant opening of the cyclic structure via productive metathesis, which in fact yields a *cis*-derived double bond in the resulting poly(norborn-2-ene). In that regards, the [1,3-H] shift and cycloreversion might proceed simultaneously in a pericyclic manner; this however is purely speculative.

3.3 Summary

In summary, the first anionic high oxidation state Mo(VI) amidato bisalkyl alkylidyne complex was presented in terms of structure and activity during ROMP and 1-alkyne

polymerization. Its activity in ROMP and 1-alkyne polymerization suggests the involvement of a mesomeric or tautomeric form that possesses an unprecedented Mo-imido alkylidenate structure. Complex **29** is inactive in alkyne metathesis and in ring-closing metathesis (RCM). The ROMP-derived polymer displays a high *cis*-content up to 96% during polymerization of NBE. However, addition of 5 equivalents of NBE to complex **29** displayed alkylidene signal which fitted with proposed mechanism. According to DFT calculations and high selectivity during ROMP, a possible mechanism was proposed. DFT calculations suggest a mesomerization between an amidato alkylidyne and imido alkylidenato complex.

3.4 References

[1] R. R. Schrock, *Chem. Commun.*, **2013**, *49*, 5529-5531.

[2] R. R. Schrock, C. Czekelius, *Adv. Synth. Catal.*, **2007**, *349*, 55-77.

[3] R. L. Gdula, M. J. A. Johnson, *J. Am. Chem. Soc.*, **2006**, *128*, 9614-9615.

[4] R. R. Schrock, *Chem. Commun.*, **2005**, 2773-2777.

[5] H. Yang, Z. Liu, W. Zhang, *Adv. Synth. Catal.*, **2013**, *355*, 885-890.

[6] S. Lysenko, C. G. Daniliuc, P. G. Jones, M. Tamm, *J. Organomet. Chem.*, **2013**, *744*, 7-14.

[7] J. Heppekausen, R. Stade, A. Kondoh, G. Seidel, R. Goddard, A. Fürstner, *Chem. Eur. J.*, **2012**, *18*, 10281-10299.

[8] X. Wu, M. Tamm, *Beilstein J. Org. Chem.*, **2011**, *7*, 82-93.

[9] B. Haberlag, X. Wu, K. Brandhorst, J. Grunenberg, C. G. Daniliuc, P. G. Jones, M. Tamm, *Chem. Eur. J.*, **2010**, *16*, 8868-8877.

[10] A. Furstner, P. W. Davies, *Chem. Commun.*, **2005**, 2307-2320.

[11] U. H. F. Bunz, *Acc. Chem. Res.*, **2001**, *34*, 998-1010.

[12] K. Jyothish, Q. Wang, W. Zhang, *Adv. Synth. Catal.*, **2012**, *354*, 2073-2078.

[13] K. Jyothish, W. Zhang, *Angew. Chem. Int. Ed.*, **2011**, *50*, 8478-8480.

[14] W. Zhang, J. S. Moore, *Adv. Synth. Catal.*, **2007**, *349*, 93-120.

[15] Z. J. Tonzetich, R. R. Schrock, P. Müller, *Organometallics*, **2006**, *25*, 4301-4306.

[16] L. J. Guggenberger, R. R. Schrock, *J. Am. Chem. Soc.*, **1975**, *97*, 2935-2935.

[17] S. M. Rocklage, R. R. Schrock, M. R. Churchill, H. J. Wasserman, *Organometallics*, **1982**, *1*, 1332-1338.

[18] R. R. Schrock, J. Y. Jamieson, J. P. Araujo, P. J. Bonitatebus Jr, A. Sinha, L. P. H. Lopez, *J. Organomet. Chem.*, **2003**, *684*, 56-67.

[19] A. Sinha, L. P. H. Lopez, R. R. Schrock, A. S. Hock, P. Müller, *Organometallics*, **2006**, *25*, 1412-1423.

[20] A. Sinha, R. R. Schrock, *Organometallics*, **2004**, *23*, 1643-1645.

[21] J. H. Oskam, H. H. Fox, K. B. Yap, D. H. McConville, R. O`Dell, B. J. Lichtenstein, R. R. Schrock, *J. Organomet. Chem.*, **1993**, *459*, 185-198.

[22] S. Sen, W. Frey, J. Meisner, J. Kästner, M. R. Buchmeiser, *J. Organomet. Chem.*, **2015**, *799–800*, 223-225.

[23] J. Y. Jamieson, R. R. Schrock, W. M. Davis, P. J. Bonitatebus, S. S. Zhu, A. H. Hoveyda, *Organometallics*, **2000**, *19*, 925-930.

[24] G. Knizia, J. E. M. N. Klein, *Angew. Chem. Int. Ed.*, **2015**, *54*, 5518-5522.

[25] T. H. Warren, R. R. Schrock, W. M. Davis, *J. Organomet. Chem.*, **1998**, *569*, 125-137.

[26] R. R. Schrock, S. Luo, J. C. Lee, N. C. Zanetti, W. M. Davis, *J. Am. Chem. Soc.*, **1996**, *118*, 3883-3895.

[27] R. R. Schrock, S. Luo, N. C. Zanetti, H. H. Fox, *Organometallics*, **1994**, *13*, 3396-3398.

[28] H. H. Fox, M. O. Wolf, R. O'Dell, B. L. Lin, R. R. Schrock, M. S. Wrighton, *J. Am. Chem. Soc.*, **1994**, *116*, 2827-2843.

Chapter 4

Experimental

4.1 Materials and Characterization

All manipulations where carried out in a N_2-filled glove box (Lab Master 130, MBraun, Garching, Germany) or by standard Schlenk techniques. CH_2Cl_2, diethyl ether, toluene, pentane and THF were dried by a solvent purification system (SPS, MBraun). Ethanol was stirred over CaH_2 and distilled under N_2. Starting materials and all reagents were purchased from Sigma-Aldrich (Munich, Germany), Alfa Aesar (Karlsruhe, Germany) and ABCR (Karlsruhe, Germany) and were dried and, where appropriate, distilled prior to use. Mo(N-2,6-Me_2-C_6H_3)(CHCMe_3)(OTf)$_2$·DME, Mo(N-3,5-Me_2-C_6H_3)(CHCMe_3)(OTf)$_2$·DME was prepared as described in the literature.[1] NMR measurements were recorded on a Bruker Avance III 400. IR spectra were measured on a Nicolet 6700 spectrometer equipped with an MCTA-detector. UV/Vis measurements were carried out in $CHCl_3$ on a Perkin Elmer Lambda 2 at room temperature. GC-MS data were recorded on an Agilent Technologies device consisting of a 7693 autosampler, a 7890A GC and a 5975C quadrupole MS. Dodecane was used as internal standard. An SPB-5 fused silica column (34.13 m x 0.25 mm x 0.25 µm film thickness) was used. The injection temperature was set to 150 °C. The column temperature ramped from 45 °C to 250 °C within eight minutes and was then held for further five minutes. The column flow was 1.05 mL per minute. GPC measurements in THF were carried out at 30 °C on a system consisting of a Waters 515 HPLC pump, a Waters 2707 autosampler, PolyPore columns (300 x 7.5 mm, Agilent technologies, Böblingen, Germany), a Waters 2489 UV/Vis- and a Waters 2414 refractive index detector. Molecular weights were determined from calibration vs. poly(styrene) (PS) standards using PS standards in the range 800 < M_n < 2000000 g/mol. GPC measurements in dimethylsulfoxide were carried out on a system consisting of a Waters 515 HPLC pump, a Waters 2707 autosampler, Polypore columns (300 x 7.5 mm, Agilent technologies, Germany) and Waters 2414 refractive index detector. For calibration, poly(methyl methacrylate) standards with 1980 < M_n < 1010000 g/mol were used.

Diallyl diphenylsilane, 1,7-octadiene, diallylether, allyltrimethysilane, 1-hexene, 1-octene, 1-nonene, 1-dodecene were distilled from CaH_2. 5,6-bis((pentyloxy)methyl)bicyclo[2.2.1]hept-2-ene, 7-oxabicyclo[2.2.1]hept-5-ene-2,3-

diylbis(methylene) diacetate[2-3] and 4,4,5,5-tetrakis(ethoxycarbonyl)-1,7-octadiyne[4] were prepared according to the literature. 1,3-Bis(2,4,6-trimethylphenyl)-2-imidazolinylidene ($IMesH_2$),[5] 1,3-bis(2,4,6-trimethylphenyl)imidazol-2-ylidene (IMes) , 5-methoxy-1,3,4–triphenyl-4,5-dihydro-1*H*-1,2,4-triazole[6] and 1,3,4–triphenyl-4,5-dihydro-1*H*-1,2,4-triazole-5-ylidene[6] were prepared according to literature procedure.

4.2 Synthesis of Complexes

Mo(N-2,6-Me_2-C_6H_3)($IMesH_2$)(CH-*t*Bu)($OTf)_2$ (**3**):

Mo(N-2,6-Me_2-C_6H_3)(CH-*t*Bu)($OTf)_2$(DME) (0.300 g, 0.445 mmol) was dissolved in benzene (8 mL) and stirred for 15 min. Then a solution of 1,3-bis(2,4,6-trimethylphenyl)-2-imidazolinylidene (0.136 g, 0.445 mmol) in benzene (5 mL) was added. Immediately, a color change from yellow to deep red was observed and a precipitate formed. The mixture was stirred for a further 3 h, the benzene was decanted and the precipitate was washed with benzene to obtain a yellow colored solid (0.320 g, 81%). The compound was dissolved in a minimum amount of CH_2Cl_2 and the solution was stored at -30 °C for 24 h to afford a yellow crystalline material in 73% yield. ^{1}H-NMR (400 MHz, CD_2Cl_2): (*syn*-isomer, 99.9%) δ = 12.76 (s, 1, C*H*CMe3, $^1J_{CH}$ =118 Hz), 7.06–6.61 (7H, Ar*H*), 3.98 (4H, CH_2NC), 2.66 (s, 3H, CH_3), 2.40-2.22 (s, 18H, CH_3), 1.70 (s, 3H, CH_3), 0.93 ppm (s, 9H, CH_3); ^{19}F-NMR (376 MHz, CD_2Cl_2): δ = -74.65 (SO_3CF_3), -76.7 ppm (SO_3CF_3). ^{13}C-NMR (100 MHz, CD_2Cl_2): δ = 320.9 (*C*H-tBu), 208.7 (*C*$N_{carbene}$), 154.6 (C_{ipso}), 140.4 (C_{ortho}), 137.1 (C_{aryl}), 136.8 (C_{aryl}), 135.7 (C_{aryl}), 131.1 (*C*H_{aryl}), 130.5 (*C*H_{aryl}), 130.1 (*C*H_{aryl}), 128.2(C_{aryl}), 120.2 (q, CF_3, J = 319 Hz), 119.8 (q, CF_3, J = 320 Hz), 53.1 (*C*Me_3), 50.7 (*C*$H_{2\text{-imidazolylene}}$), 30.5 (C*Me*$_3$), 21.3(*C*$H_3$), 19.0(*C*$H_3$), 18.9 ppm (*C*$H_3$). Elemental analysis calcd (%) for $C_{36}H_{45}F_6MoN_3O_6S_2\cdot CH_2Cl_2$: C 45.54, H 4.96, N 4.31; found: C 45.52, H 4.75, N 4.37.

Mo(N-2,6-Me_2-C_6H_3)(I-*t*Bu)(CH-*t*Bu)($OTf)_2$ (**4**):

[Mo(N-2,6-Me_2-C_6H_3)(CH-*t*Bu)($OTf)_2$(DME)] (0.100 g, 0.148 mmol) was dissolved in benzene (3 mL). Then a benzene solution (1 mL) of 1,3-di-*tert*-butylimidazol-2-ylidene (0.027 g, 0.15 mmol) was added under stirring. Immediately, a color change from

yellow to deep red was observed and a precipitate formed. The mixture was stirred for a further 3 h; then, the benzene was decanted and the precipitate was washed with benzene to obtain a yellow colored solid (0.060 g, 65%). The yellow solid was dissolved in a minimum amount of CH_2Cl_2 and stored at -30 °C for 24 h to afford a yellow crystalline material in 60% yield. ^{1}H-NMR (400 MHz, CD_2Cl_2): δ = 14.60 (s, 1H, C*H*CMe$_3$, J_{CH} = 121 Hz, *syn*-isomer), 7.12–6.95 (3H, Ar*H*), 2.60 (2H, C*H*NC), 1.80–1.67 (brs, 24H, Me), 1.32 (s, 9H, CH_2C*Me*$_3$); ^{19}F-NMR (376 MHz, CD_2Cl_2): δ = -77.68, -77.69, -77.70, -77.71 (CF_3SO_3), -78.06, -78.07, -78.08, -78.09 ppm (CF_3SO_3); ^{13}C-NMR (101 MHz,CD_2Cl_2): δ = 329.6 (*C*H-tBu), 175.4 (*C*N$_{carbene}$), 154.3 (C$_{ipso}$), 142.2 (*C*$_{aryl}$), 136.9 (*C*$_{aryl}$), 129.7 (*C*$_{aryl}$), 129.6 (*C*$_{aryl}$), 128.9 (C$_{aryl}$), 121.7 (*C*$_{C=C}$), 120.6 (*C*$_{C=C}$), 119.8 (q, CF_3, J = 318 Hz), 119.7 (q, CF_3, J = 319 Hz), 61.7 (N*C*Me$_3$), 61.3 (C*Me*$_3$), 32.8 (C*Me*$_3$), 30.5 (C*Me*$_3$), 30.1 (C*Me*$_3$), 21.1 (CH_3), 18.4 ppm (CH_3). Elemental analysis calcd (%) for $C_{26}H_{39}F_6MoN_3O_6S_2$: C 40.84, H 5.27, N 5.50; found: C 40.88, H 5.20, N 5.56.

Mo(N-2,6-Me$_2$-C$_6$H$_3$)(IMesH$_2$)(CHCMe$_2$Ph)(OTf)$_2$ (5):

Mo(N-2,6-Me$_2$-C$_6$H$_3$)(CHCMe$_2$Ph)(OTf)$_2$(DME) (**2**, 0.200 g, 0.272 mmol) was dissolved in benzene (8 mL). A solution of 1,3-bis(2,4,6-trimethylphenyl)-2-imidazolidin-2-ylidene (0.083 g, 0.272 mmol) in benzene (1 mL) was added and an immediate color change from yellow to deep red was observed as a precipitate formed. The mixture was stirred for 3 h. Then, the benzene was decanted and the residue was washed with benzene until the washing were colorless and dried *in vacuo* to afford the product as a yellow solid (0.150 g, 81%). Alternatively, the yellow solid can be dissolved in a minimum amount of dichloromethane followed by storage at -30 °C for 24 h to afford product as a yellow crystalline material in (69% yield). ^{1}H-NMR (400 MHz, CD_2Cl_2): δ = 13.11 (s, 1H, C*H*CMe$_2$Ph, $^1J_{CH}$ = 114 Hz), 7.19-6.95 (m, 10H, Ar*H*), 6.51 (s, 2H, Ar*H*), 3.97 (s, 4H, C*H*NC), 2.69-1.71 (s, 27*H*, Me), 1.25 (s, 3*H*, CHC*Me*$_2$Ph); ^{19}F-NMR (CD_2Cl_2): δ -74.59 (s, CF_3SO_3), -76.53 (s, CF_3SO_3); ^{13}C-NMR (101 MHz, CD_2Cl_2): δ = 317.4 (*C*HCMe$_3$), 208.7 (*C*N$_{carbene}$), 154.6 (C$_{ipso}$),149.0, 140.4 (*C*$_{ortho}$), 137.0 (*C*$_{aryl}$), 136.4 (*C*$_{aryl}$), 135.6 (*C*$_{aryl}$), 130.9 (*C*$_{aryl}$), 130.5 (*C*$_{aryl}$), 130.2 (*C*$_{aryl}$), 128.4 (*C*$_{aryl}$), 128.2 (*C*$_{aryl}$), 126.9 (*C*$_{aryl}$), 125.9 (*C*$_{aryl}$), 121.1 (q, CF_3, *J* = 323 Hz), 119.8 (q, CF_3, *J* = 320 Hz), 56.8 (*C*Me$_2$Ph), 53.1 (*C*H$_{2\text{-imidazolydene}}$), 32.9 (C*Me*$_2$Ph), 29.6

(C*Me*$_2$Ph), 21.3 (*C*H$_3$), 19.0 (*C*H$_3$), 18.9 ppm (*C*H$_3$). Elemental analysis calcd. (%) for $C_{41}H_{47}F_6MoN_3O_6S_2$: C 51.68, H 5.02, N 4.41; Found: C 51.81, H 4.88, N 4.35.

Mo(N-2,6-Me$_2$-C$_6$H$_3$)(IMes)(CHCMe$_2$Ph)(OTf)$_2$ (**6**):

Mo(N-2,6-Me$_2$-C$_6$H$_3$)(CHCMe$_2$Ph)(OTf)$_2$(DME) (**2**, 0.150 g, 0.204 mmol) was dissolved in benzene (6 mL). A solution of 1,3-bis(2,4,6-trimethylphenyl)imidazol-2-ylidene (0.062 g, 0.204 mmol) in benzene (1 mL) was added and an immediate color change from yellow to deep red was observed while a precipitate formed. The mixture was stirred for 3 h, the benzene was decanted and the residue was washed with benzene until the washing were colorless and dried *in vacuo* to get a yellow colored solid (0.130 g, 85%). Alternatively, the yellow solid can be dissolved in a minimum amount of dichloromethane followed by storage at -30 °C for 24 h to afford a yellow crystalline material (ca. 65% yield).^{1}H-NMR (400 MHz, CD_2Cl_2): δ = 13.18 (s, 1H, C*H*CMe$_2$Ph, J_{CH} = 118 Hz), 7.21-6.95 (m, 12H, Ar*H*), 6.56 (s, 2*H*), 2.60-1.97 (s, 27*H*, Me), 1.29 (s, 3*H*, CHC*Me*$_2$Ph); ^{19}F-NMR (376 MHz, CD_2Cl_2): δ = -74.92 (s, C*F*$_3$SO$_3$), -76.53 (s, C*F*$_3$SO$_3$); ^{13}C NMR (CD_2Cl_2): δ = 317.0 (*C*HCMe$_3$, J_{CH} =124 Hz), 184.3 (*C*N$_{carbene}$), 154.8 (C$_{ipso}$), 149.0, 141.3 (C$_{ortho}$), 136.4 (*C*$_{aryl}$), 135.9 (*C*$_{aryl}$), 135.5 (*C*$_{aryl}$), 130.6 (*C*$_{aryl}$), 130.1 (*C*$_{aryl}$), 130.0 (*C*$_{aryl}$), 128.6 (*C*$_{aryl}$), 128.2 (*C*$_{aryl}$), 126.9 (*C*$_{aryl}$), 126.4 (*C*=*C*), 125.9 (*C*=*C*), 120.0 (q, *C*F$_3$, J = 320 Hz), 119.8 (q, *C*F$_3$, J = 316 Hz), 56.8 (*C*Me$_2$Ph), 33.2 (C*Me*$_2$Ph), 29.8 (C*Me*$_2$Ph), 21.4 (*C*H$_3$), 20.6 (*C*H$_3$), 18.7 ppm (*C*H$_3$). Elemental analysis calcd. (%) for $C_{41}H_{45}F_6MoN_3O_6S_2$: C 51.79, H 4.88, N 4.42; Found: C 51.73, H 4.80, N 4.39.

Mo(N-2,6-Me$_2$-C$_6$H$_3$)(IMesH$_2$)(CHCMe$_2$Ph)(OTf)(OCH(CF$_3$)$_2$) (**7**):

A solution of **5** (0.040 g, 0.042 mmol) in a minimum amount (~ 2 mL) of $C_2H_4Cl_2$ was cooled to -30 °C; then LiOCH(CF$_3$)$_2$ (0.005 g, 0.042 mmol) was added. The mixture was stirred for a further 2 h, then filtered through celite and the solvent was removed under reduced pressure to afford a yellow solid. It was dissolved in a minimum amount of CH_2Cl_2 and the solution was stored at -30 °C for several days to afford a yellow crystalline material in 63% yield. ^{1}H-NMR (400 MHz, CD_2Cl_2): δ = 13.49 (s, 1H, C*H*CMe$_2$Ph, J_{CH} = 114 Hz), 7.28-6.41 (m, 12H, Ar*H*), 3.97-3.82 (m, 4H, C*H*$_2$NC), 2.32-

1.79 (brs, 30H, Me); ^{13}C-NMR (101 MHz, CD_2Cl_2): δ = 323.8 (*C*HCMe$_2$Ph), 210.0 (*C*N$_{carbene}$), 155.2 (C$_{ipso}$), 150.7, 139.5 (C$_{ortho}$), 136.9 (*C*$_{aryl}$), 135.8 (*C*$_{aryl}$), 135.2 (*C*$_{aryl}$), 130.1 (*C*$_{aryl}$), 129.9 (*C*$_{aryl}$), 129.1 (*C*$_{aryl}$), 128.6 (*C*$_{aryl}$), 127.8 (*C*$_{aryl}$), 126.6 (*C*$_{aryl}$), 125.8 (*C*$_{aryl}$), 120.0 (q, *C*F$_3$, J = 317 Hz), 76.07-75.11 (q, O*C*H(CF$_3$)$_2$), 56.1 (*C*Me$_2$Ph), 51.9 (*C*H$_{2\text{-imidazolydene}}$), 37.2 (C*Me*$_2$Ph), 29.3 (C*Me*$_2$Ph), 21.5 (*C*H$_3$), 21.3 (*C*H$_3$), 19.0 (*C*H$_3$), 18.9 (CH$_3$); ^{19}F-NMR (376 MHz, CD_2Cl_2): δ = - 73.12 (q, *C*F$_3$, *J* = 11 Hz), -73.35 (q, *C*F$_3$, *J* = 11 Hz), -78.07 (s, CF$_3$SO$_3$, *trans* to NHC ligand). Elemental analysis calcd. (%) for $C_{44}H_{50}Cl_2F_9MoN_3O_4S$: C 50.05, H 4.87, N 3.98; found: C 50.51, H 4.85, N 4.07.

Mo(N-2,6-Me$_2$-C$_6$H$_3$)(IMesH$_2$)(CH-*t*Bu)(OTf)(OEt) (**9**):

Mo(N-2,6-Me$_2$-C$_6$H$_3$)(IMesH$_2$)(CH-*t*Bu)(OTf)$_2$ (0.080 g, 0.090 mmol) was added into a suspension of NaOEt (0.0120 g, 0.184 mmol) in a minimum amount (~ 2 mL) of solvent (diethyl ether:tetrahydrofuran, 1:1); the reaction mixture turned immediately to light red. The mixture was stirred for 2 h. The solvent was removed under reduced pressure and the residue was extracted with dichloromethane. The dichloromethane extract was filtered through celite, and the dichloromethane was removed *in vacuo* to afford a yellow solid, which was dissolved in a minimum amount of dichloromethane and stored at -20 °C for several days to afford a crystalline material in 71% yield (0.05 g). ^{1}H NMR (CD_2Cl_2): δ = 12.30 (s, 1H, C*H*CMe$_3$), 6.94-6.65 (overlapping resonance, 7H, Ar*H*), 4.15 (4H, C*H*$_2$NC), 3.69 (2H, OC*H*$_2$CH$_3$), 2.53-2.24 (24H, Me), 1.82 (3H, OCH$_2$C*H*$_3$), 1.14 (S, 9H, CH$_2$C*Me*$_3$); ^{19}F NMR (CD_2Cl_2): δ -79.05 (CF$_3$SO$_3$, *trans* to imido ligand).
N.B: During singel crystal X-ray mesurment the crystal decomposed

Mo(N-2,6-Me$_2$-C$_6$H$_3$)(IMesH$_2$)(CHCMe$_2$Ph)(OTf)(OC$_6$F$_5$) (**10**)**:**

A solution of Mo(N-2,6-Me$_2$-C$_6$H$_3$)(IMesH$_2$)(CHCMe$_2$Ph)(OTf) (0.1500 g, 0.1580 mmol) in a minimum amount of $C_2H_4Cl_2$ (~ 2 mL) was cooled to -30 °C; then LiOC$_6$F$_5$ (0.0300 g, 0.1580 mmol) was added. The mixture was stirred for a further 3 h, then filtered through celite. The solvent was removed *in vacuo* to afford a yellow solid. It was dissolved in a minimum amount of CH_2Cl_2 and the solution was stored at -30 °C for several days to afford a yellow crystalline material in 60% (0.094 g) isolated yield. ^{1}H-NMR (400 MHz, CD_2Cl_2): δ = 13.81 (s, 1H, C*H*CMe$_2$Ph, $^1J_{CH}$ = 124 Hz), 7.40-6.41

(m, 14H, Ar*H*), 4.04-3.83 (m, 4H, C*H*$_2$NC), 2.27 (s, 6H, C*H*$_3$), 2.18 (s, 3H, C*H*$_3$), 2.01 (s, 12H, C*H*$_3$), 1.86 (s, 3H, C*H*$_3$), 0.90 (s, 3H, C*H*$_3$); ^{19}F-NMR (376 MHz, CD_2Cl_2): δ = -78.99 (s, C*F*$_3$SO$_3$), -162.37 (2,6-F, d, $^3J_{F\text{-}F}$ = 23 Hz, C$_6$*F*$_5$), -168.99 (3,5-F, t, $^3J_{F\text{-}F}$ = 23 Hz, C$_6$*F*$_5$), -174.47 (4-F, tt, $^3J_{F\text{-}F}$ = 23 Hz, $^4J_{F\text{-}F}$ = 7.5 Hz, C$_6$*F*$_5$); ^{13}C-NMR (101 MHz, CD_2Cl_2): δ = 321.8 (*C*HCMe$_2$Ph,), 211.8 (*C*N$_{carbene}$), 154.6 (*C*$_{ipso}$), 150.8 (*C*$_{aryl}$), 141.8(*C*$_{ortho}$), 139.6 (*C*$_{aryl}$), 137.3 (*C*$_{aryl}$), 136.6 (*C*$_{aryl}$), 135.9 (*C*$_{aryl}$), 135.5 (*C*$_{aryl}$), 135.0 (*C*$_{aryl}$), 130.8 (*C*$_{aryl}$), 130.2 (*C*$_{aryl}$), 129.8 (*C*aryl), 128.9 (*C*$_{aryl}$), 128.8 (*C*$_{aryl}$), 127.7 (*C*$_{aryl}$), 126.8 (*C*$_{aryl}$), 126.4 (*C*$_{aryl}$), 126.1 (*C*$_{aryl}$), 119.7 (q, *C*F$_3$SO$_3$, *J* = 330 Hz), 56.2 (*C*Me$_2$Ph), 52.0 (*C*H$_{2\text{-imidazolidinylidene}}$), 37.2 (C*Me*$_2$Ph), 30.3 (C*Me*$_2$Ph), 21.3 (*C*H$_3$), 21.2 (*C*H$_3$), 19.0 (*C*H$_3$), 18.8 ppm (*C*H$_3$). Elemental analysis calcd. (%) for $C_{46}H_{47}F_8MoN_3O_4S$: C 56.04, H 4.81, N 4.26; found: C 56.15, H 4.82, N 4.35.

Mo(N-2,6-Me$_2$-C$_6$H$_3$)(IMesH$_2$)(CHCMe$_2$Ph)(OTf)(OC(CF$_3$)$_3$) (11):

A solution of Mo(N-2,6-Me$_2$C$_6$H$_3$)(IMesH$_2$)(CHCMe$_2$Ph)(OTf) (0.131 g, 0.138 mmol) in a minimum amount of $C_2H_4Cl_2$ (~ 5 mL) was cooled to -30 °C; then LiOC(CF$_3$)$_3$ (0.034 g, 0.138 mmol) was added. The mixture was stirred overnight, then filtered through celite. The solvent was removed *in vacuo* to afford a yellow colored gummy solid in 80% (0.115 g) isolated yield. All efforts to obtain a solid or crystalline material failed. ^{1}H-NMR (400 MHz, CD_2Cl_2): δ = 12.53 (s, 1H, C*H*CMe$_2$Ph, $^1J_{CH}$ = 120 Hz), 7.26-6.83 (m, 14H, Ar*H*), 4.34-4.27 (m, 4H, C*H*$_2$NC), 2.36 (s, 6H, C*H*$_3$), 2.34 (s, 6H, C*H*$_3$), 2.31 (s, 6H, C*H*$_3$), 2.11 (s, 6H, C*H*$_3$), 2.01 (s, 3H, C*H*$_3$), 0.91 (s, 3H, C*H*$_3$); ^{19}F-NMR (376 MHz, CD_2Cl_2): δ = -73.39 (s, C*F*$_3$), -78.94 (s, C*F*$_3$SO$_3$); ^{13}C-NMR (101 MHz, CD_2Cl_2): δ = 313.6 (*C*HCMe$_2$Ph,), 201.2 (*C*N$_{carbene}$), 157.0 (*C*$_{ipso}$), 147.0 (*C*$_{aryl}$), 141.6 (*C*$_{ortho}$), 138.5 (*C*$_{aryl}$), 136.6 (*C*$_{aryl}$), 136.3 (*C*$_{aryl}$), 131.7 (*C*$_{aryl}$), 131.5 (*C*$_{aryl}$) 130.8 (*C*$_{aryl}$), 129.6 (*C*aryl), 128.8 (*C*$_{aryl}$), 128.5 (*C*$_{aryl}$), 127.4 (*C*$_{aryl}$), 121.4 (q, *C*F$_3$SO$_3$, *J* = 298 Hz), 120.9 (q, *C*F$_3$, *J* = 295 Hz), 57.8 (*C*Me$_2$Ph), 52.4 (*C*H$_{2\text{-imidazolidinylidene}}$), (*C*Me$_2$Ph), 44.5 (C*Me*$_2$Ph), 32.0 (C*Me*$_2$Ph), 21.3 (*C*H$_3$), 19.5 (*C*H$_3$), 18.6 ppm (*C*H$_3$). Elemental analysis calcd. (%) for $C_{44}H_{47}F_{12}MoN_3O_4S$: C 50.92, H 4.56, N 4.05; found: C 50.73, H 5.07, N 4.92.

Mo(N-2,6-Me_2-C_6H_3)($IMesH_2$)($CHCMe_2Ph$)(OTf)($OC(CF_3)_2CH_3$) (12):

A solution of Mo(N-2,6-Me_2-C_6H_3)($CHCMe_2Ph$)(OTf)($IMesH_2$) (0.0500 g, 0.5042 mmol) in a minimum amount (~ 2 mL) of $C_2H_4Cl_2$ was cooled to -30 °C; then $LiOC(CF_3)_2CH_3$ (0.0094 g, 0.5042 mmol) was added. The mixture was stirred for a overnight, then filtered through celite. The solvent was removed *in vacuo* to afford a yellow solid. It was dissolved in a minimum amount of CH_2Cl_2 and the solution was stored at -30 °C for several days to afford a yellow crystalline material in 40% yield. ^{1}H NMR (CD_2Cl_2): δ = 12.34 (s, 1H, C*H*CMe_2Ph), 7.34-6.82 (m, 14H, Ar*H*), 4.04-3.83 (m, 4H, C*H*$_2$NC), 2.37-1.38(s, 33H, Me); ^{19}F NMR (CD_2Cl_2): δ = -77.00 (q, 3F, CF_3), -77.75 (q, 3F, CF_3), -78.93 (s, 3F, CF_3).

Mo(N-2,6-Me_2-C_6H_3)(IMes)($CHCMe_2Ph$)(OTf)(OC_6F_5) (13):

A solution of Mo(N-2,6-Me_2-C_6H_3)($IMesH_2$)($CHCMe_2Ph$)(OTf) (0.1500 g, 0.1580 mmol) in a minimum amount of $C_2H_4Cl_2$ (~ 2 mL) was cooled to -30 °C; then $LiOC_6F_5$ (0.0300 g, 0.1580 mmol) was added. The mixture was stirred for a further 3 h, then filtered through celite. The solvent was removed *in vacuo* to afford a yellow solid. It was dissolved in a minimum amount of CH_2Cl_2 and the solution was stored at -30 °C for several days to afford a yellow crystalline material in 60% (0.094 g) isolated yield. ^{1}H-NMR (400 MHz, CD_2Cl_2): δ = 13.70 (s, 1H, C*H*CMe_2Ph), 7.34 (d, 2H, *J* = 4 Hz, Ar*H*), 7.28-7.26 (q, 3H, *J* = 4 Hz, Ar*H*), 7.07-7.03 (m, 1H, Ar*H*), 6.94-6.88 (m, 3H, Ar*H*), 6.92 (s, 2H, Ar*H*), 6.41 (s, 2H, C*H*NC), 2.43 (s, 3H, C*H*$_3$), 2.08 (s, 3H, C*H*$_3$), 2.07 (s, 6H, C*H*$_3$), 2.02 (s, 6H, C*H*$_3$),1.84 (s, 3H, C*H*$_3$), 1.77 (s, 6H, C*H*$_3$) 0.90 (s, 3H, C*H*$_3$); ^{19}F-NMR (376 MHz, CD_2Cl_2): δ = -78.93 (s, C*F*$_3$SO$_3$), -162.37 (2,6-F, d, $^3J_{F\text{-}F}$ = 23 Hz, C_6F_5), -168.95 (3,5-F, t, $^3J_{F\text{-}F}$ = 19 Hz, C_6F_5), -174.44 ppm (4-F, tt, $^3J_{F\text{-}F}$ = 23 Hz, $^4J_{F\text{-}F}$ = 7.5 Hz, C_6F_5).

[Mo(N-2,6-Me_2-C_6H_3)($CHCMe_3$)(OTf)($IMesH_2$)$^+$B(Ar^F)$_4^-$] (14):

A solution of **5** (0.0837 g, 0.0879 mmol) in a minimum amount (~2 mL) of $C_2H_4Cl_2$ was cooled to -30 °C; then solution of [Ag(CH_3CN)$_2$B(Ar^F)$_4$] (0.0926 g, 0.0879 mmol) in a minimum amount of $C_2H_4Cl_2$ (~ 1 mL) was added. The mixture was stirred overnight, then filtered through celite and solvent was removed *in vacuo* to afford a yellow solid.

It was dissolved in a minimum amount of CH_2Cl_2 and the solution was stored at -30 °C for several days to afford a yellow crystalline material (ca. 60% yield). ^{1}H NMR (400 MHz, CD_2Cl_2): δ = 12.90 (s, 1H, C*H*CMe$_2$Ph, $^1J_{CH}$ = 127 Hz), 7.72-6.97 (m, 20H, Ar*H*), 4.06(s, 4H, C*H*$_2$NC), 2.37-0.92 (s, 33H, CH_3); ^{13}C NMR (101 MHz, CD_2Cl_2): δ = 325.0 (*C*HCMe$_3$), 206.7 (*C*N$_{Carben}$), 163.1-162.59 (q, $^1J_{B-C}$ = 50 Hz), 154.0 (*C*$_{ipso}$), 144.3 (*C*$_{aryl}$), 143.2(*C*$_{aryl}$) , 142.4 (*C*$_{aryl}$), 141.3 (*C*$_{ortho}$), 137.1 (*C*$_{aryl}$), 135.4 (*C*$_{aryl}$), 132.5 (*C*$_{aryl}$), 131.6 (*C*$_{aryl}$), 130.6 (*C*$_{aryl}$), 130.0 (*C*$_{aryl}$), 129.6 (*C*$_{aryl}$), 129.2 (*C*$_{aryl}$), 129.0 (*C*$_{aryl}$) 128.8 (*C*$_{aryl}$), 128.6 (C$_{aryl}$), 127.8 (*C*$_{aryl}$), 126.7 (*C*$_{aryl}$), 126.3 (*C*$_{aryl}$), 125.2 (q, *C*F$_3$, ^1J = 270 Hz), 118.1 (sept, ^2J = 3Hz), 57.5 (*C*Me$_2$Ph), 52.8 (*C*H$_{2Imidazolyden}$), 28.8 (C*Me*$_2$Ph), 21.4 (*C*H$_3$), 21.3 (*C*H$_3$), 20.7 (*C*H$_3$), 19.8 (*C*H$_3$), 18.7 (*C*H$_3$), 18.0 (*C*H$_3$); ^{19}F NMR (376 MHz, CD_2Cl_2): δ = - 62.89 (s, 24F), -75.66 (s, CF_3SO_3, *trans* to the imido ligand). Elemental analysis calcd. (%) for $C_{74}H_{62}BF_{27}MoN_4O_3S$: C 52.02, H 3.66, N 3.28; found: C 51.71, H 3.33, N 3.26.

[Mo(N-2,6-Me$_2$-C$_6$H$_3$)(IMes)(CHCMe$_2$Ph)(OTf)(CH$_3$CN)$^+$B(Ar^F)$_4^-$] (15):

A solution of **6** (0.094 g, 0.089 mmol) in a minimum amount of $C_2H_4Cl_2$ (~ 2 mL) was cooled to -30 °C; then solution of [Ag(CH$_3$CN)$_2$B(Ar^F)$_4$] (0.095 g, 0.089 mmol) in a minimum amount of $C_2H_4Cl_2$ (~1 mL) was added. The mixture was stirred overnight, then filtered through celite and solvent was removed *in vacuo* to afford a yellow solid. It was dissolved in a minimum amount of CH_2Cl_2 and the solution was stored at -30 °C for several days to afford a yellow crystalline material in ~ 60% (0.091 g) yield. ^{1}H-NMR (400 MHz, CD_2Cl_2): δ = 12.96 (s, 1H, C*H*CMe$_2$Ph, $^1J_{CH}$ = 125 Hz), 7.72-7.02 (m, 20H, Ar*H*), 2.56 (s, 3H, C*H*$_3$), 2.30 (s, 6H, C*H*$_3$), 2.12 (s, 6H, C*H*$_3$), 1.91 (s, 6H, C*H*$_3$), 1.84 (s, 3H, C*H*$_3$), 1.71 (s, 3H, C*H*$_3$), 1.00 (s, 3H, C*H*$_3$); ^{19}F-NMR (376 MHz, CD_2Cl_2): δ = - 62.9 (s, 24*F*), -75.6 (s, C*F*$_3$SO$_3$); ^{13}C-NMR (101 MHz, CD_2Cl_2): δ = 324.1 (*C*HCMe$_2$Ph), 183.2 (*C*N$_{carbene}$), 162.3 (q, $^1J_{B-C}$ = 50 Hz, B(Ar^F)$_4$), 154.0 (*C*$_{ipso}$), 141.9 (*C*$_{ortho}$), 136.3 (*C*$_{aryl}$), 135.4 (B(Ar^F)$_4$), 134.7 (*C*$_{aryl}$), 134.1 (*C*$_{aryl}$), 131.5 (*C*$_{aryl}$), 130.8 (*C*$_{aryl}$), 130.3 (*C*$_{aryl}$), 129.9 (*C*$_{aryl}$), 129.6 (B(Ar^F)$_4$), 129.0 (*C*$_{aryl}$), 128.5 (*C*$_{aryl}$), 127.9 (*C*$_{aryl}$), 126.3 (*C*$_{C=C}$), 124.2 (q, *C*F$_3$, 274 Hz), 118.0 (B(Ar^F)$_4$), 57.4 (C*Me*$_2$Ph), 29.0 (C*Me*$_2$Ph), 21.4 (*C*H$_3$), 20.7 (*C*H$_3$), 18.4 (*C*H$_3$), 17.6 ppm (*C*H$_3$). Elemental analysis calcd. (%) for $C_{74}H_{62}BF_{27}MoN_4O_3S1.5\ CH_2Cl_2$: C 49.46, H 3.52, N 3.06; found: C 49.35; H 3.44; N 3.27.

[Mo(N-2,6-Me$_2$-C$_6$H$_3$)(IMesH$_2$)(CHCMe$_2$Ph)(OC$_6$F$_5$)(CH$_3$CN)$^+$B(Ar^F)$_4^-$] (16):

A solution of **10** (0.040 g, 0.039 mmol) in a minimum amount of CH_2Cl_2 (~ 1 mL) was cooled to -30 °C; then [Ag(CH$_3$CN)$_2$B(Ar^F)$_4$] (0.041g, 0.039 mmol) was added. The mixture was stirred for a further 3 h, then filtered through celite. The solvent was removed *in vacuo* to afford a yellow solid. It was dissolved in a minimum amount of CH_2Cl_2 and the solution was stored at -30 °C for several days to afford a yellow crystalline material in 70% (0.048 g) isolated yield. ^{1}H-NMR (400 MHz, CD_2Cl_2): δ = 13.46 (s, 1H, C*H*CMe$_2$Ph), 7.72 (m, 8H, Ar*H*), 7.56 (s, 4H, Ar*H*), 7.28-6.51 (m, 12H, Ar*H*), 4.04-3.93 (m, 4H, C*H*$_2$NC), 2.33 (s, 3H, C*H*$_3$), 2.21 (s, 15H, C*H*$_3$), 2.15 (s, 9H, C*H*$_3$), 1.86 (s, 3H, C*H*$_3$); ^{19}F-NMR (376 MHz, CD_2Cl_2): δ = -62.90 (s, *C*F$_3$), -160.86 (2,6-F, d, $^3J_{F\text{-}F}$ = 23 Hz), -165.77 (3,5-F, t, $^3J_{F\text{-}F}$ = 23 Hz), -170.74 (4-F, tt, $^3J_{F\text{-}F}$ = 23 Hz, $^4J_{F\text{-}F}$ = 7.5 Hz); ^{13}C-NMR (101 MHz, CD_2Cl_2): δ = 324.8 (*C*HCMe$_2$Ph), 208.6 (*C*N$_{carbene}$), 152.3 (q, ^1J(B, C) = 49 Hz), 154.6 (*C*$_{ipso}$), 146.4 (*C*$_{aryl}$) , 140.3 (*C*$_{ortho}$), 136.8 (*C*$_{aryl}$), 135.4 (*C*$_{aryl}$), 130.7 (*C*$_{aryl}$), 130.2 (*C*$_{aryl}$), 129.6 (*C*$_{aryl}$), 129.3 (*C*$_{aryl}$), 128.9 (*C*$_{aryl}$), 128.5 (*C*$_{aryl}$), 127.3 (*C*$_{aryl}$), 126.8 (*C*$_{aryl}$), 126.4 (*C*$_{aryl}$),126.1 (*C*$_{aryl}$), 122.5 (q, *C*F$_3$, *J* = 280 Hz), 56.2 (*C*Me$_2$Ph), 52.1 (*C*H$_{2\text{-imidazolidinylidene}}$), 31.3 (*C*Me$_2$Ph), 29.8 (*C*Me$_2$Ph), 21.3 (*C*H$_3$), 20.9 (*C*H$_3$), 19.9 (*C*H$_3$), 18.4 ppm (*C*H$_3$). Elemental analysis calcd. (%) for C$_{79}$H$_{62}$BF$_{29}$MoN$_4$O 2.5 CH_2Cl_2 : C 50.11, H 3.43, N 3.49; found: C 50.37, H 3.46, N 3.61.

[Mo(N-2,6-Me$_2$-C$_6$H$_3$)(IMes)(CHCMe$_2$Ph)(OC$_6$F$_5$)(CH$_3$CN)$^+$B(Ar^F)$_4^-$] (17):

A solution of **13** (0.057 g, 0.058 mmol) in a minimum amount of CH_2Cl_2 (~ 1 mL) was cooled to -30 °C; then [Ag(CH$_3$CN)$_2$B(Ar^F)$_4$] (0.061g, 0.058 mmol) was added. The mixture was stirred for a further 3 h, then filtered through celite. The solvent was removed *in vacuo* to afford a yellow solid. It was dissolved in a minimum amount of CH_2Cl_2 and the solution was stored at -30 °C for several days to afford a yellow crystalline material (ca. 67% isolated yield). ^{1}H-NMR (400 MHz, CD_2Cl_2): δ = 13.47 (s, 1H, C*H*CMe$_2$Ph), 7.72 (m, 8H, Ar*H*), 7.56 (s, 4H, Ar*H*), 7.27-7.23 (t, 3H, *J* = 8 Hz, Ar*H*), 7.19 (d, 1H, *J* = 4 Hz, Ar*H*), 7.09-7.06 (t, 3H, *J* = 8 Hz, Ar*H*), 6.98 (d, 2H, *J* = 8 Hz, Ar*H*),6.82 (s, 2H, Ar*H*), 6.73 (s, 2H, C*H*NC), 2.38 (s, 3H, C*H*$_3$), 2.22 (s, 9H, C*H*$_3$), 2.00 (s, 6H, C*H*$_3$), 1.96 (s, 6H, C*H*$_3$), 1.89 (s, 6H, C*H*$_3$); ^{19}F-NMR (376 MHz, CD_2Cl_2): δ = -

62.89 (s, *C*F_3), -161.25 (2,6-F, d, $^3J_{F\text{-}F}$ = 19 Hz, C_6F_5), -165.78 (s, 3,5-F, C_6F_5), -170.81 (4-F, C_6F_5).

Mo(N-2,6-Me_2-C_6H_3)((1-*R*-phenethyl)-3-mesitylimidazolidin-2-ylidene)-(CHCMe_2Ph)$(OTf)_2$ (18):

1-(*R*-Phenylethyl)-3-mesityl-4,5-dihydro-1*H*-imidazol-3-ium tetrafluoroborate (0.082 g, 0.216 mmol) was suspended in benzene (2 mL). Potassium hexamethyldisilazide (KHMDS, 0.043 g, 0.216 mmol) was added. After 1 h, the clear benzene solution was filtered through celite. Mo(N-2,6-Me_2-C_6H_3)(CHCMe_2Ph)$(OTf)_2$·DME (0.159 g, 0.216 mmol) dissolved in benzene (8 mL) was added and the color immediately changed from yellow to deep red. The mixture was stirred for 3 h, then the benzene was removed and the yellow colored residue was washed with *n*-pentane and dried *in vacuo* to get a yellow colored solid (0.170 g, 85%). The compound was dissolved in a minimum amount of CH_2Cl_2 and the solution was stored at -30 °C for several days to afford a yellow crystalline material (ca. 60% isolated yield). ^{1}H-NMR (400 MHz, CD_2Cl_2): δ = 14.73 (s, 1H, C*H*CMe$_2$Ph, $^1J_{CH}$ = 126 Hz), 7.36-6.99 (m, 14H, Ar*H*), 6.29 (s, 1H, Ar*H*), 4.08-3.80 (m, 4H, CH_2NC), 2.46 (s, 3H, CH_3), 2.22 (s, 3H, CH_3), 1.82 (s, 3H, CH_3), 1.78 (s, 3H, CH_3), 1.76 (s, 3H, CH_3), 1.59 (s, 3H, CH_3), 1.54 (s, 3H, CH_3), 1.39 (s, 3H, CH_3); ^{19}F-NMR (376 MHz, CD_2Cl_2): δ = -77.06 (s, CF_3SO_3), -77.77 (s, CF_3SO_3, *trans* to NHC ligand); ^{13}C-NMR (101 MHz, CD_2Cl_2): δ = 316.3 (*C*HCMe$_2$Ph), 316.1 (*C*HCMe$_2$Ph), 205.3 (*C*$N_{carbene}$), 153.2 (C_{ipso}), 146.7 (C_{aryl}), 142.8 (C_{aryl}), 141.3 (C_{ortho}), 140.4 (C_{aryl}), 139.0 (C_{aryl}), 138.2 (C_{aryl}), 137.4 (C_{aryl}), 131.3 (C_{aryl}), 131.0 (C_{aryl}), 130.3 (C_{aryl}), 129.4 (C_{aryl}), 129.1 (C_{aryl}), 128.8 (C_{aryl}), 128.1 (C_{aryl}), 127.1 (C_{aryl}), 126.8 (C_{aryl}), 126.4 (C_{aryl}), 120.0 (q, *C*F_3SO_3, *J* = 321 Hz), 60.1 (*C*$H_{2\text{-imidazolidinylidene}}$), 58.0 (*C*$H_{2\text{-imidazolidinylidene}}$), 51.2 (*C*Me$_2$Ph), 46.9 ((*C*Me$_2$Ph), 31.2 (C*Me*$_2$Ph), 30.1 (C*Me*$_2$Ph), 21.2 (*C*$H_3$), 20.5 (*C*$H_3$), 19.4 (*C*$H_3$), 18.2 ppm (*C*$H_3$). Elemental analysis (%) calcd. for $C_{41}H_{47}Cl_2F_6MoN_3O_6S_2$: C 48.14, H 4.73, N 4.10; found: C 48.17, H 4.68, N 4.06.

Mo(N-3,5-Me_2-C_6H_3)(IMesH_2)(CHCMe_2Ph)$(OTf)_2$ (19):

Mo(N-3,5-Me_2-C_6H_3)(CHCMe_2Ph)$(OTf)_2$·DME (0.055 g, 0.075 mmol) was dissolved in benzene (3 mL). A benzene solution (1 mL) of 1,3-bis(2,4,6-trimethylphenyl)-2-imidazolidin-2-ylidene (0.023 g, 0.076 mmol) was added and an immediate color

change from yellow to light orange was observed while a precipitate formed. The mixture was stirred for 3 h, and then benzene was removed *in vacuo* to get a yellow colored solid (0.055 g, 80%). Alternatively, the yellow solid can be dissolved in a minimum amount of CH_2Cl_2 followed by storage at -30 °C for 24 h to afford a yellow crystalline material in 46% isolated yield. ^{1}H-NMR (400 MHz, C_6D_6): δ = 14.33 (s, 1H, C*H*CMe$_2$Ph), 7.35-6.49 (m, 12H, Ar*H*), 2.94 (s, br, 4H, C*H*$_2$NC), 2.47-1.90 (24H, C*H*$_3$), 1.32 (s, 3H, C*H*$_3$), 1.21 (s, 3H, C*H*$_3$); ^{19}F-NMR (376 MHz, C_6D_6): δ = -76.89 ppm (SO_3CF_3). ^{13}C-NMR (101 MHz, CD_2Cl_2): δ = 316.54 (*C*HCMe$_2$Ph), 206.4 (*C*N$_{carbene}$), 159.7 (*C*$_{aryl}$), 154.6 (*C*$_{aryl}$), 147.3 (*C*$_{aryl}$), 140.7 (*C*$_{aryl}$), 138.2 (*C*$_{aryl}$), 137.4 (*C*$_{aryl}$), 135.6 (*C*$_{aryl}$), 132.4 (*C*$_{aryl}$), 130.8 (*C*$_{aryl}$), 128.9 (*C*$_{aryl}$), 128.1 (*C*$_{aryl}$), 126.8 (*C*$_{aryl}$), 126.6 (*C*$_{aryl}$), 119.9 (q, *C*F$_3$SO$_3$, *J* = 320.2 Hz), 57.3 (*C*Me$_2$Ph), 52.8 (*C*H$_{2\text{-imidazolidinylidene}}$), 32.3 (C*Me*$_2$Ph), 28.9 (C*Me*$_2$Ph), 21.4 (*C*H$_3$), 19.1 (*C*H$_3$), 18.7 ppm (*C*H$_3$). Elemental analysis (%) calcd. for $C_{41}H_{47}F_6MoN_3O_6S_2$: C 51.73, H 4.98, N 4.41; found: C 51.72, H 5.09, N 4.43.

Mo(N-3,5-Me$_2$-C$_6$H$_3$)(IMes)(CHCMe$_2$Ph)(OTf)$_2$ (20):

Mo(N-3,5-Me$_2$-C$_6$H$_3$)(CHCMe$_2$Ph)(OTf)$_2$·DME (0.1400 g, 0.191 mmol) was dissolved in 4 mL of benzene. A benzene (1 mL) solution of 1,3-bis(2,4,6-trimethylphenyl)imidazol-2-ylidene (0.064 g, 0.210 mmol) was added and an immediate color change from yellow to light orange was observed. The mixture was stirred for 3 h; then the benzene was removed *in vacuo* to get a yellow-colored solid (0.120 g, 80%). Alternatively, the yellow solid can be dissolved in a minimum amount of CH_2Cl_2 followed by storage at -30 °C for 24 h to afford a yellow crystalline material in 65% isolated yield (0.115 g). ^{1}H-NMR (400 MHz, C_6D_6): δ = 14.40 (s, 1H, C*H*CMe$_2$Ph), 7.27-6.49 (m, 12H, Ar*H*), 5.91 (s, 2H, C*H*NC), 2.13-2.02 (24H, C*H*$_3$), 1.39 (s, 3H, C*H*$_3$), 1.31 (s, 3H, C*H*$_3$). ^{19}F-NMR (376 MHz, C_6D_6): δ = -76.73 (s, C*F*$_3$SO$_3$). ^{13}C-NMR (101 MHz, CD_2Cl_2): δ = 316.8 (*C*HCMe$_2$Ph), 182.7 (*C*N$_{carbene}$), 154.7 (*C*$_{aryl}$), 147.4 (*C*$_{aryl}$), 141.4 (*C*$_{aryl}$), 141.39 (*C*$_{aryl}$), 138.2 (*C*$_{aryl}$), 136.5 (*C*$_{aryl}$), 135.7 (*C*$_{aryl}$), 134.2 (*C*$_{aryl}$), 132.3 (*C*$_{aryl}$), 130.4 (*C*$_{aryl}$), 127.8 (*C*$_{aryl}$), 126.9 (*C*$_{aryl}$), 126.6 (*C*$_{aryl}$), 125.9 (C=C), 119.9 (*C*F$_3$SO$_3$, *J* = 320 Hz), 57.4 (*C*Me$_2$Ph), 32.6 (*C*H$_3$), 29.0 (*C*H$_3$), 21.4 (*C*H$_3$), 21.4 (*C*H$_3$), 18.7 (*C*H$_3$), 18.5 ppm (*C*H$_3$). Elemental analysis (%) calcd. for $C_{41}H_{45}F_6MoN_3O_6S_2$ 0.5 CH_2Cl_2: C 50.23, H 4.67, N 4.23; found: C 50.46, H 4.83, N 4.22.

Mo(N-3,5-Me_2-C_6H_3)($IMesH_2$)($CHCMe_2Ph$)(OTf)(O-2,6-Ph_2-C_6H_3) (21):

A solution of Mo(N-3,5-Me_2-C_6H_3)($IMesH_2$)($CHCMe_2Ph$)$(OTf)_2$ (0.149 g, 0.156 mmol) in a minimum amount of toluene/1,2-dichloroethane (5/2 mL) was cooled to -30 °C; then $LiOC_3H_3(C_6H_5)_2$ (0.038 g, 0.156 mmol) was added. The mixture was stirred for a further 3 h, then filtered through celite. The solvent was removed *in vacuo* to afford a yellow solid. It was washed with diethyl ether and dissolved in a minimum amount of CH_2Cl_2 and the solution was stored at -30 °C for several days to afford a yellow crystalline material in 80% (0.130 g) isolated yield. ^{1}H-NMR (400 MHz, C_6D_6,): δ = 13.59 (s, 1H, C*H*CMe_2Ph), 8.05 (s, 2H, Ar*H*), 7.64 (s, 2H, Ar*H*), 7.47-6.83 (m, 21H, Ar*H*), 2.75 (t, 2H, CH_2NC, J = 12 Hz), 2.55 (t, 2H, CH_2NC, J = 12 Hz), 2.33 (s, 3H, CH_3), 2.15 (s, 6H, CH_3), 2.09 (s, 6H, CH_3), 1.93 (s, 6H, CH_3), 1.36 (s, 3H, CH_3), 1.22 (s, 6H, CH_3); ^{19}F-NMR (376 MHz, CD_2Cl_2): δ = -77.60 (s, CF_3SO_3); ^{13}C-NMR (101 MHz, CD_2Cl_2): δ = 323.5 (*C*$HCMe_2Ph$), 213.2 (*C*$N_{carbene}$), 159.1 (C_{aryl}), 155.0 (C_{aryl}), 148.7 (C_{aryl}), 138.3 (C_{aryl}), 137.4 (C_{aryl}), 135.6 (C_{aryl}), 135.2 (C_{aryl}), 133.7 (C_{aryl}), 132.2 (C_{aryl}), 131.1 (C_{aryl}), 130.1 (C_{aryl}), 129.9 (C_{aryl}), 129.5 (C_{aryl}), 128.7 (C_{aryl}), 127.5 (C_{aryl}), 126.5 (C_{aryl}), 126.3 (C_{aryl}), 119.8 (CF_3SO_3), 54.7 (*C*Me_2Ph), 52.1 ($CH_{2\text{-imidazolidinylidene}}$), 31.0 (C*Me*$_2$Ph), 31.0 (C*Me*$_2$Ph), 21.2 ($CH_3$), 21.0 ($CH_3$), 19.2 ppm ($CH_3$). Elemental analysis (%) calcd. for $C_{58}H_{60}F_3MoN_3O_4SCH_2Cl_2$: C 62.54, H 5.60, N 3.71; found: C 63.43, H 5.91, N 4.49.

Mo(N-3,5-Me_2-C_6H_3)($IMesH_2$)($CHCMe_2Ph$)(OTf)($OC(CF_3)_3$) (22):

A solution of Mo(N-3,5-Me_2-C_6H_3)($IMesH_2$)($CHCMe_2Ph$)$(OTf)_2$ (0.072 g, 0.076 mmol) in a minimum amount of 1,2-dichloroethane (2 mL) was cooled to -30 °C; then $LiOC(CF_3)_3$ (0.018 g, 0.076 mmol) was added. The mixture was stirred for a further 3 h, then filtered through celite. The solvent was removed *in vacuo* to afford a yellow solid. It was washed with diethyl ether and dissolved in a minimum amount of CH_2Cl_2 and the solution was stored at -30 °C for several days to afford a yellow crystalline material in 70% isolated yield (0.060 g). ^{1}H-NMR (400 MHz, C_6D_6): δ = 14.09 (s, 1H, C*H*CMe_2Ph), 7.32-7.30 (d, 2H, J_{HH} = 8 Hz, Ar*H*), 7.09-7.05 (t, 1H, J_{HH} = 8 Hz Ar*H*), 6.97-6.93 (t, 1H, J_{HH} = 8 Hz Ar*H*), 6.80 (s, 2H, Ar*H*), 6.69 (s, 2H, Ar*H*), 6.62 (s, 1H, Ar*H*), 6.52 (s, 2H, Ar*H*), 3.12 (brs, 4H, CH_2NC), 2.46 (s, 6 H, CH_3), 2.09 (s, 15H, CH_3),

1.36 (s, 6 H, C*H*$_3$), 1.01 (s, 3 H, C*H*$_3$); ^{19}F-NMR (376 MHz, CD_2Cl_2): δ = - 73.70 (s, C*F*$_3$), -77.60 (s, C*F*$_3$SO$_3$); ^{13}C-NMR (101 MHz, CD_2Cl_2): δ = 302.9 (*C*HCMe$_2$Ph), 209.3 (*C*N$_{carbene}$), 154.1 (*C*$_{ipso}$), 147.6 (*C*$_{aryl}$) , 139.2 (*C*$_{ortho}$), 138.1 (*C*$_{aryl}$), 137.3 (*C*$_{aryl}$), 136.5 (*C*$_{aryl}$), 131.7 (*C*$_{aryl}$), 130.9 (*C*$_{aryl}$), 127.0 (*C*$_{aryl}$), 126.4 (*C*$_{aryl}$), 123.60 (*C*F$_3$), 120.7 (*C*F$_3$SO$_3$), 55.5 (*C*Me$_2$Ph), 52.5 (CH$_{2\text{-imidazolidinylidene}}$), 30.8 (C*Me*$_2$Ph), 20.8 (*C*H$_3$), 19.8 (*C*H$_3$), 19.3 ppm (*C*H$_3$). Elemental analysis (%) calcd. for $C_{44}H_{47}F_{12}MoN_3O_4S$: C 50.87, H 4.66, N 4.05; found: C 51.11, H 4.89, N 4.03.

Mo(N-2,6-Me$_2$-C$_6$H$_3$)(IMes)(CHCMe$_2$Ph)(OTf)((1R,2S,5R)-2-isopropyl-5-methylcyclo-hexan-1-olate) (**23**)**:**

A solution of Mo(N-2,6-Me$_2$-C$_6$H$_3$)(CHCMe$_2$Ph)(OTf)(IMes) (0.083 g, 0.0873 mmol) in a minimum amount (~ 5 mL) of $C_2H_4Cl_2$ was cooled to -30 °C; then Li(-)-menthol (0.0142 g, 0.0873 mmol) was added. The mixture was stirred for a further overnight, then filtered through celite. The solvent was removed *in vacuo* to afford a yellow colour gummy solid in 80% yield. ^{1}H-NMR (400 MHz, CD_2Cl_2): δ = 12.03 (s, 1H, C*H*CMe$_2$Ph), 7.12-6.85 (m, 12H, Ar*H*), 4.11-4.08 (m, 0.5H, menthol), 3.91-3.85 (m, 0.5H, menthol), 3.76 (s, 1H, OC*H*-Cyclohexyl), 2.29-1.98 (s, 30H, CH$_3$), 1.62 (t, 4H,cyclohexyl), 1.04-0.62 (m, 13H, menthol); ^{19}F-NMR (376 MHz, CD_2Cl_2): δ = -78.91 ppm (s, 3F, *C*F$_3$).

[(1,3-(2-*i*Pr)$_2$-tetrahydropyrimidin-2-ium)$^+$(Mo(N-2-*t*Bu-C$_6$H$_4$)(CHCMe$_2$Ph)-(OTf)(μ^2-(CF$_3$-SO$_3$)$_2$(μ^2-F)$^-$] (**24**):

Mo (N-2-*t*Bu-C$_6$H$_4$)(CHCMe$_2$Ph)(OTf)$_2$·DME (0.0500 g, 0.0750 mmol) was dissolved in 3 mL of toluene. A 1,3-diisopropylhexahydropyrimidine-2-carboxylate (0.0234 g, 0.0760 mmol) was added and heated the suspended reaction mixture at 60 °C. The mixture was stirred for 3 h, then the toluene was removed *in vacuo* to get a yellow colored solid (0.4 g, 80%). Alternatively, the yellow solid can be dissolved in a minimum amount of CH_2Cl_2/Et_2O (1:2) followed by storage at -30 °C for 24 h to afford a yellow crystalline material.^{1}H NMR (CD_2Cl_2): δ = 14.48 (s, 1H, CHCMe$_2$Ph), 14.44 (s, 1H, CHCMe$_2$Ph) 7.72-7.06 (m, 20H, ArH), 6.23 (s, 1H, NCHN) 4.18 (m, 2H, CH(CH$_3$)$_2$), 4.18-2.93 (m, 6H, CH$_2$), 1.92-1.27 (s, 42*H*, Me); ^{19}F NMR (CD_2Cl_2): δ -76.75 (s, CF_3SO_3);

Mo(N-2,6-Me_2-C_6H_3)(1,3,4–triphenyl-4,5-dihydro-1H-1,2,4-triazole-5-ylidene)-(CHCMe_2Ph)(OTf)$_2$ (25):

Mo(N-2,6-Me_2-C_6H_3)(CHCMe_2Ph)(OTf)$_2$(DME) (0.400 g, 0.5437 mmol) was dissolved in 8 mL of benzene. A benzene solution (1 mL) of 1,3,4–triphenyl-4,5-dihydro-1H-1,2,4-triazole-5-ylidene (0.162 g, 0.5437 mmol) was added. The mixture was stirred for 18 h, then the benzene was removed *in vacuo* and the residue was washed with diethyl ether and dried *in vacuo* to get a yellow coloured solid (0.360 g, 81%). Alternatively, the yellow solid can be dissolved in a minimum amount of ether followed by storage at -30 °C for 24 h to afford a yellow crystalline material (ca. 69% yield).^{1}H-NMR (400 MHz, CD_2Cl_2): δ = 14.37 (s, 1H, C*H*CMe$_2$Ph), 14.08 (s, 0.57H, C*H*CMe$_2$Ph), 8.09-6.24 (m, 35H, Ar*H*), 1.95 (s, 6*H*, CH_3), 1.58 (s, 3*H*, CH_3), 1.12-1.10 (s, 5*H*, CH_3), 0.78 (s, 5*H*, CH_3); ^{19}F-NMR (376 MHz, CD_2Cl_2): δ = – 77.41, 77.46 (d, C*F*$_3$SO$_3$); -77.79, -77.85 (d, C*F*$_3$SO$_3$). ^{13}C-NMR (101 MHz, CD_2Cl_2): δ = 322.9 (*C*HCMe$_2$Ph), 320.7 (*C*HCMe$_2$Ph), 186.0 (*C*N$_{carbene}$), 185.0 (*C*N$_{carbene}$), 146.8 (*C$_{ipso}$*), 139.6 (*C$_{ortho}$*), 135.3 (*C$_{aryl}$*), 132.7 (*C$_{aryl}$*), 132.3 (*C$_{aryl}$*), 132.1 (*C$_{aryl}$*), 131.9 (*C$_{aryl}$*), 131.6 (*C$_{aryl}$*), 131.3 (*C$_{aryl}$*), 130.7 (*C$_{aryl}$*), 130.5 (*C$_{aryl}$*), 129.8 (*C$_{aryl}$*), 129.6 (*C$_{aryl}$*), 129.0 (*C$_{aryl}$*), 128.5 (*C$_{aryl}$*), 128.2 (*C$_{aryl}$*), 127.3 (*C$_{aryl}$*), 126.8 (*C$_{aryl}$*), 123.2(C*F*$_3$), 120.1(q, C*F*$_3$, *J* = 319 Hz), 57.8 (*C*Me$_2$Ph), 57.4 (*C*Me$_2$Ph), 30.7 (C*Me*$_2$Ph), 28.0 (C*Me*$_2$Ph), 27.2 (C*Me*$_2$Ph), 19.4 (*C*H$_3$), 18.2(*C*H$_3$). Elemental analysis calcd. (%) for $C_{40}H_{36}F_6MoN_4O_6S_2$: C 50.96, H 3.85, N 5.94; Found: C 54.90, H 4.47, N 6.37.

[Mo(N-2,6-Me_2-C_6H_3)(1,3,4–triphenyl-4,5-dihydro-1H-1,2,4-triazole-5-ylidene)-(CHCMe_2Ph)(OTf)(OC(CF_3)$_3$)] (26) :

A solution of Mo(N-2,6-Me_2-C_6H_3)(1,3,4–triphenyl-4,5-dihydro-1H-1,2,4-triazole-5-ylidene)(CHCMe_2Ph)(OTf)$_2$ (1) (0.1020 g, 0.1040 mmol) in a minimum amount (~ 5mL) of $C_2H_4Cl_2$ was cooled to -30 °C; then LiOC(CF_3)$_3$ (0.0252 g, 0.1040 mmol) was added. The mixture was stirred for a further overnight, then filtered through celite. The solvent was removed *in vacuo* to afford a yellow solid. It was dissolved in a minimum amount of diallylether and the solution was stored at -30 °C for several days to afford a yellow crystalline material (ca. 55% yield). ^{1}H-NMR (400 MHz, CD_2Cl_2): δ = 14.54, 14.23 (s, 1.56 H, C*H*CMe$_2$Ph, *major isomer*), 13.75, 13.53 (s, 0.65H, C*H*CMe$_2$Ph, *minor isomer*), 8.02-6.70 (m, 51 H, Ar*H*), 2.11-0.81 (s, 27 H, Me); ^{19}F-NMR (376 MHz,

CD_2Cl_2): *major isomer*: δ = – 72.97(s, CF_3SO_3), 73.04 (s, CF_3SO_3), -73.35 to -73.37 (q, J = 3.76 Hz, CF_3SO_3), -73.41 to -73.43 (q, J = 3.76 Hz, CF_3SO_3), *minor isomer* : -76.81 to -76.84 (q, J = 3.76 Hz, CF_3SO_3), -76.93 to -76.95 (q, J = 3.76 Hz, CF_3SO_3) -77.38 (s, CF_3SO_3) , -77.46 (s, CF_3SO_3) . ^{13}C NMR (101 MHz, CD_2Cl_2): δ = 323.0 (*C*HCMe$_2$Ph, major isomer), 321.6 (*C*HCMe$_2$Ph, minor isomer), 187.8 (*C*N$_{carbene}$), 186.8 (*C*N$_{carbene}$), 154.3, 153.3 ($C_{ipso,}$ *major isomer*), 153.3 ($C_{ipso,}$ *minor isomer*), 147.8 ($C_{aryl,}$ *major*), 147.6 ($C_{aryl,}$ *minor)*, 141.0 (C_{aryl}), 140.6 (C_{aryl}), 139.9 (C_{aryl}), 139.4 (C_{aryl}), 136.4 (C_{aryl}), 135.4 (C_{aryl}), 134.6 (C_{aryl}), 132.1 (C_{aryl}), 131.9 (C_{aryl}), 131.4 (C_{aryl}), 131.2 (C_{aryl}), 131.1 (C_{aryl}), 130.9 (C_{aryl}), 130.8 (C_{aryl}), 130.6 (C_{aryl}), 130.5 (C_{aryl}), 130.1 (C_{aryl}), 130.0 (C_{aryl}), 129.6 (C_{aryl}), 129.5 (C_{aryl}), 128.9 (C_{aryl}), 128.5 (C_{aryl}), 128.0 (C_{aryl}), 127.3 (C_{aryl}), 127.0 (C_{aryl}), 126.6 (C_{aryl}), 126.4 (C_{aryl}), 125.5 (C_{aryl}), 121.5 (*C*F$_3$), 121.0(*C*F$_3$), 119.4 (*C*F$_3$),118.5 (*C*F$_3$), 57.2 (*C*Me$_2$Ph, major isomer), 56.8 (*C*Me$_2$Ph, major isomer), 56.5 (*C*Me$_2$Ph, minor isomer), 56.1 (*C*Me$_2$Ph, minor isomer), 31.7 (C*Me$_2$*Ph), 31.5 (C*Me$_2$*Ph), 30.9 (C*Me$_2$*Ph), 30.3 (C*Me$_2$*Ph), 29.5 (C*Me$_2$*Ph), 29.2 (C*Me$_2$*Ph), 27.7 (C*Me$_2$*Ph), 27.4 (C*Me$_2$*Ph), 20.0 (CH_3), 19.8 (CH_3), 18.8 (CH_3), 18.5 ppm (CH_3).

[(1,3,4–Triphenyl-4,5-dihydro-1H-1,2,4-triazole-4-ium)$^+$Mo(N-2,6-Me$_2$-C$_6$H$_3$)-(CHCMe$_2$Ph)(OTf)(μ^2-(OCH$_3$)$_2$(μ^2-CF$_3$SO$_3$)$^-$] (27):

Mo(N-2,6-Me$_2$-C$_6$H$_3$)(CHCMe$_2$Ph)(OTf)$_2$(DME) (0.151 g, 0.2053 mmol) was dissolved in 4 mL of toluene. A toluene solution (2 mL) of 5-methoxy-1, 3, 4–triphenyl-4,5-dihydro-1*H*-1,2,4-triazole (0.0676 g, 0.2053 mmol) was added. After some minutes, white precipitate formed. The mixture was stirred for 3 h, filtered over celite and then the toluene was removed *in vacuo* and the residue was washed with diethyl ether and dried *in vacuo* to get a yellow coloured solid (0.2100 g, 76%). Alternatively, the yellow solid can be dissolved in a minimum amount of toluene followed by storage at -30 °C for several days to afford a yellow crystalline material (ca. 54% yield). ^{1}H-NMR (400 MHz, CD_2Cl_2): δ = 13.67 (s, 2H, C*H*CMe$_2$Ph), 10.28 (s, 1H, NC*H*N), 8.11-6.80 (m, 31H, Ar*H*), 3.58 (s, 6H, OC*H*$_3$), 2.34-1.44 (s, 24*H*, C*H*$_3$); ^{19}F-NMR (376 MHZ, CD_2Cl_2): δ = – 77.73 (s, CF_3SO_3), -77.80 (s, CF_3SO_3). ^{13}C-NMR (101 MHz, CD_2Cl_2): δ = 322.0 (*C*HCMe$_2$Ph), 155.1 (N*C*$_{carbene}$), 154.9 (C_{ipso}), 150.2 (C_{aryl}), 141.5 (C_{aryl}), 138.3 (C_{ortho}), 135.2 (C_{aryl}), 133.4 (C_{aryl}), 132.5 (C_{aryl}), 132.0 (C_{aryl}), 131.2 (C_{aryl}), 130.9 (C_{aryl}), 129.9 (C_{aryl}), 129.5 (C_{aryl}), 128.7 (C_{aryl}), 128.3 (C_{aryl}), 128.2 (C_{aryl}), 127.3 (C_{aryl}), 126.8 (C_{aryl}), 126.6 (C_{aryl}), 126.4 (C_{aryl}), 126.0 (C_{aryl}), 125.8 (C_{aryl}), 122.3(*C*F$_3$), 119.9 (q, CF_3, J =

330 Hz), 70.7 (O*C*H_3), 55.9 (*C*Me_2Ph), 31.2 (C*Me*$_2$Ph), 30.6 (C*Me*$_2$Ph), 21.7 (*C*H_3), 19.1 ppm (*C*H_3). Elemental analysis calcd. (%) for $C_{68}H_{72}F_9Mo_2N_5O_{11}S_3$: C 51.22, H 4.55, N 4.39; Found: C 50.87, H 4.63, N 4.17.

[Mo(N-2,6-Me_2-C_6H_3)(CH_2CMe_3)$_2$($CCMe_3$)($Mg{\cdot}Et_2O$-*μ*-Cl)$_2$] (29):

A solution of neopentylmagnesium chloride in diethyl ether (1.0 M, 2.1 mL, 2.1 mmol) was added drop wise to a prechilled solution of Mo(N-2,6-Me_2-C_6H_3)(CHCMe_2Ph)(OTf)$_2$(DME) (0.508 g, 0.69 mmol) in 2 mL of diethyl ether. The color changed from yellow to red-brown as a precipitate formed. The mixture was stirred overnight, the ether was removed *in vacuo* and the residue was extracted with pentane. The pentane extract was filtered through celite, and the pentane was removed *in vacuo* to yield a sticky orange compound. Recrystallization from diethyl ether allowed for isolating 160 mg of **29** (56% yield). ^{1}H NMR (400 MHz, C_6D_6): *δ* = 7.40 (dd, *J* = 7.3, 1.2 Hz, 2H, CHCMe_2*Ph*), 7.25 (dd, *J* = 7.4, 1.9 Hz, 2H, CHCMe_2*Ph*), 7.12 (tt, *J* = 7.3, 1.2 Hz,1, CHCMe_2*Ph*), 7.02 (d, *J* = 7.4Hz, 2H, NAr-*H*), 6.78 (t, *J* = 7.4 Hz ,1H, NAr-*H*), 2.36 (d, *J* = 12 Hz, 2H, C*H*HCMe_3), 2.32 (s, 6, C*H*$_3$), 1.66 (s, 6, CHC*Me*$_2$Ph), 1.28 (s, 18, CH_2C*Me*$_3$), 0.95 (d, J = 12 Hz, 2H, C*H*HCMe_3); ^{13}C NMR (101 MHz, C_6D_6): *δ* = 307.2 (CMe_2Ph), 161.8 (*C*$_{aryl}$), 148.8 (*C*$_{aryl}$), 129.5 (*C*$_{aryl}$), 128.9 (*C*$_{aryl}$), 128.5 (*C*$_{aryl}$), 127.4, 125.6 (*C*$_{aryl}$), 121.5 (*C*$_{aryl}$), 76.9 (*C*H_2CMe_3), 68.0 (CH_3-*C*H_2O*C*H_2-CH_3), 59.7 (C*C*Me_2Ph), 35.1 (CH_2*C*Me_3), 34.3 (CH_2*C*Me_3), 30.4 (CC*Me*$_2$Ph), 22.0 (CH_3), 13.9 ppm (*C*H_3-CH_2OCH_2-*C*H_3). Elemental analysis (%) calcd. for $C_{60}H_{104}Cl_2Mg_2Mo_2N_2O_2{\cdot}CH_2Cl_2$: C 58.75, H 8.04, N 2.11; found: C 58.51, H 7.94, N 2.22.

Mo(N-2,6-Me_2-C_6H_3)($IMesH_2$)(CHCMe_2Ph)(OTf)(OCN):

Mo(N-2,6-Me_2-C_6H_3)($IMesH_2$)(CHCMe_2Ph)(OTf)$_2$ (0.0500 g, 0.05250 mmol) was dissolved in a minimum amount (~ 2 mL) of CH_2Cl_2 , then AgOCN (0.0070 g, 0.05250 mmol) was added portion wise to the reaction mixture. The mixture was stirred for a further 2 h, then filtered through celite, and solvent removed in vacuo to afford a yellow solid. The compound was dissolved in a minimum amount of dichloromethane and the solution was stored at -30 °C for several days to afford a yellow crystalline material (ca. 60% yield). ^{1}H-NMR (400 MHz, CD_2Cl_2): *δ* = 14.09 (s, 1H, C*H*CMe_2Ph), 7.36-6.72

(m, 12H, Ar*H*), 3.85 (s, 4H, C*H*$_2$NC), 2.38-2.30 (s, 24H, CH_3), 1.51 (s, 3H, CH_3), 1.47 (s, 3H, CH_3); ^{19}F-NMR (376 MHz, CD_2Cl_2): δ = -77.66 (s, CF_3SO_3), -78.20-78.23 (d, CF_3SO_3).

4.3 Polymerization Procedures

ROMP of 5,6-bis((pentyloxy)methyl)bicyclo[2.2.1]hept-2-ene (poly(M1)):

A prechilled solution of catalyst **3** (0.0048 g, 0.0054 mmol) in CH_2Cl_2 (0.5 mL) was added at once to a solution of the monomer (0.0802 g, 0.2716 mmol) in CH_2Cl_2 (2 mL) at -30 °C. The mixture was stirred over 4 h at room temperature and then precipitated from pentane. The washing phase was concentrated and precipitated again. The polymer was washed with pentane and dried for analysis. A white polymer was obtained in 90% yield (0.072 g). FT-IR (ATR, cm^{-1}): 2929 (s), 2852 (s), 1465 (m), 1366 (m), 1104 (s), 1010 (w), 805 (w), 642 (m); ^{1}H-NMR (400 MHz, $CDCl_3$): δ 5.27-5.15 (m, 2H), 3.34 (brs, 10H), 2.67 (brs, 1H), 2.32 (brs, 1 H), 1.93 (brs, 2H), 1.54 (brs, 4H), 1.32 (brs, 8H), 0.89 (brs, 6H). ^{13}C-NMR (101 MHz, $CDCl_3$): δ = 133.9, 71.1 (m), 50.9-39.91 (m), 29.6, 28.7, 22.7, 14.2. M_n = 9,000 g/mol, PDI = 1.2, σ_{trans} = 90%. A k_p/k_i value of 35 was calculated.[5] In the polymerization triggered by catalyst **4**, the polymer prepared from 0.050 g (0.169 mmol) monomer and 2.6 mg (0.0034 mmol) of **4** was obtained in 60% isolated yield (M_n = 8,500 g/mol), PDI = 1.1, σ_{trans} = 50%). A solution of catalyst **5** (0.0032 g, 0.0033 mmol) in CH_2Cl_2 (0.5 mL) was added at once to a solution of the monomer (0.05 g, 0.167 mmol) in CH_2Cl_2 (2 mL) at room temperature. The mixture was stirred over 4 h at room temperature and then precipitated from pentane. The washing phase was concentrated and precipitated again. The polymer was washed with pentane and dried for analysis. A white polymer was obtained in 84% isolated yield (0.042 g). ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 5.27-5.15 (m, 2H), 3.34 (brs, 10H), 2.70 (brs, 1H), 2.31 (brs, 1 H), 1.93 (brs, 2H), 1.54 (brs, 4H), 1.32 (brs, 8H), 0.89 (brs, 6H). ^{13}C-NMR (101 MHz, $CDCl_3$): δ 134, 133.7, 71.25-70.25 (m), 50.9-39.91 (m), 29.7, 29.6, 28.7, 22.7, 14.2; FT-IR (ATR, cm^{-1}): 2928 (s), 2854 (s), 1460 (m), 1369 (m), 1104 (s), 967 (w), 734(w); M_n= 8,300 g/mol, PDI = 1.1, σ_{trans} = 95%. With catalyst **6** (0.0032 g, 0.0033 mmol) in CH_2Cl_2 (0.5 mL) and the monomer (0.05 g, 0.167 mmol) in CH_2Cl_2 (2 mL) the polymer was obtained in 86% isolated yield (0.042 g). ^{1}H-NMR

(400 MHz, $CDCl_3$): δ = 5.27-5.17 (m, 2H), 3.34 (brs, 10H), 2.70 (brs, 1H), 2.31 (brs, 1 H), 1.93 (brs, 2H), 1.54 (brs, 4H), 1.32 (brs, 8H), 0.89 (brs, 6H). ^{13}C-NMR (101 MHz, $CDCl_3$): δ = 134, 133.7, 71.12-70.63 (m), 47.60-39.92 (m), 29.7, 28.7, 22.7, 14.2; FT-IR (ATR, cm^{-1}): 2928 (s), 2854 (s), 1460 (m), 1369 (m), 1104 (s), 967 (w), 733(w); M_n= 8,200 g/mol, PDI = 1.1, σ_{trans} = 97%. With catalyst **7** (0.0026 g, 0.00271 mmol) in CH_2Cl_2 (0.5 mL) and the monomer (0.04 g, 0.1358 mmol) in CH_2Cl_2 (2 mL) the polymer was obtained in 28% isolated yield (0.012 g). ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 5.27-5.17 (m, 2H), 3.34 (brs, 10H), 2.70 (brs, 1H), 2.31 (brs, 1 H), 1.93 (brs, 2H), 1.54 (brs, 4H), 1.32 (brs, 8H), 0.89 (brs, 6H). ^{13}C-NMR (101 MHz, $CDCl_3$): δ = 134, 133.6, 71.11-70.11 (m), 47.60-39.78 (m), 29.6, 29.5 28.5, 22.6, 22.5, 14.2; FT-IR (ATR, cm^{-1}): 2928 (s), 2854 (s), 1460 (m), 1369 (m), 1104 (s), 966 (w), 737(w); M_n = 11,400 g/mol, PDI = 1.2 , σ_{trans} = 64%.

ROMP of 7-oxabicyclo[2.2.1]hept-5-ene-2,3-diylbis(methylene)diacetate (poly(M2)):

A prechilled solution of **3** (0.0045 g, 0.0050 mmol) in CH_2Cl_2 (0.5 mL) was added at once to a solution of monomer (0.0600 g, 0.2520 mmol) in CH_2Cl_2 (2 mL) at -30 °C. The mixture was stirred for 24 h at room temperature and then precipitated from pentane. After drying *in vacuo*, 0.058g of polymer (97%) were obtained. FT-IR (ATR, cm^{-1}): 2902 (m), 1732 (s), 1431 (w), 1366 (s), 1220 (s), 1104 (w), 1029 (s), 968 (s), 728 (m).^{1}H-NMR (400 MHz, $CDCl_3$): δ = 5.72-5.58 (m, 2 H), 4.49 (brs, 1 H), 4.18 (m, 5 H), 2.40 (brs, 2 H), 2.03 (brs, 6 H); ^{13}C-NMR (101 MHz, $CDCl_3$): δ = 170.8, 133.1, 81.4, 61.9, 45.8, 20.9. M_n = 13,000 g/mol, PDI = 1.7, σ_{trans} = 85%. For the polymerization a k_p/k_i value of 11 was calculated.[5] In the polymerization triggered by catalyst **4**, the polymer was prepared from 0.050 g (0.209 mmol) monomer and 3.2 mg (0.0042 mmol) of **2** were obtained in 35% isolated yield (M_n = 1,800 g/mol), PDI = 1.2, σ_{trans} = 33%). All the other polymerization processes were triggered by different catalysts in the same way.

ROMP of bicyclo[2.2.1]hept-2-ene-2,3-diyldimethanol (poly(M3)) using Catalyst 3:

A solution of Catalyst **3** (0.0173 g, 0.0194 mmol) in $CHCl_3$ (1.5 mL) was added at once to a solution of the monomer (0.0300 g, 0.1940 mmol) in $CHCl_3$ (2 mL) at room temperature. The mixture was stirred over 5 h at 55 °C (some yellow coloured polymer sticked to the schlenk tube) and then precipitated from pentane. The polymer was washed with pentane, dichloromethane and dried for analysis. A white-yellow polymer was obtained in 80% yield (0.024 g). FT-IR (ATR, cm^{-1}): 3373 (s), 2930 (s), 2884 (s), 1477 (m), 1261 (s), 1109 (s), 1023 (s), 921 (w), 632 (s); ^{1}H-NMR (400 MHz, DMSO-d_6): δ = 5.48-5.40 (m, 2H), 3.86 (brs, 2H), 3.44 (brs, 4H), 2.45 (brs, 1H), 2.10(brs, 1H), 1.83 (brs, 1H), 1.57(brs, 1H), 1.33 (brs, 1H), ^{13}C-NMR (101 MHz, DMSO-d_6): δ = 134.8, 132.0, 60.76, 59.29, 47.77, 47.03, 43.77, 43.39, 32.29, 29.63 ppm; M_n = 2,800 g/mol, PDI = 1.1, σ_{trans} = 47%.

ROMP of bicyclo[2.2.1]hept-5-ene-2-carboxaldehyde (poly(M4)) using Catalyst 3:

A solution of Catalyst **3** (0.006 g, 0.0068 mmol) in CH_2Cl_2 (1.0 mL) was added at once to a solution of the monomer (0.0400 g, 0.3438 mmol) in CH_2Cl_2 (1.0 mL) at room temperature. The mixture was stirred over 20h at room temperature, quenched with MeOH-HCl (10%) solution and then precipitated from pentane. The polymer was washed with pentane and dried for analysis. A grey coloured polymer was obtained in 55% isolated yield (0.022 g). FT-IR (ATR, cm^{-1}): 2942 (s), 2830 (m), 1720 (s), 1630 (s), 1470 (s), 1255 (s), 1158 (s), 1026 (s), 719 (s), 636 (s); ^{1}H-NMR (400 MHz, THF-d8): δ = 7.70, 6.75, 5.32, 5.19, 5.04, 4.26, 4.11, 2.78, 1.41, 0.90, 0.60, 0.41; ^{13}C-NMR (101 MHz, THF-d_8): δ = 204.6, 141.2, 136.8, 131.9, 130.7, 128.7, 43.1, 30.3, 26.0, 23.4, 21.1, 18.9, 17.8; M_n = 5,000 g/mol, PDI = 2.1 ($M_{n,\ theor.}$ = 6,100 g/mol).

ROMP of bicyclo[2.2.1]hept-5-en-2-ylmethyl cyclohexanamine (poly(M5)):

A solution of Catalyst **3** (0.0174 g, 0.0195 mmol) in CH_2Cl_2 (1.5 mL) was added at once to a solution of the monomer (0.0400 g, 0.1951 mmol) in $CHCl_3$ (2 mL) at room temperature. The mixture was stirred for 5 h at 70 °C, then the polymer was

precipitated from pentane. The polymer was washed with pentane and dried for modification. An orange polymer was obtained in 90% isolated yield (0.036 g). The brown polymer was dissolved in methanol (2-3 mL) and 1 mL of concentrated HCl was added. The mixture was stirred for 5 minute, then NaOH pellets were added to precipitate the polymer. The polymer was washed with pentane, dichloromethane and dried for analysis. FT-IR (ATR, cm^{-1}): 3421 (m), 2935 (s), 2858 (m), 2424 (m), 1630 (m), 1454 (s), 1222 (s), 1155 (s), 1030 (s), 724 (s), 637 (s); ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 6.97, 6.17, 6.07, 5.79, 5.77, 5.35, 5.33, 4.54, 3.45, 3.18, 2.96, 2.82, 2.64, 2.36, 2.31, 1.81, 1.60, 1.24; ^{13}C-NMR (101 MHz, $CDCl_3$): δ = 140.7, 138.5, 137.1, 136.6, 135.2, 132.3, 130.3, 58.2, 48.7, 45.0, 42.8, 42.6, 36.2, 31.5, 29.0, 24.8, 21.0, 17.5, 14.4. M_n = 13,100 g/mol, PDI = 1.10. All the other polymerization processes were triggered by different catalysts in the same way.

ROMP of bicyclo[2.2.1]hept-5-en-2-yl-N,N-dimethylmethanamine (poly(M6)):

A solution of Catalyst **3** (0.0194 g, 0.0218 mmol) in CH_2Cl_2 (1.5 mL) was added at once to a solution of the monomer (0.0300 g, 0.1983 mmol) in $CHCl_3$ (2 mL) at room temperature. The mixture was stirred for 3 h at 75 °C, then the polymer was precipitated from pentane. The polymer was washed with pentane, dichloromethane and dried for modification. A brown polymer was obtained in 90% isolated yield (0.027 g). The brown polymer was dissolved in methanol (2 mL) and 1 ml concentrated HCl were added. The mixture was stirred for 5 min, then NaOH pellets were added to precipitate the polymer. The polymer was washed with pentane, dichloromethane and dried for analysis. FT-IR (ATR, cm^{-1}): 2955 (s), 1629 (s), 1464 (s), 1259 (s), 1151 (s), 1029 (s), 636 (s); ^{1}H-NMR (400 MHz, DMSO-d_6): δ = 6.98, 5.42, 3.14, 2.66, 2.32, 2.20, 2.17, 2.05, 0.85; M_n = 10,500 g/mol, PDI = 1.21.

General Procedure for Cyclopolymerizations:

All cyclopolymerizations were performed under a nitrogen atmosphere in a glove box. The CH_2Cl_2 used for polymerization was passed over Al_2O_3. Initiators were dissolved in 1 mL of the respective solvent. This solution was added quickly to a solution of the monomer in the same solvent. Reactions were terminated by addition of methanol and stirred for another 10 minutes. Then the solution was concentrated and precipitated in

methanol or pentane. The precipitate was dissolved in $CHCl_3$ and precipitated again. The resulting polymers were dried *in vacuo*.

Poly(4,4-bis(ethoxycarbonyl)-1,6-heptadiyne) (poly(M7)):

The polymer was prepared from **3** (4.5 mg, 0.0051 mmol) and the monomer (60 mg, 0.2540 mmol) in 89% isolated yield (53 mg). Polymerization was started at -30 °C and allowed to run for 1 h. ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 6.95-6.83 (s, 1H, CH), 6.45 (s, 1H, CH), 4.10-3.37 (bm, 6H, CH_2), 2.82 (s, 1H, CH), 2.05-1.80 (m, 2H, CH_2), 1.17 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 170.9,170.8, 169.0, 137.0, 123.2, 61.9, 58.2, 58.0, 57.3, 57.1, 54.3, 54.1, 41.5, 29.7, 14.1; IR (ATR, cm^{-1}): 3367 (m), 2969 (s), 2929 (s), 2864 (s), 1673 (s), 1519 (m), 1453 (m), 1366 (s), 1337 (w),1258 (w), 1190 (w), 1125 (s), 1077 (s), 947 (m), 770 (s), 690 (w); UV/Vis ($CHCl_3$): λ_{max} = 548, 584 nm, M_n = 9,600 g/mol, PDI = 1.6, α-insertion: 81%, k_p/k_i = 7. With **4** only 46% yield was obtained, M_n = 1600 g/mol, PDI = 2.7. The polymer was prepared from **5** (0.004 g, 0.0042 mmol) and the monomer (0.05 g, 0.213 mmol) in 84% isolated yield (0.042 g). Polymerization was started at -30 °C and allowed to run for 1 h. ^{13}C-NMR (101 MHZ, $CDCl_3$): δ = 172.1, 137.1, 128.4, 126.3, 123.4, 62.1, 57.0, 41.6, 14.2; FT-IR (ATR, cm^{-1}): 2977 (m), 1720 (s), 1444 (w), 1367 (s), 1245 (s), 1157 (w), 1065 (s), 946 (s), 629 (m). UV/Vis ($CHCl_3$): λ_{max} = 592, 547 nm, M_n = 8,500 g/mol, PDI = 2.1, α-insertion: ≥ 95%. In case the polymer was prepared from **6** (0.0040 g, 0.0042 mmol) and the monomer (0.0500 g, 0.212 mmol) poly-DEDPM was obtained in 86% isolated yield (0.043 g). ^{13}C-NMR (101 MHz, $CDCl_3$): δ = 172.1, 138.7, 128.0, 125.8, 122.9, 62.1, 57.4, 41.5, 14.2; FT-IR (ATR, cm^{-1}): 2979 (m), 1722 (s), 1446 (w), 1367 (s), 1248 (s), 1158 (w), 1067 (s), 947 (s), 631 (m). UV/Vis ($CHCl_3$): λ_{max} = 591, 552 nm, M_n = 84,000 g/mol, PDI = 2.3, α-insertion: ≥ 99%. In case the polymer was prepared from **7** (0.0040 g, 0.0042 mmol) and the monomer (0.0500 g, 0.212 mmol) poly-DEDPM was obtained in 54% isolated yield (0.043 g); ^{13}C-NMR ($CDCl_3$): δ = 172.1, 137.1, 128.2, 126.4, 123.3, 62.1, 57.4, 41.6, 14.2; FT-IR (ATR, cm^{-1}): 2977 (m), 1721 (s), 1444 (w), 1367 (s), 1248 (s), 1158 (w), 1067 (s), 947 (s), 631 (m). UV/Vis ($CHCl_3$): λ_{max} = 591, 552 nm, M_n = 67,400 g/mol, PDI = 2.7, α-insertion: ≥ 96%.

Poly(4,4-bis[(diethoxybenzoyloxy)methyl]-1,6-heptadiyne) (poly(M8)):

The polymer was prepared from **3** (1.9 mg, 0.0022 mmol) and the monomer (60 mg, 0.1120 mmol) in 94% isolated yield (57 mg). Polymerization was started at -30 °C and allowed to run for 1 h. ^{1}H-NMR ($CDCl_3$): δ = 7.04-6.92 (m, 4H), 6.71-6.60 (m, 2H), 6.45-6.31 (m, 2H), 4.44-4.31 (m, 4H), 3.90-3.81 (m, 8H), 2.89-2.82 (m, 4H), 1.40-1.25 (m, 12H); ^{13}C-NMR ($CDCl_3$): δ = 168.3,159.3, 138.2, 131.2, 107.7, 107.6, 106.3, 63.6, 40.7, 27.1, 14.7; IR (ATR, cm^{-1}): 3367 (m), 2969 (s), 2929 (s), 2864 (s), 1673 (s), 1519 (m), 1453 (m), 1366 (s), 1337 (w),1258 (w), 1190 (w), 1125 (s), 1077 (s), 947 (m), 770 (s), 690 (w); UV/Vis ($CHCl_3$): λ_{max} = 550, 590 nm, *α*-insertation: > 91%, k_p/k_i = 33. The polymer was prepared from **5** (0.0014 g, 0.0015 mmol) and the monomer (0.04 g, 0.0745 mmol) in ~ 100% isolated yield (0.0392 g). Polymerization was started at -30 °C and was allowed to run for 1 h at 80 °C. ^{1}H-NMR ($CDCl_3$): *δ* = 6.90 (br, m, 4H), 6.36 (br, m, 4H), 4.30 (br, s, 4H), 3.85 (br, s, 8H), 2.81 (br, s, 4H), 1.29 (br, s, 12H); ^{13}C-NMR ($CDCl_3$): *δ* = 166.5, 159.9, 138.3, 131.1, 123.4, 107.7, 106.4, 69.6, 63.7, 43.4, 40.8, 14.8; FT-IR (ATR, cm^{-1}): 2978 (w), 1788 (w), 1716 (s), 1592 (s), 1446 (m), 1385 (w), 1296 (m), 1216 (s), 1166 (s), 1101 (m), 1051 (m), 990 (w), 817 (w), 757 (m), 675 (w), 619 (m); UV/Vis ($CHCl_3$): λ_{max} = 591, 550 nm, M_n = 11,600 g/mol, PDI = 1.82, *α*-insertion: ≥ 93%. All the other polymerization processes were triggered by different catalysts in the same way.

Poly(4,4,5,5-tetrakis(ethoxycarbonyl)-1,7-octadiyne) ((poly(M11)):

The polymer was prepared from **3** (3.6 mg, 0.004 mmol) and the monomer (80 mg, 0.203 mmol) in 81% isolated yield (64 mg). Polymerization was started at -30 °C and allowed to run for 1 h. IR (cm^{-1}): 2901 (m), 1730 (ss), 1461 (m), 1444 (m), 1387 (m), 1363 (m), 1265 (s), 1198 (m), 1122 (w),1095 (m), 1052 (m), 1027 (s), 941 (m), 856 (m), 781 (w), 703 (w);^{1}H-NMR ($CDCl_3$): *δ* = 6.71 (s, 2H, C*H*), 4.41-4.25 (bs, 8H, CH_2), 3.25-3.18(bs, 4H, CH_2), 1.38-1.23 (bs, 12H, CH_3); ^{13}C-NMR ($CDCl_3$): *δ* = 169.7, 130.8, 124.7, 61.7, 56.9, 32.5, 13.7; UV/Vis ($CHCl_3$): λ_{max} =484 nm. M_n = 13,200 g/mol, PDI = 1.9 ($M_{n,\ theor.}$ = 19,700 g/mol). The polymer was prepared from **5** (0.0036 g, 0.004 mmol) and the monomer (80 mg, 0.203 mmol) in 81% isolated yield (64 mg). Polymerization was started at -30 °C and allowed to run for 1 h at 80 °C. ^{1}H-NMR ($CDCl_3$): *δ* = 7.01 (br, m, 2H), 4.21 (br, m, 8H), 3.18 (br, m, 4H), 1.28 (br, m, 12H); ^{13}C-

NMR ($CDCl_3$): δ = 169.9, 131.0, 125.0, 61.9, 57.1, 32.7, 14.0; FT-IR (ATR, cm^{-1}): 2981 (m), 1729 (s), 1444 (w), 1368 (s), 1262 (s), 1199 (w), 1092 (s), 1027 (w), 945 (s), 862(w), 700 (w), 636 (w), 579(w). UV/Vis ($CHCl_3$): λ_{max} = 483 nm, M_n = 15,000 g/mol, PDI = 2.2, α-insertion: ≥ 96%. All the other polymerization processes were triggered by different catalysts in the same way.

Poly(2,2-di(prop-2-yn-1-yl)propane-1,3-diol) (poly(M9)):

The polymer was obtained in 80% isolated yield (0.030 g) with catalysts **3** .^{1}H NMR (400 MHz, DMSO-d_6): δ 7.09-6.66 (m, 2H), 4.60 (brs, 2H), 3.17 (s, 2H), 2.08 (s, 2H). UV-Vis: λ_{max} = 593, 554 nm (DMSO). The polymer was prepared from **5** (0.010 g, 0.0105 mmol) and the monomer (0.04 g, 0.2628 mmol) in ~70% isolated yield (0.027 g). Polymerization was started at room temperature and allowed to run for 1 h. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 7.1-6.7 (b, m, olefinic carbons, 2H), 4.42 (s, 4H); IR (ATR-mode, cm^{-1}): 3400 (w), 2977 (w), 1444 (w), 1367 (w), 1247 (m), 1159 (m), 1065 (m), 946 (w), 856 (w), 629 (w). UV-Vis: λ_{max} = 593, 554 nm (DMSO); M_n = 5,000 g/mol, PDI = 2.1.
All the other polymerization processes were triggered by different catalysts in the same way.

Poly(4,4-dicyano-1,7-heptadiyne) (poly(M10)):

A prechilled solution of catalyst **3** (0.016 g, 0.0211 mmol) in CH_2Cl_2 (0.5 mL) was added at once to a solution of the monomer (0.0300 g, 0.211 mmol) in CH_2Cl_2 (2 mL) at -30 °C. The mixture was stirred over 2 h at room temperature, quenched with MeOH-HCl (10%) solution and then precipitated from pentane. The polymer was washed with pentane and dried for analysis. A red-violet polymer was obtained in 60% isolated yield (0.018 g). IR (cm^{-1}): 2960 (m), 2252 (w), 1588 (w), 1484 (m), 1267 (s), 1232 (s), 1027 (s), 810 (w), 636 (s); ^{1}H-NMR (DMSO-d_6): δ = 7.0, 6.78, 6.11, 5.76, 4.43, 3.97, 3.18, 2.75, 2.34, 2.29, 2.11, 1.14; ^{13}C-NMR (DMSO-d_6): δ = 160.1, 139.6, 135.5, 130.8, 129.4, 129.0, 122.2, 119.0, 115.8, 50.8, 20.5, 17.6, 17.7, 13.8; UV/Vis (DMSO): λ_{max} = 530 nm. M_n = 1,100, PDI = 1.2 ($M_{n,\ theor.}$ = 1,420 g/mol).

Poly(4,5-bis(carboxylic acid)-1,7-octadiyne) (poly(M12)):

A prechilled solution of Catalyst **3** (0.0137 g, 0.0154 mmol) in CH_2Cl_2 (1.0 mL) was added at once to a solution of the monomer (0.0300 g, 0.1956 mmol) in THF (2 mL) at -30 °C. The mixture was stirred over 1h at room temperature and then precipitated from pentane. The polymer was washed with pentane and dried for analysis. A red polymer was obtained in 90% yield (0.027 g). IR (cm^{-1}): 3288 (m), 2918 (m), 1702 (s), 1431 (m), 1213 (s), 1168 (s), 1026 (s), 946 (m), 634 (s); ^{13}C-NMR (101 MHz, THF-d_8): δ = 174.7, 136.6, 130.84, 47.81, 40.41; UV/Vis (THF): λ_{max} = 432 nm. M_n = 2,600 g/mol, PDI = 1.3 ($M_{n,\ theor.}$ = 2,500 g/mol).

Poly(2-(prop-2-yn-1-yl)pent-4-ynoic acid) (poly(M13)):

The polymer was prepared from **3** (0.0055 g, 0.0059 mmol) and the monomer (0.004 g, 0.294 mmol) in 65% isolated yield (0.0260 g). Polymerization was started at -30 °C and allowed to run for 4 h at 80 °C. ^{1}H-NMR (400 MHz, DMSO-d_6): δ = 12.27 (b, s, COO<u>H</u>, 1H), 67.3-6.8 (b, m, olefinic protons, 2 H), 3.23, 2.34; ^{13}C-NMR (400 MHz, DMSO-d_6): δ = 176.2 (<u>C</u>OOH), 136.0 (b, C=C); FT-IR (ATR, cm^{-1}): 2981 (m), 1729 (s), 1444 (w), 1368 (s), 1262 (s), 1199 (w), 1092 (s), 1027 (w), 945 (s), 862 (w), 700 (w), 636 (w), 579(w). UV/Vis ($CHCl_3$): λ_{max} = 587, 547 nm, M_n = 6,200 g/mol, PDI = 1.5. All the other polymerization processes were triggered by different catalysts in the same way.

Copolymerization of NBE and CPE:

NBE (80 mg, 0.84 mmol) and CPE (405 mg, 5.88 mmol) were dissolved in CH_2Cl_2 (7 mL). A solution of **3** (0.0020 g, 0.0022 mmol) in CH_2Cl_2 was added to this solution The mixture was stirred over 1h at room temperature. The polymer was precipitated in 50 mL of methanol and dried *in vacuo*. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 5.37–5.20 (brm, 4H), 2.77 (br s, 1H), 2.43 (br s, 1H), 1.93–1.77 (brm, 7H), 1.44–1.33 (br s, 4H); 1.09–1.00 ppm (m, 1H); ^{13}C-NMR (150.93 MHz, $CDCl_3$): δ = 135.4, 135.2, 133.9 (poly(NBE)), 133.0 (poly(NBE)), 130.3 (poly(CPE)),129.8 (poly(CPE)), 128.3, 128.2, 43.5, 43.3, 41.7, 41.3, 38.2, 38.0, 32.6,32.3, 32.2, 32.0, 29.8, 29.5, 27.1, 26.9 ppm.

Kinetics

Kinetic investigations on the cyclopolymerization of monomers by the action of **3** were done in THF and CH_2Cl_2 at room temperature. The monomer conversion was detected using GC-MS. Dodecane was used as an internal standard.

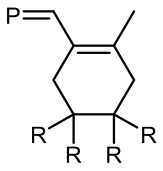
MALDI-TOF Analysis

Calculation of repeat units and end groups of the **oligo-M11-3** by MALDI-TOF mass analysis.

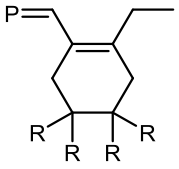
rep.unit	resid.	end1	end2	cation	Mn	Mw	pd	DP
394.163	-0.21234	70.0783	end2a	22.9898	3480.38	3951.33	1.13531	8.82982
394.163	-0.23859	70.0783	end2b	22.9898	3327.99	3789.57	1.13870	8.44319
394.163	-0.22298	70.0783	end2b	22.9898	4551.40	4667.09	1.02542	11.5470
394.163	-0.07599	70.0783	end2b	22.9898	2920.01	3165.15	1.08395	7.40814

End1: -neopentyl

End2:

end 2a 

R= $COOC_2H_5$
Mw: 396,178

end 2b 

R= $COOC_2H_5$
Mw: 410,194

Positive ion MALDI-TOF (matrix-assisted laser desorption ionization time-of-flight) measurements were performed on Bruker Autoflex III with a smart ion beam laser (337 nm). Measurements were carried out in the reflector mode. Samples were prepared from THF solution by mixing matrix dithranol (10 mg/ml), polymer (5 mg/ml), and sodium trifluoromethan sulfonate (17 mg/ml) in a ratio of 25:5.2.

4.4 General Procedure for RCM, HM and CM

1. Ca. 20-25 mg of substrate (or of both substrates in CM) were transferred into a 10 mL dram vial. 1 mL of solvent was added. Subsequently, 50 µL of dodecane (internal standard) were added to the substrate solution. An aliquot with 1 mg of substrate was taken for the t_0 sample. A stock solution of the catalyst was prepared. The corresponding amount of stock solution was added to the substrate solution and the mixture was placed inside an aluminum block for heating and stirred at the indicated temperature for the indicated time period with the caps closed. Reactions were quenched by exposure to air and an aliquot was taken for GC-MS analysis.

2. For reactions with very low catalyst loading around 1.5 g of substrate were used. All reactions were run inside Schlenk tubes under an Ar-atmosphere. All substrates were passed over fresh activated neutral Al_2O_3 (minimum twice) prior to use. 8 mL of the corresponding solvent were added to the substrate. Subsequently, 150 µL of dodecane (internal standard) were added to the substrate solution. An aliquot with 10 mg of substrate was taken for the t_0 sample. A stock solution of the catalyst was prepared. The corresponding amount of catalyst stock solution was added to the substrate(s) and the mixture was placed inside an aluminum block for heating and stirred at the indicated temperature for the indicated time period with the caps closed. Reactions were quenched by exposure to air and an aliquot was taken for GC-MS analysis.

3. Reactions at 140 °C were conducted in a Schlenk tube with periodical opening of the valve to release built-up pressure.

4.5 General Procedure for Ethenolysis

A solution of the corresponding catalyst in CH_2Cl_2 (0.3 mL) was added at once to a solution of *cis*-cyclooctene (1.000 g, 9.07 mmol) in toluene (20 mL) at room temperature (add 0.3 mL *n*-dodecane as internal slandered) to a high pressure stainless steel reactor. The mixture was stirred at the indicated temperature for the indicated time period with continuous fixed ethylene pressure.

n.b: After finishing reaction, some of the reaction mixture was slowly poured into the methanol but no precipitation was observed, means no poly(cyclooctene) formed.

4.6 X-ray Measurements and Structure Determination

X-ray measurements of single-crystals and the corresponding structure determination were carried out by Dr. Wolfgang Frey at the Institute of Organic Chemistry, University of Stuttgart, Germany. Data were collected on a Bruker Kappa Apex 2 duo diffractometer at 100 K. The structures were solved using direct methods with refinement by full matrix least-squares of F2, with the program system SHELXL 97 in connection with a multi-scan absorption correction. All non-hydrogen atoms were refined anisotropically.

4.7 DFT Calculation

Density functional theory (DFT) calculations on structure **29** (dimeric form) as well as in its monomeric form after dissociation of $Mg_2Cl_2^{2+}$ were performed by the group of Prof. Kastner, Institute of Theoretical Chemistry, University of Stuttgart. All DFT calculations used the BP86 functional[7-8] in Turbomole version 6.2.[11] The def2-SVP basis set was used for all atoms. The density was expressed on an m^3 grid. A relativistic effective core potential with 14-electrons was used for molybdenum.[9] Energies were converged to changes below 10^{-7} Hartree per iteration. The CH_2Cl_2 solvent was modeled using COSMO with a relative dielectric constant of 8.93. Geometries were optimized using DL-FIND[10] in ChemShell[11] with default tolerances. Orbital plots were generated from intrinsic bond orbitals calculated with molpro.[12]

General Polymerization Procedure with 29:

Both the monomer (0.531 mmol) and **29** (0.0136 g, 0.011 mmol, monomer:**29** = 1:50) were dissolved in a minimum amount of CH_2Cl_2. Both solutions were prechilled to -30 °C and the catalyst solution was added to the one of the monomer. After 3 h of stirring, the polymerization reaction was quenched by addition of ferocenaldehyde, then the polymer was precipitated from methanol, washed with pentane and dried *in vacuo*.

4.8 References

[1] J. H. Oskam, H. H. Fox, K. B. Yap, D. H. McConville, R. O`Dell, B. J. Lichtenstein, R. R. Schrock, *J. Organomet. Chem.*, **1993**, *459*, 185-198.

[2] D. Wang, K. Wurst, W. Knolle, U. Decker, L. Prager, S. Naumov, M. R. Buchmeiser, *Angew. Chem. Int. Ed.*, **2008**, *47*, 3267-3270.

[3] D. Wang, K. Wurst, M. R. Buchmeiser, *Chem. Eur. J.*, **2010**, *16*, 12928-12934.

[4] J. Unold, D. Wang, W. Frey, M. R. Buchmeiser, *Polym. Chem.*, **2013**, *4*, 4219-4233.

[5] M. Iglesias, D. J. Beetstra, J. C. Knight, L.-L. Ooi, A. Stasch, S. Coles, L. Male, M. B. Hursthouse, K. J. Cavell, A. Dervisi, I. A. Fallis, *Organometallics*, **2008**, *27*, 3279-3289.

[6] D. Enders, K. Breuer, U. Kallfass, T. Balensiefer, *Synthesis*, **2003**, *2003*, 1292-1295.

[7] A. D. Becke, *Phys. Rev. A*, **1988**, *38*, 3098-3100.

[8] J. P. Perdew, *Phys. Rev. B*, **1986**, *33*, 8822-8824.

[9] D. Andrae, U. Häußermann, M. Dolg, H. Stoll, H. Preuß, *Theor. Chem. Acc.*, *77*, 123-141.

[10] J. Kästner, J. M. Carr, T. W. Keal, W. Thiel, A. Wander, P. Sherwood, *J. Phys. Chem. A*, **2009**, *113*, 11856-11865.

[11] S. Metz, J. Kästner, A. A. Sokol, T. W. Keal, P. Sherwood, *Rev. Comput. Mol. Sci.*, **2014**, *4*, 101-110.

[12] H.-J. Werner, P. J. Knowles, G. Knizia, F. R. Manby, M. Schütz, *Rev. Comput. Mol. Sci.*, **2012**, *2*, 242-253.

Appendix I

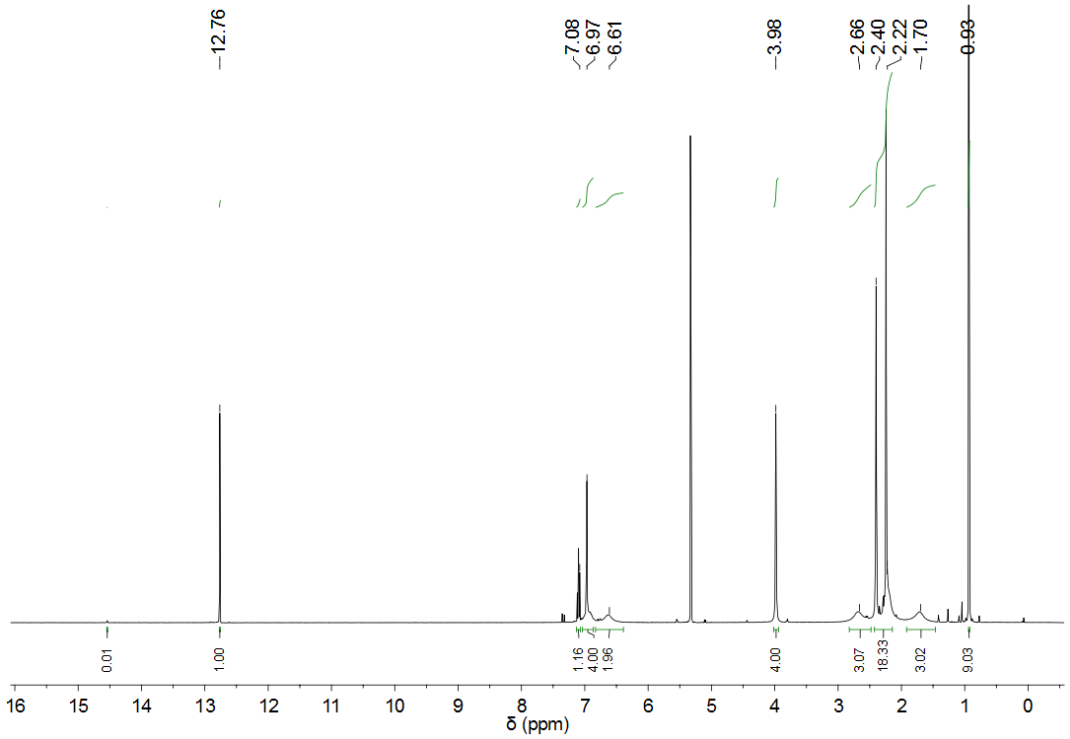


Figure S1. ^{1}H-NMR spectrum (400 MHz, CD_2Cl_2) of **3**.

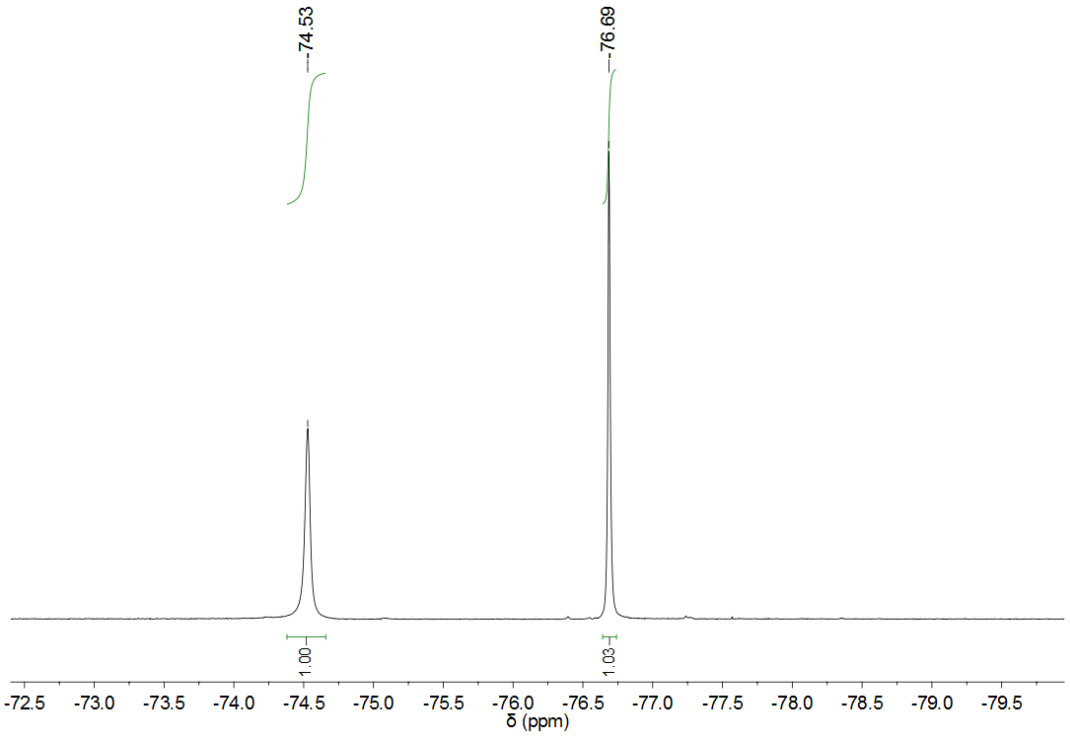


Figure S2. ^{19}F-NMR spectrum (376 MHz, CD_2Cl_2) of **3**.

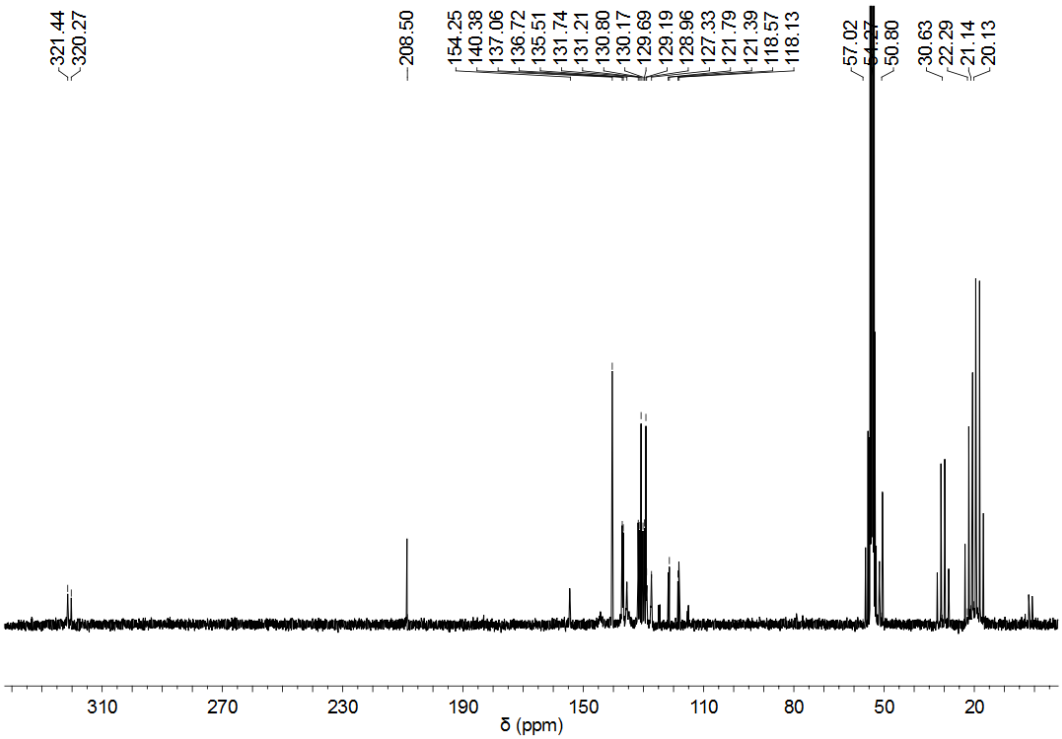


Figure S3. ^{13}C (gated decoupling) NMR spectrum (101 MHz, CD_2Cl_2) of **3**.

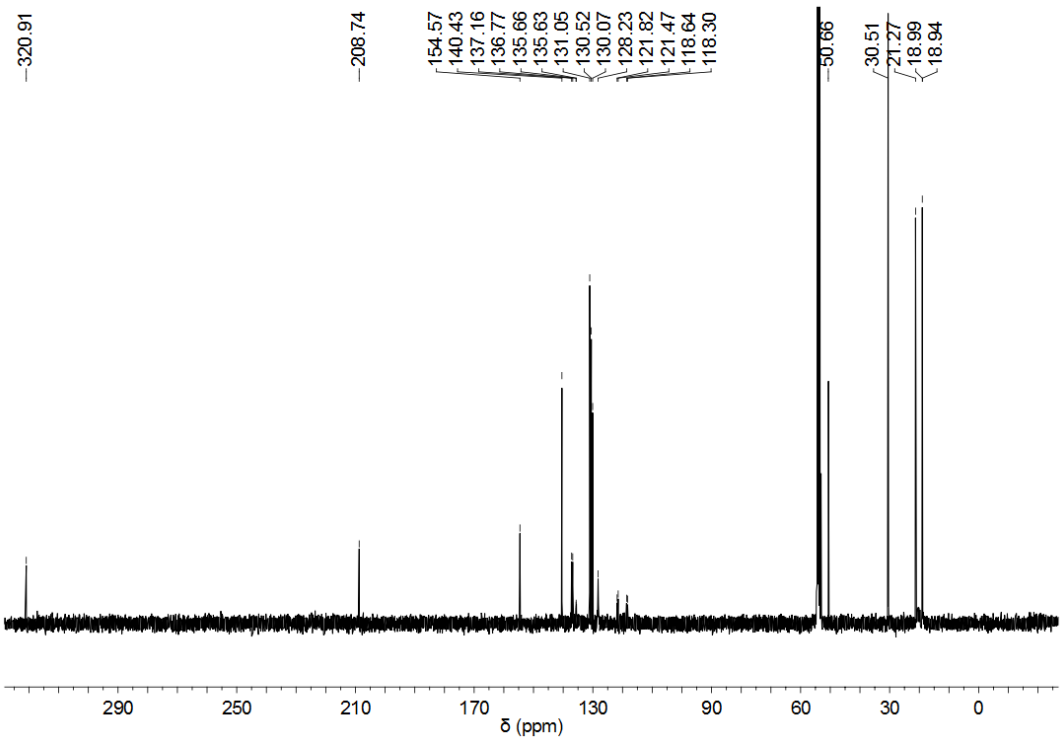


Figure S4. ^{13}C NMR spectrum (101 MHz, CD_2Cl_2) of **3**.

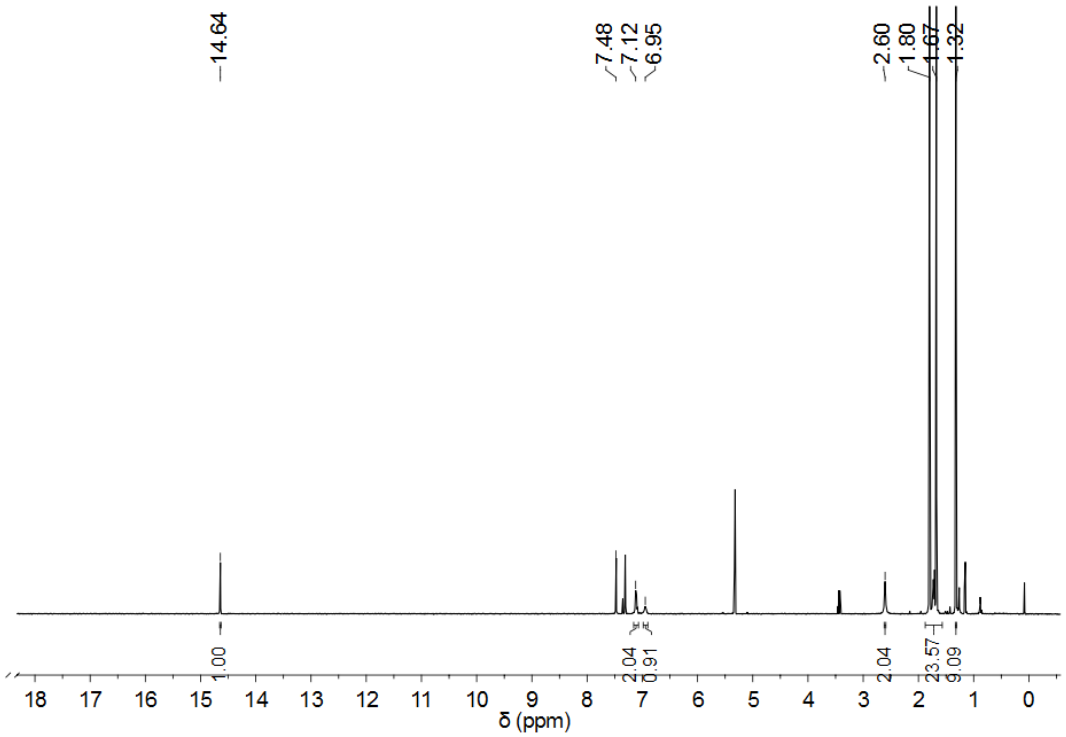


Figure S5. ^{1}H-NMR spectrum (400 MHz, CD_2Cl_2) of **4**.

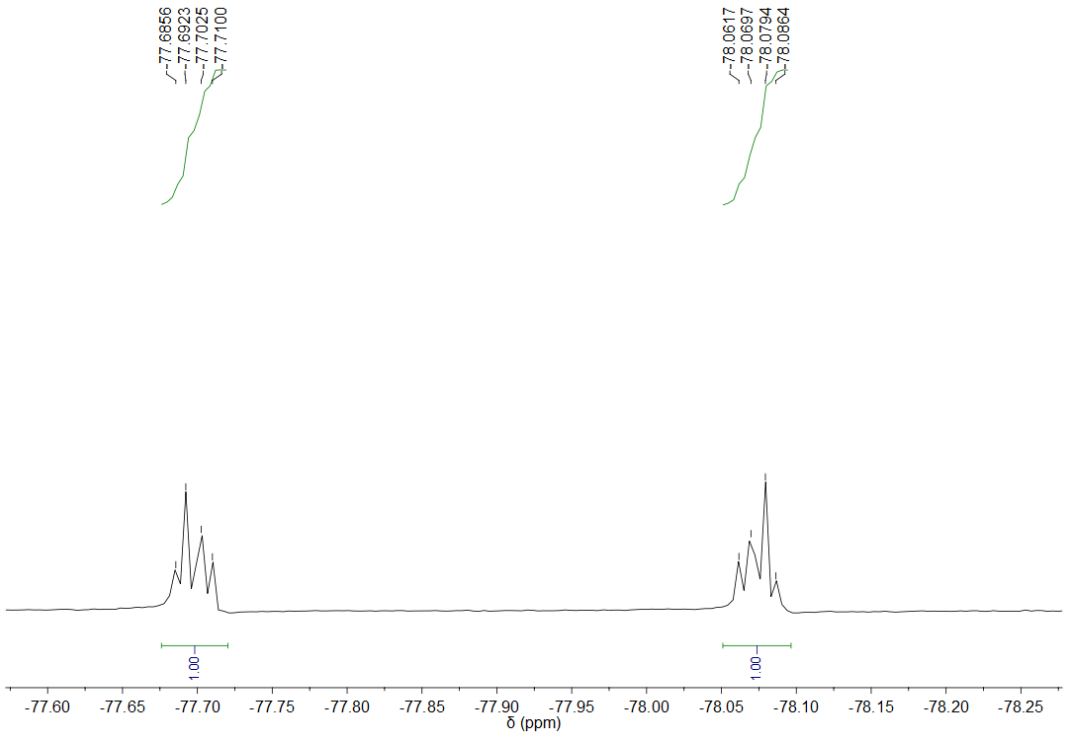


Figure S6. ^{19}F-NMR spectrum (376 MHz, CD_2Cl_2) of **4**.

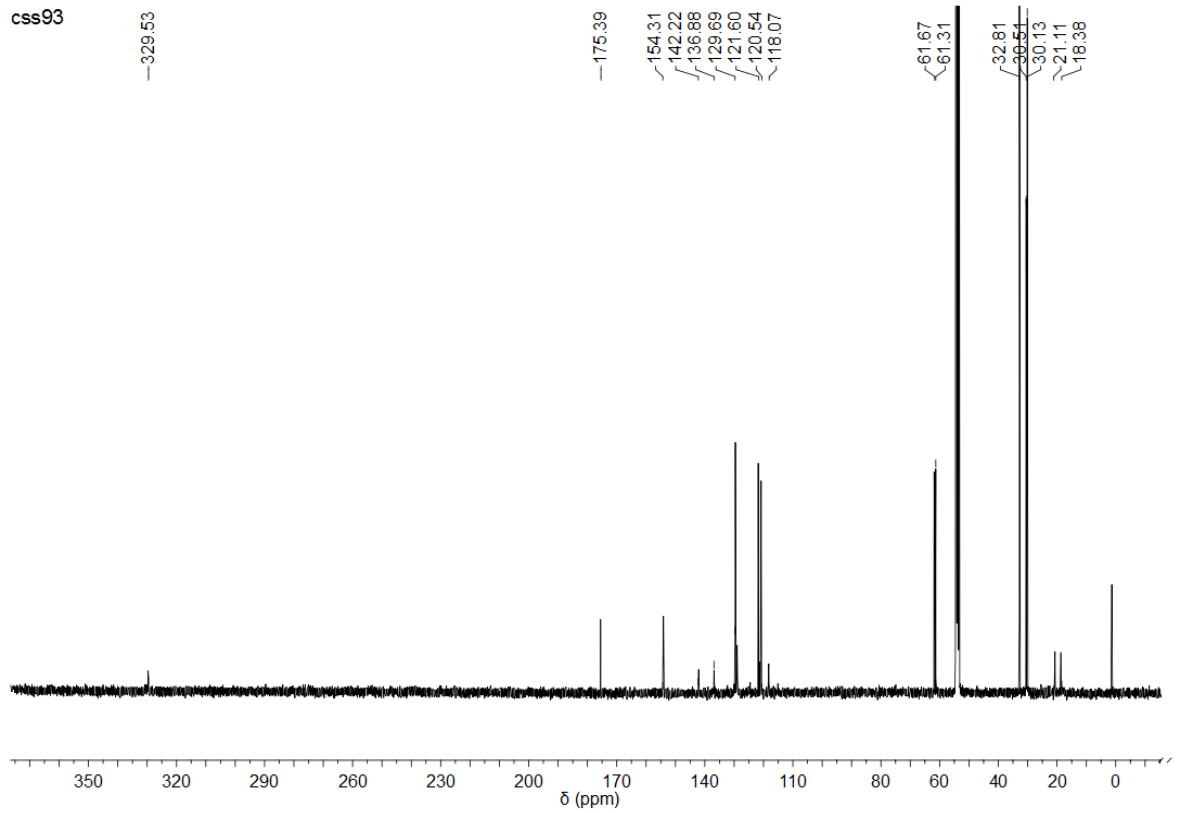


Figure S7. ^{13}C-NMR spectrum (101 MHz, CD_2Cl_2) of **4**.

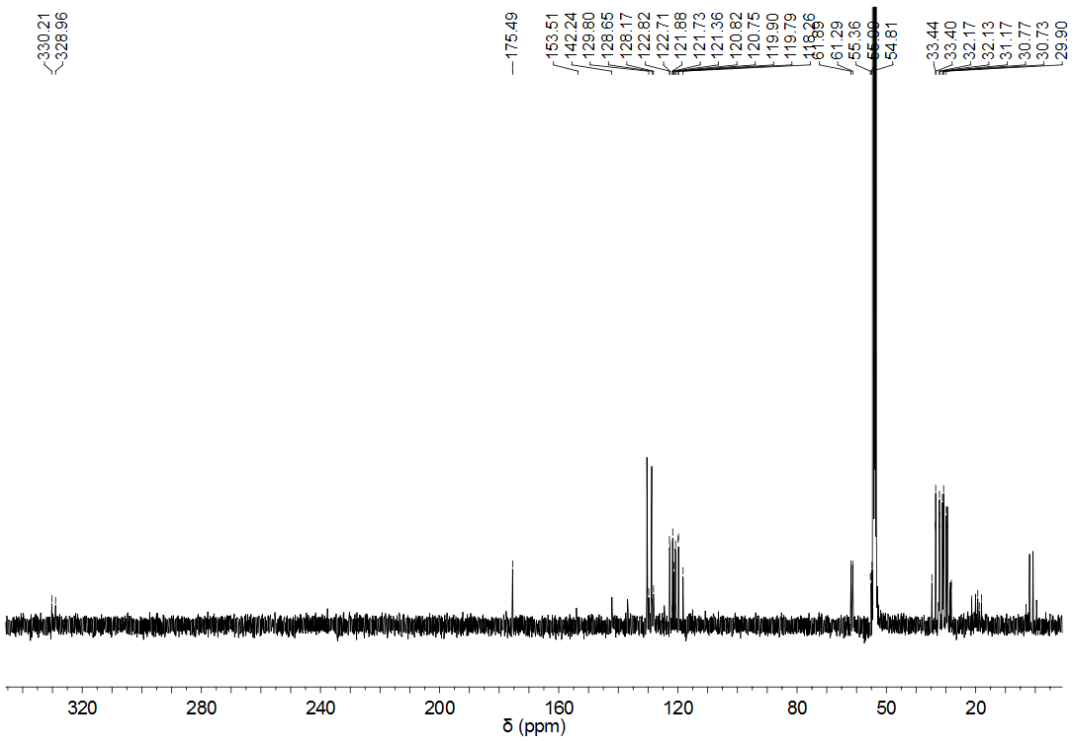


Figure S8. ^{13}C (gated decoupling) NMR spectrum (101 MHz, CD_2Cl_2) of **4**.

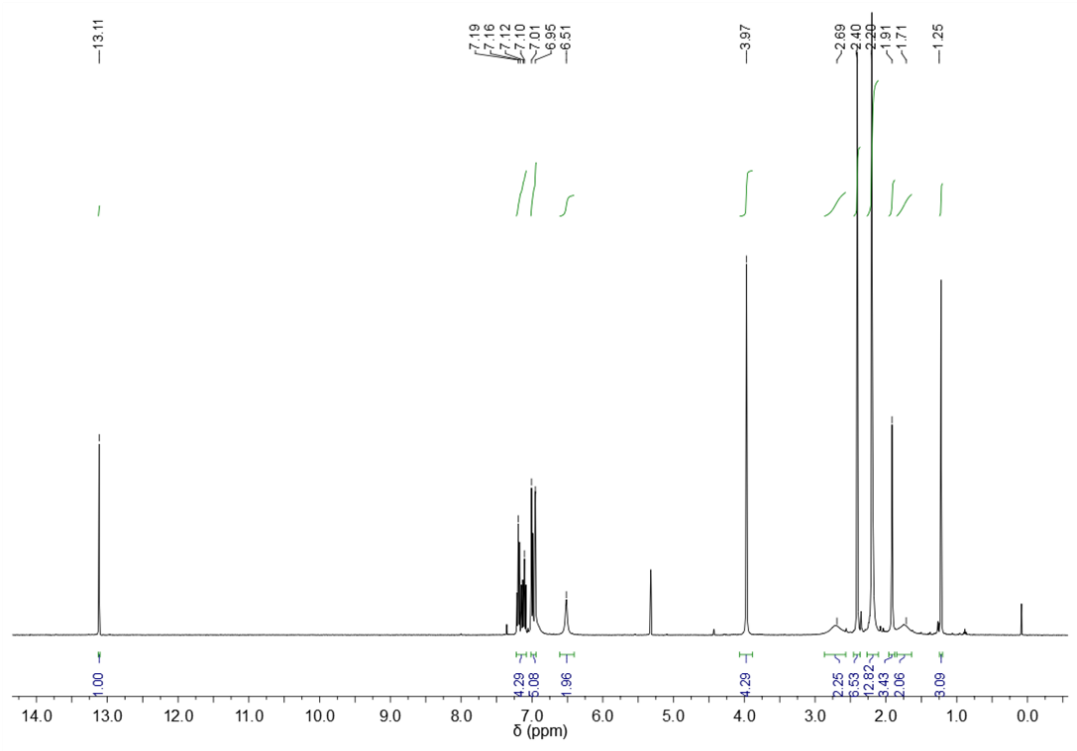


Figure S9. ^{1}H-NMR spectrum (400 MHz,CD_2Cl_2) of **5**.

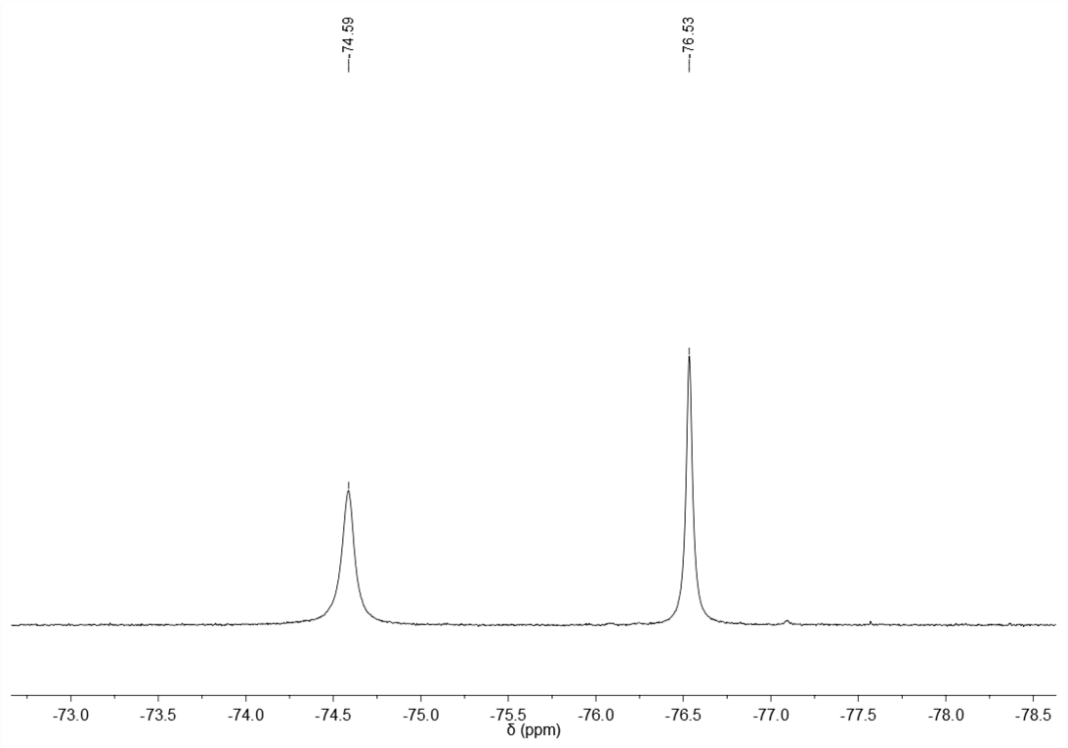


Figure S10. ^{19}F-NMR spectrum (376 MHz, CD_2Cl_2) of **5**.

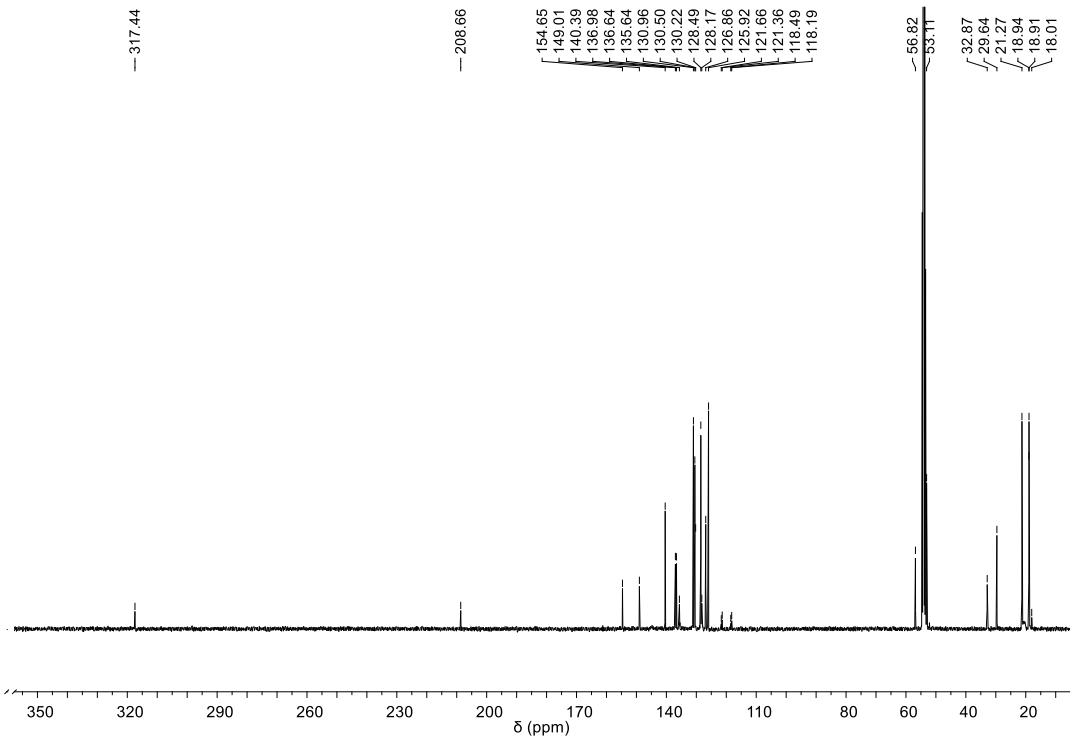


Figure S11. ^{13}C-NMR spectrum (101 MHz,CD_2Cl_2) of **5**.

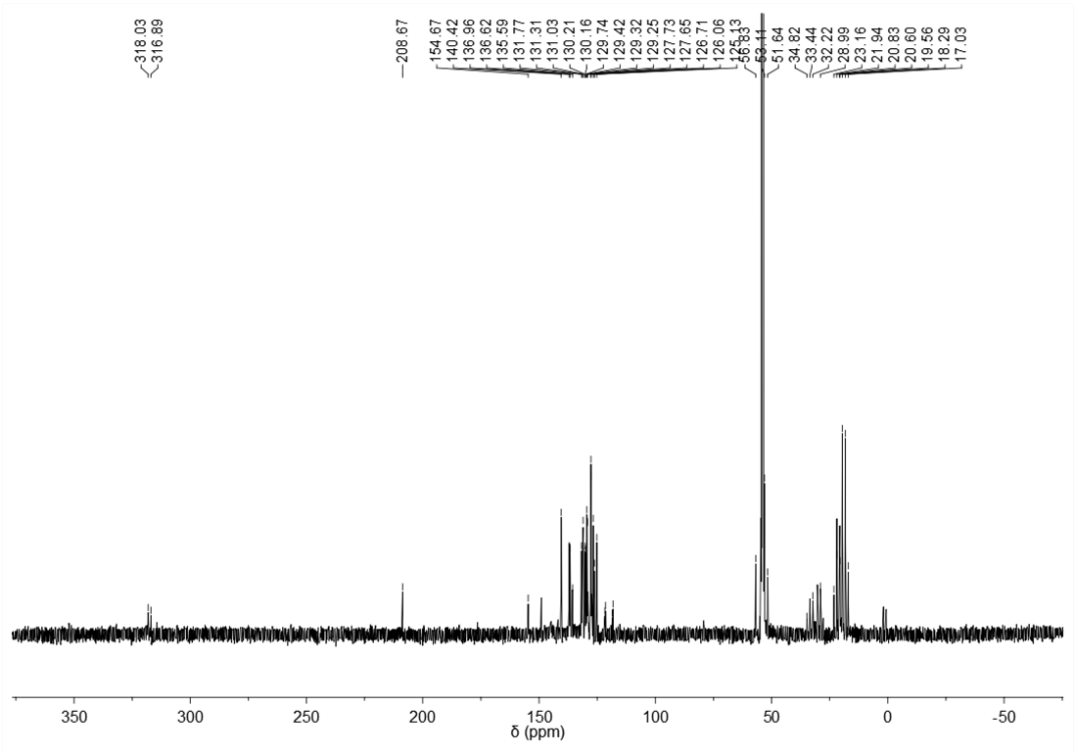


Figure S12. ^{13}C (gated decoupling) NMR spectrum (101 MHz,CD_2Cl_2) of **5**.

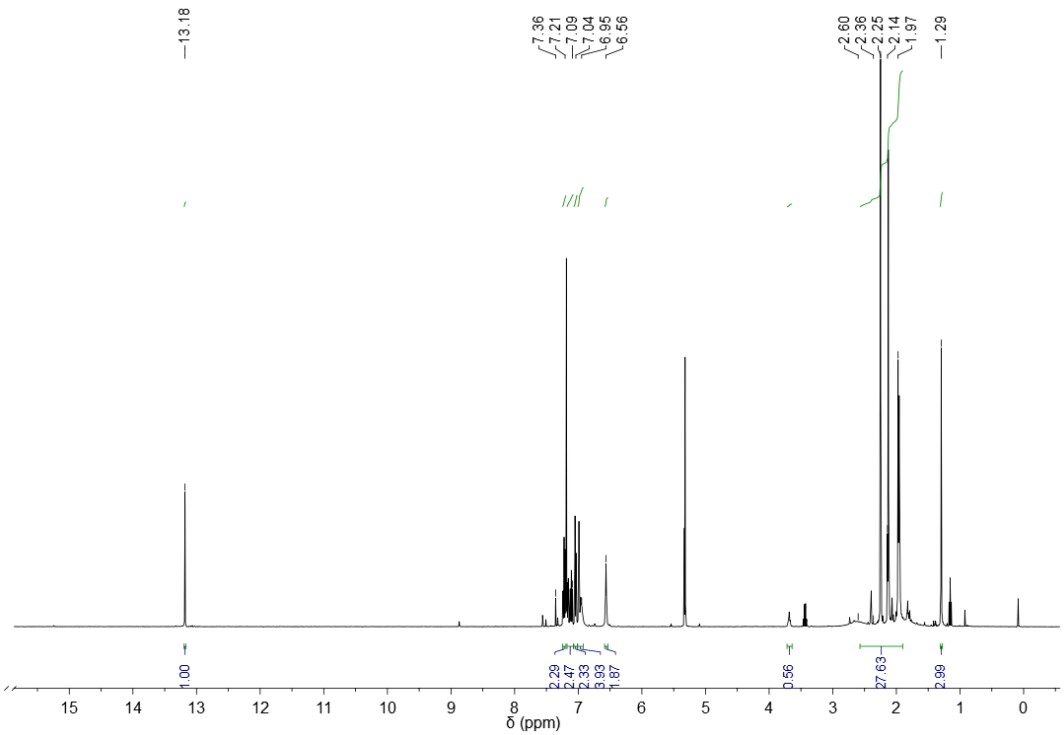


Figure S13. ^{1}H-NMR spectrum (400 MHz,CD_2Cl_2) of **6**.

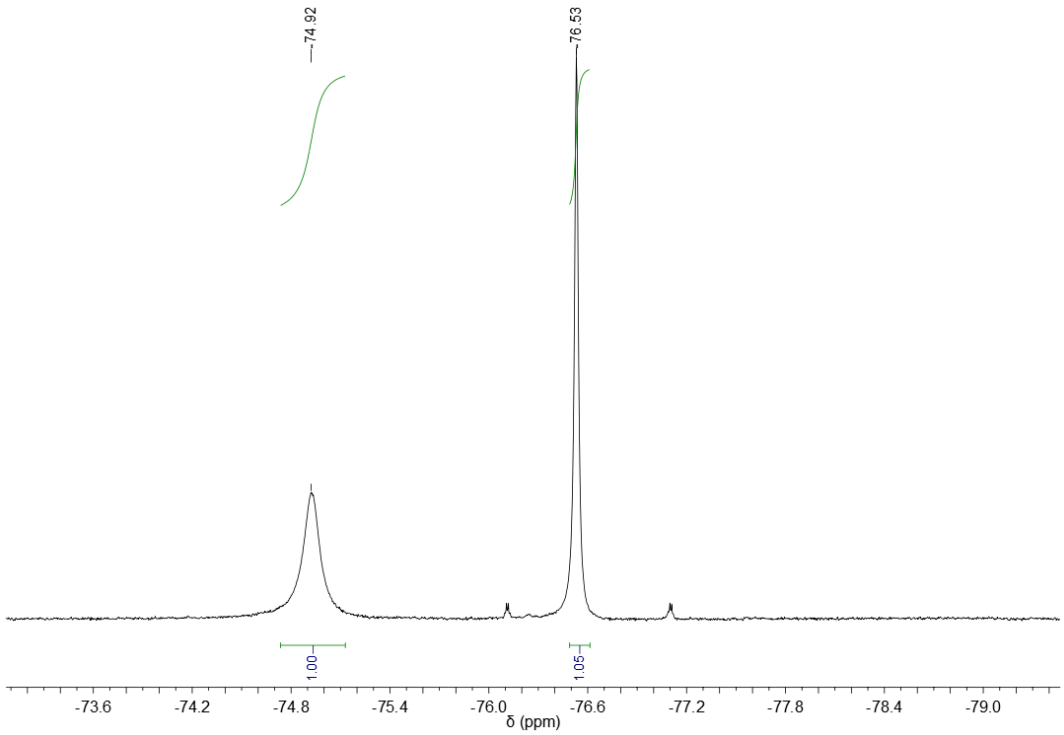


Figure S14. ^{19}F-NMR spectrum (376 MHz, CD_2Cl_2) of **6**.

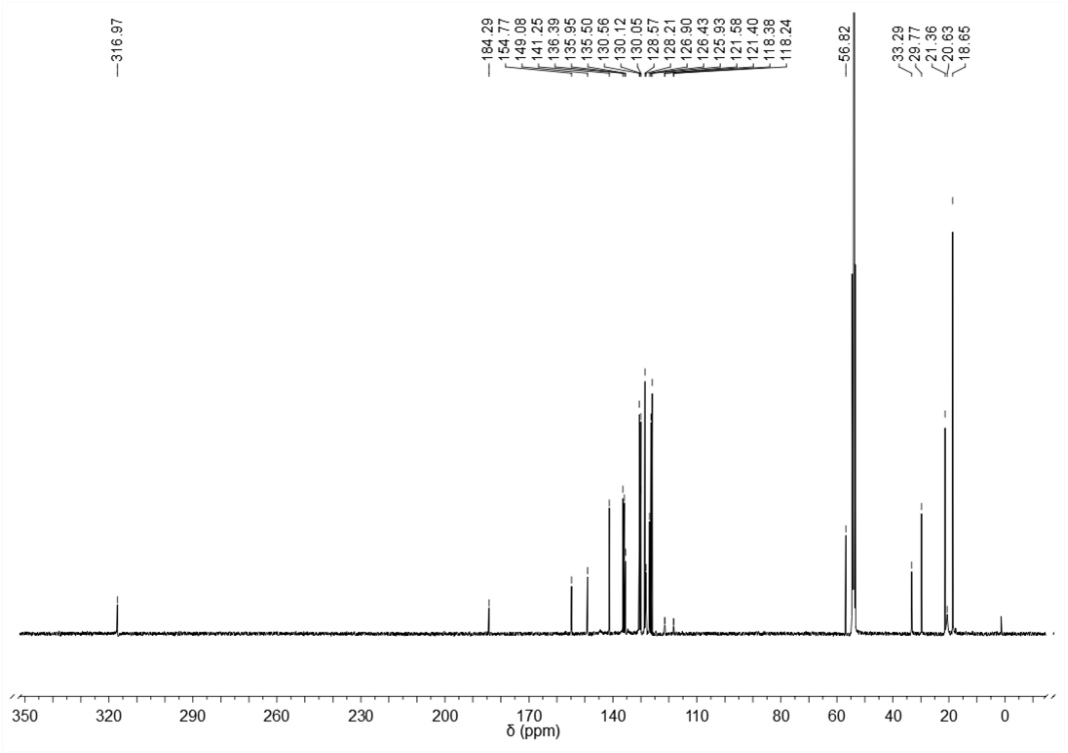


Figure S15. ^{13}C-NMR spectrum (101 MHz,CD_2Cl_2) of **6**.

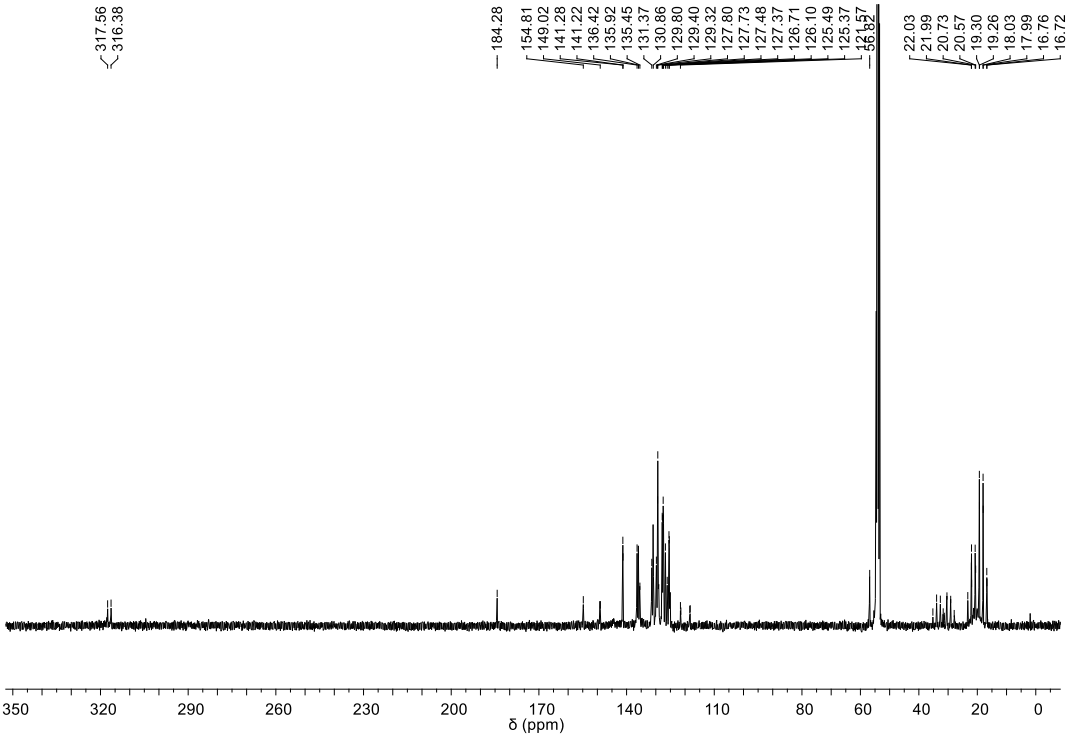


Figure S16. ^{13}C (gated decoupling) NMR spectrum (101 MHz,CD_2Cl_2) of **6**.

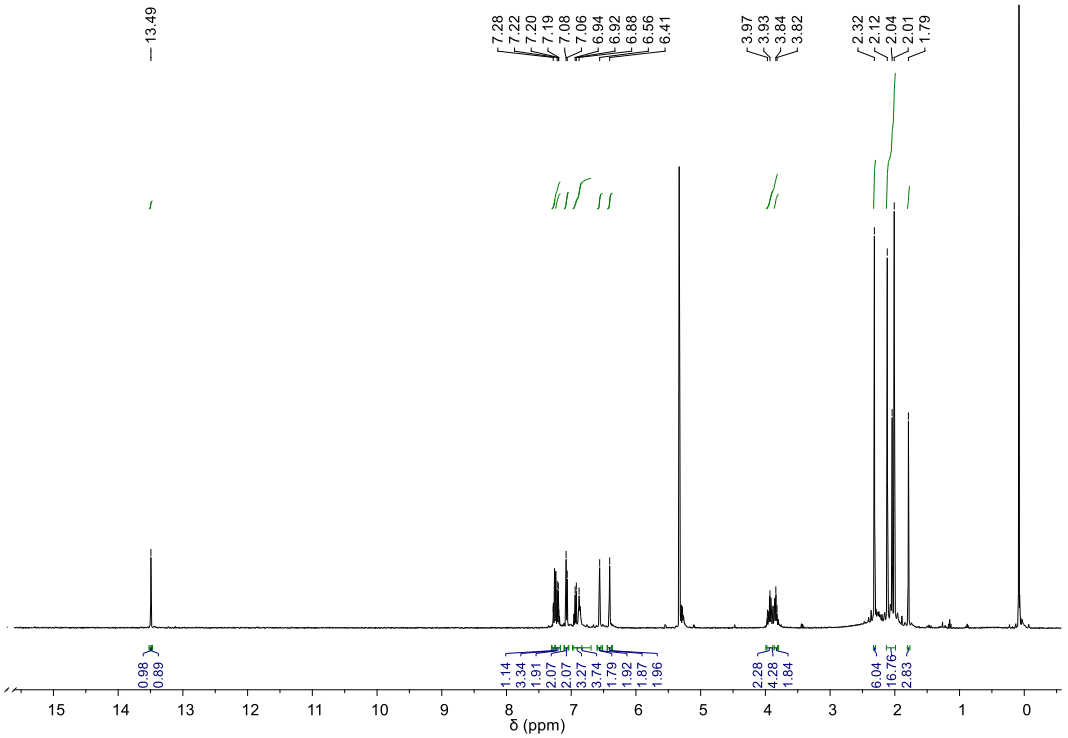


Figure S17. ^{1}H-NMR spectrum (400 MHz, CD_2Cl_2) of **7**.

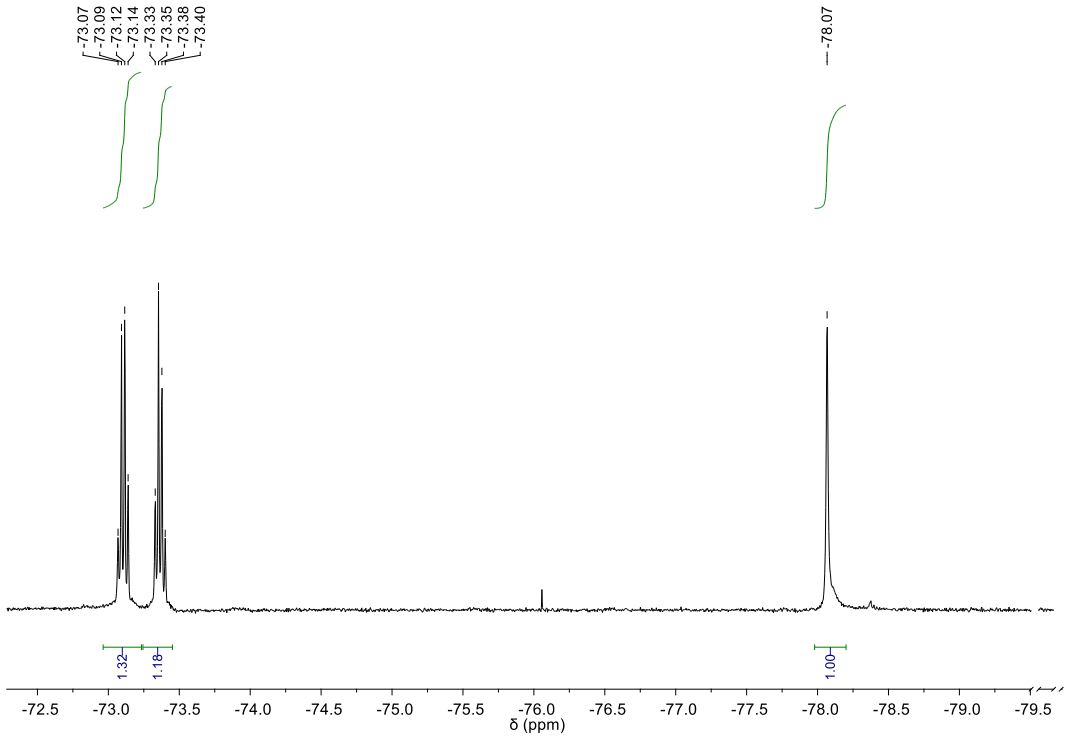


Figure S18. ^{19}F-NMR spectrum (376 MHz, CD_2Cl_2) of **7**.

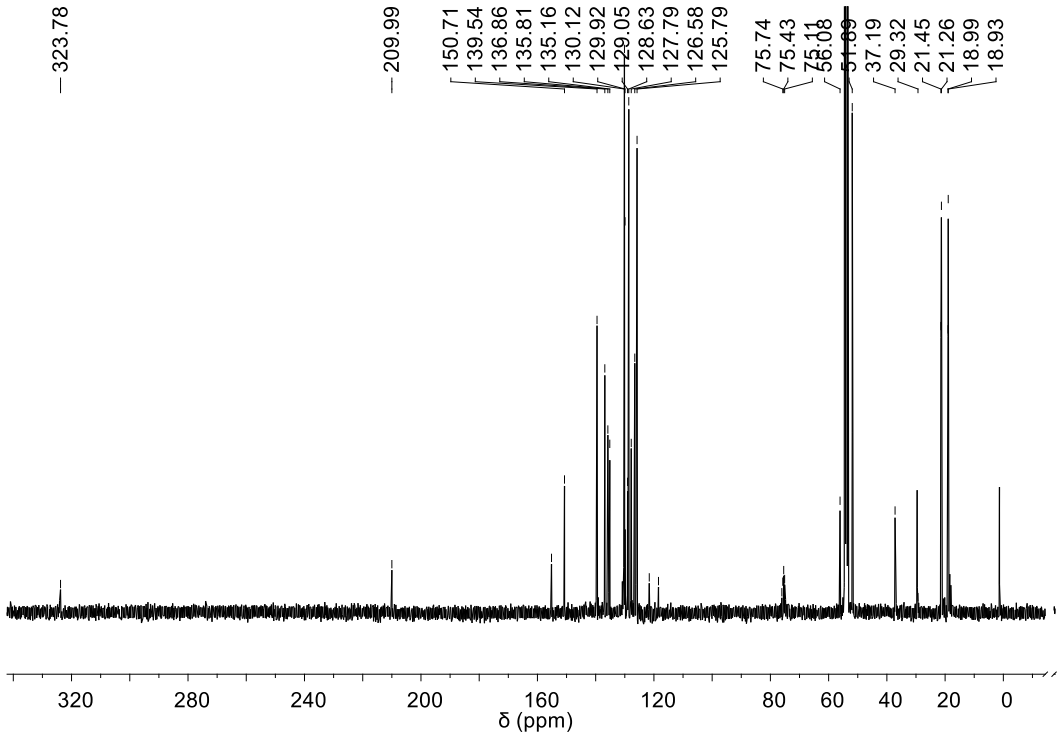


Figure S19. ^{13}C-NMR spectrum (101 MHz,CD_2Cl_2) of **7**.

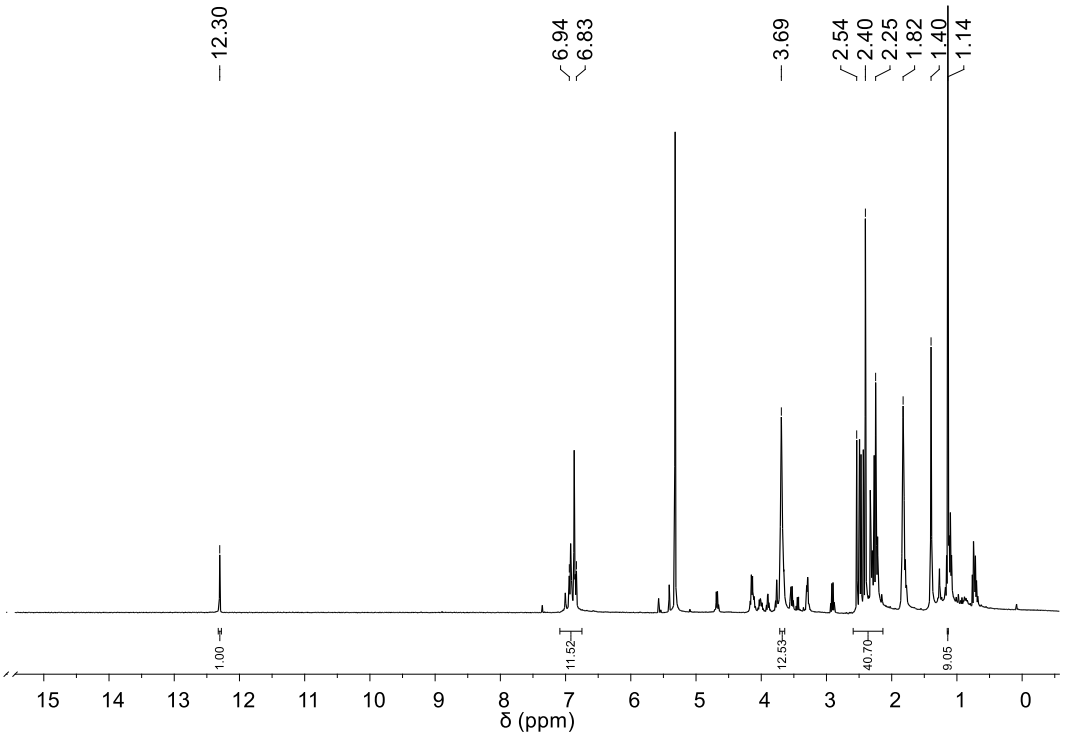


Figure S20. ^{1}H NMR spectrum (400 MHz, CD_2Cl_2) of **9**.

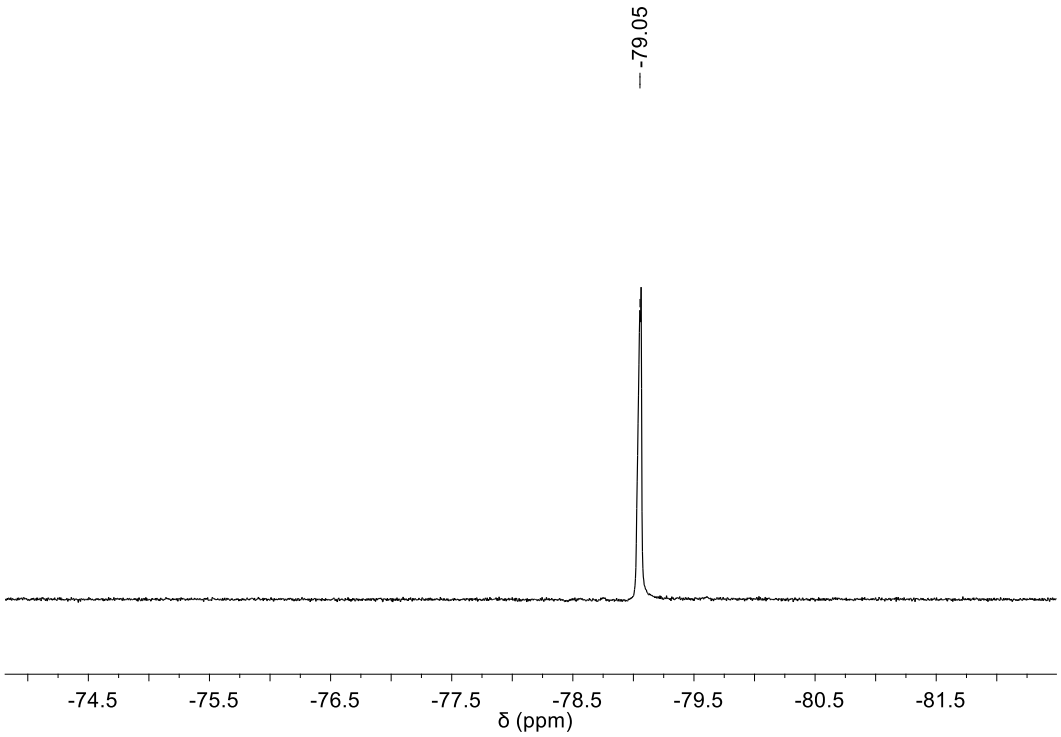


Figure S21. ^{19}F NMR spectrum (376 MHz, CD_2Cl_2) of **9**.

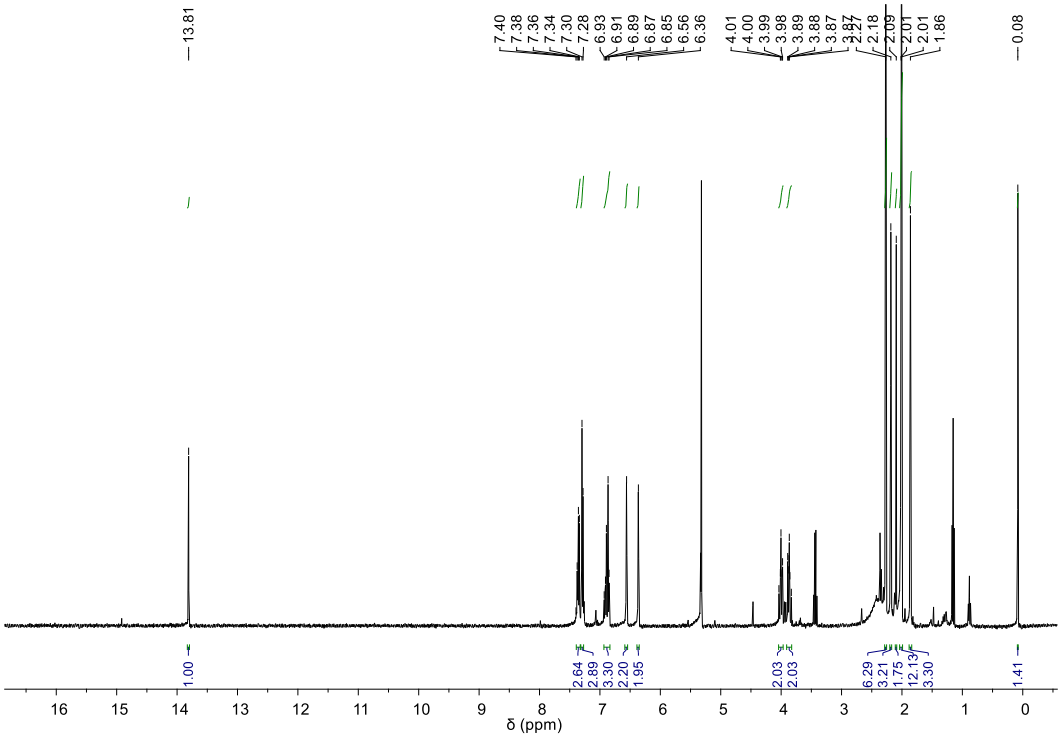


Figure S22. ^{1}H-NMR spectrum (400 MHz,CD_2Cl_2) of **10**.

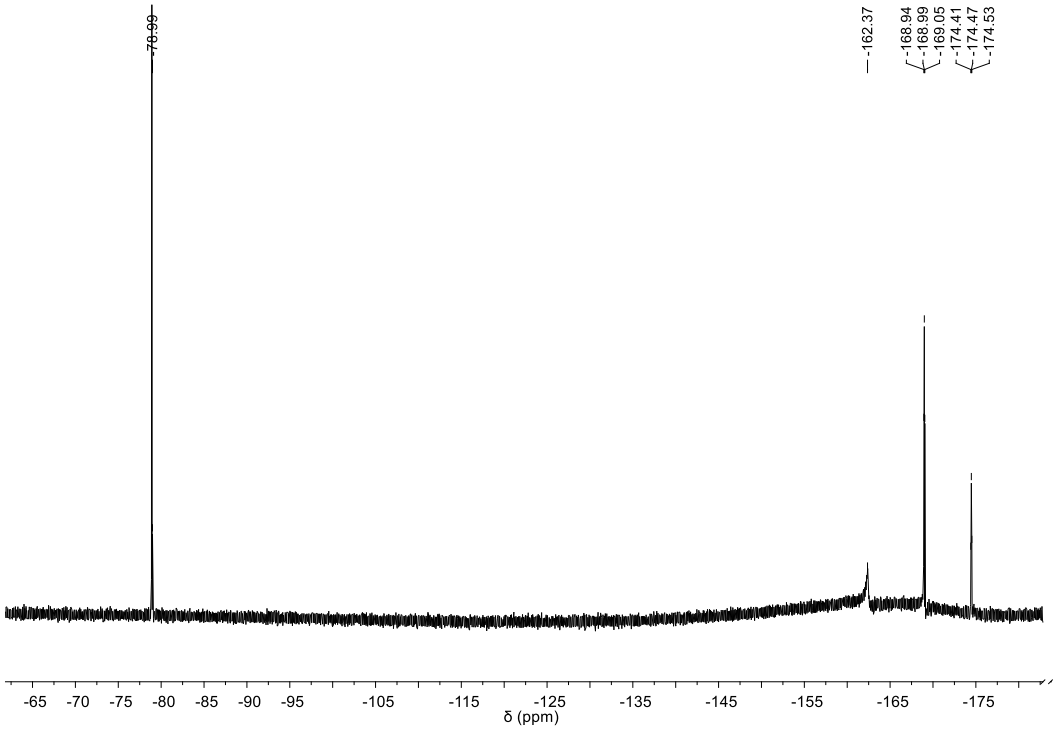


Figure S23. ^{19}F-NMR spectrum (376 MHz, CD_2Cl_2) of **10**.

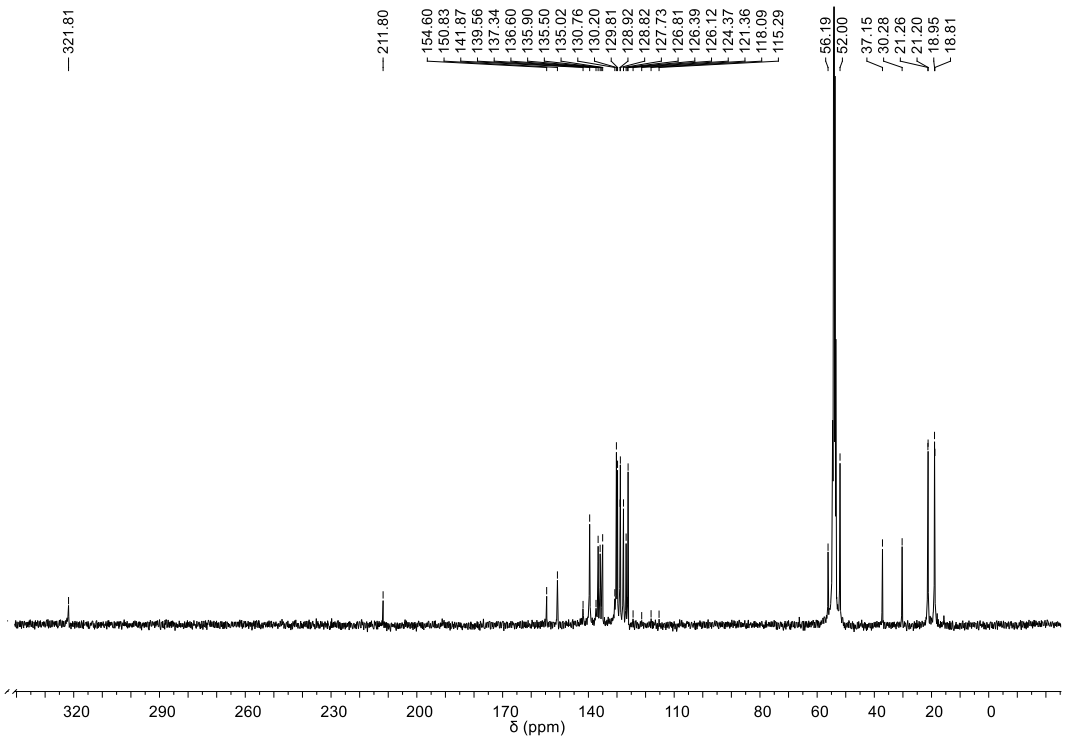


Figure S24. ^{13}C-NMR spectrum (101 MHz, CD_2Cl_2) of **10**.

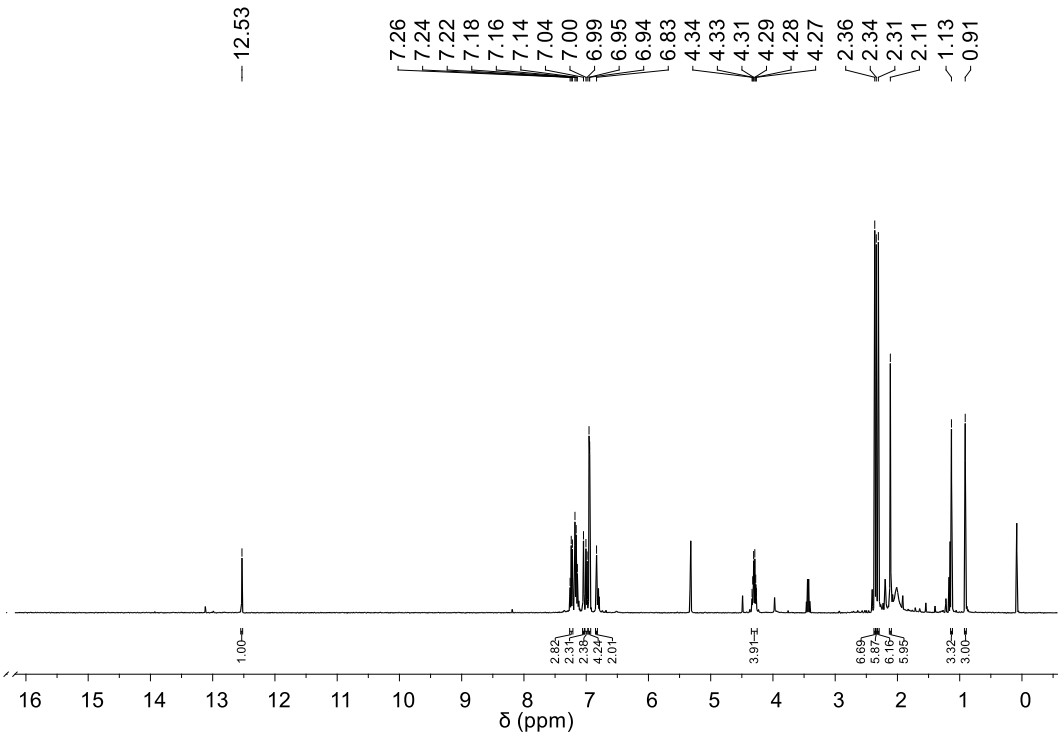


Figure S25. ^{1}H-NMR spectrum (400 MHz, CD_2Cl_2) of **11**.

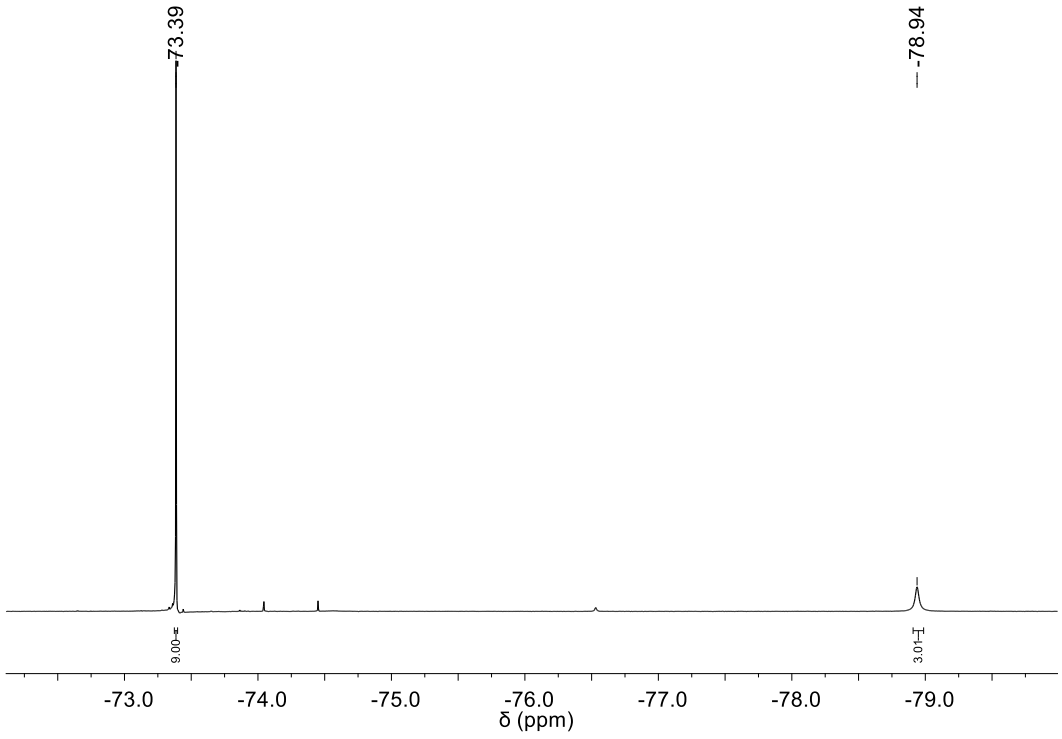


Figure S26. ^{19}F-NMR spectrum (376 MHz, CD_2Cl_2) of **11**.

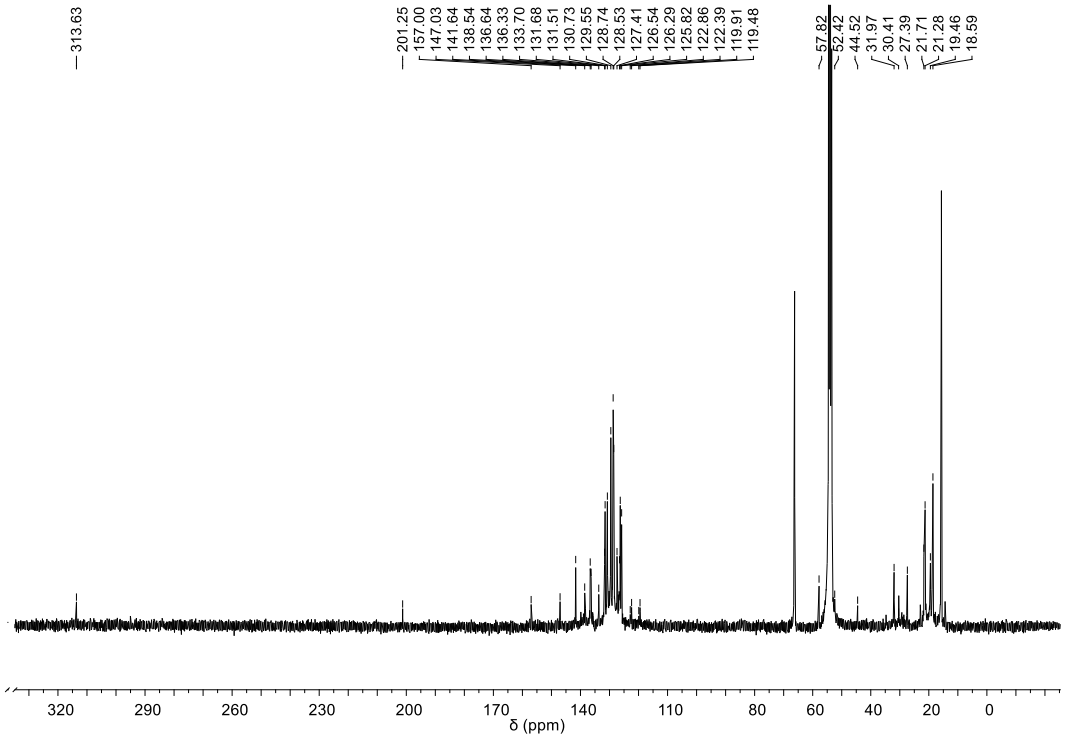


Figure S27. ^{13}C-NMR spectrum (101 MHz, CD_2Cl_2) of **11**.

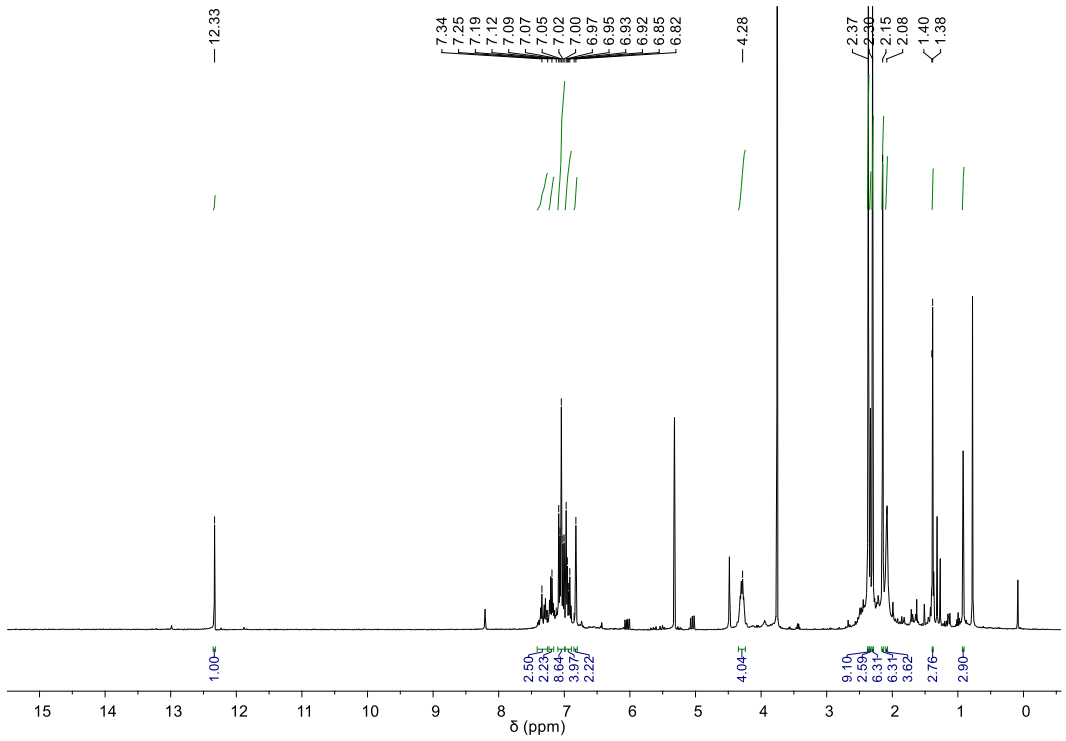


Figure S28. ^{1}H-NMR spectrum (400 MHz, CD_2Cl_2) of **12**.

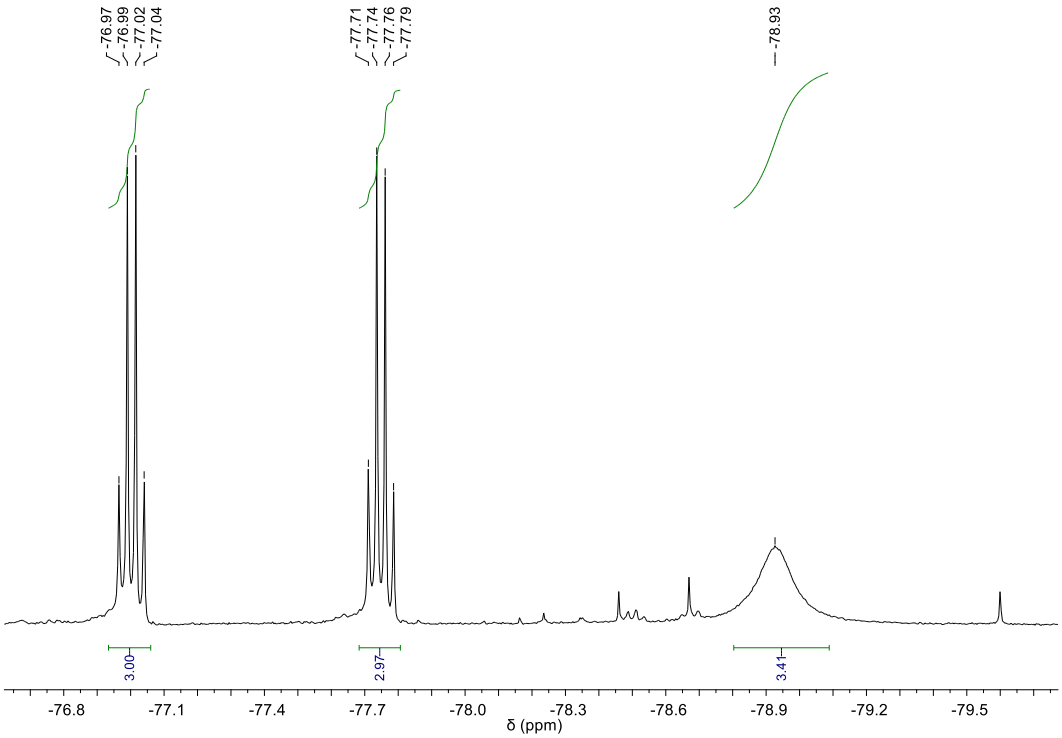


Figure S29. ^{19}F-NMR spectrum (376 MHz, CD_2Cl_2) of **12**.

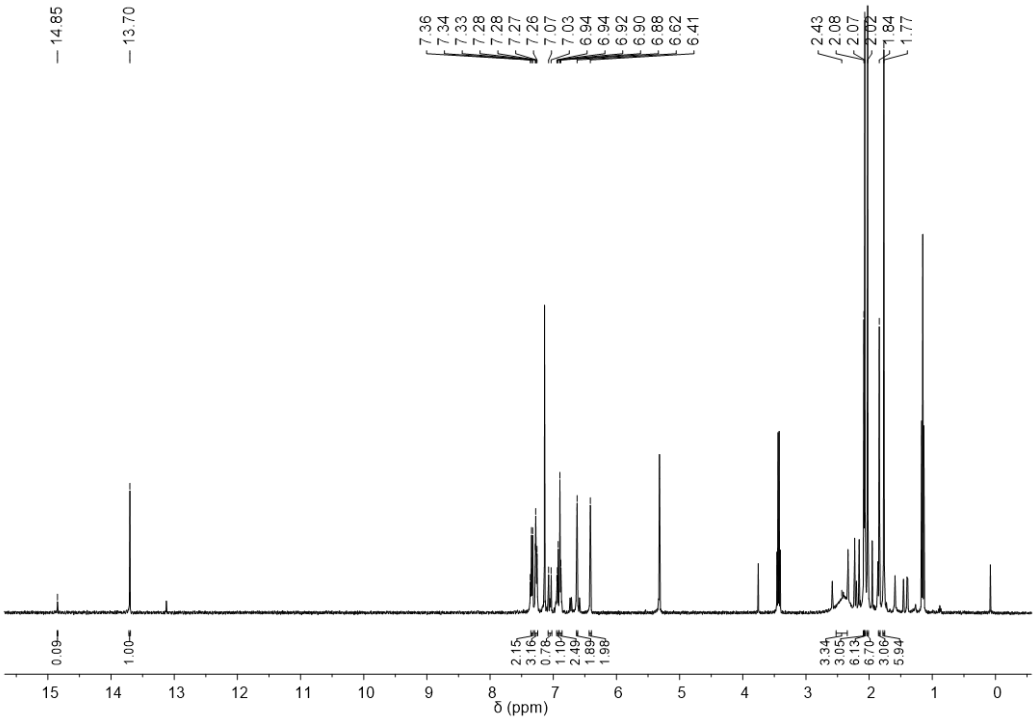


Figure S30. ^{1}H-NMR spectrum (400 MHz, CD_2Cl_2) of **13**.

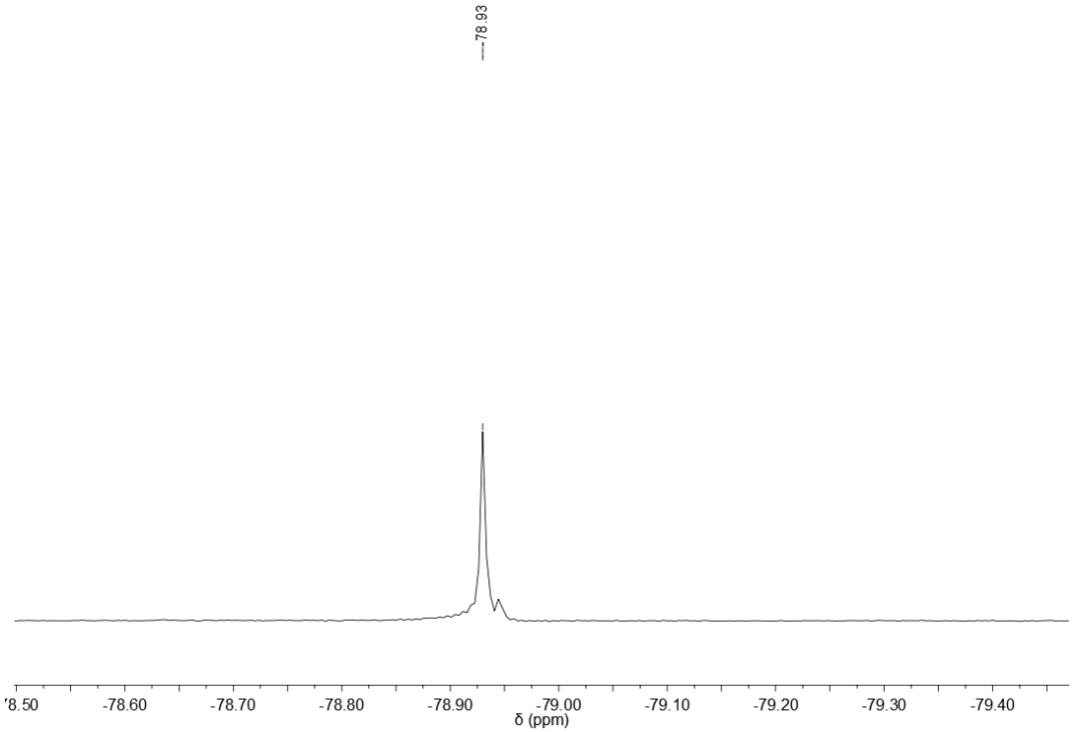


Figure S31. ^{19}F-NMR spectrum (376 MHz, CD_2Cl_2) of **13**.

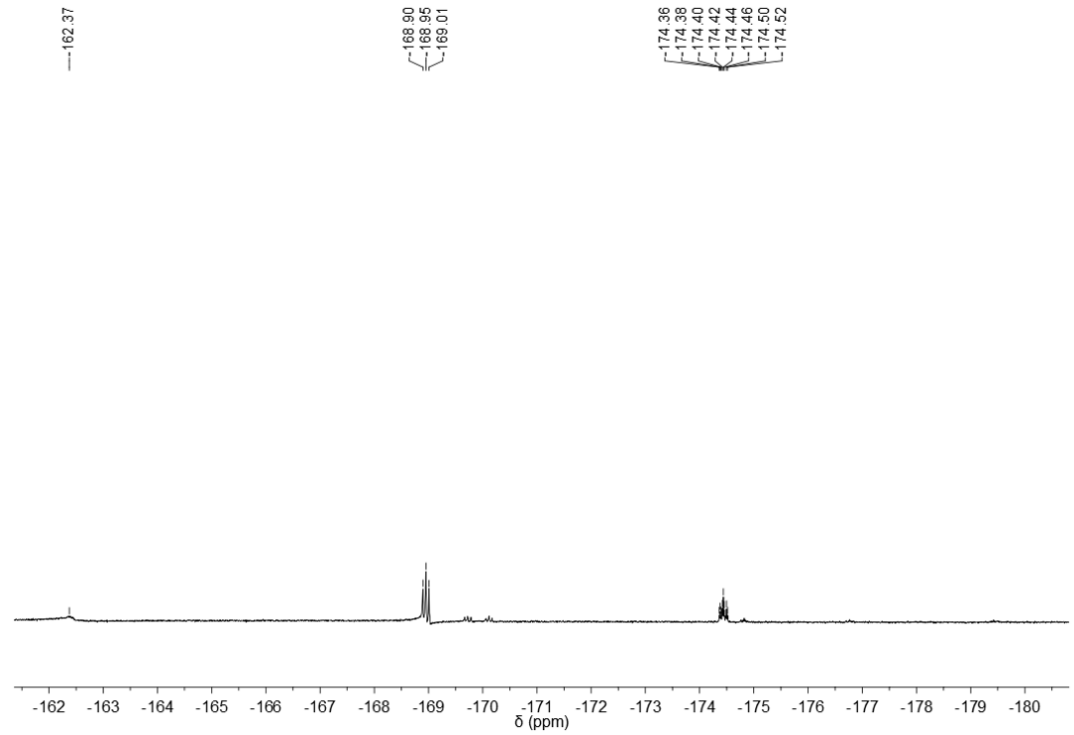


Figure S32. ^{19}F-NMR spectrum (376 MHz, CD_2Cl_2) of **13**.

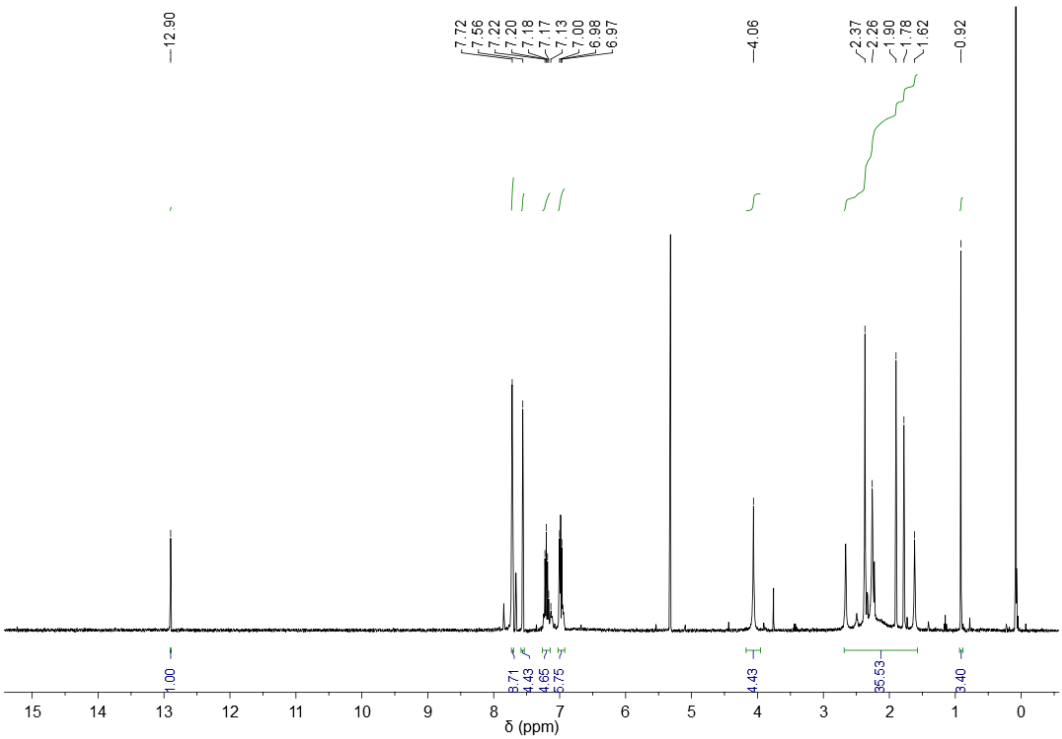


Figure S33. ^{1}H-NMR spectrum (400 MHz, CD_2Cl_2) of **14**.

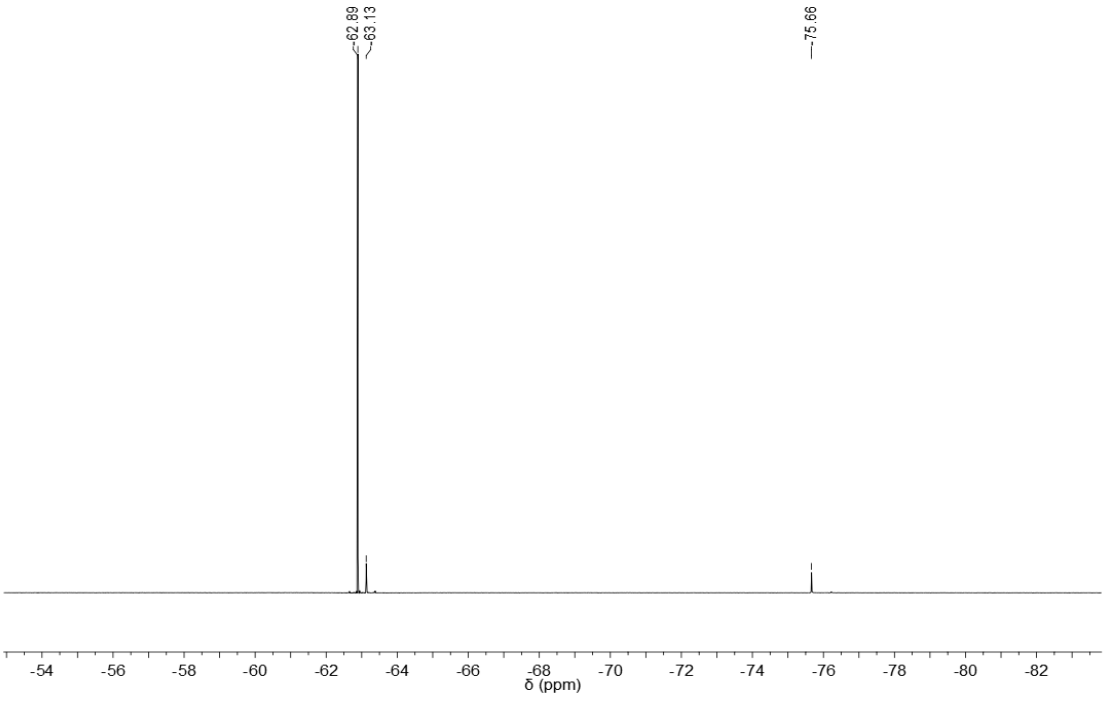


Figure S34. ^{19}F-NMR spectrum (376 MHz, CD_2Cl_2) of **14**.

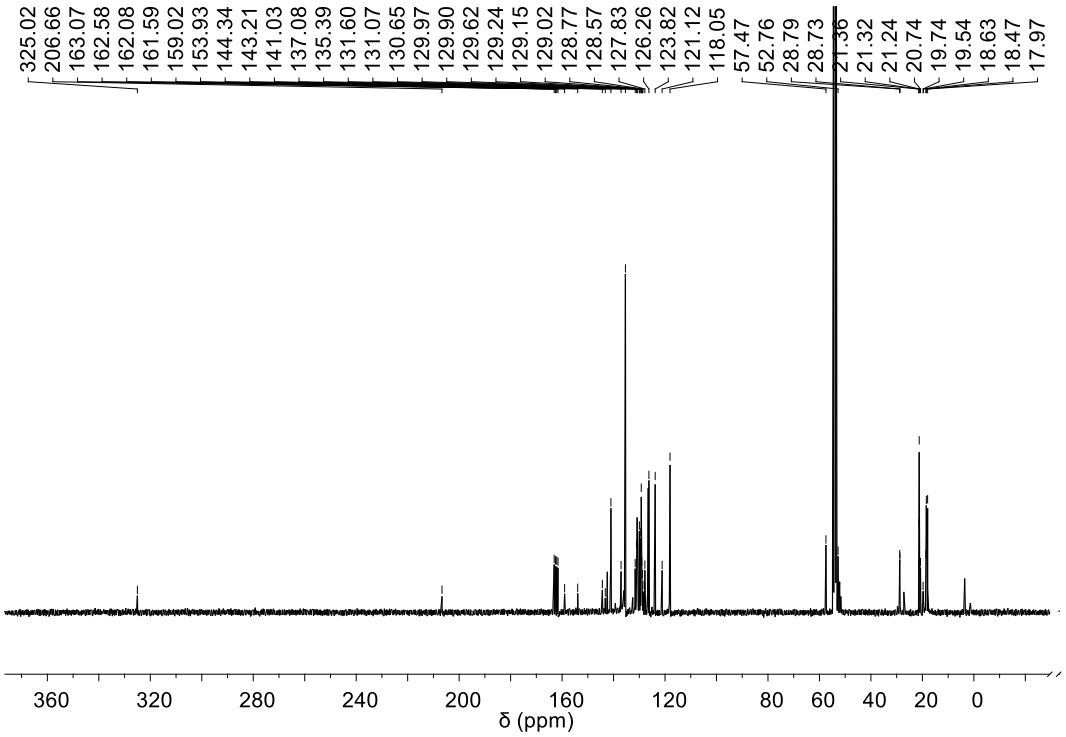


Figure S35.[13]C-NMR spectrum (101 MHz, CD_2Cl_2) of **14**.

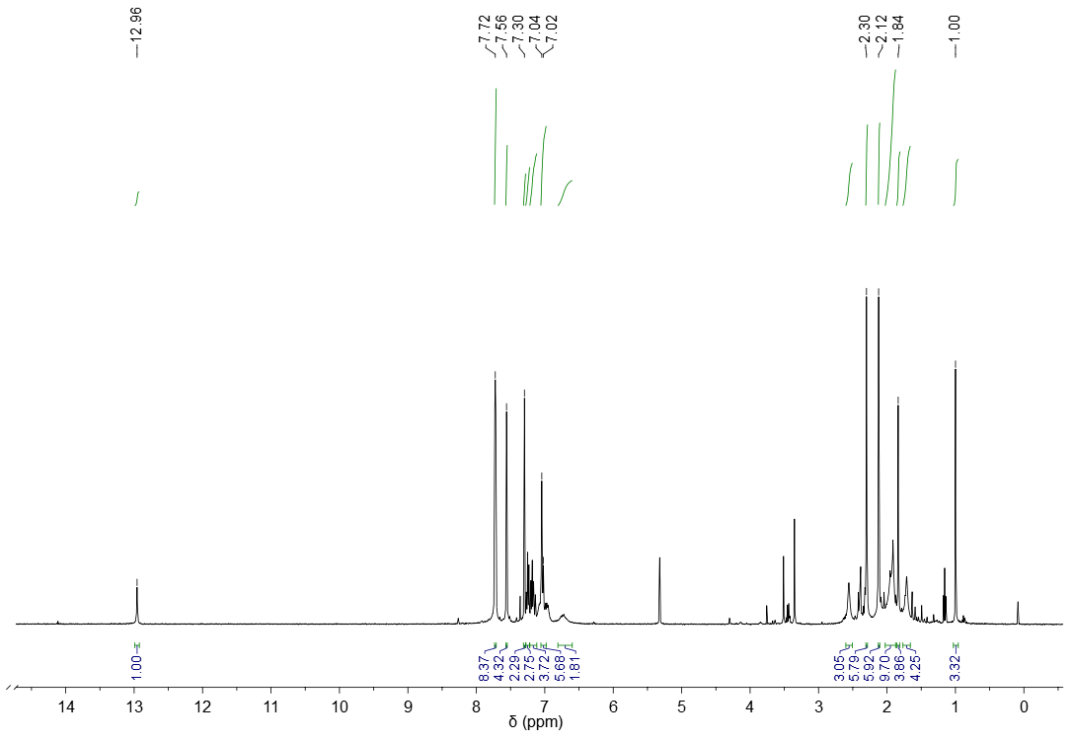


Figure S36. [1]H-NMR spectrum (400 MHz, CD_2Cl_2) of **15**.

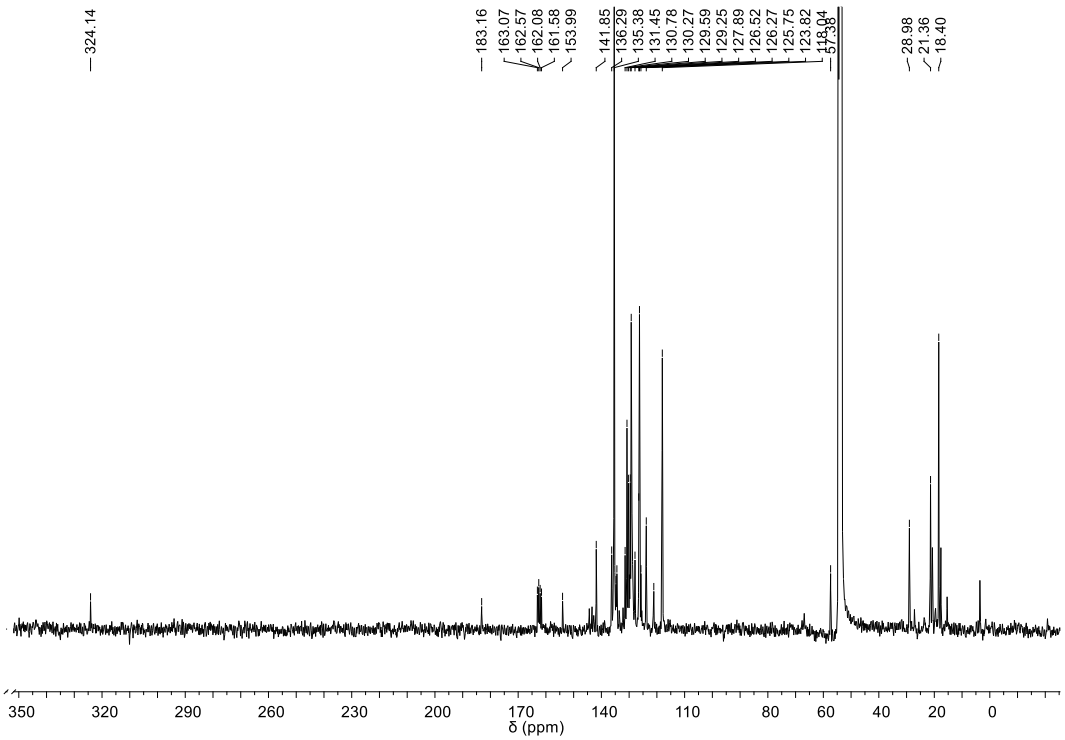


Figure S37. ^{13}C-NMR spectrum (101 MHz, CD_2Cl_2) of **15**.

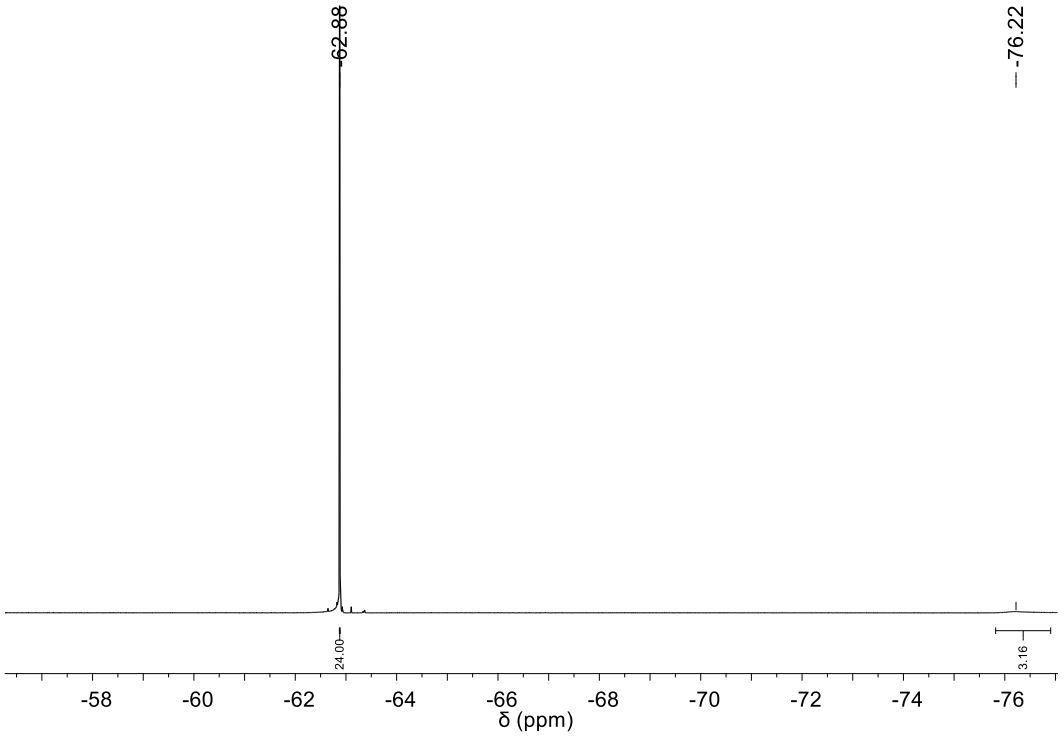


Figure S38. ^{19}F-NMR spectrum (376 MHz, CD_2Cl_2) of **15**.

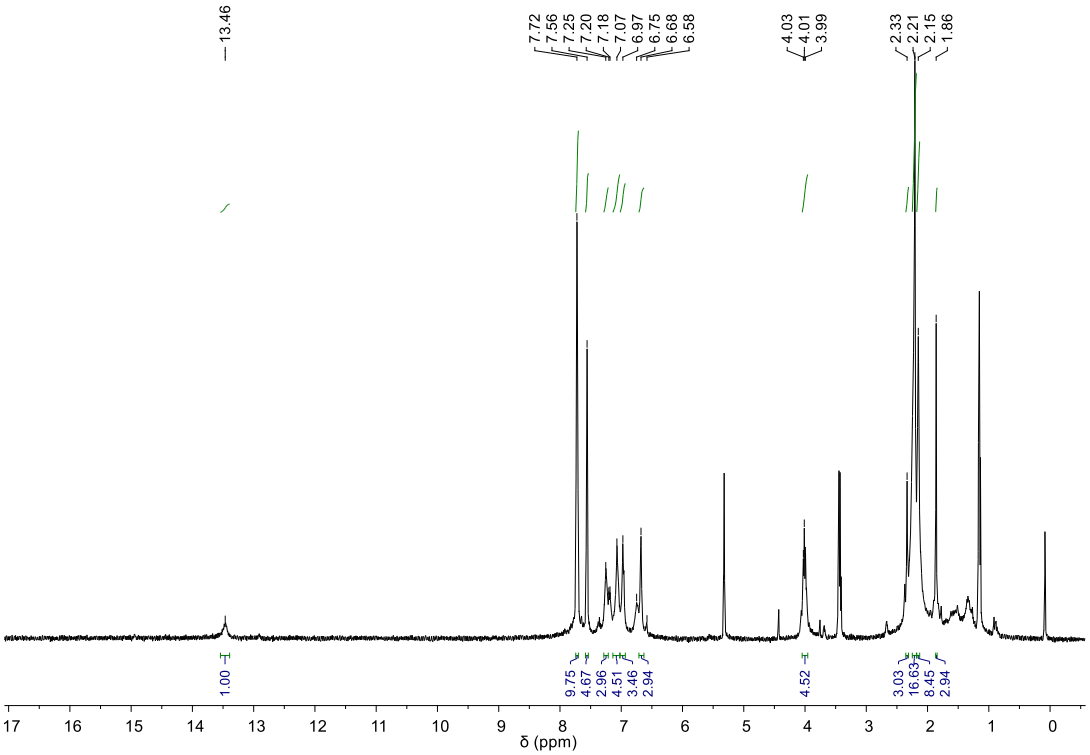


Figure S39. ^{1}H-NMR spectrum (400 MHz, CD_2Cl_2) of **16**.

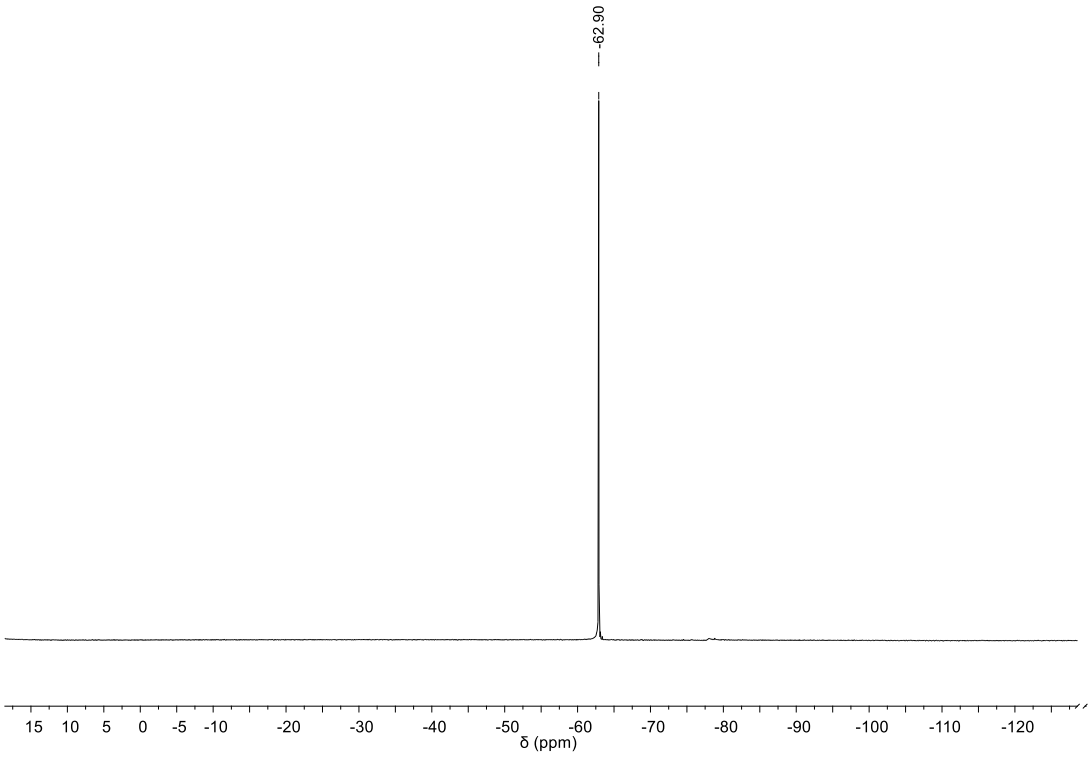


Figure S40. ^{19}F-NMR spectrum (376 MHz, CD_2Cl_2) of **16**.

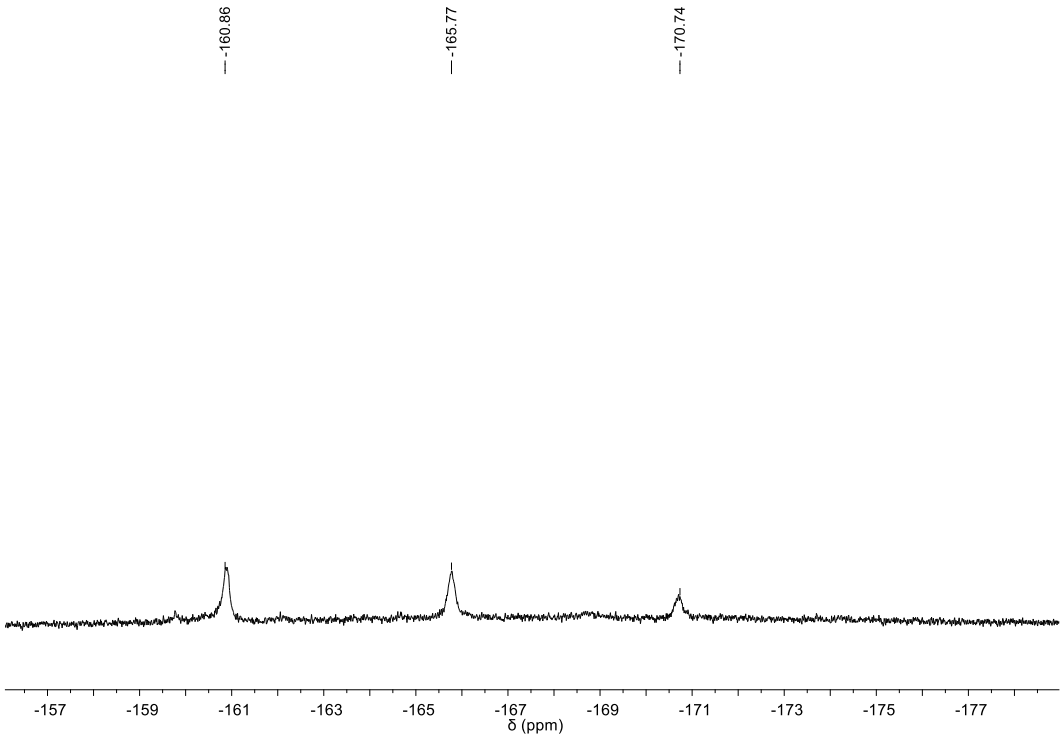


Figure S41. ^{19}F-NMR spectrum (376 MHz, CD_2Cl_2) of **16**.

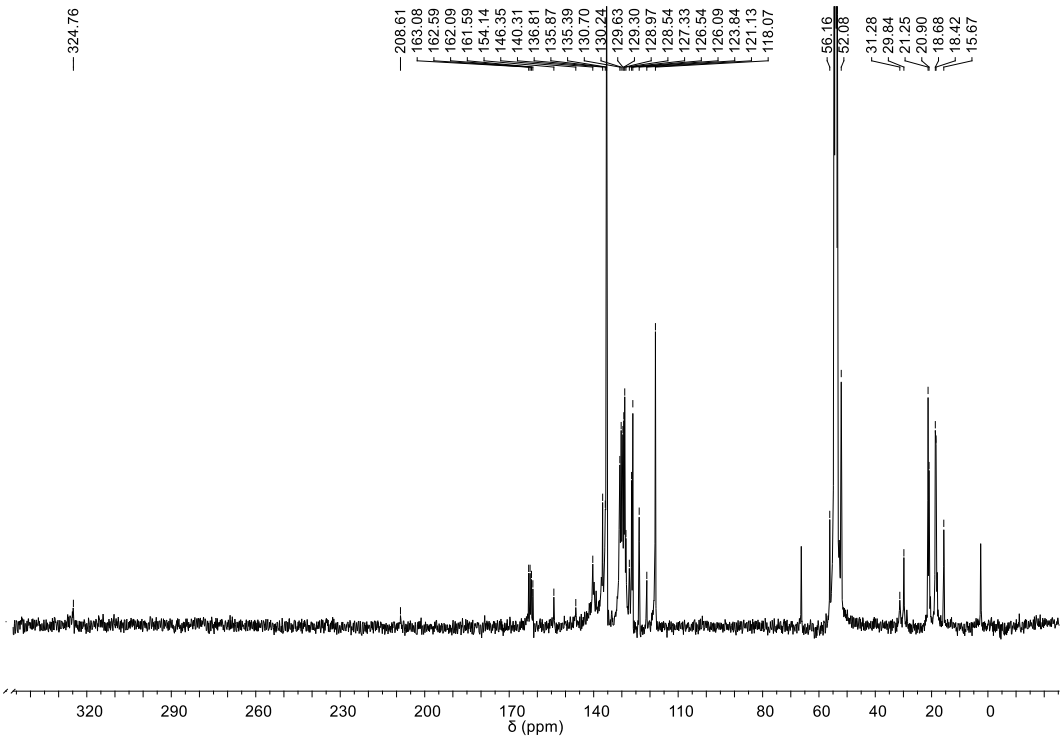


Figure S42. ^{13}C-NMR spectrum (101 MHz, CD_2Cl_2) of **16**.

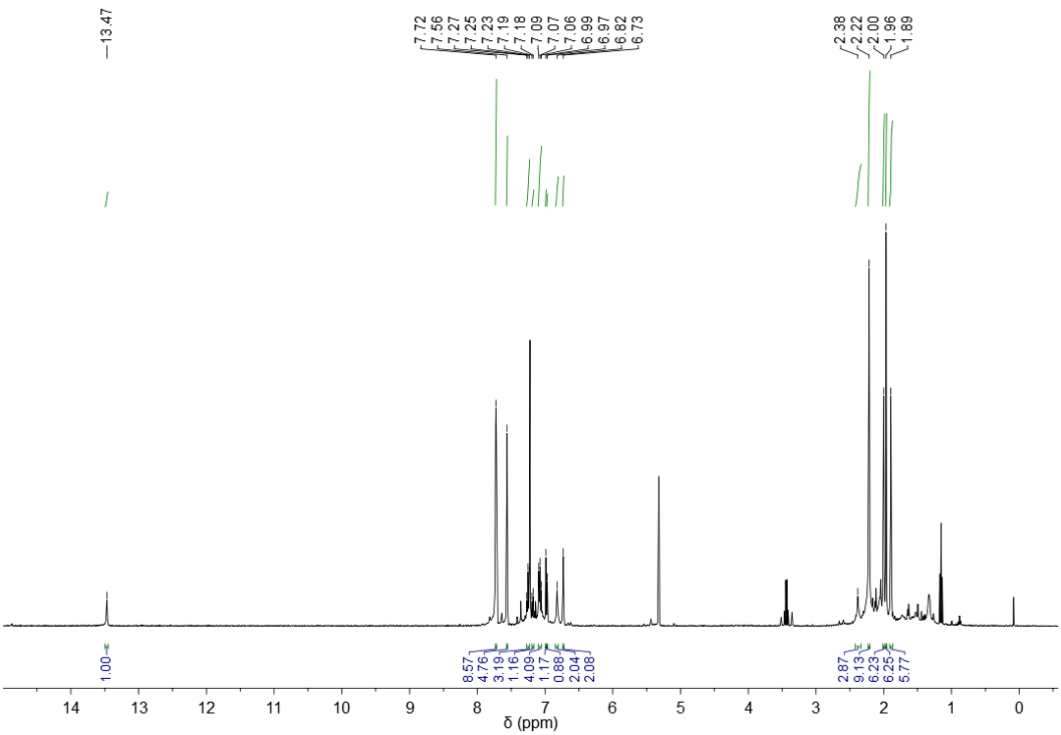


Figure S43. ^{1}H-NMR spectrum (400 MHz, CD_2Cl_2) of **17**.

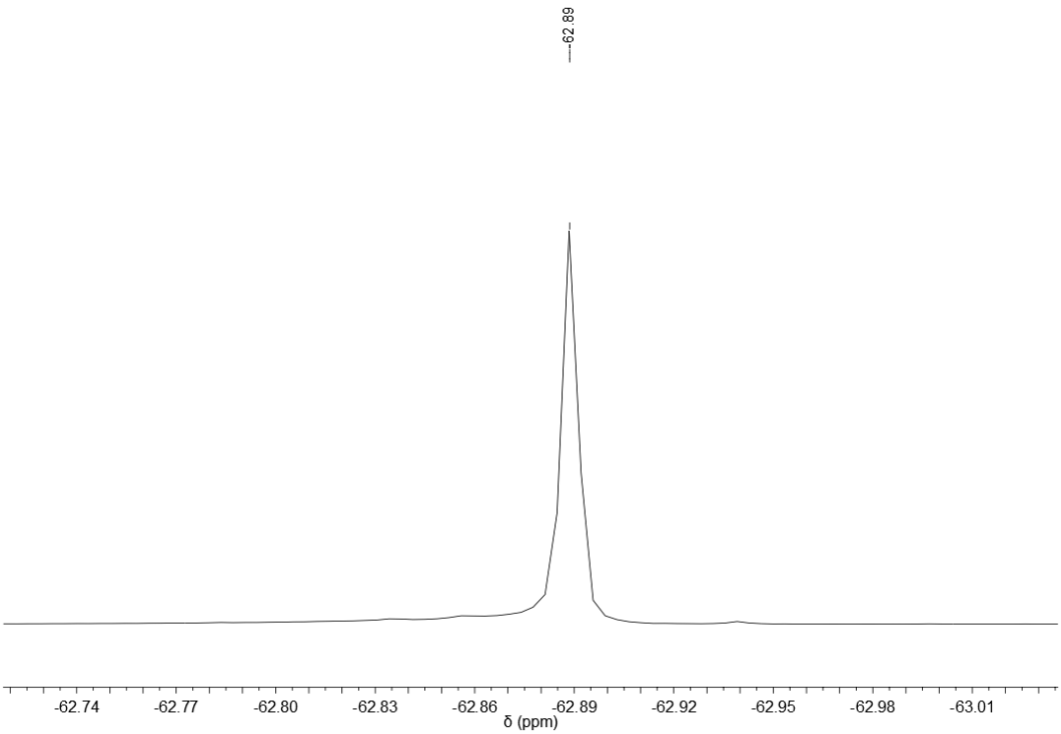


Figure S44. ^{19}F-NMR spectrum (376 MHz, CD_2Cl_2) of **17**.

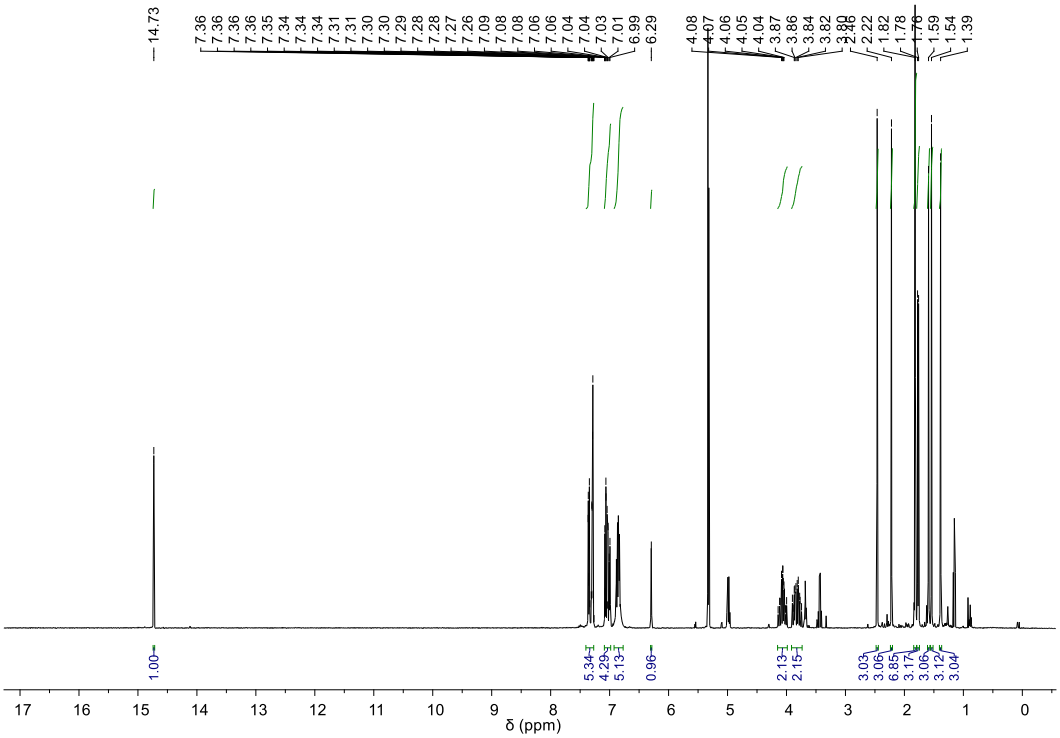


Figure S45. ^{1}H-NMR spectrum (400 MHz,CD_2Cl_2) of **18**.

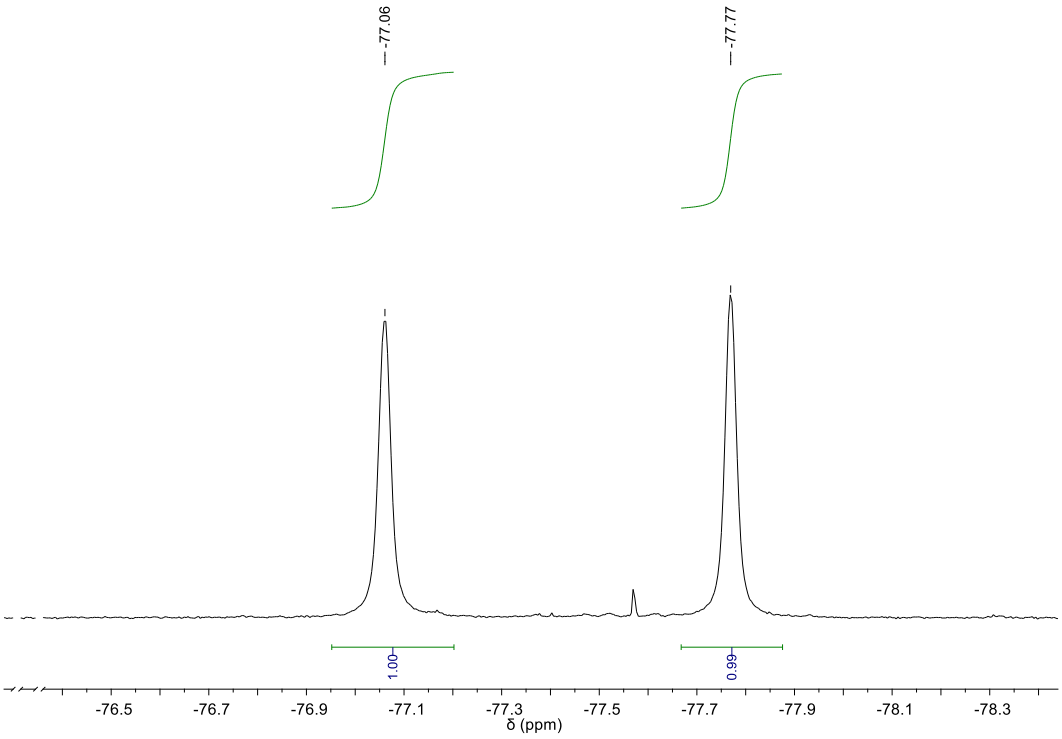


Figure S46. ^{19}F-NMR spectrum (376 MHz, CD_2Cl_2) of **18**.

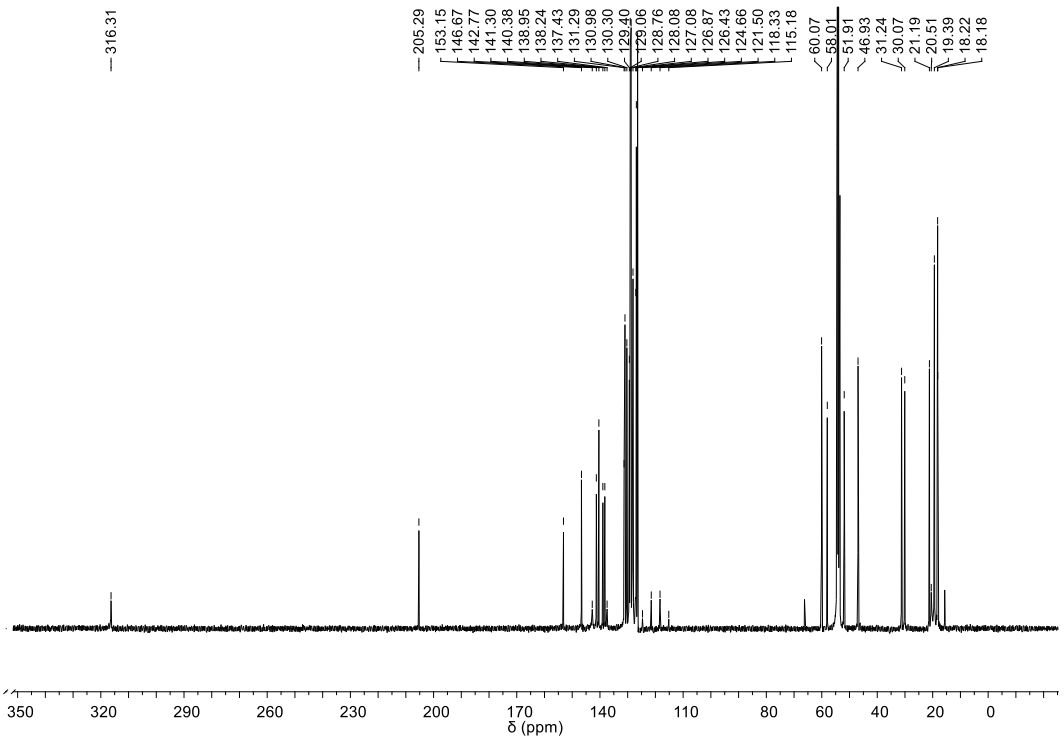


Figure S47. ^{13}C-NMR spectrum (101 MHz, CD_2Cl_2) of **18**.

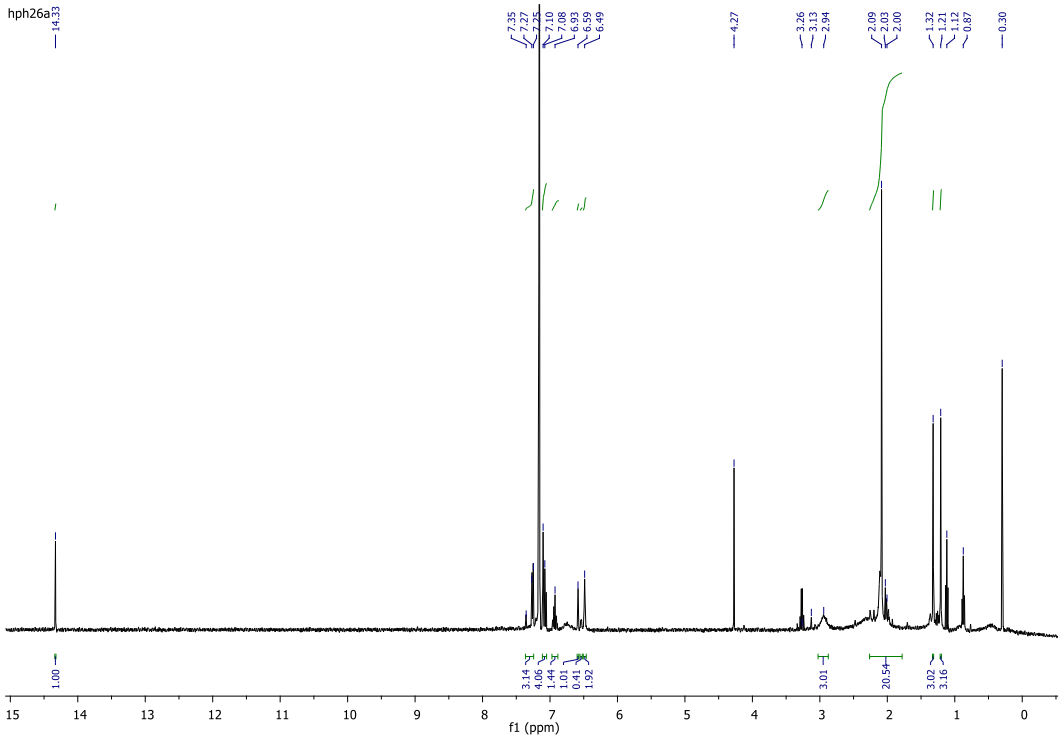


Figure S48. ^{1}H-NMR spectrum (400 MHz, C_6D_6) of **19**.

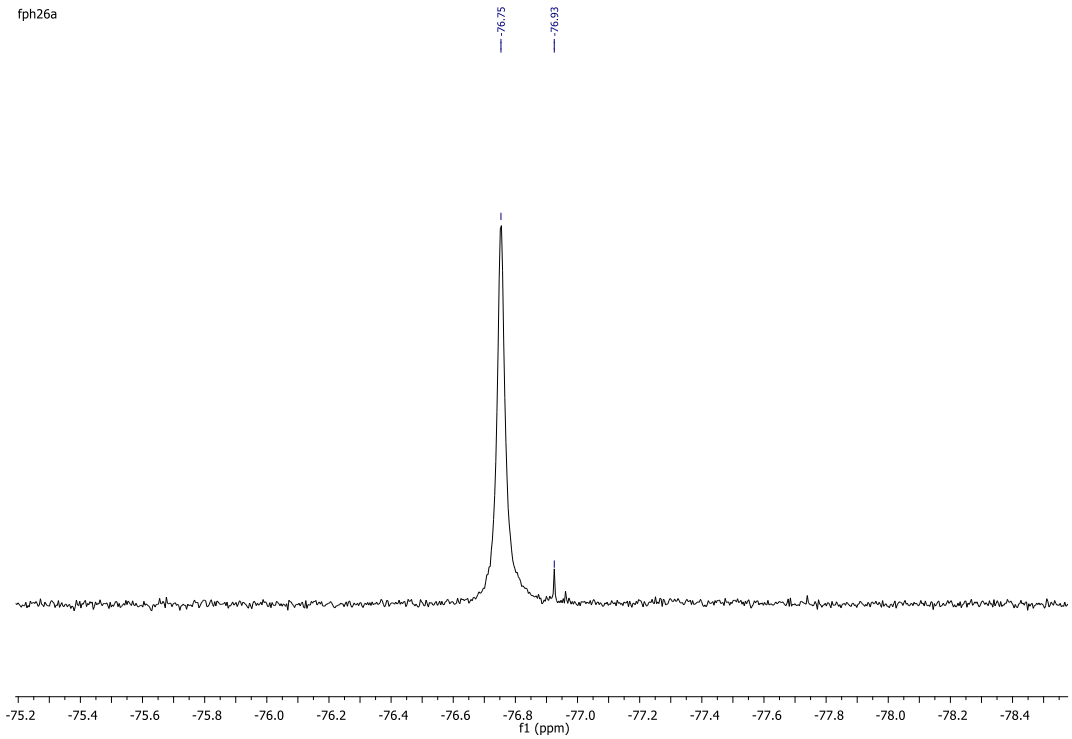


Figure S49. ^{19}F-NMR spectrum (376 MHz, C_6D_6) of **19**.

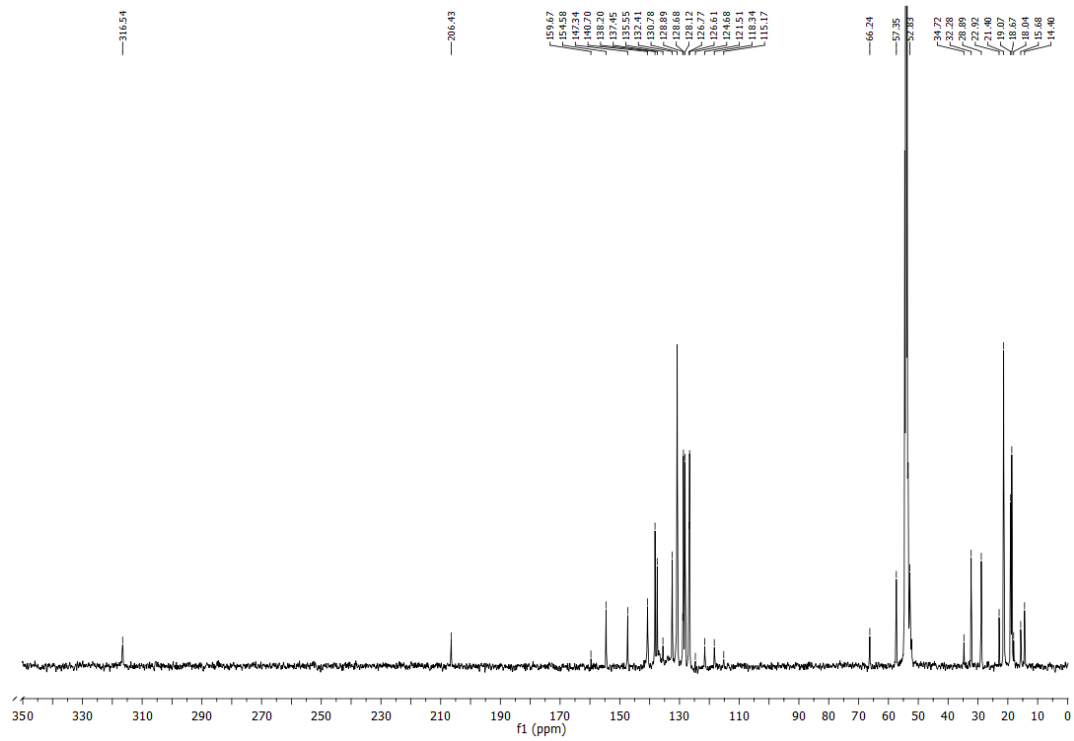


Figure S50. ^{13}C-NMR spectrum (CD_2Cl_2) of **19**.

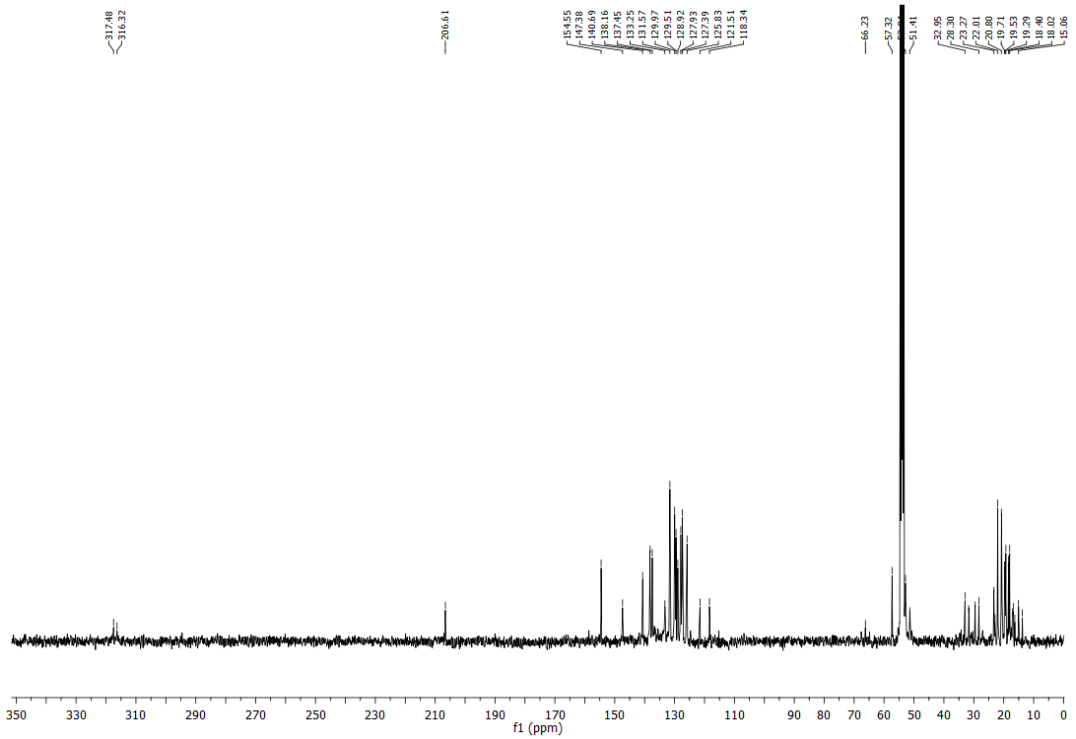


Figure S51. ^{13}C-(gated decoupling) NMR spectrum (101 MHz, CD_2Cl_2) of **19**.

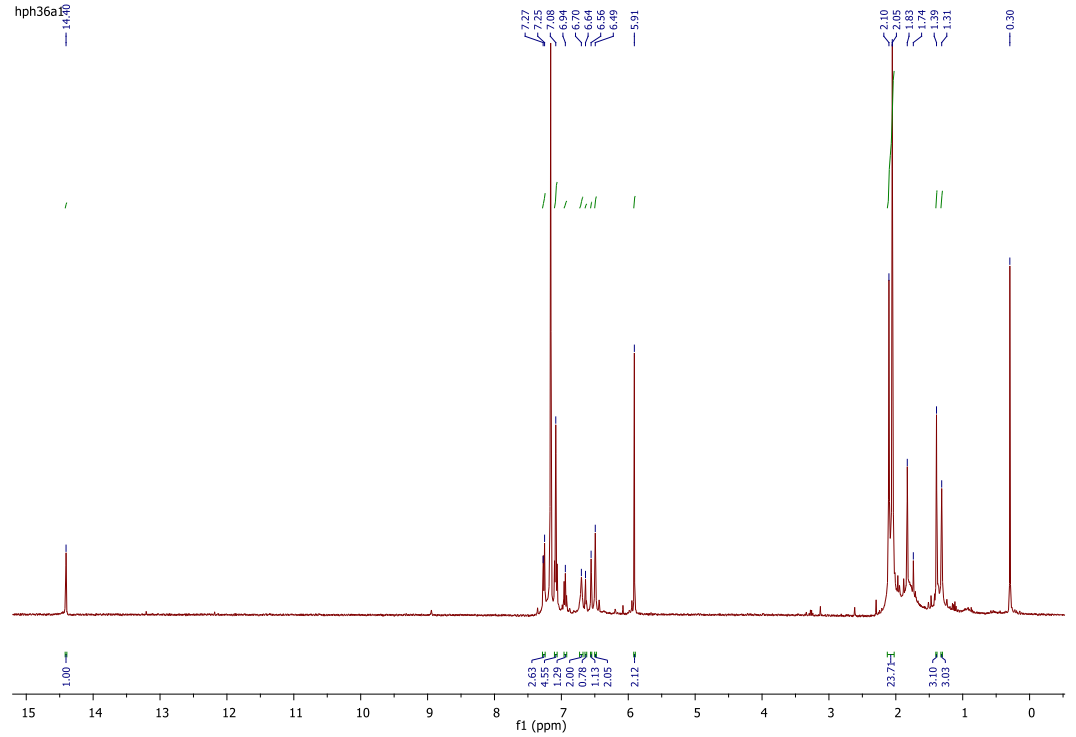


Figure S52. ^{1}H-NMR spectrum (400 MHz, C_6D_6) of **20**.

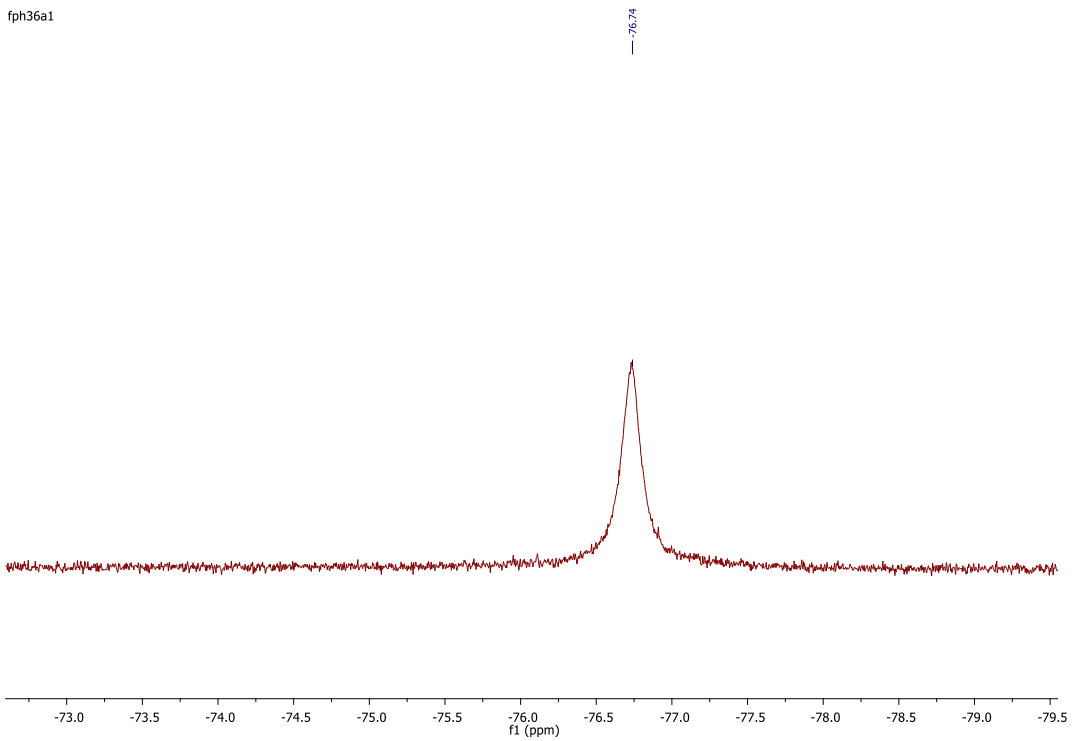


Figure S53. ^{19}F-NMR spectrum (376 MHz, C_6D_6) of **20**.

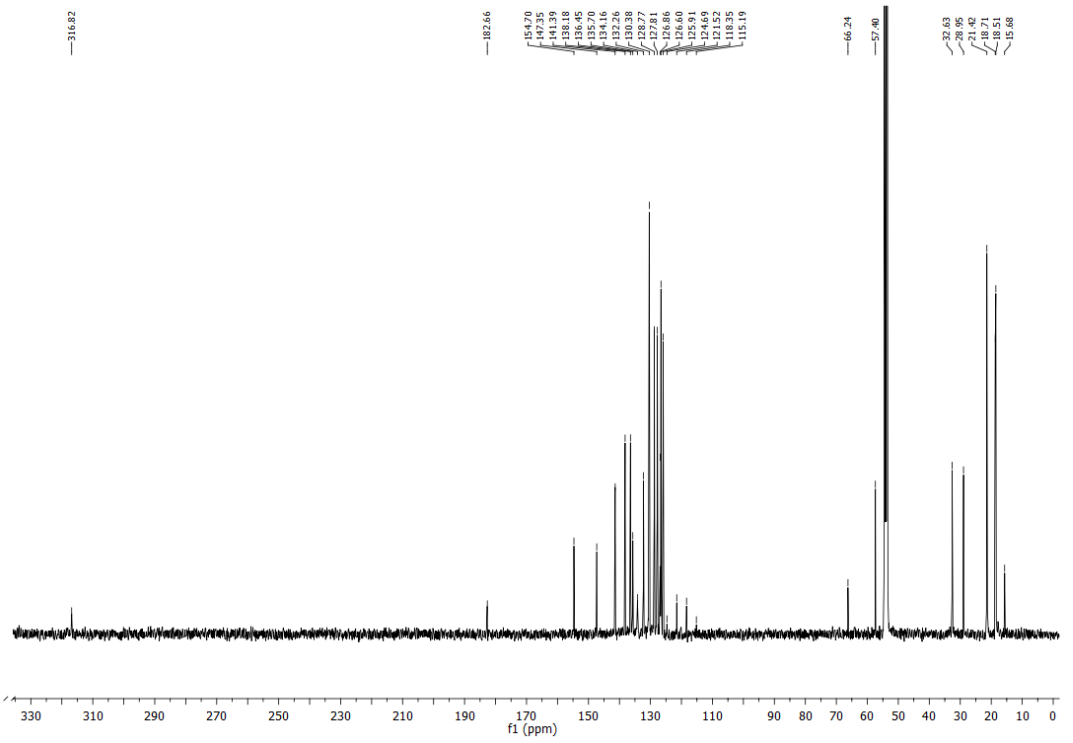


Figure S54. ^{13}C-NMR spectrum (101 MHz, CD_2Cl_2) of **20**.

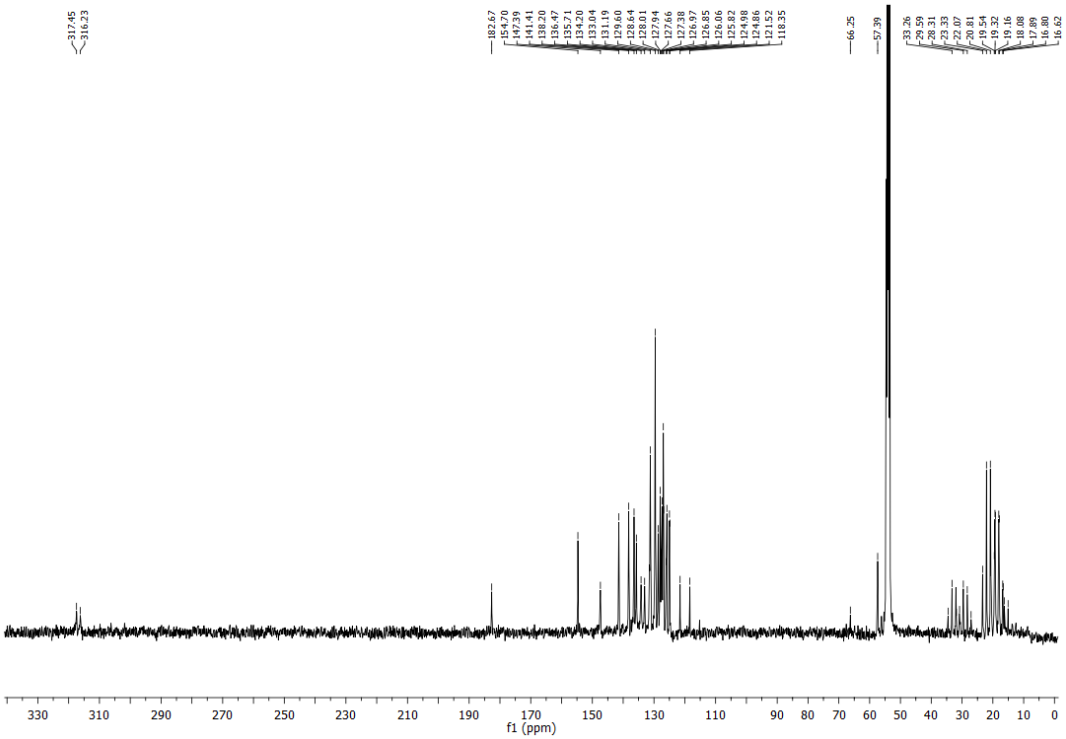


Figure S55. ^{13}C-(gated decoupling) NMR spectrum (101 MHz, CD_2Cl_2) of **20**.

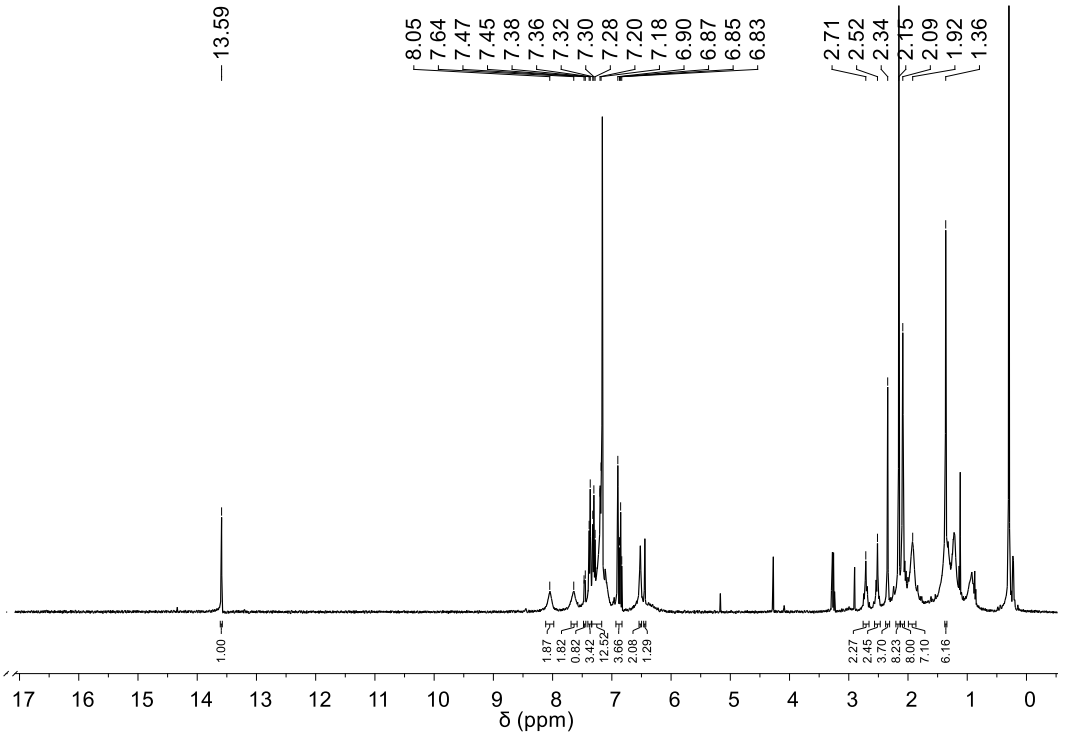


Figure S56. ^{1}H-NMR spectrum (400 MHz, C_6D_6) of **21**.

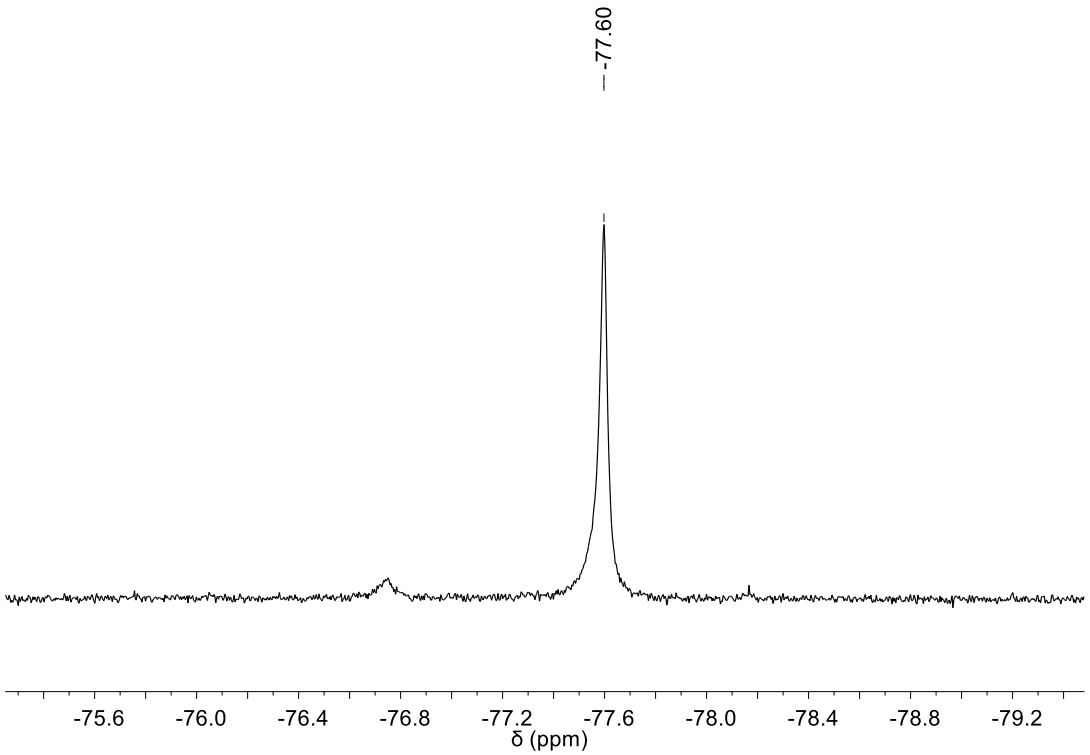


Figure S57. ^{19}F-NMR spectrum (376 MHz, C_6D_6) of **21**.

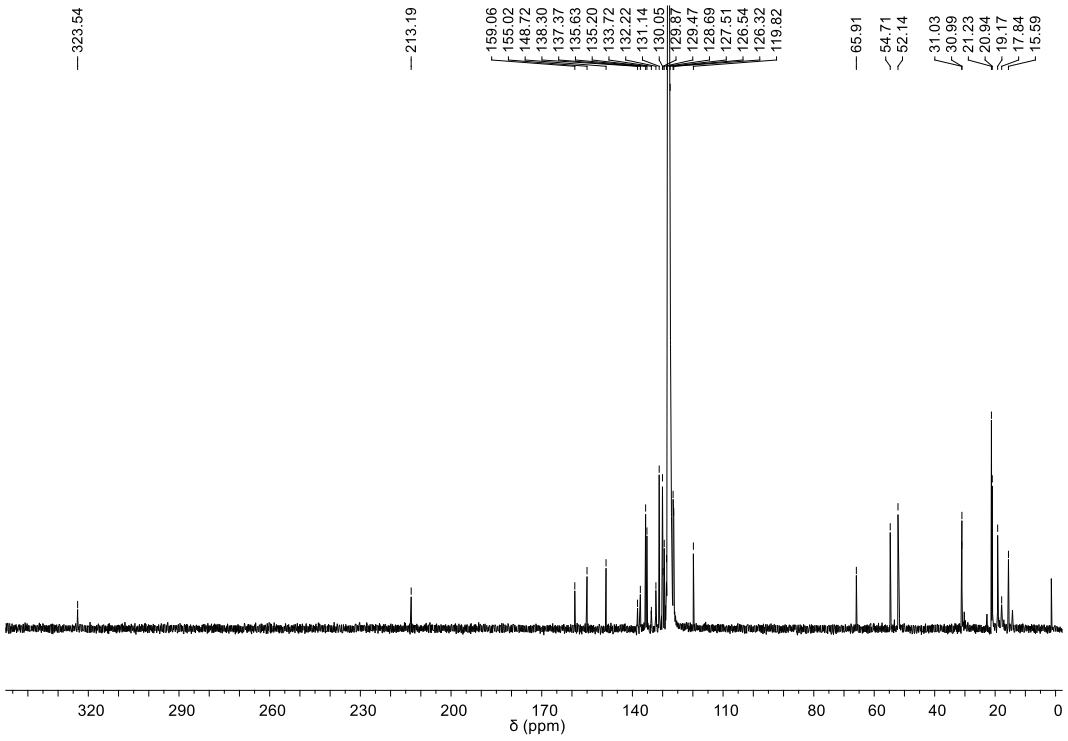


Figure S58. ^{13}C-NMR spectrum (101 MHz, CD_2Cl_2) of **21**.

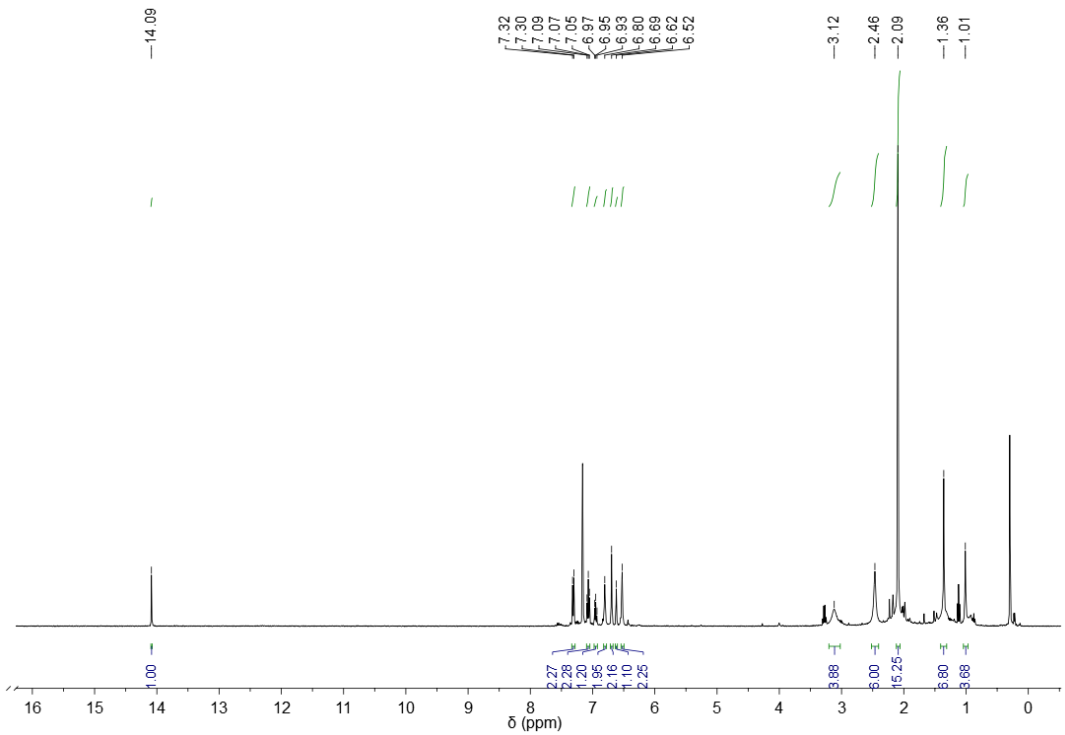


Figure S59. ^{1}H-NMR spectrum (400 MHz,C_6D_6) of **22**.

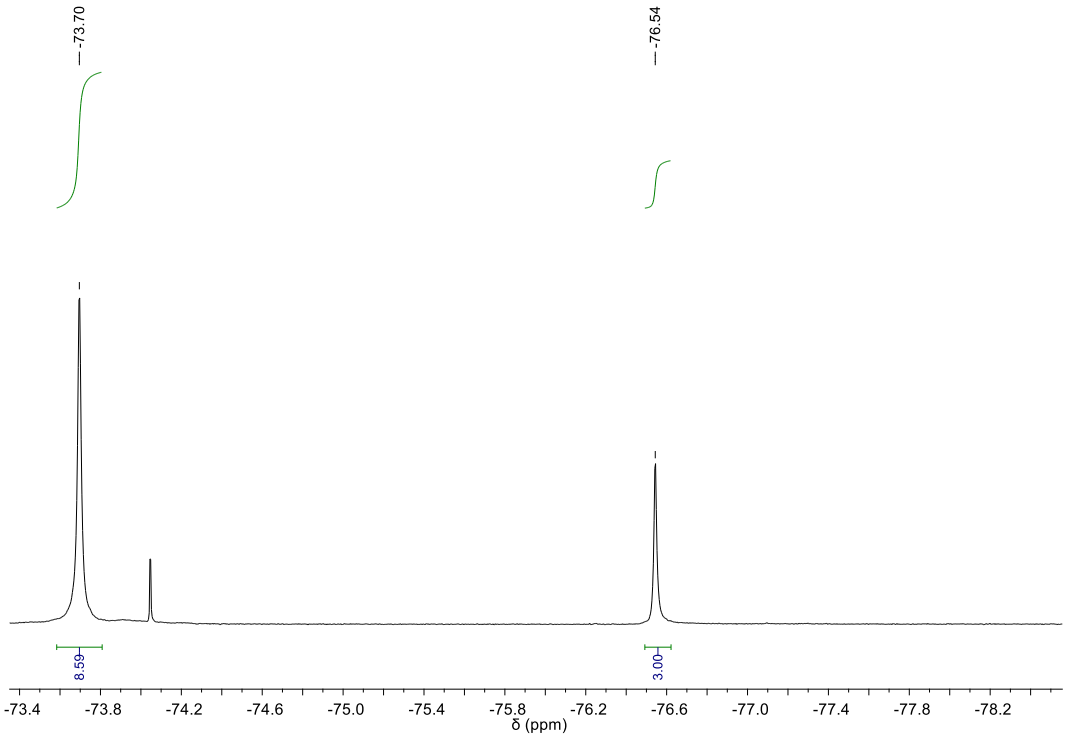


Figure S60. ^{19}F-NMR spectrum (376 MHz,C_6D_6) of **22**.

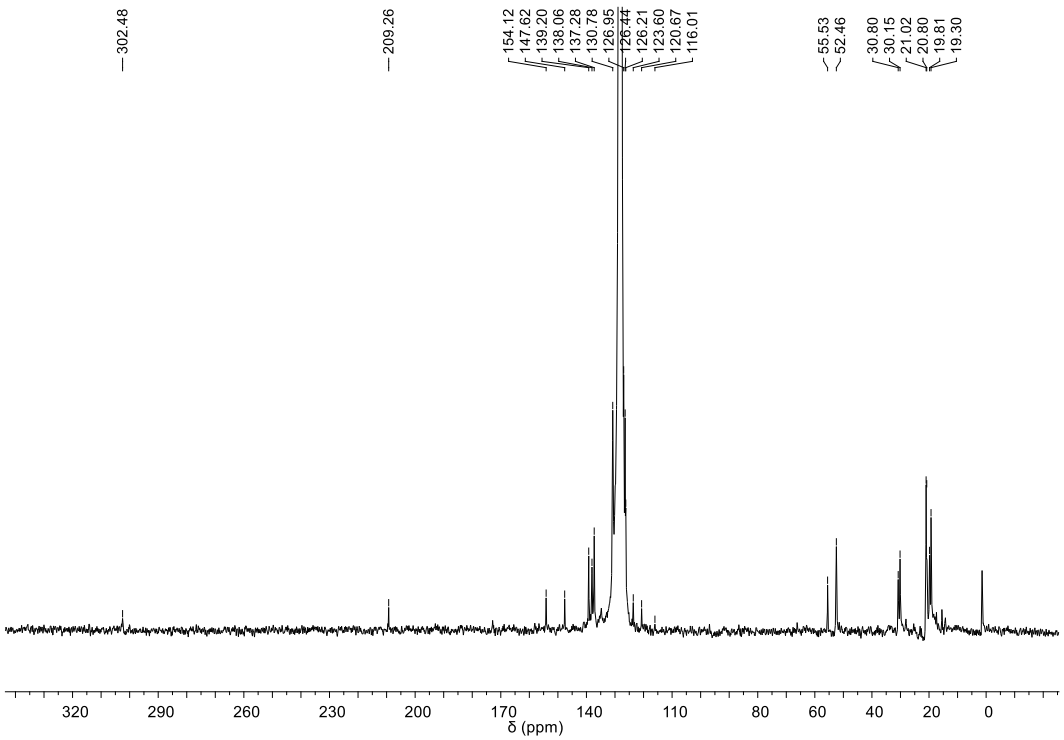


Figure S61. ^{13}C-NMR spectrum (101 MHz,C_6D_6) of **22**.

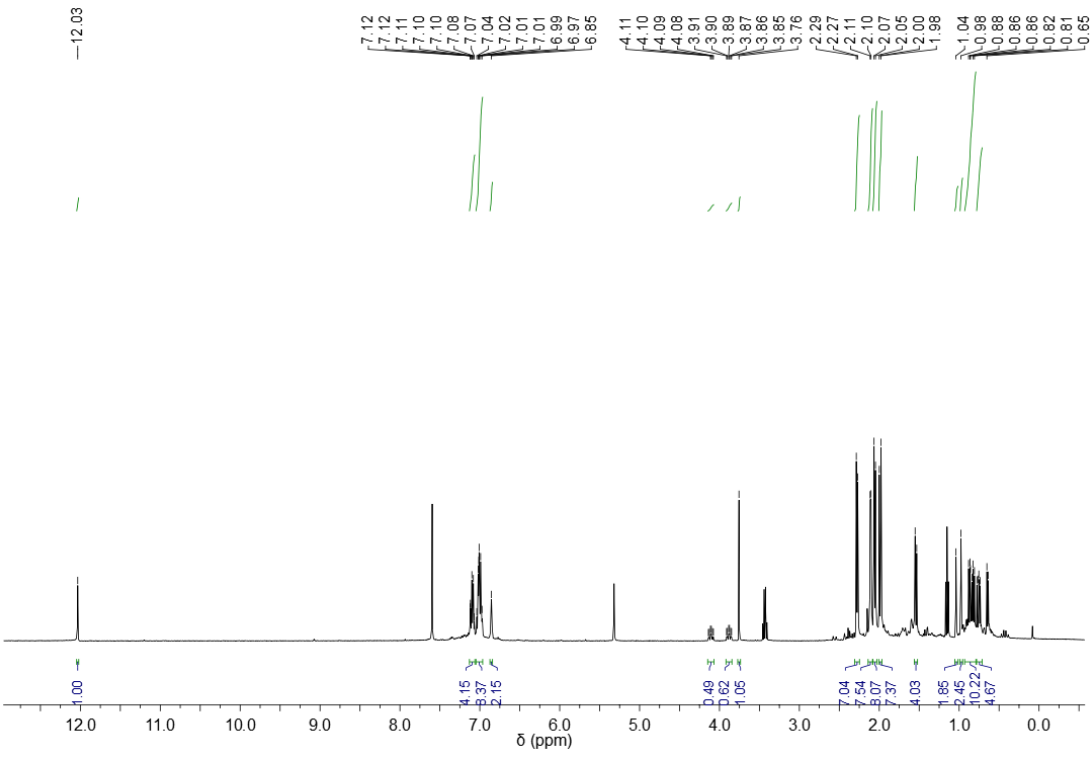


Figure S62. ^{1}H-NMR spectrum (400 MHz, CD_2Cl_2) of **23**.

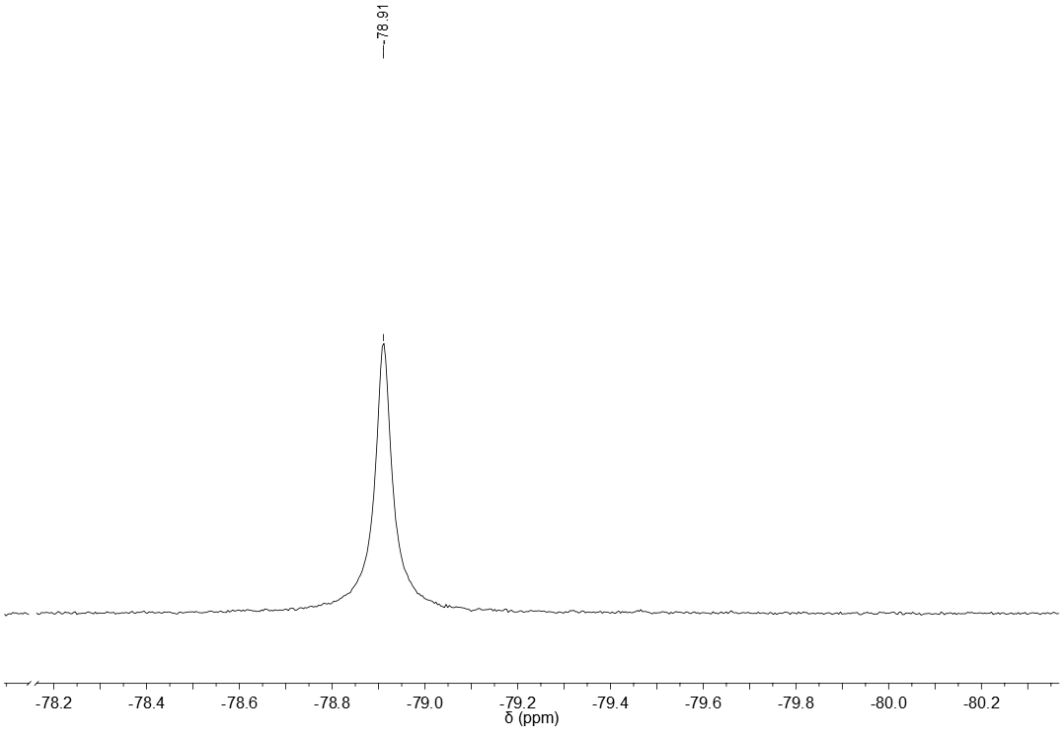


Figure S63. ^{19}F-NMR spectrum (376 MHz, CD_2Cl_2) of **5**.

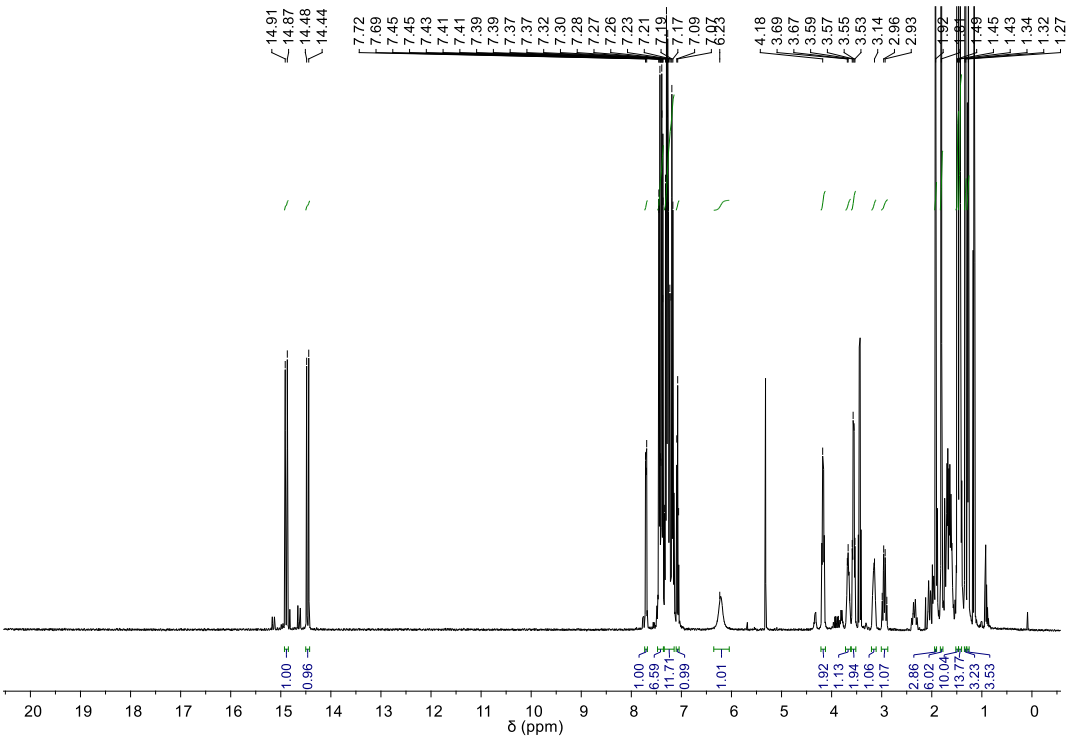


Figure S64. ^{1}H-NMR spectrum (400 MHz,CD_2Cl_2) of **24**.

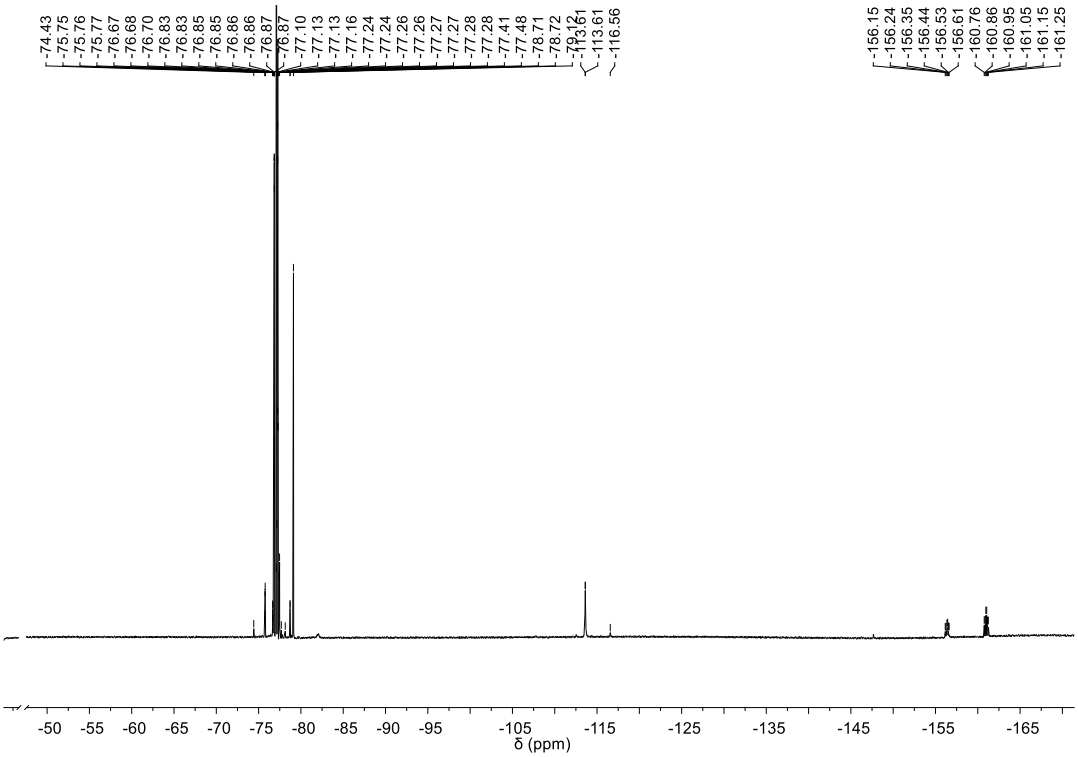


Figure S65. ^{19}F-NMR spectrum (CD_2Cl_2) of **24**.

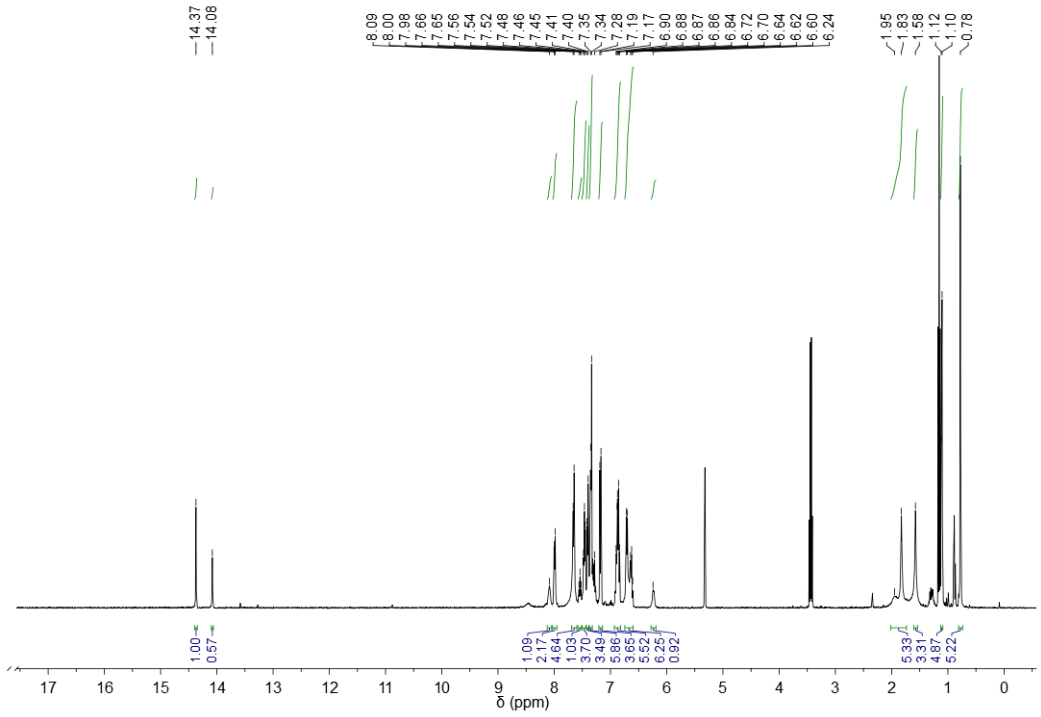


Figure S66. ^{1}H-NMR spectrum (400 MHz, CD_2Cl_2) of **25**.

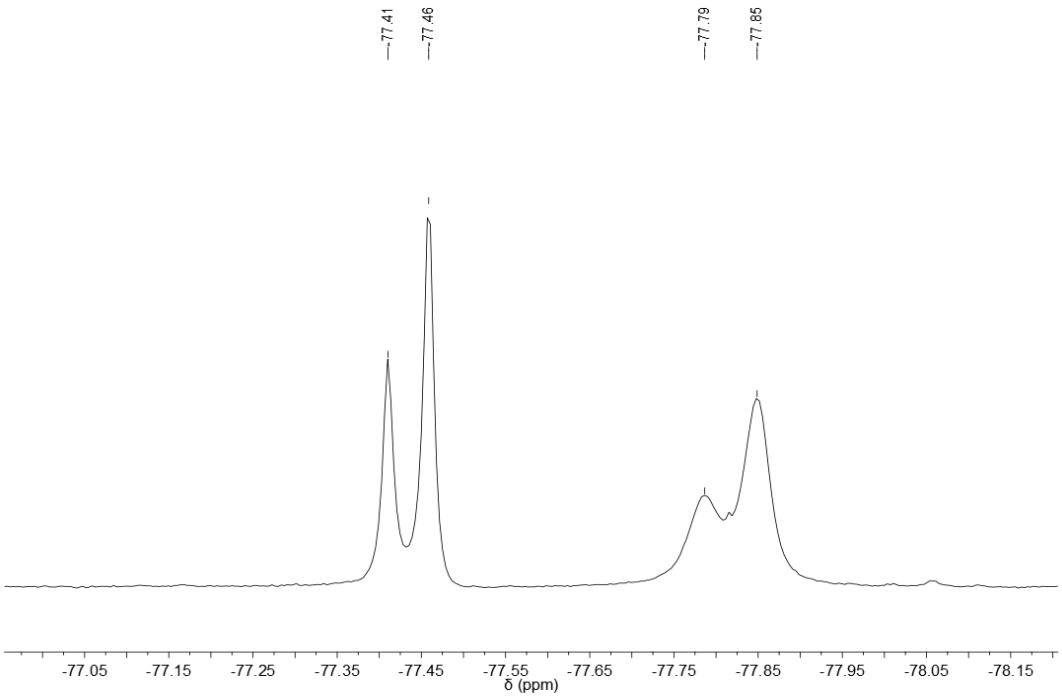


Figure S67. ^{19}F-NMR spectrum (376 MHz, CD_2Cl_2) of **25**.

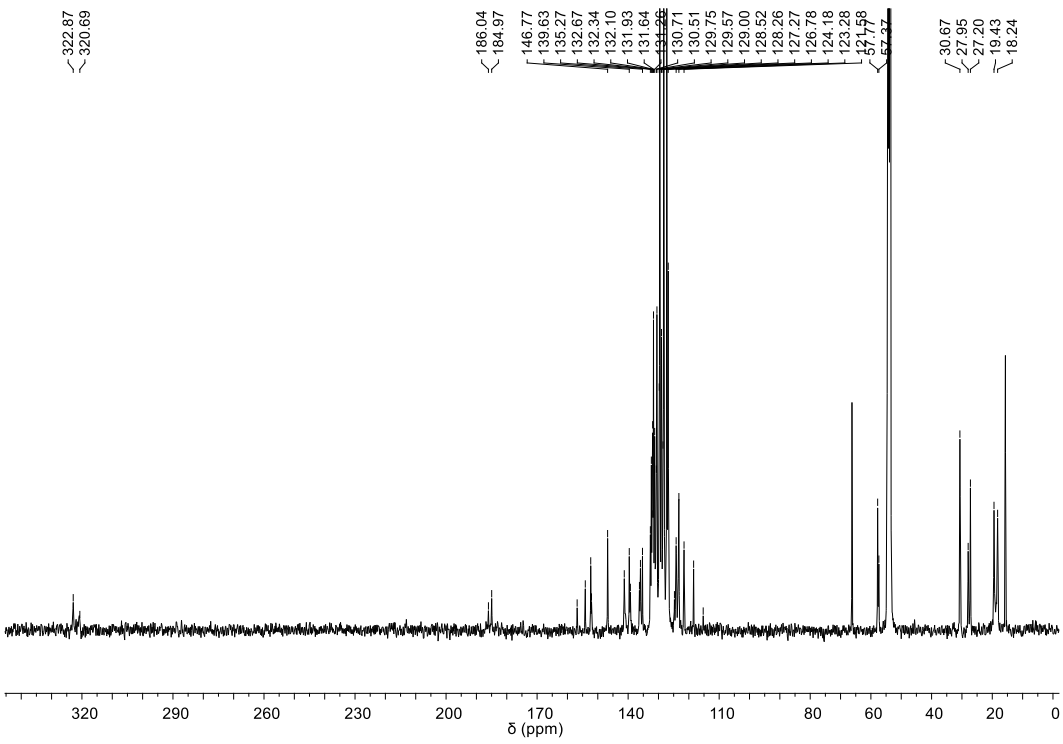


Figure S68. ^{13}C-NMR spectrum (101 MHz, CD_2Cl_2) of **25**.

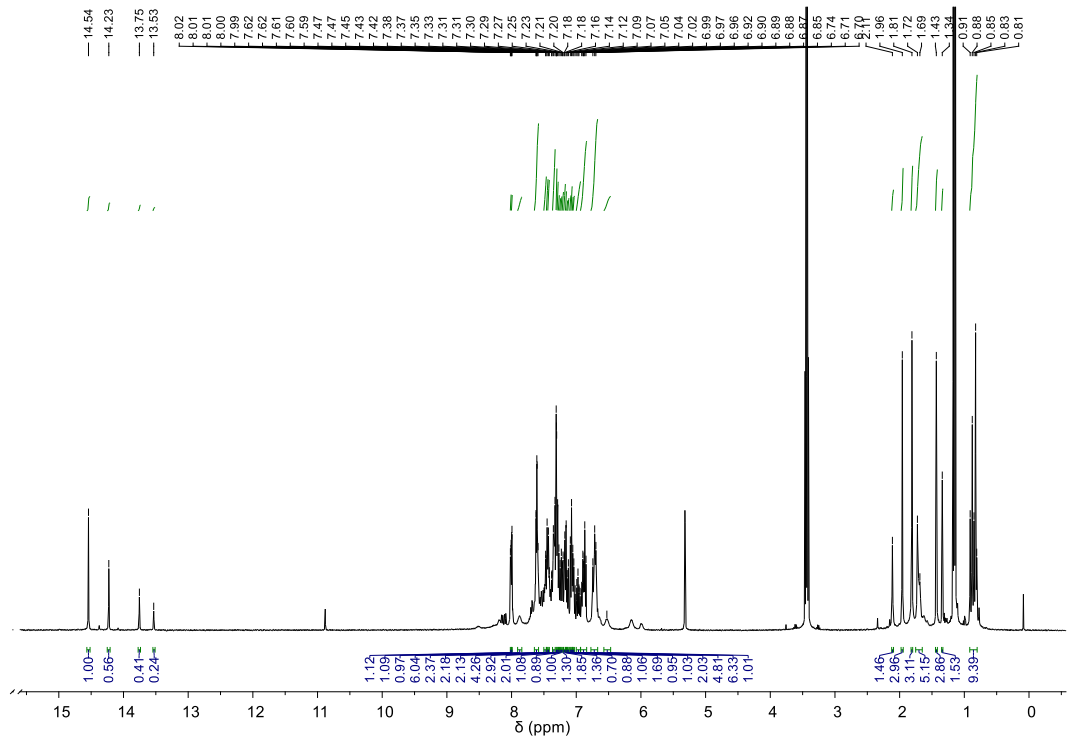


Figure S69. ^{1}H-NMR spectrum (400 MHz, CD_2Cl_2) of **26**.

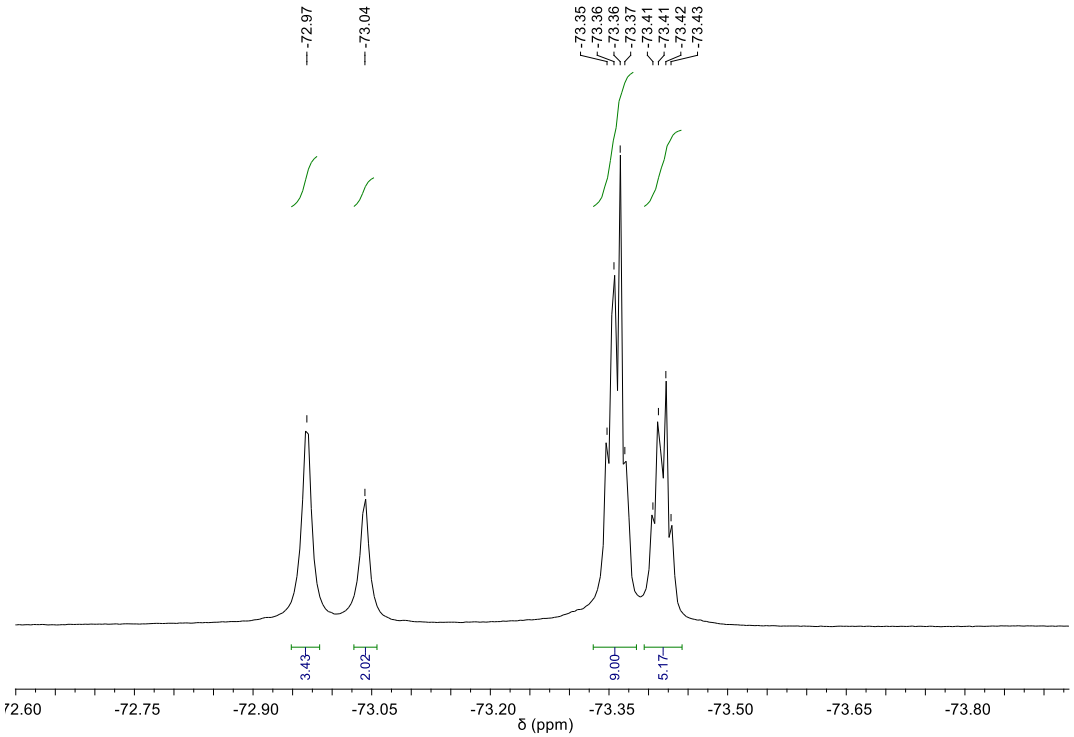


Figure S70. ^{19}F-NMR spectrum (376 MHz, CD_2Cl_2) of **26**.

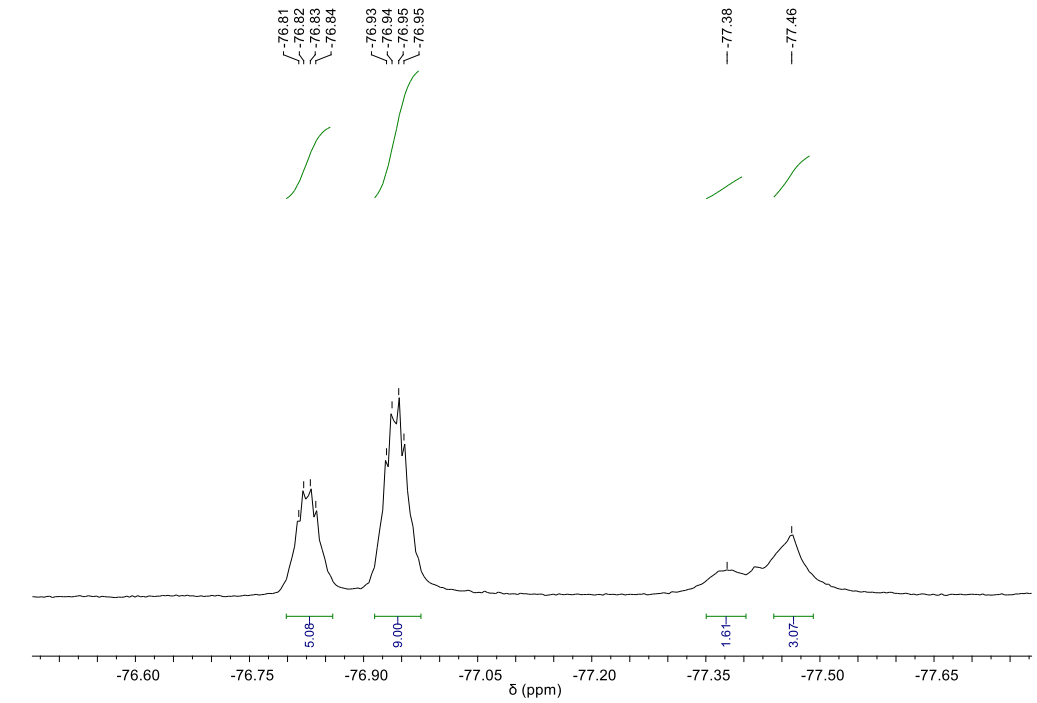


Figure S71. ^{19}F-NMR spectrum (376 MHz, CD_2Cl_2) of **26**.

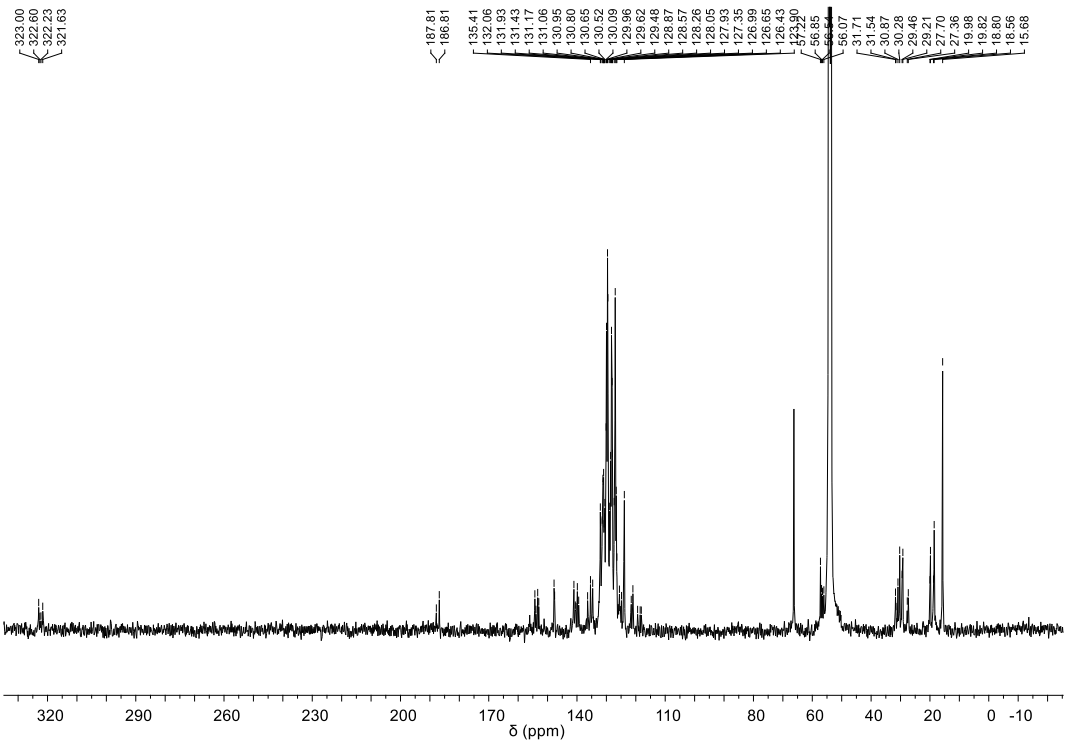


Figure S72. ^{13}C-NMR spectrum (101 MHz,CD_2Cl_2) of **26**.

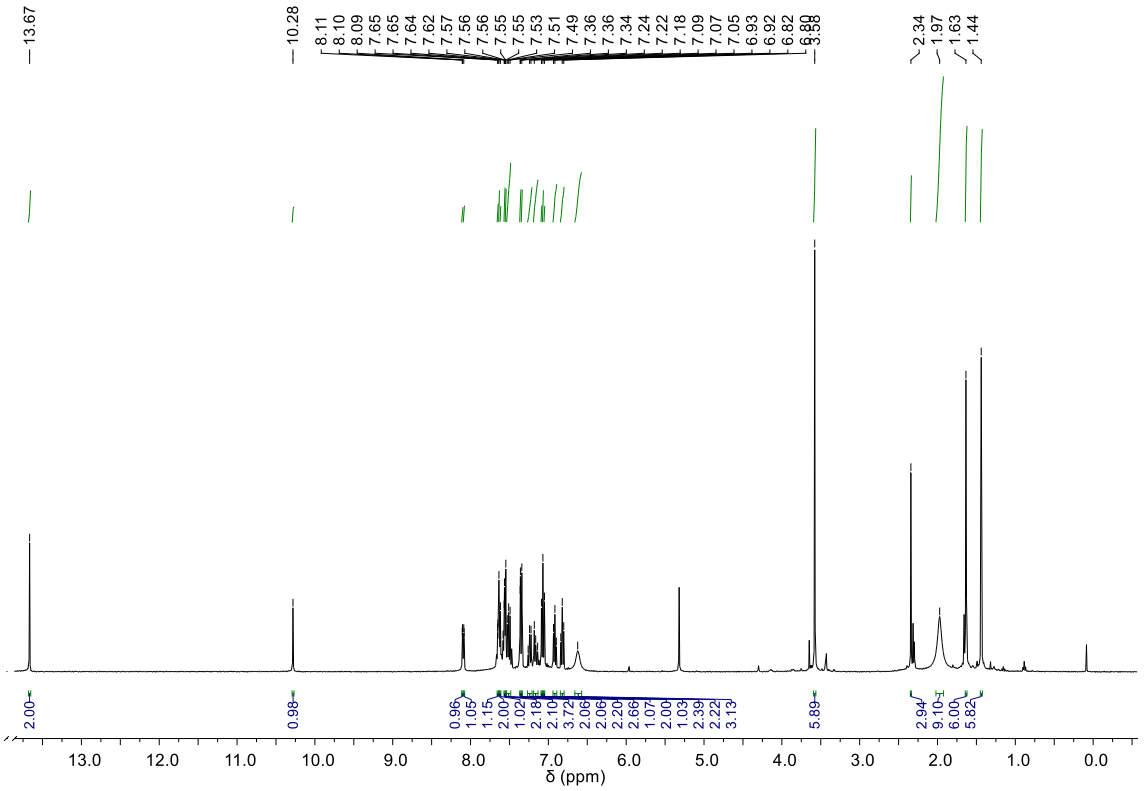


Figure S73. ^{1}H-NMR spectrum (400 MHz, CD_2Cl_2) of **27**.

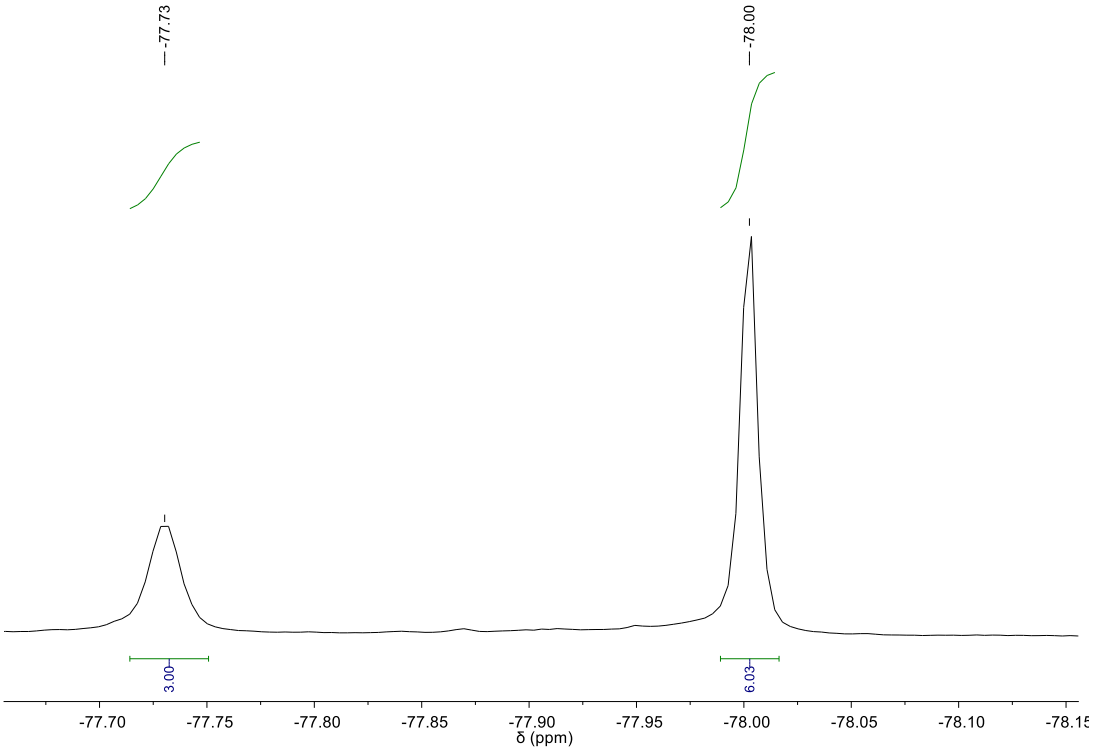


Figure S74. ^{19}F-NMR spectrum (376 MHz, CD_2Cl_2) of **27**.

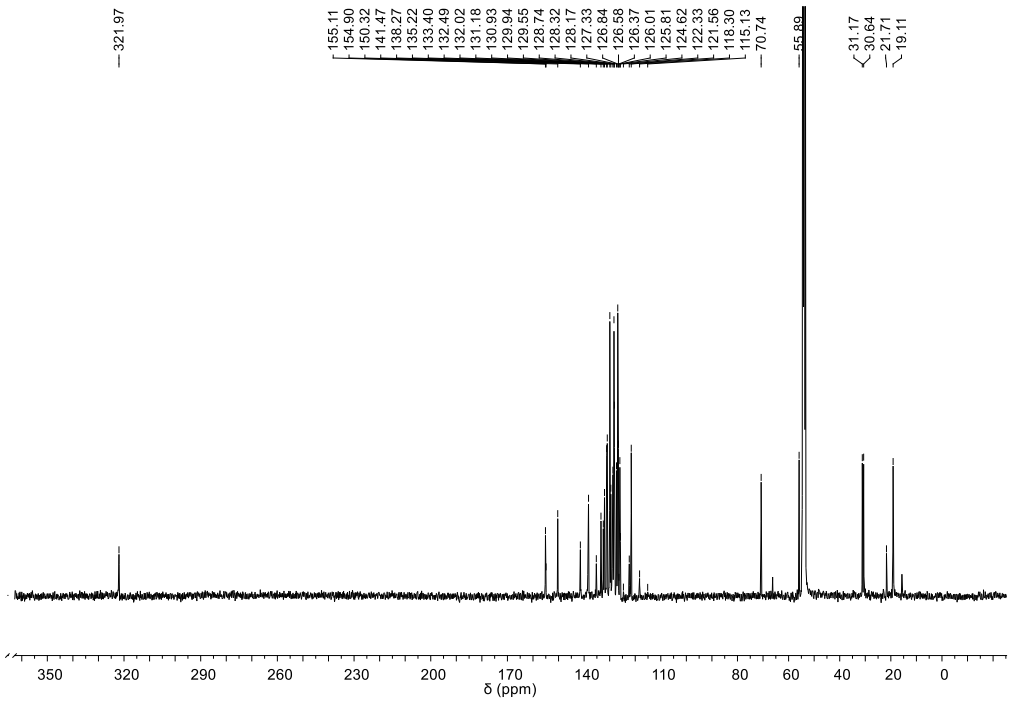


Figure S75. ^{13}C-NMR spectrum (101 MHz, CD_2Cl_2) of **27**.

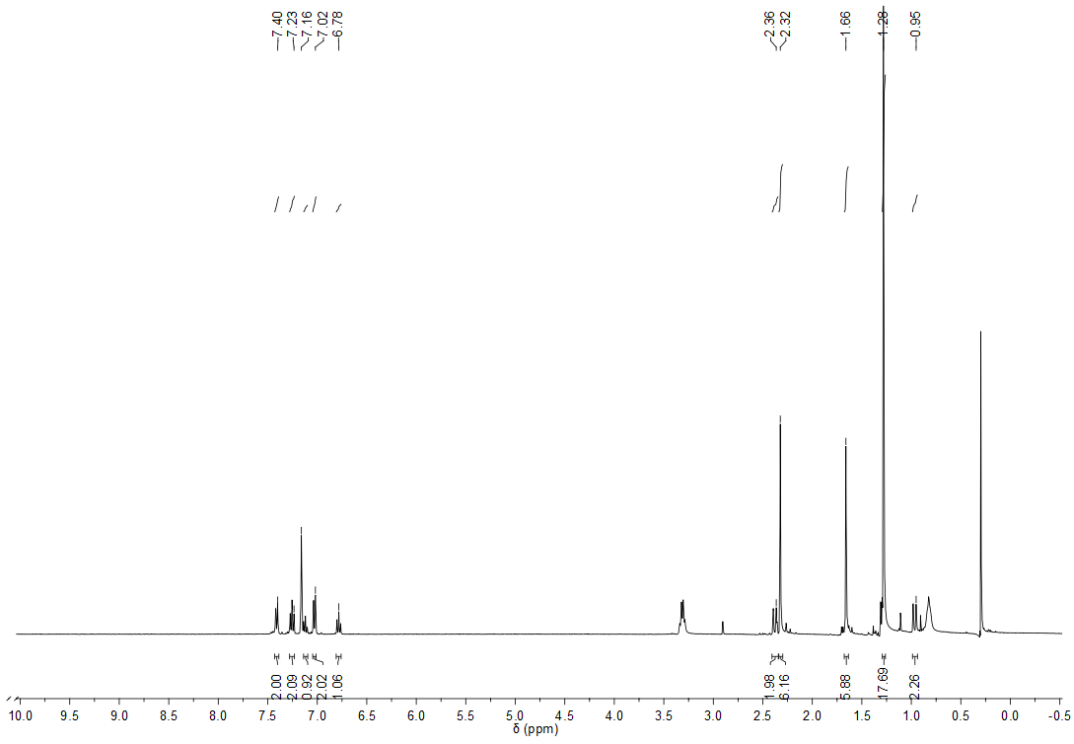


Figure S76. ^{1}H-NMR (400 MHz, C_6D_6) spectrum of **29**.

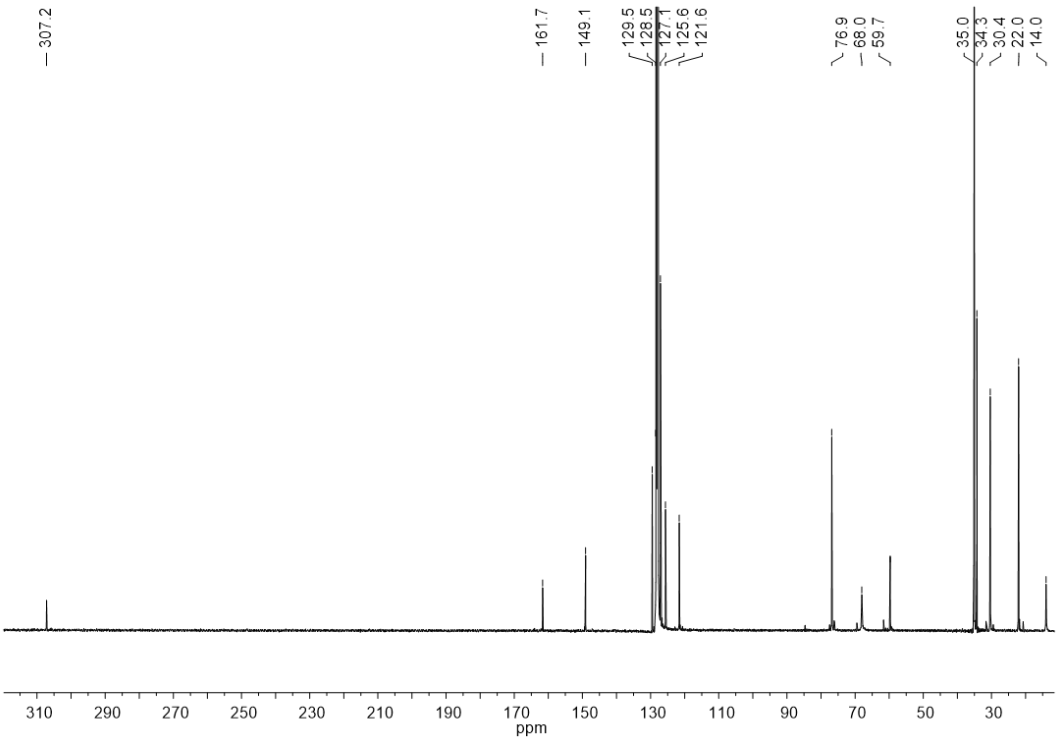


Figure S77. ^{13}C-NMR (101 MHz, C_6D_6) spectrum of **29**.

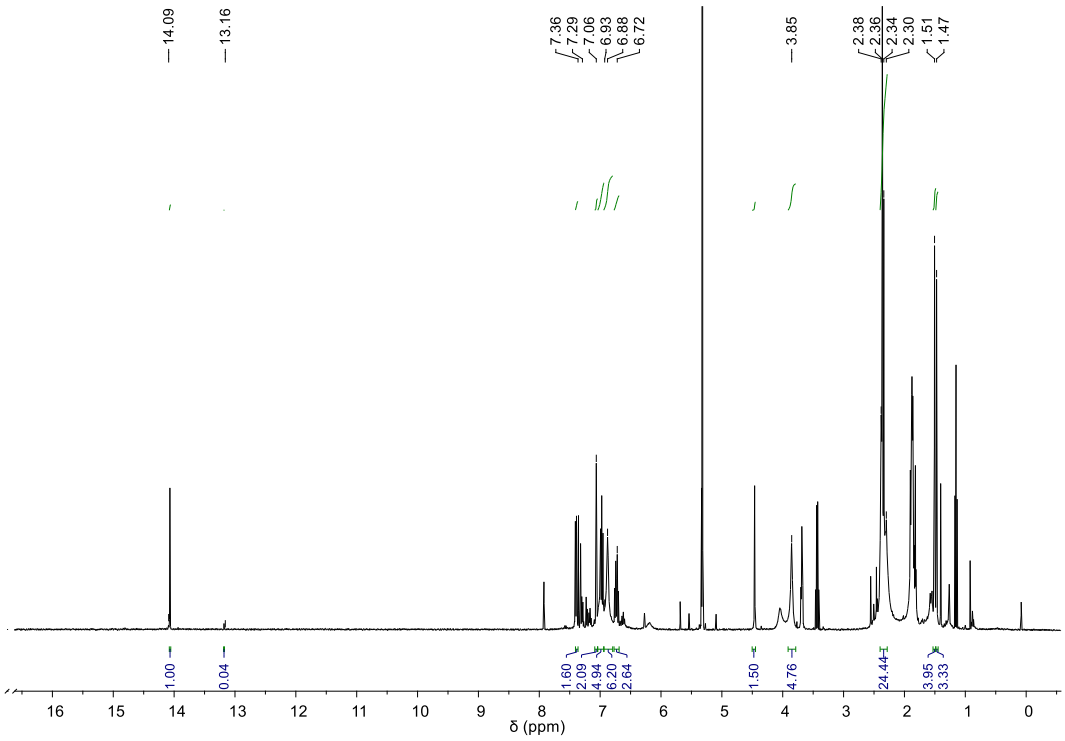


Figure S78. ^{1}H-NMR spectrum (400MHz, CD_2Cl_2) of Mo (N-2,6-Me_2-C_6H_3)(IMesH_2)(CHCMe_2Ph)(OTf)(OCN).

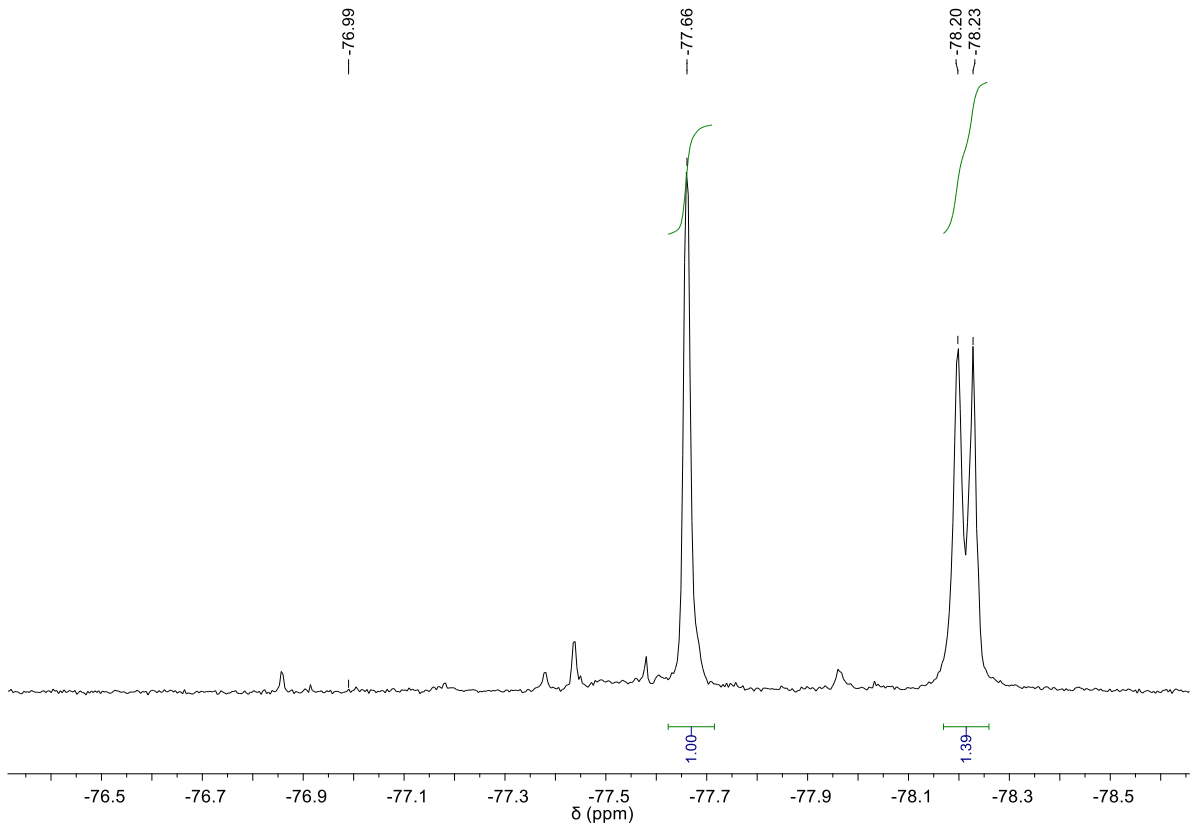


Figure S79. ^{19}F-NMR spectrum (376 MHz, CD_2Cl_2) of Mo (N-2,6-Me_2-C_6H_3)($IMesH_2$)($CHCMe_2Ph$)(OTf)(OCN).

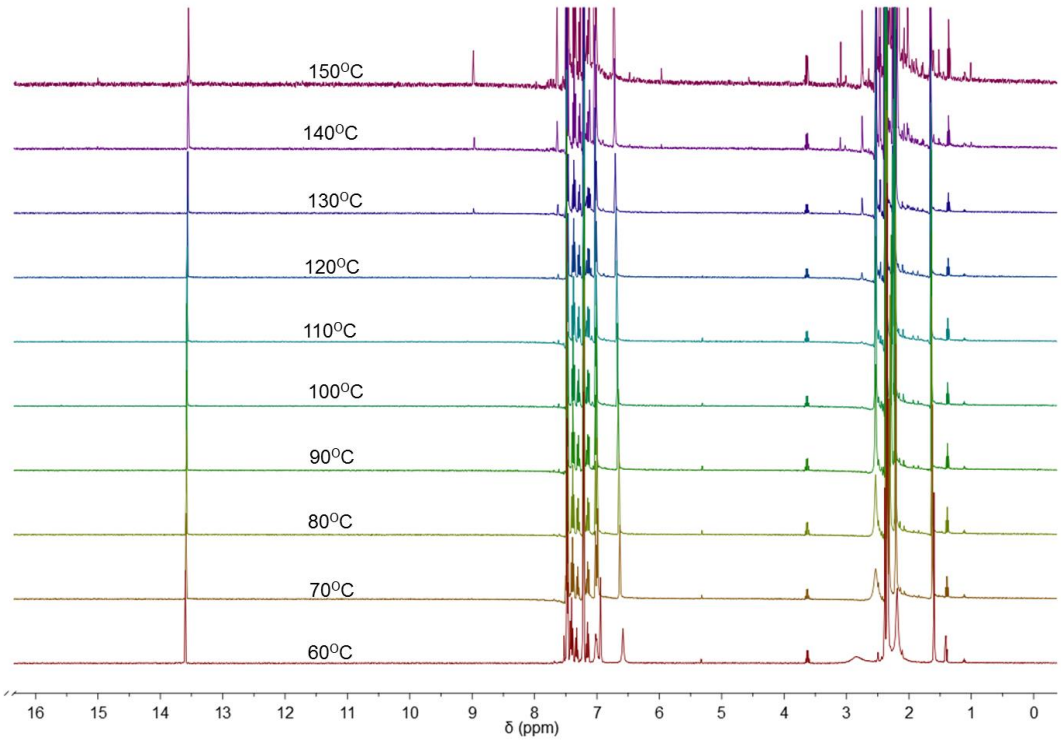


Figure S80. VT ^{1}H-NMR spectra (400 MHz, 1,2-dichlorobenzene-d_4) of **6**.

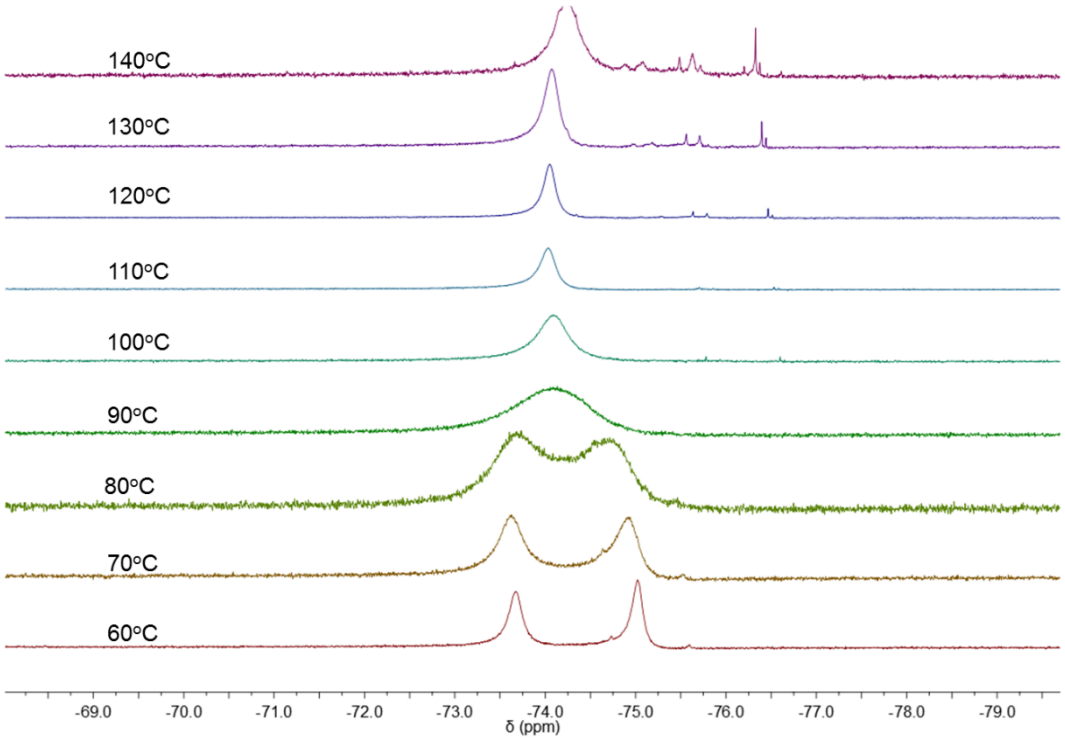


Figure S81. VT ^{19}F-NMR spectra (376 MHz, 1,2-dichlorobenzene-d_4) of **6**.

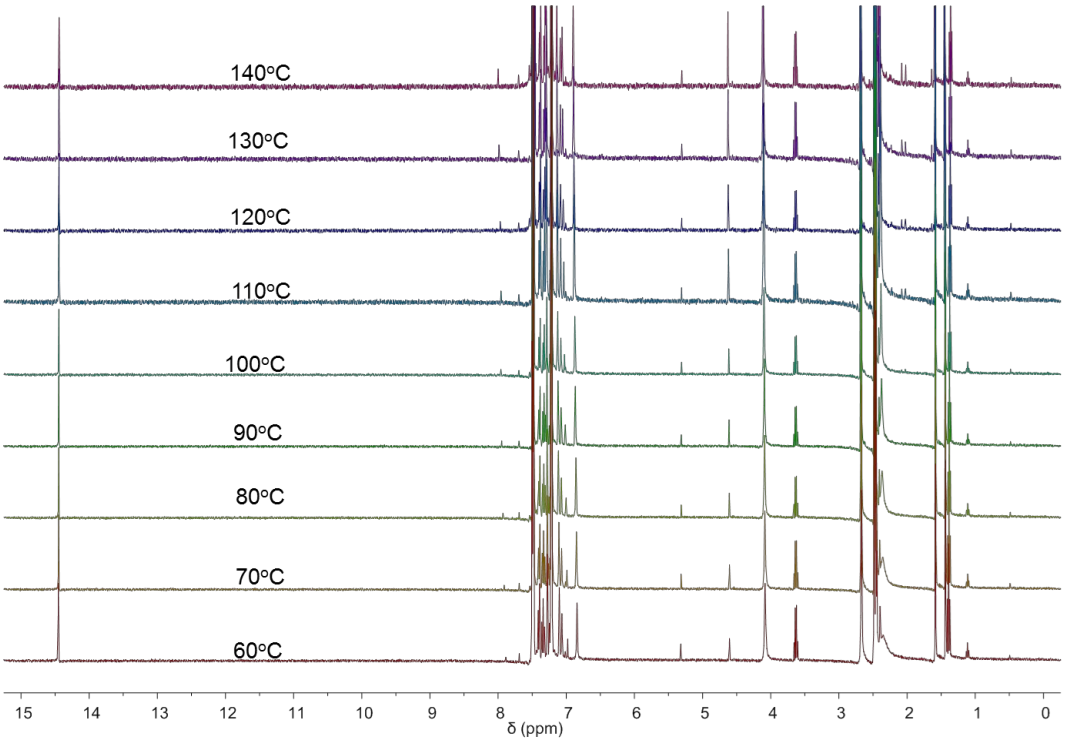


Figure S82. VT ^{1}H-NMR spectra (400 MHz, 1,2-dichlorobenzene-d_4) of **19**.

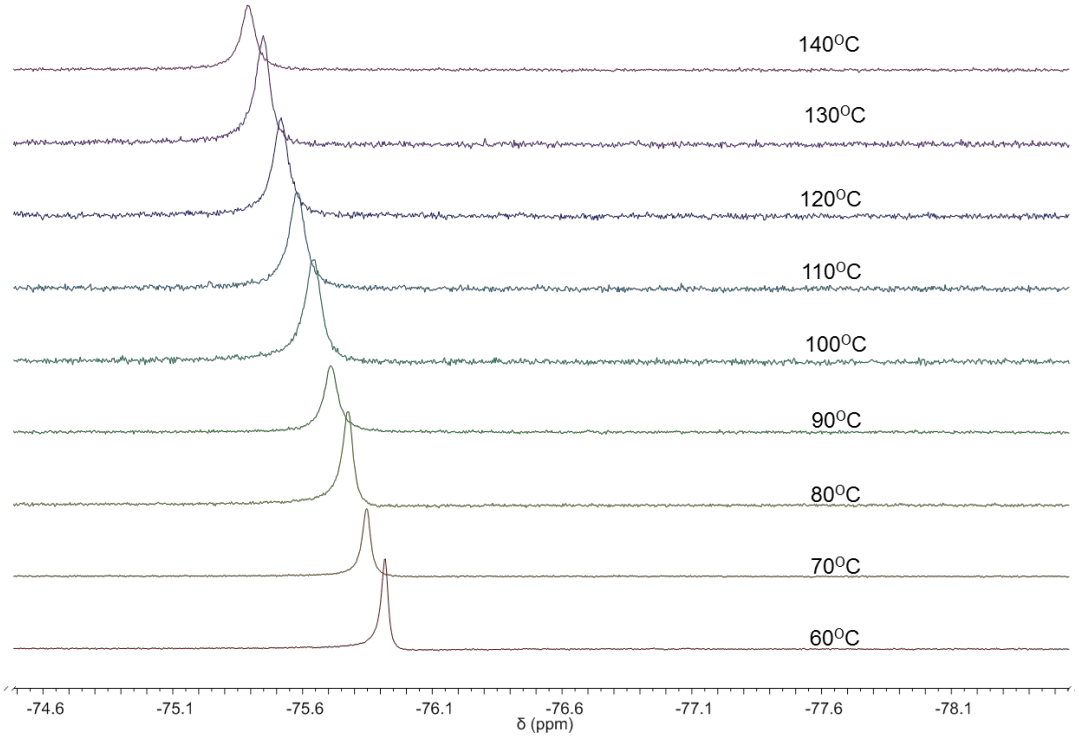


Figure S83. VT ^{19}F-NMR spectra (376 MHz, 1,2-dichlorobenzene-d_4) of **19**.

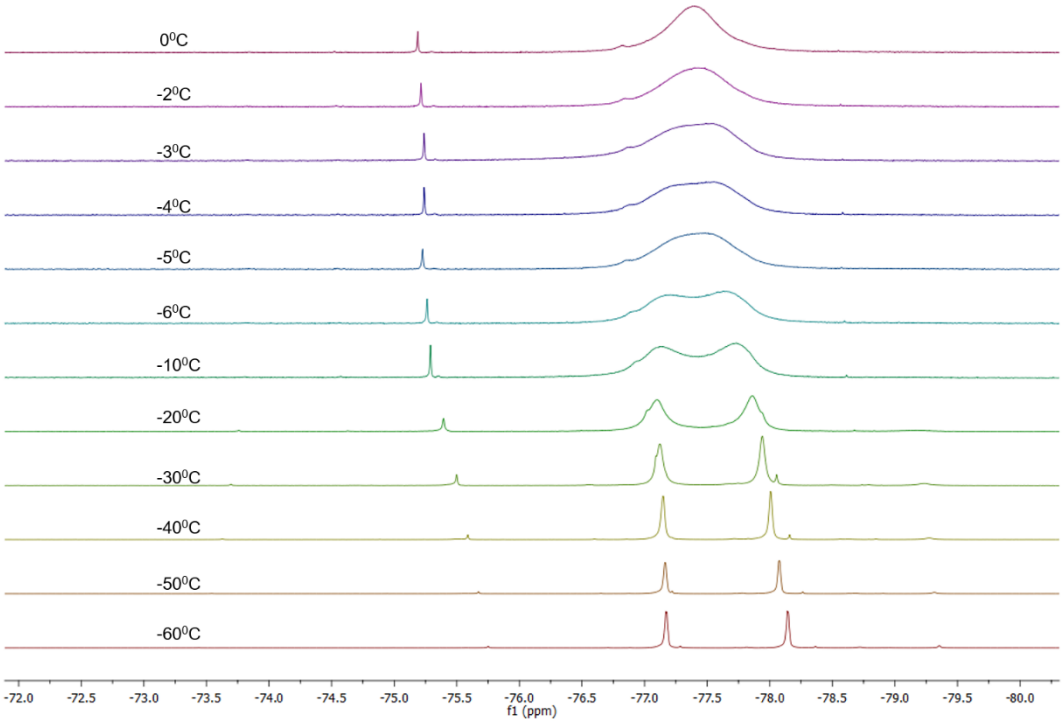


Figure S84. VT ^{19}F-NMR spectra (376 MHz, CD_2Cl_2) of **19**.

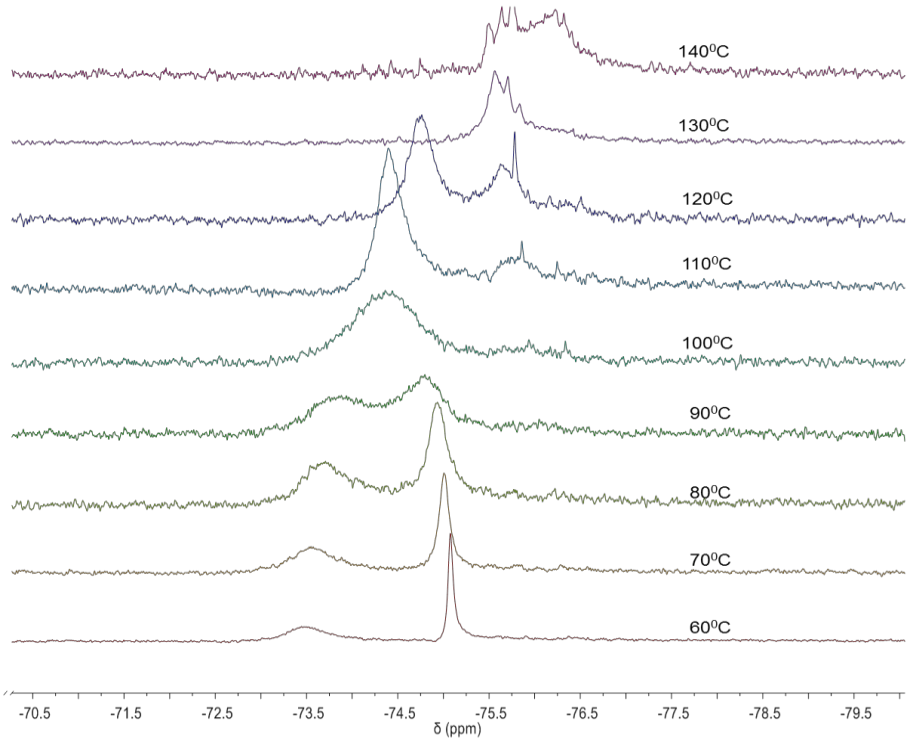


Figure S85. VT ^{19}F-NMR spectra (376 MHz, 1,2-dichlorobenzene-d_4) of **5**.

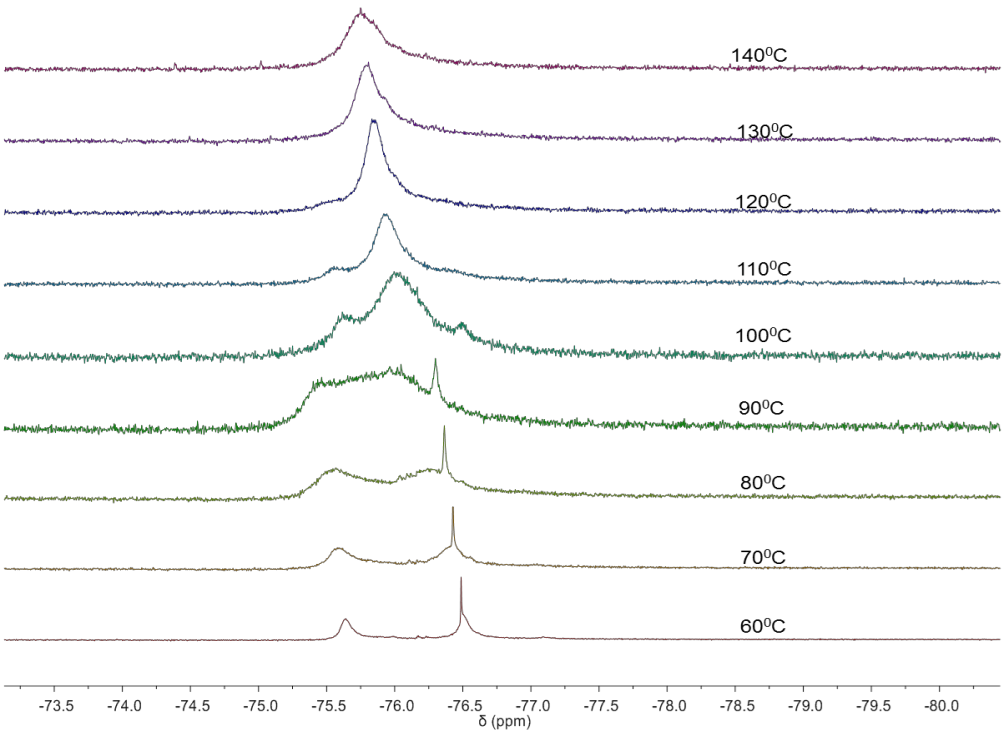


Figure S86. VT ^{19}F-NMR spectra (376 MHz, 1,2-dichlorobenzene-d_4) of **18**.

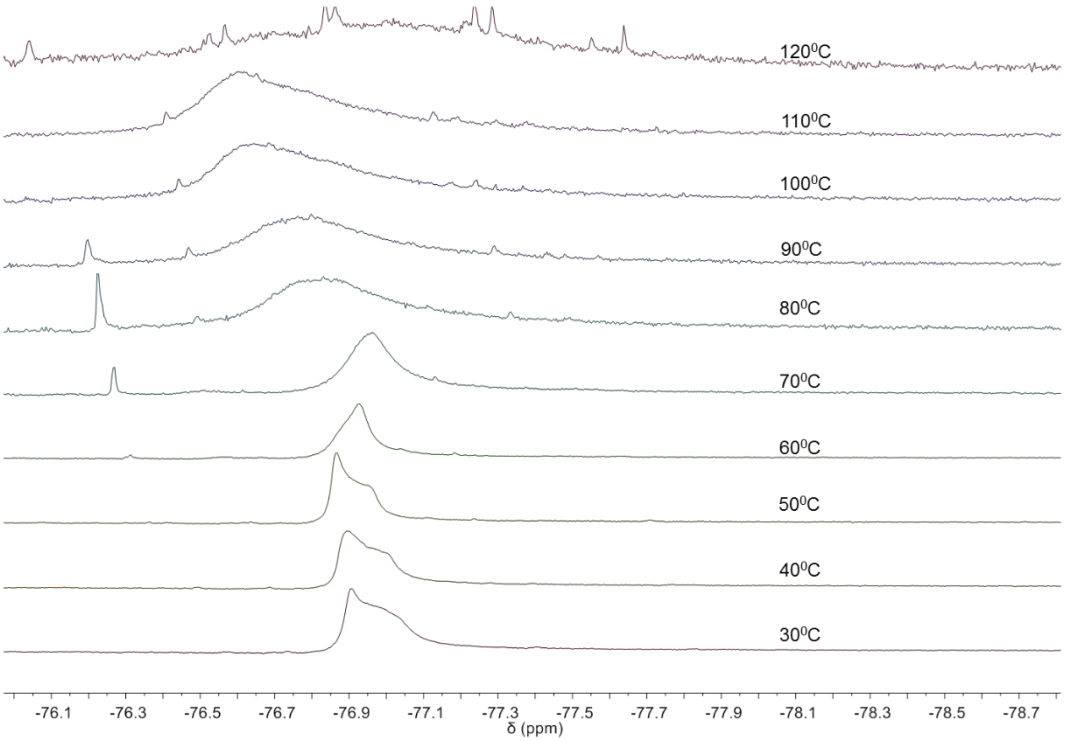


Figure S87. VT-^{19}F NMR spectra (376 MHz, toluene-d_8) of compound **20**.

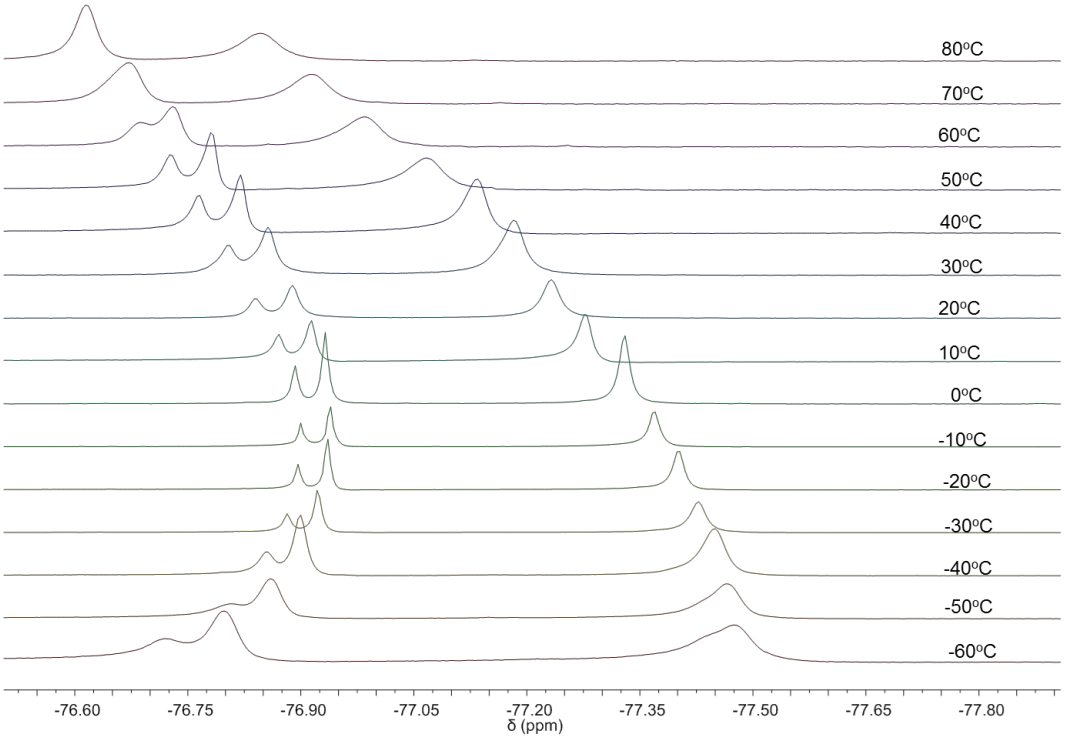


Figure S88. VT ^{19}F-NMR (376 MHz, Toluene-d_8) spectra of **25**.

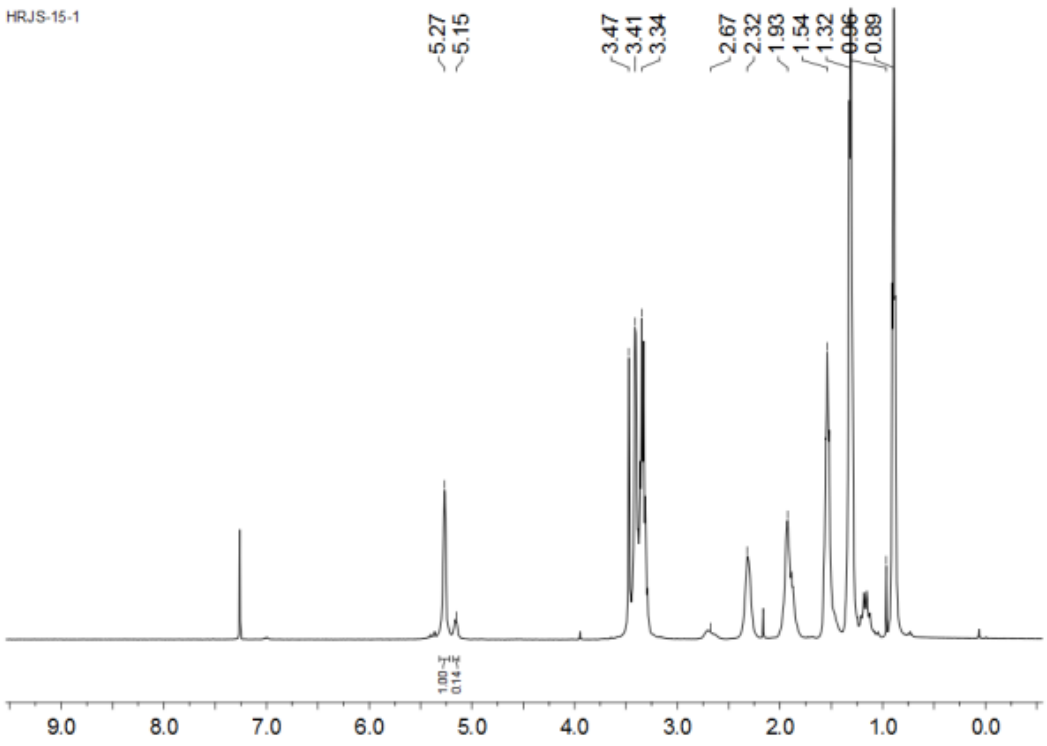


Figure S89. ^{1}H-NMR (400MHz, $CDCl_3$) of poly(2,3-bis(pentyloxymethyl)bicyclo-[2.2.1]hept-5-ene) prepared by the action of **3**. σ_{trans} = 90%.

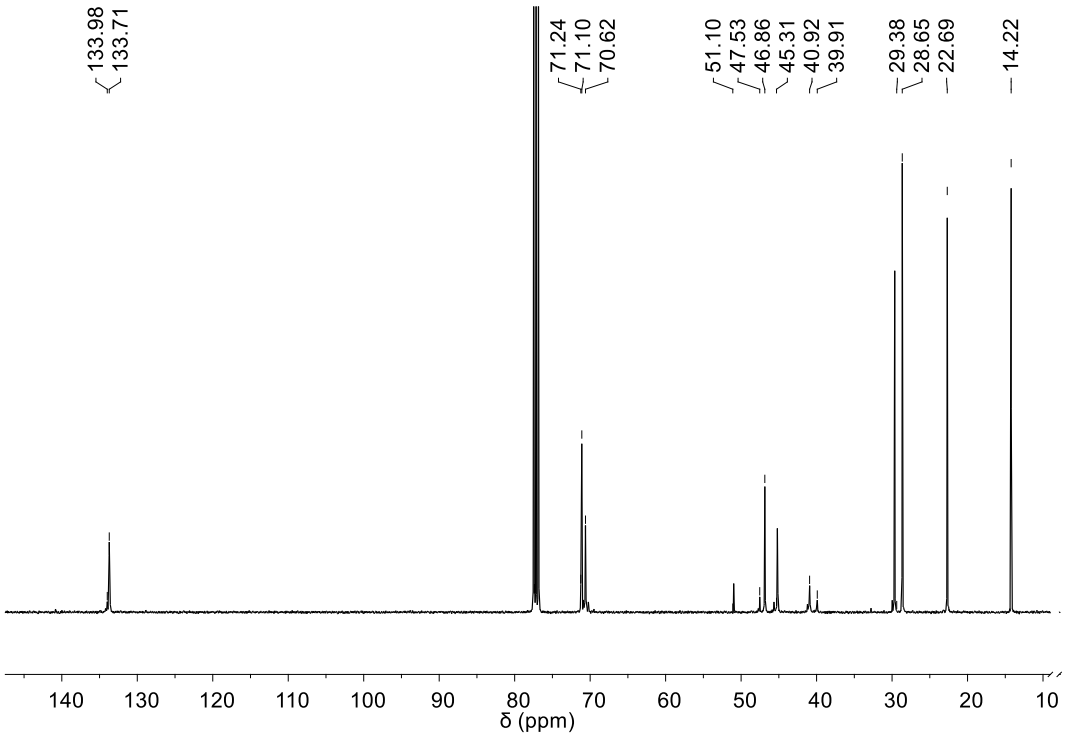


Figure S90. ^{13}C-NMR (101 MHz, $CDCl_3$) of poly(2,3-bis(pentyloxymethyl)bicyclo-[2.2.1]hept-5-ene) prepared by the action of **3**.

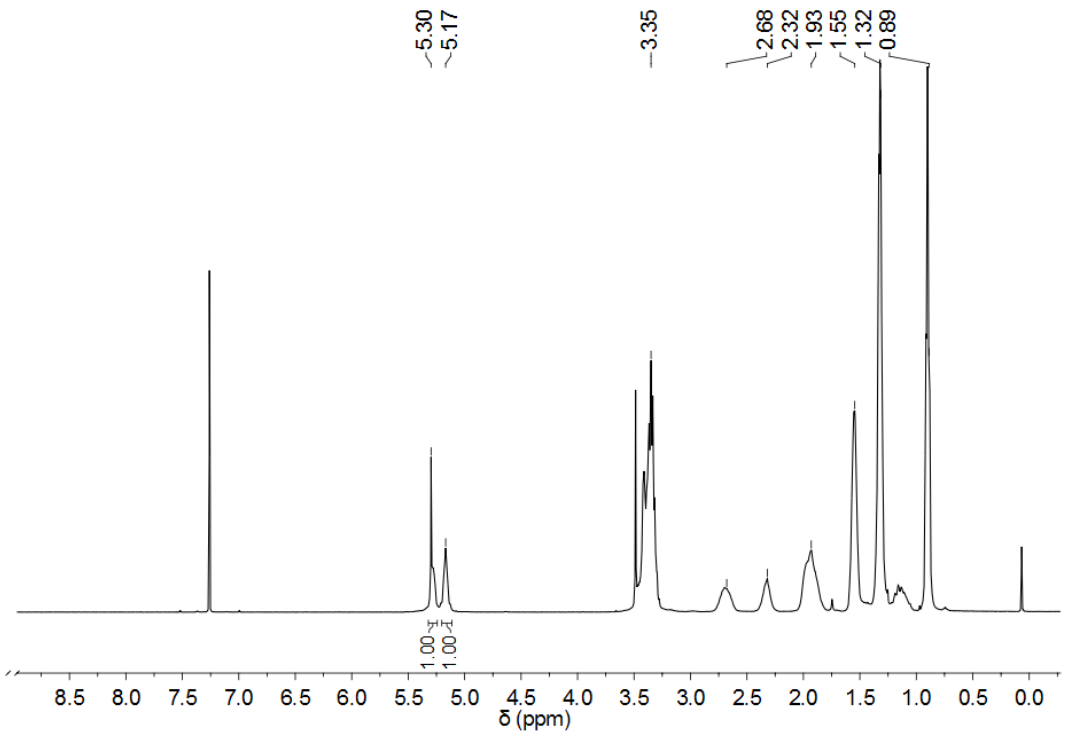


Figure S91. ^{1}H-NMR (400MHz, $CDCl_3$) of poly(2,3-bis(pentyloxymethyl)bicyclo-[2.2.1]hept-5-ene) prepared by the action of **4**. σ_{trans} = 50%.

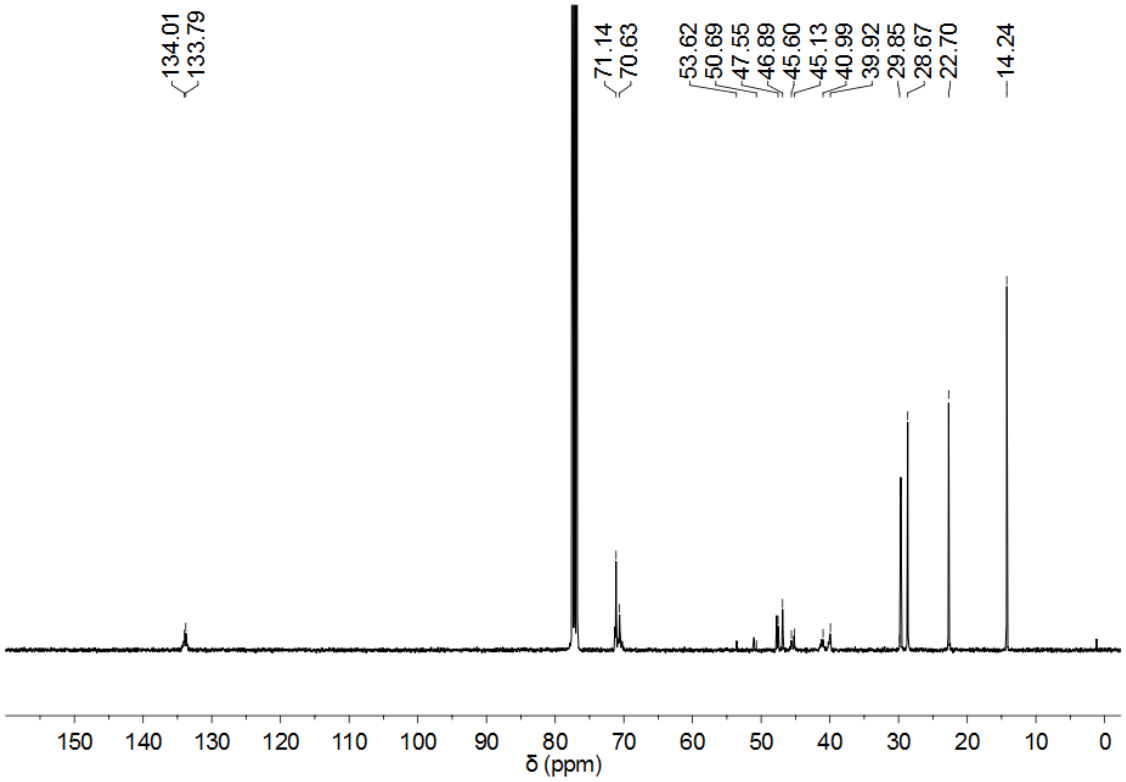


Figure S92. ^{13}C-NMR (101 MHz, $CDCl_3$) of poly(2,3-bis(pentyloxymethyl)bicyclo-[2.2.1]hept-5-ene) prepared by the action of **4**.

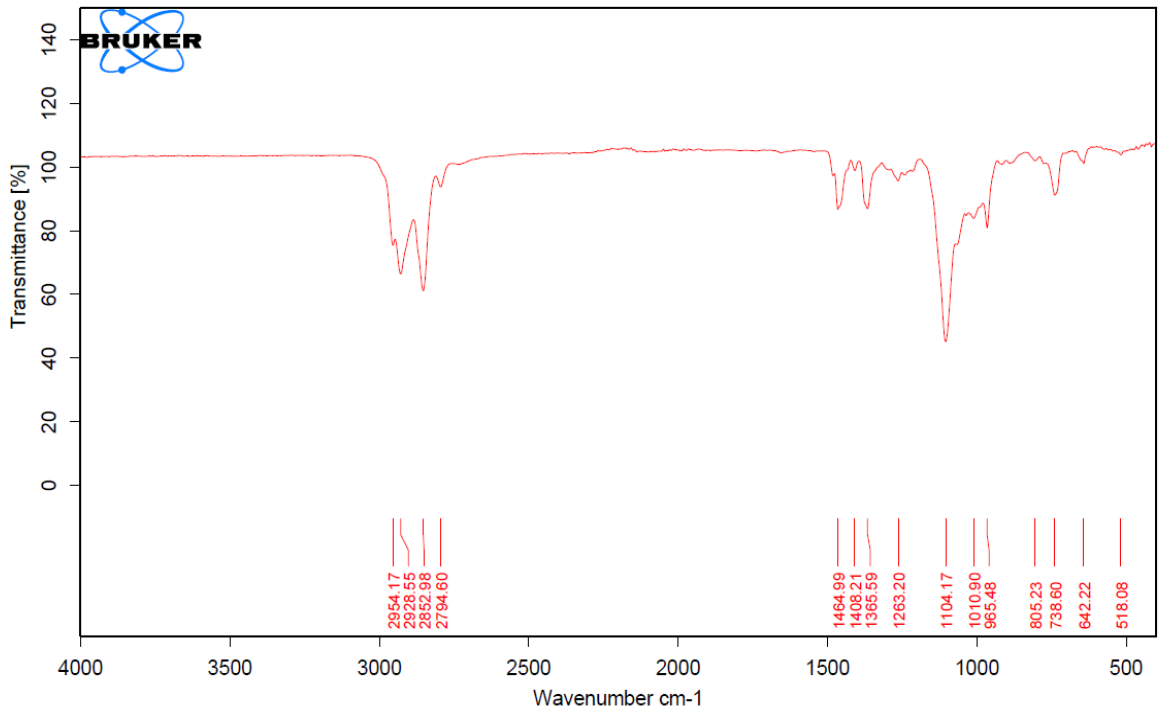


Figure S93. IR spectrum of poly(2,3-bis((pentyloxy)methyl)bicyclo[2.2.1]hept-2-ene) prepared by the action of **4**.

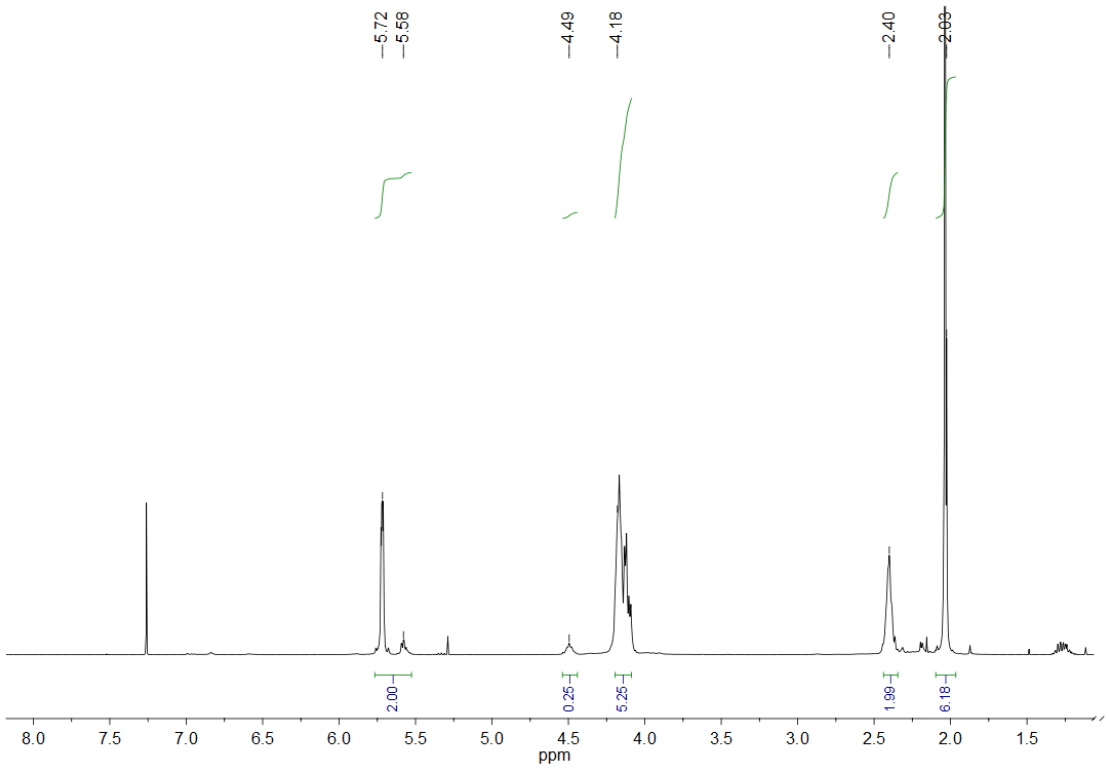


Figure S94. ^{1}H-NMR (400 MHz, $CDCl_3$) of poly(7-oxabicyclo[2.2.1]hept-5-ene-2,3-diylbis(methylene)diacetate) obtained by the action of **3**. σ_{trans}=85%.

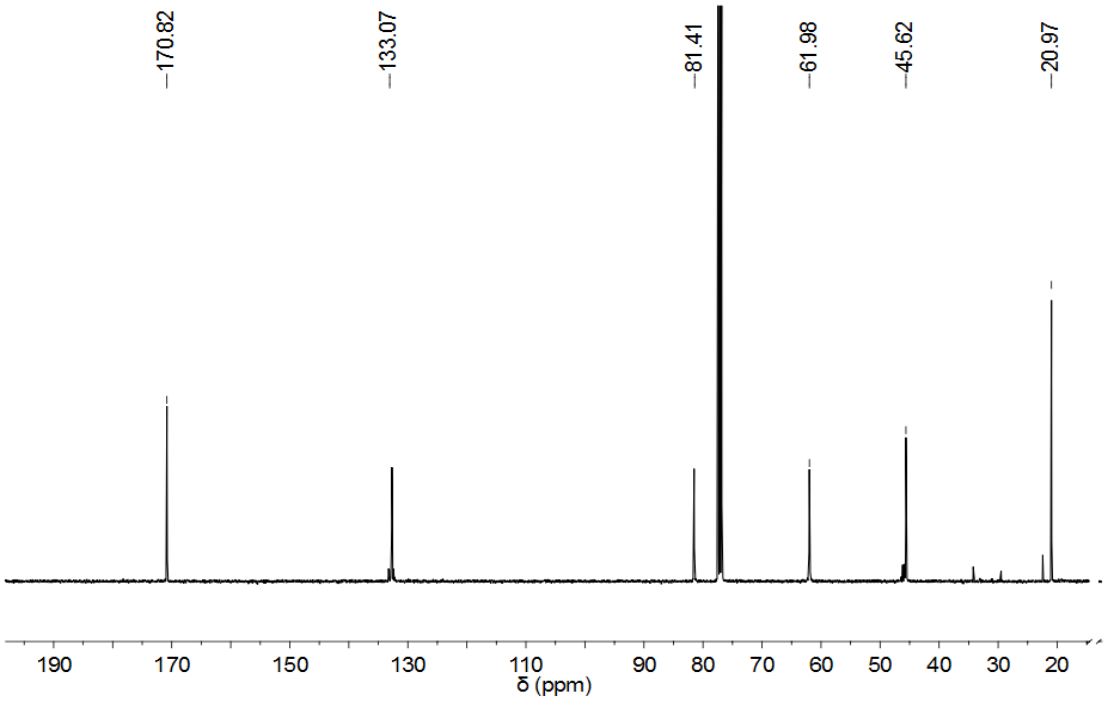


Figure S95. ^{13}C-NMR (101 MHz, $CDCl_3$) of poly(7-oxabicyclo[2.2.1]hept-5-ene-2,3-diylbis(methylene)diacetate) obtained by the action of **3**.

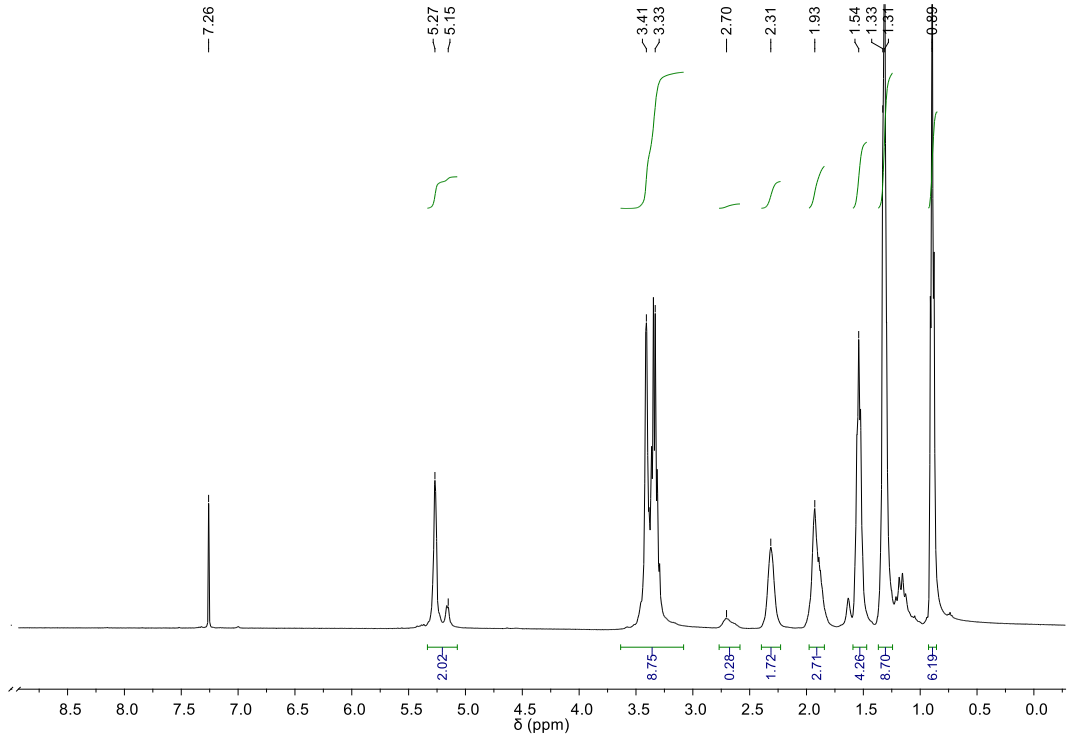


Figure S96. ^{1}H-NMR (400MHz, $CDCl_3$) of poly(2,3-bis(pentyloxymethyl)bicyclo-[2.2.1]hept-5-ene) prepared by the action of **5**. σ_{trans} = 95%.

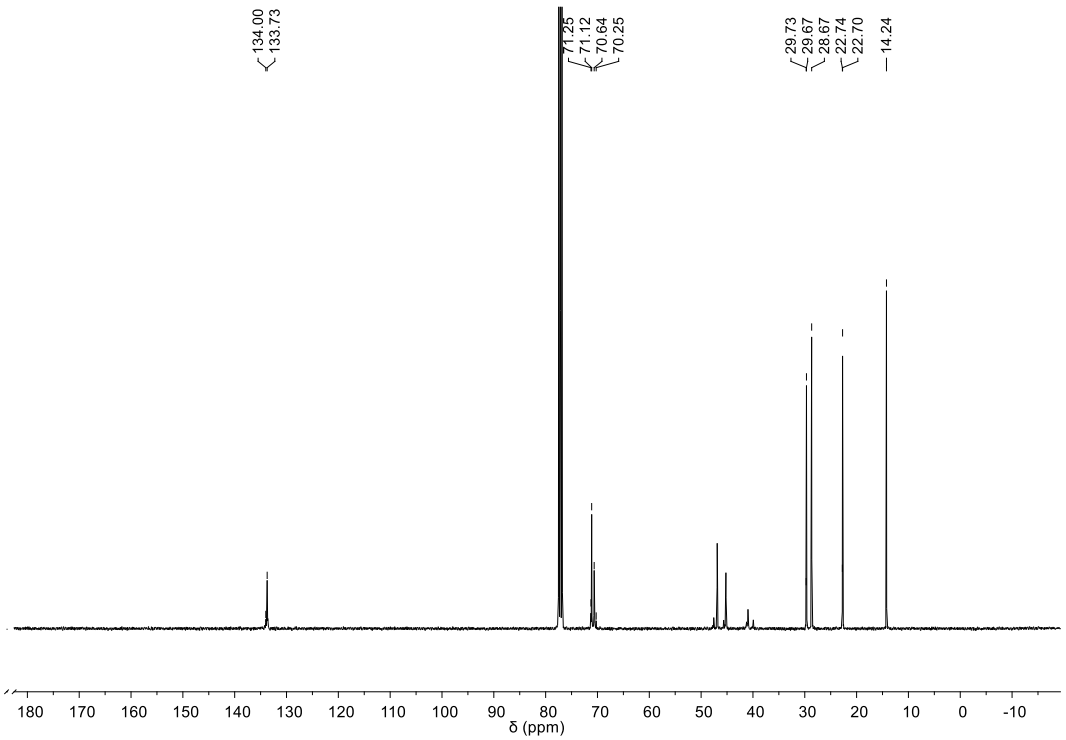


Figure S97. ^{13}C-NMR (101 MHz, $CDCl_3$) of poly(2,3-bis(pentyloxymethyl)bicyclo-[2.2.1]hept-5-ene) prepared by the action of **5**.

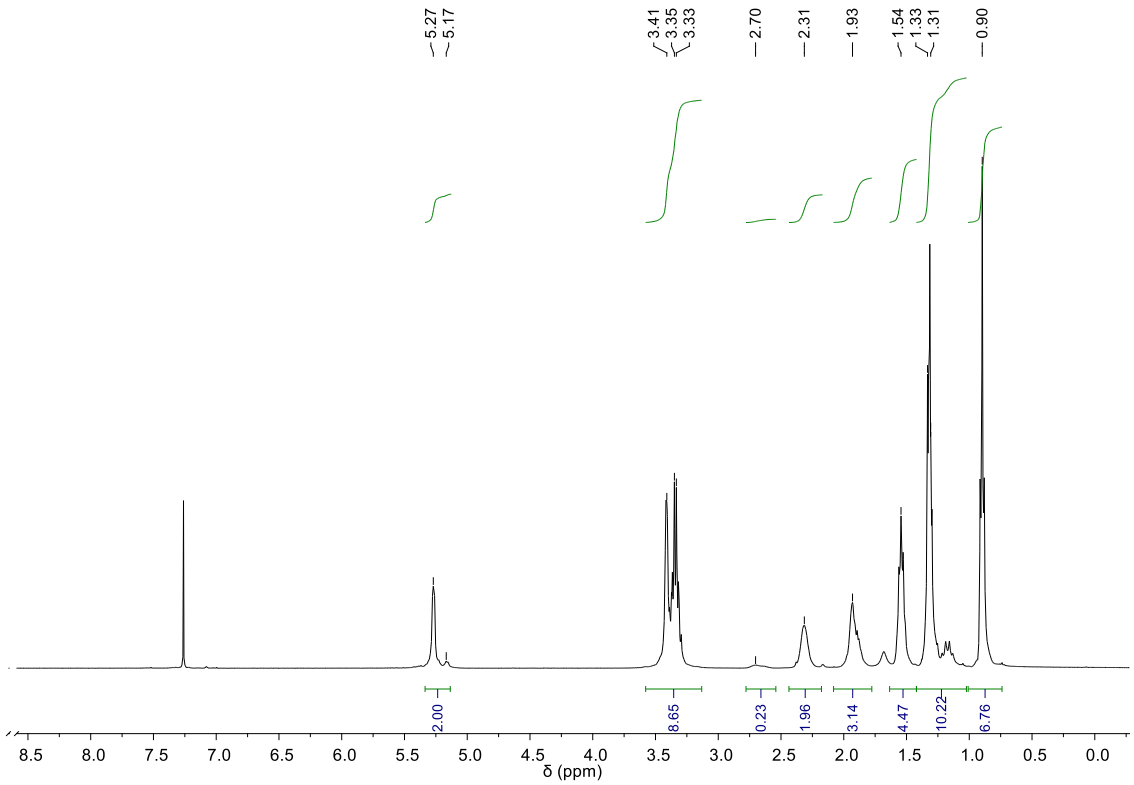


Figure S98. ^{1}H-NMR (400MHz, $CDCl_3$) of poly(2,3-bis(pentyloxymethyl)bicyclo-[2.2.1]hept-5-ene) prepared by the action of **6**. σ_{trans} = 95%.

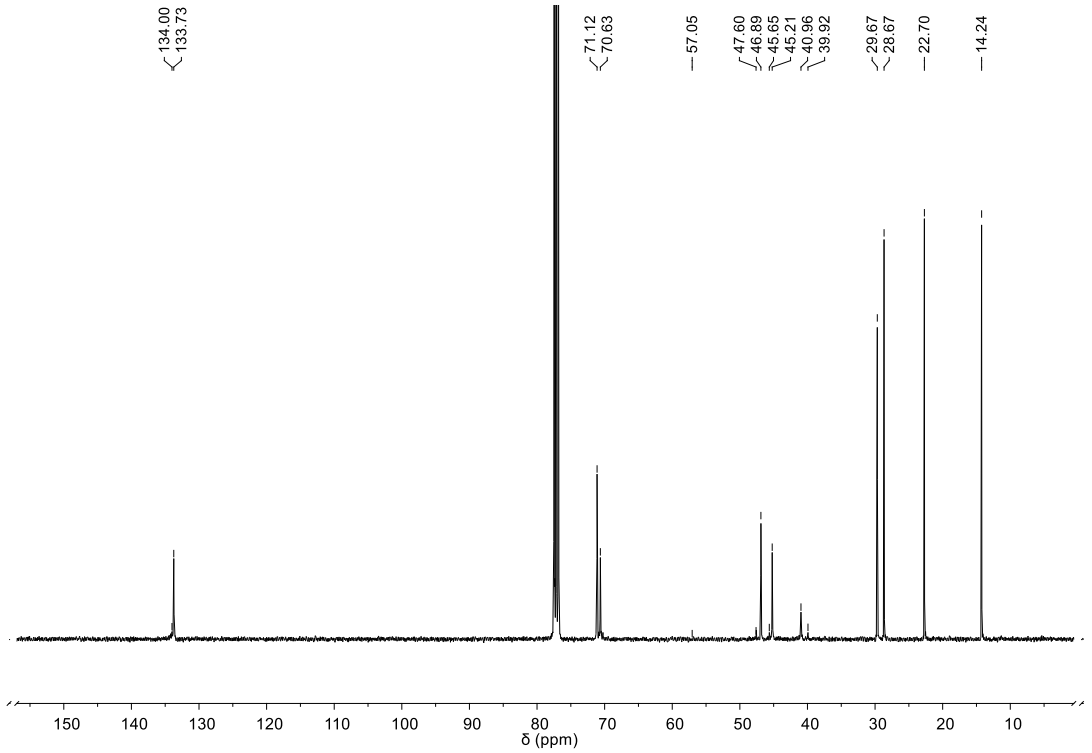


Figure S99. ^{13}C-NMR (101 MHz, $CDCl_3$) of poly(2,3-bis(pentyloxymethyl)bicyclo-[2.2.1]hept-5-ene) prepared by the action of **6**.

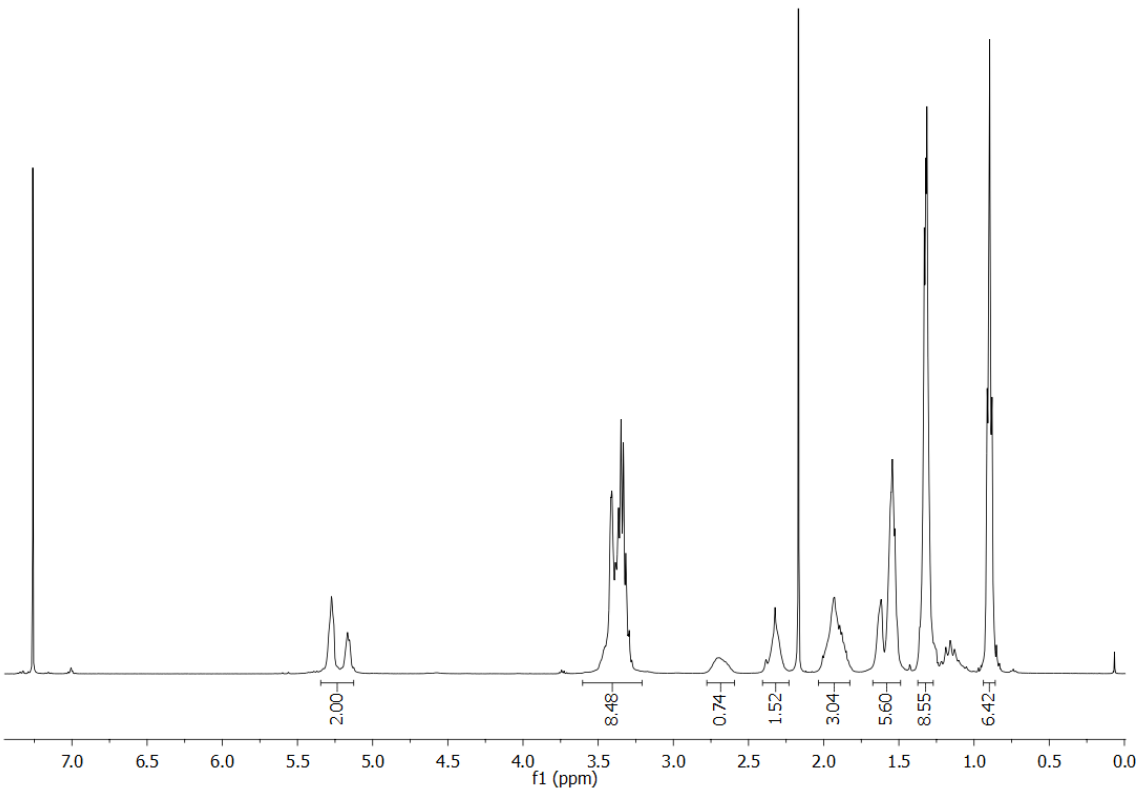


Figure S100. ^{1}H-NMR (400MHz, $CDCl_3$) of poly(2,3-bis(pentyloxymethyl)bicyclo-[2.2.1]hept-5-ene) prepared by the action of **7**. σ_{trans} = 64%.

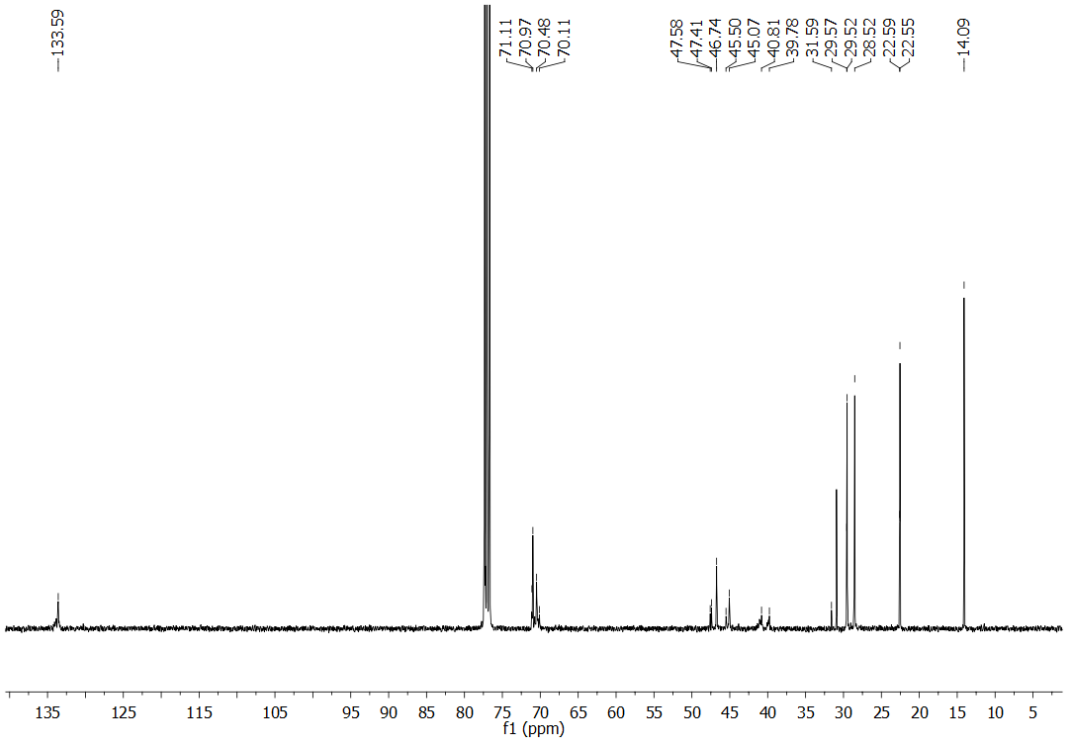


Figure S101. ^{13}C-NMR (101 MHz, $CDCl_3$) of poly(2,3-bis(pentyloxymethyl)bicyclo-[2.2.1]hept-5-ene) prepared by the action of **7**.

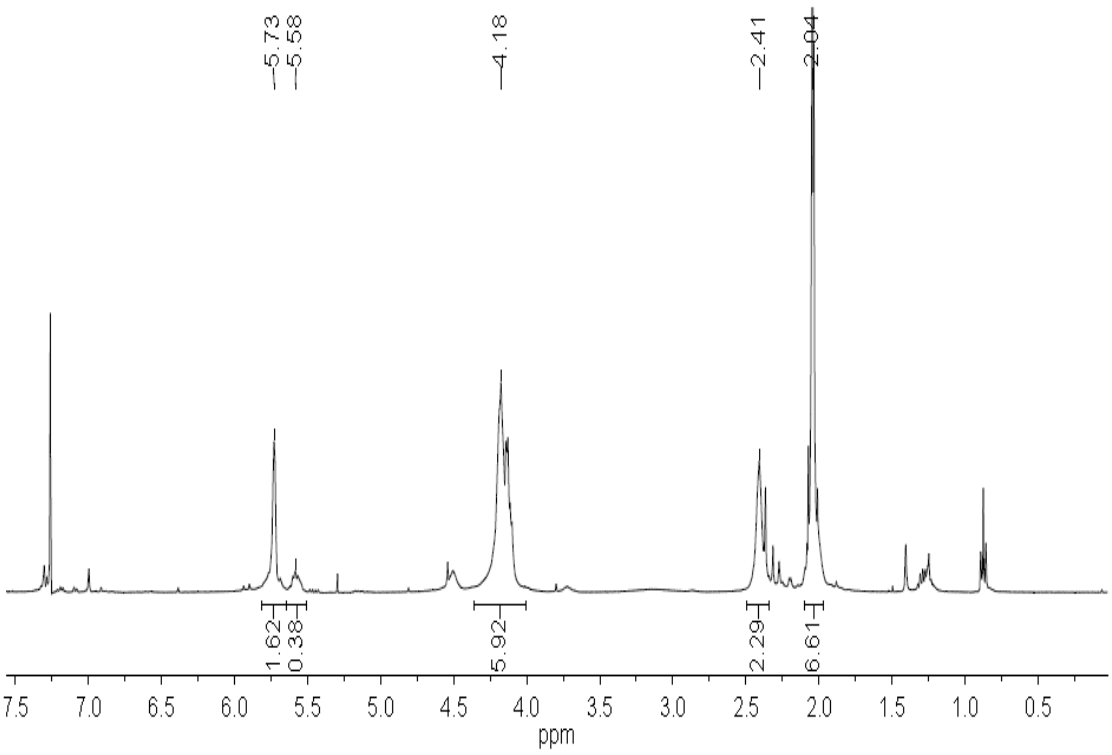


Figure S102. ^{1}H-NMR (400 MHz, $CDCl_3$) of poly(7-oxabicyclo[2.2.1]hept-5-ene-2,3-diylbis(methylene)diacetate) obtained by the action of **5**. σ_{trans} = 81%.

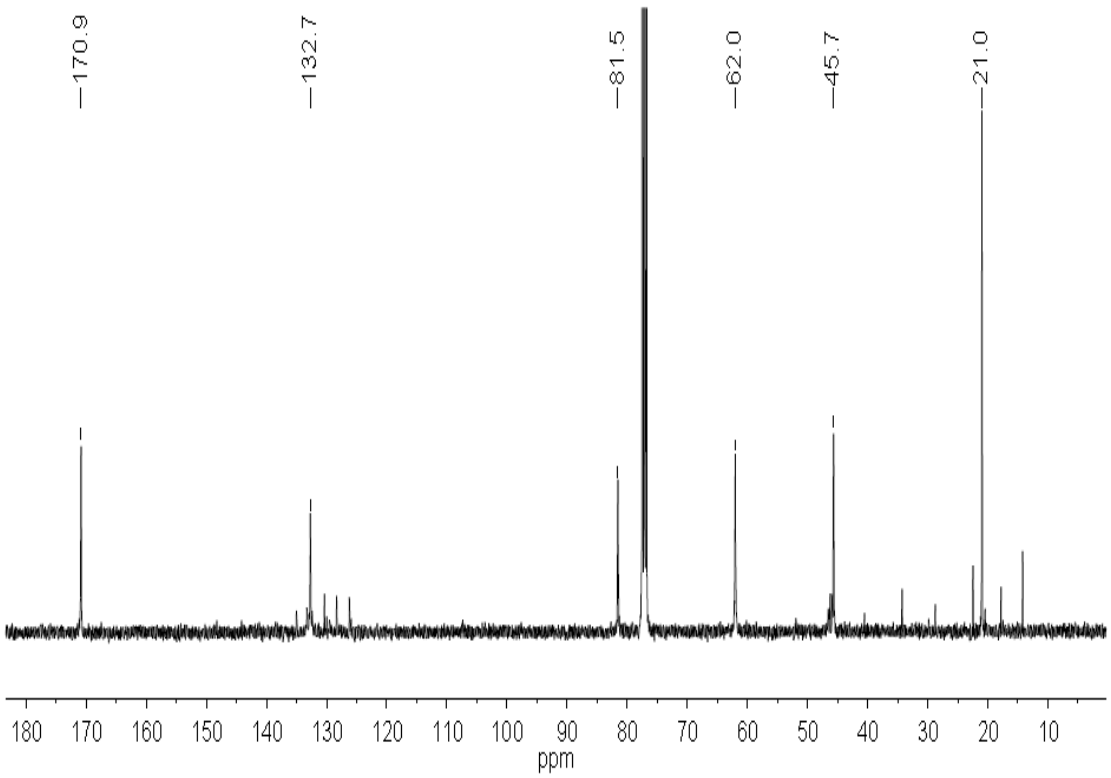


Figure S103. ^{13}C-NMR (101 MHz, $CDCl_3$) of poly(7-oxabicyclo[2.2.1]hept-5-ene-2,3-diylbis(methylene)diacetate) obtained by the action of **5**.

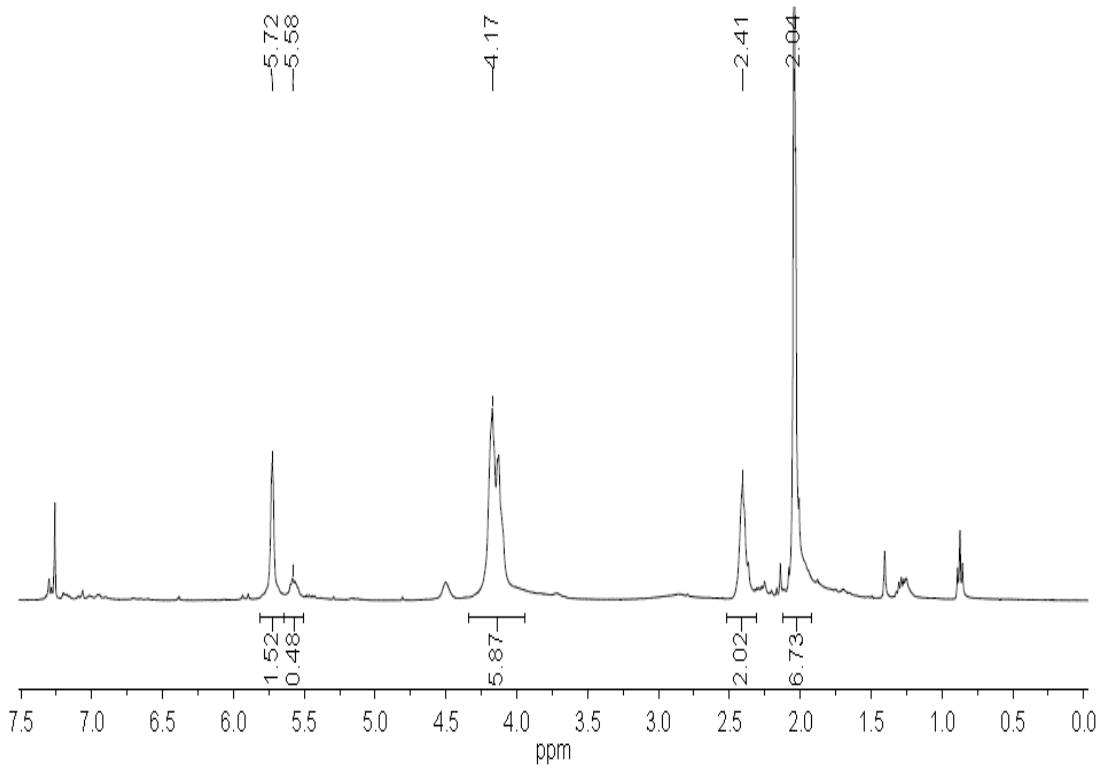


Figure S104. ^{1}H-NMR (400 MHz, $CDCl_3$) of poly(7-oxabicyclo[2.2.1]hept-5-ene-2,3-diylbis(methylene)diacetate) obtained by the action of **6**. σ_{trans} = 76%.

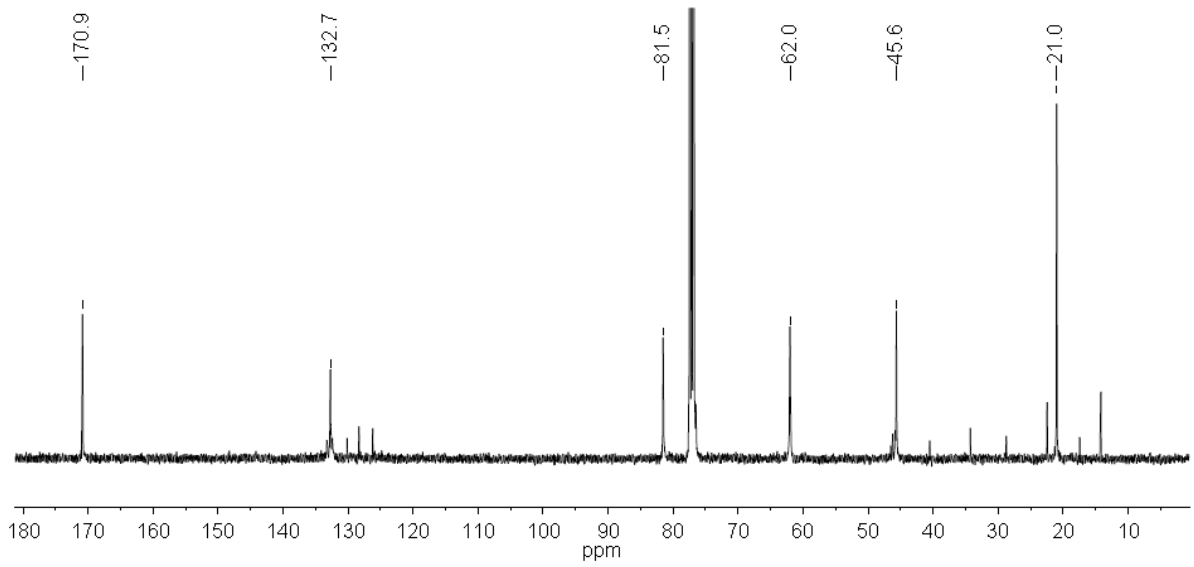


Figure S105. ^{13}C-NMR (101 MHz, $CDCl_3$) of poly(7-oxabicyclo[2.2.1]hept-5-ene-2,3-diylbis(methylene)diacetate) obtained by the action of **6**.

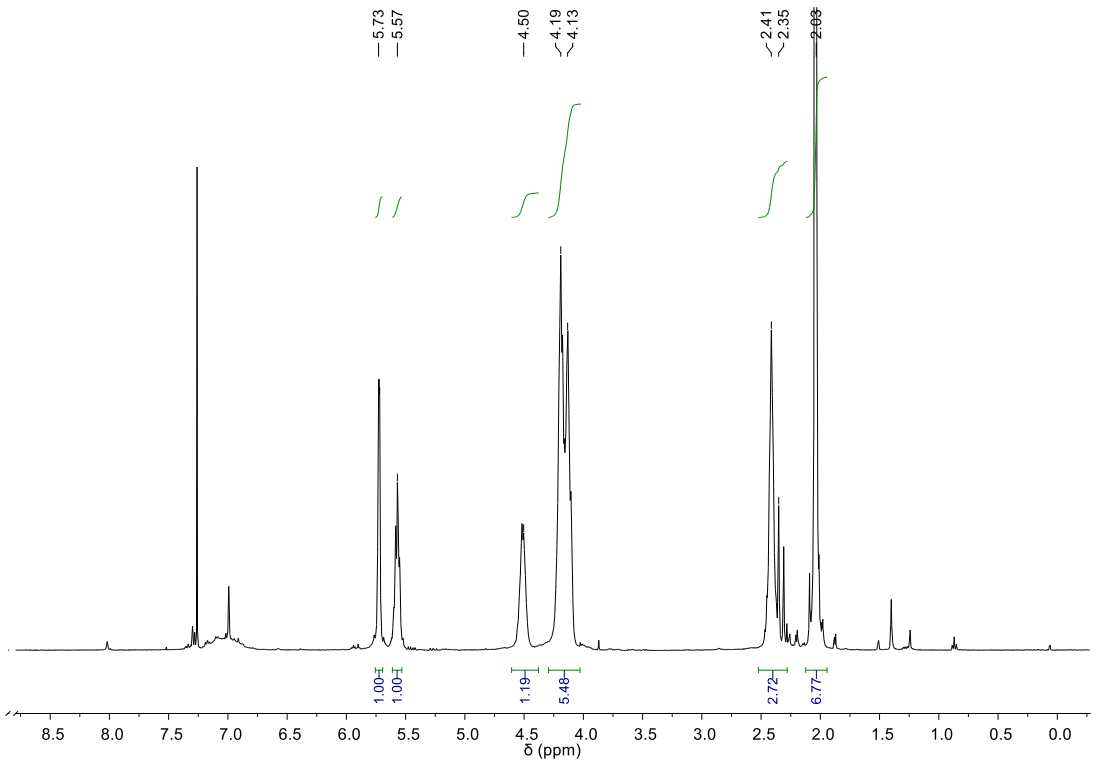


Figure S106. ^{1}H-NMR (400 MHz, $CDCl_3$) of poly(7-oxabicyclo[2.2.1]hept-5-ene-2,3-diylbis(methylene)diacetate) obtained by the action of **7**. σ_{trans} = 50%.

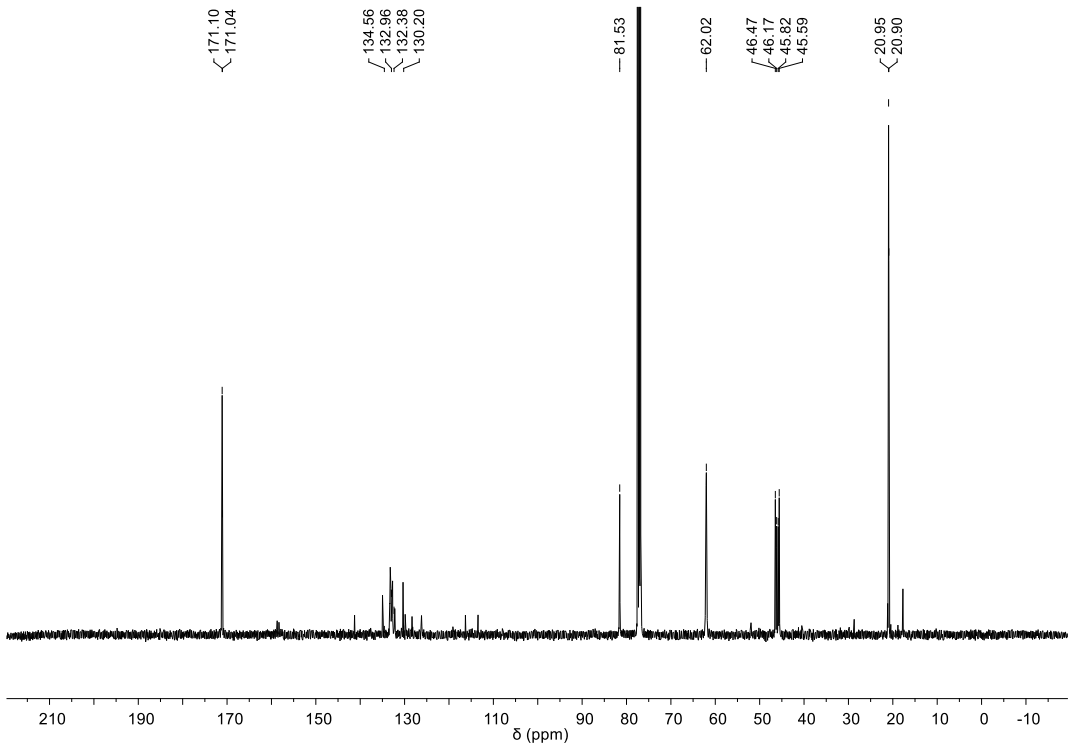


Figure S107. ^{13}C-NMR (101 MHz, $CDCl_3$) of poly(7-oxabicyclo[2.2.1]hept-5-ene-2,3-diylbis(methylene)diacetate) obtained by the action of **7**

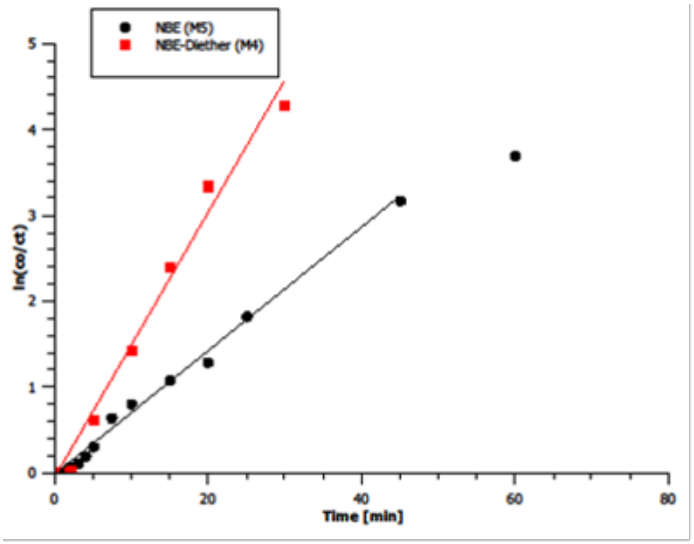


Figure S108. Kintecis of 2,3-bis(pentyloxymethyl)bicyclo-[2.2.1]hept-5-ene) during polymerzation by action of **3**.

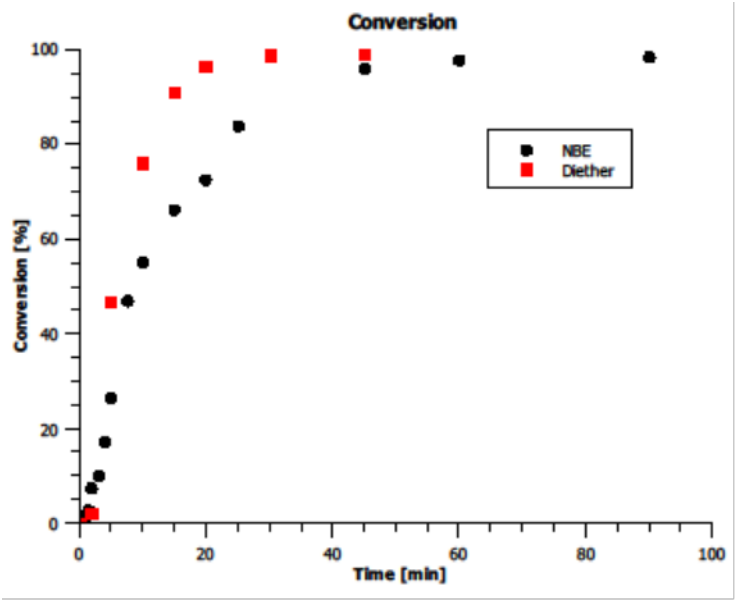


Figure S109. Conversion of of 2,3-bis(pentyloxymethyl)bicyclo-[2.2.1]hept-5-ene) during polymerzation by action of **3**.

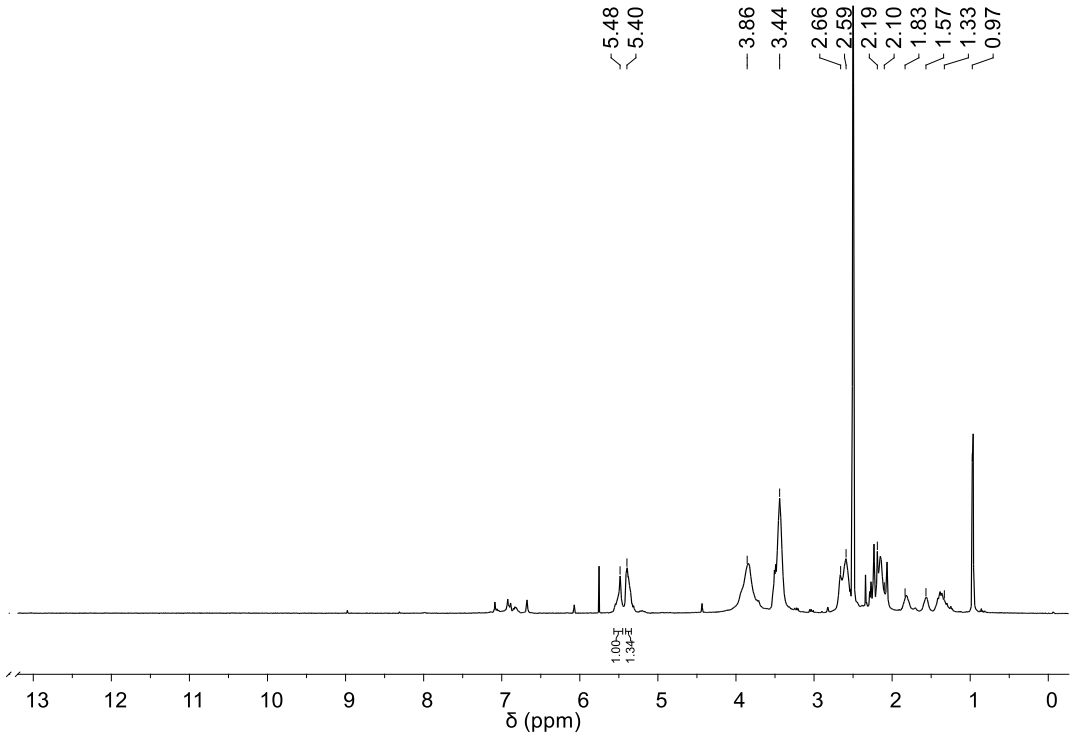


Figure S110. ^{1}H-NMR (400 MHz, DMSO-d_6) of poly(bicyclo [2.2.1]hept-2-ene-2,3-diyldimethanol) obtained by the action of **3**.

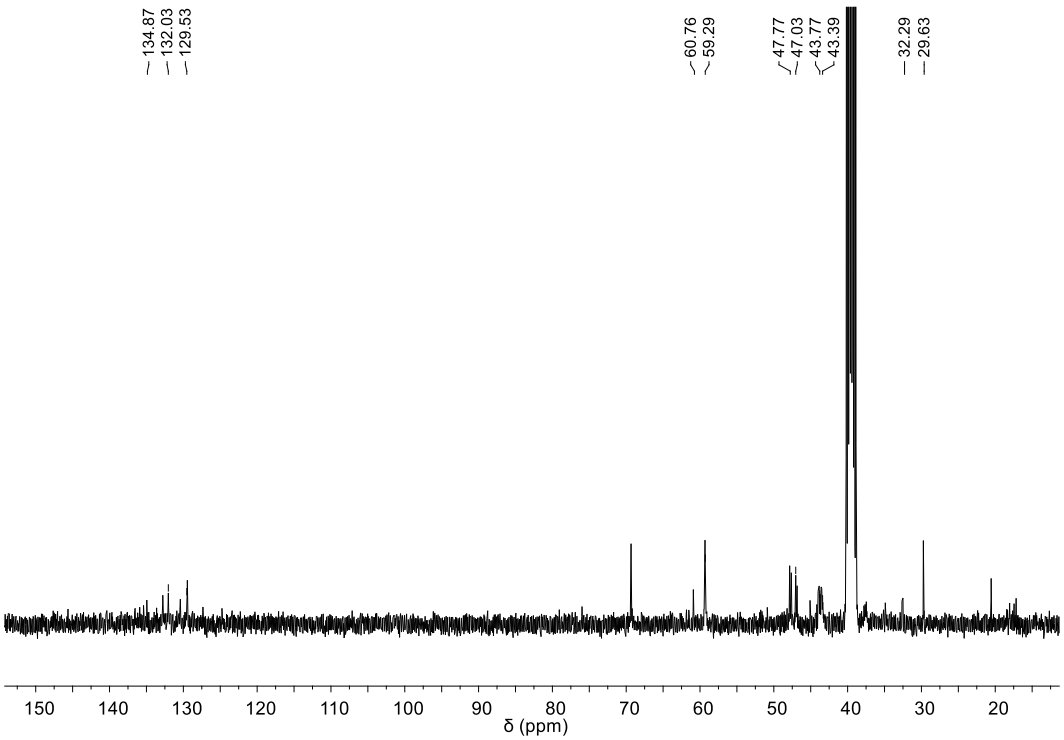


Figure S111. ^{13}C-NMR (101 MHz, DMSO-d_6) of of poly (bicyclo[2.2.1]hept-2-ene-2,3-diyldimethanol) obtained by the action of **3**.

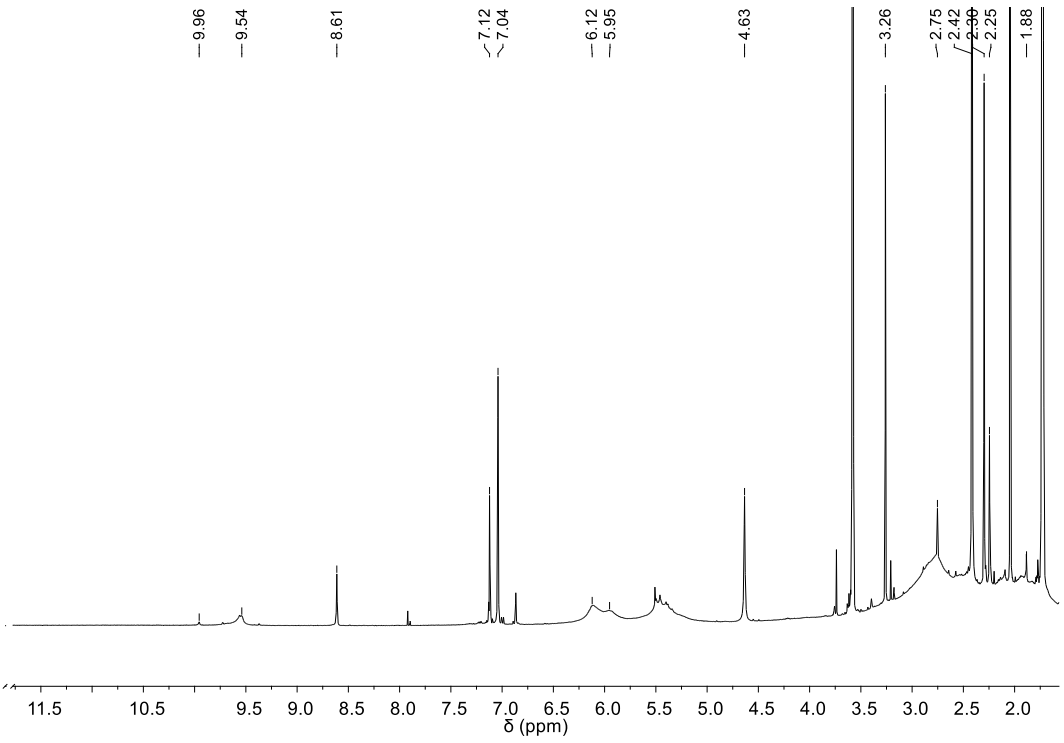


Figure S112. ^{1}H-NMR (400 MHz, THF-d_8) of poly (bicyclo[2.2.1]hept-5-ene-2-carboxaldehyde) obtained by action of **3**.

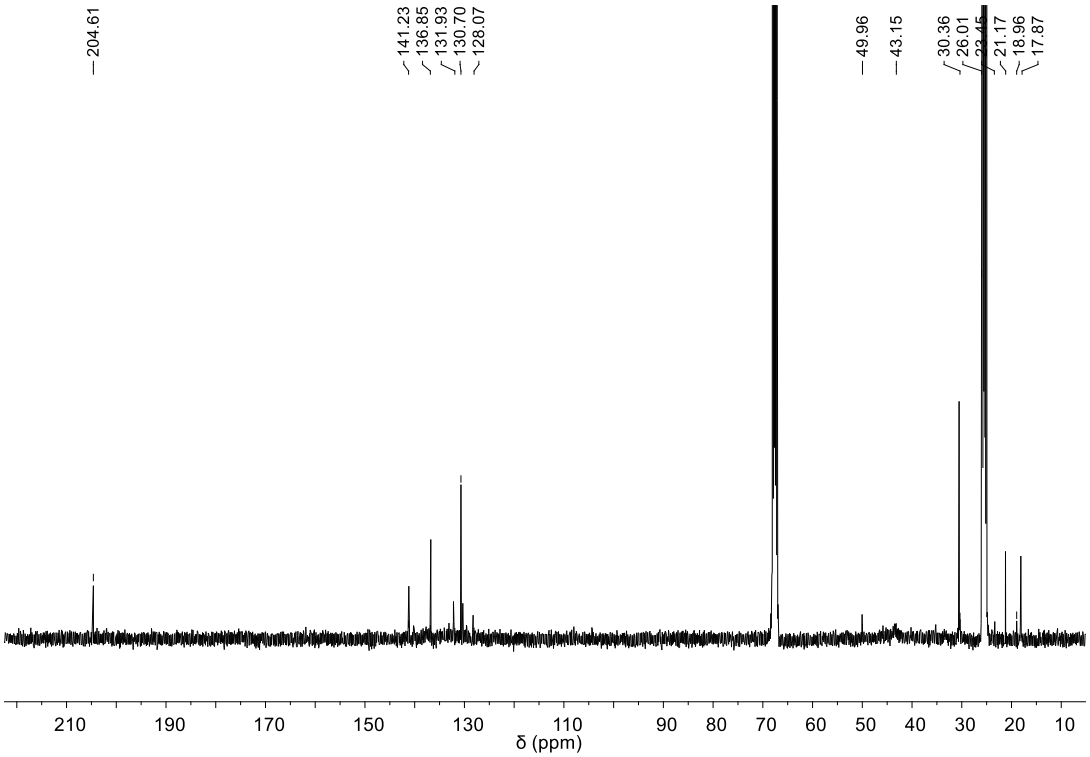


Figure S113. ^{13}C-NMR (101 MHz, THF-d_8) of poly (bicycle [2.2.1]hept-5-ene-2-carboxaldehyde) obtained by action of **3**.

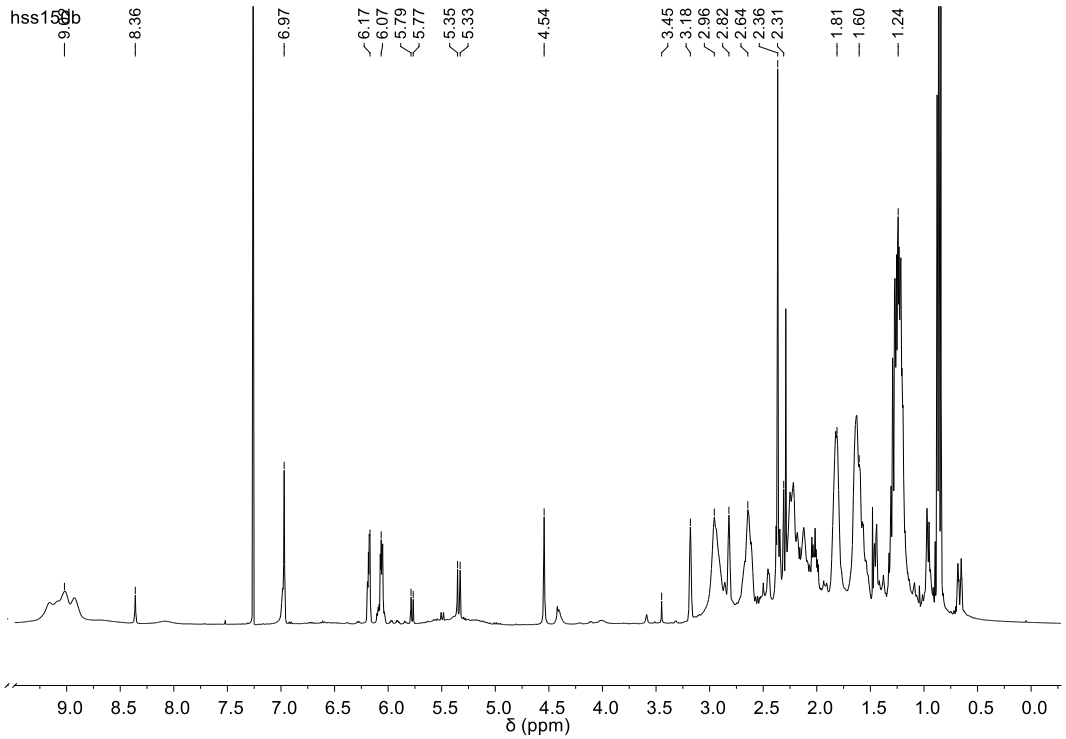


Figure S114. ^{1}H-NMR (400 MHz, $CDCl_3$) of poly(bicyclo[2.2.1]hept-5-ene-2-ylmethyl) cyclohexanamine) obtained by action of **3**.

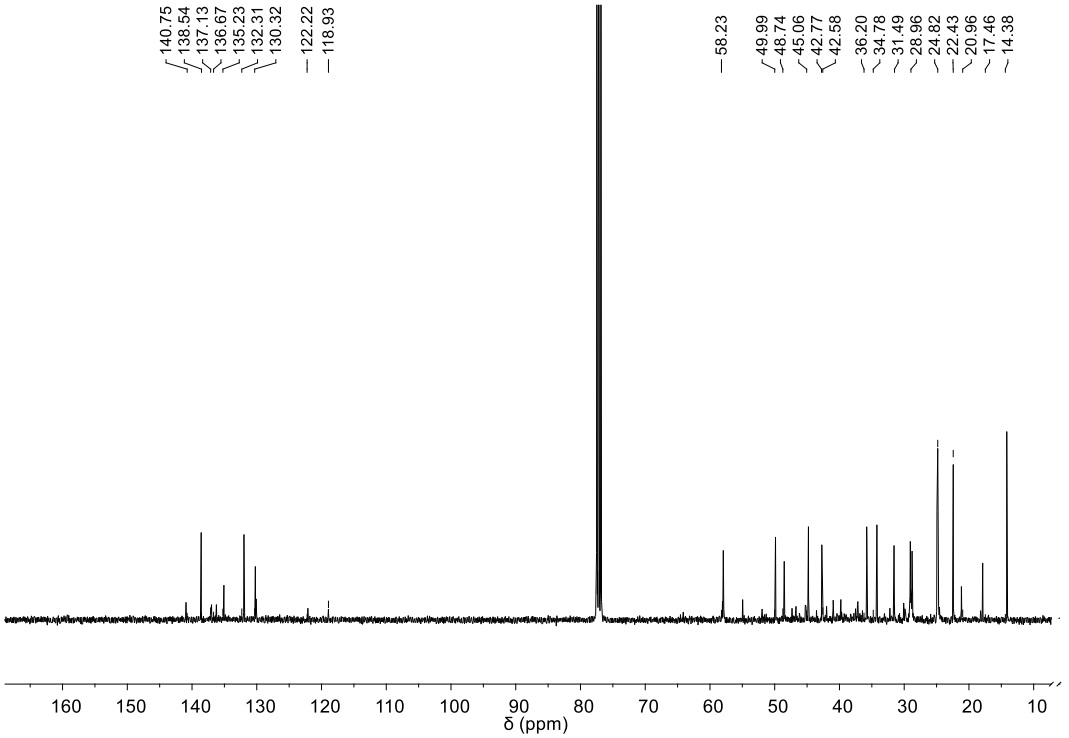


Figure S115. ^{13}C-NMR (101 MHz, $CDCl_3$) of poly (bicyclo[2.2.1]hept-5-ene-2-ylmethyl)cyclohexanamine) obtained by action of **3**.

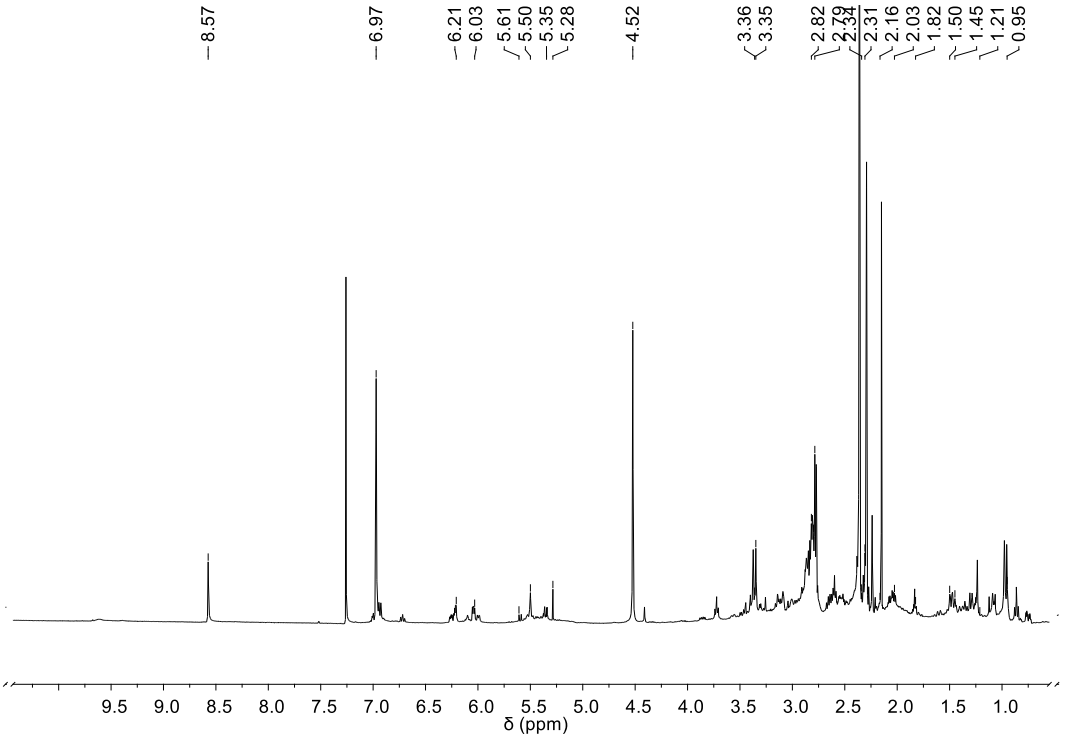


Figure S116. ^{1}H-NMR (400 MHz, $CDCl_3$) of poly (bicyclo[2.2.1]hept-5-ene-2-yl)-N,N-dimethylmethanamine) obtained by action of **3**.

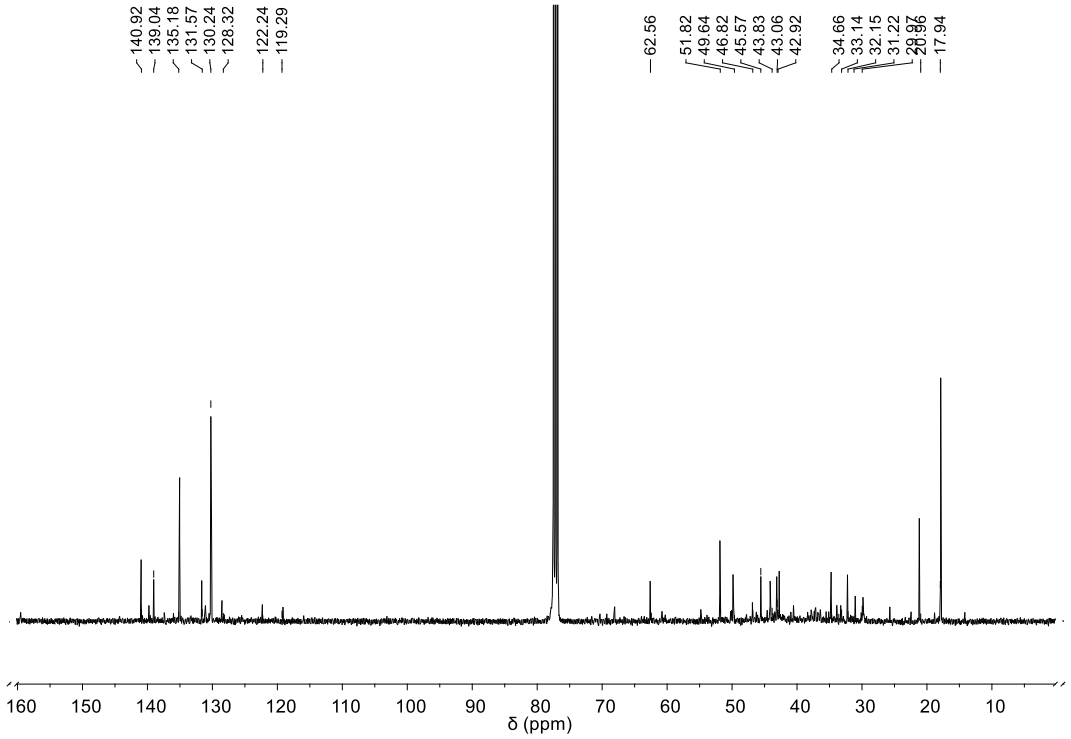


Figure S117. ^{13}C-NMR (101 MHz, $CDCl_3$) of poly(bicyclo[2.2.1]hept-5-ene-2-yl)-N,N-dimethylmethanamine) obtained by action of **5**

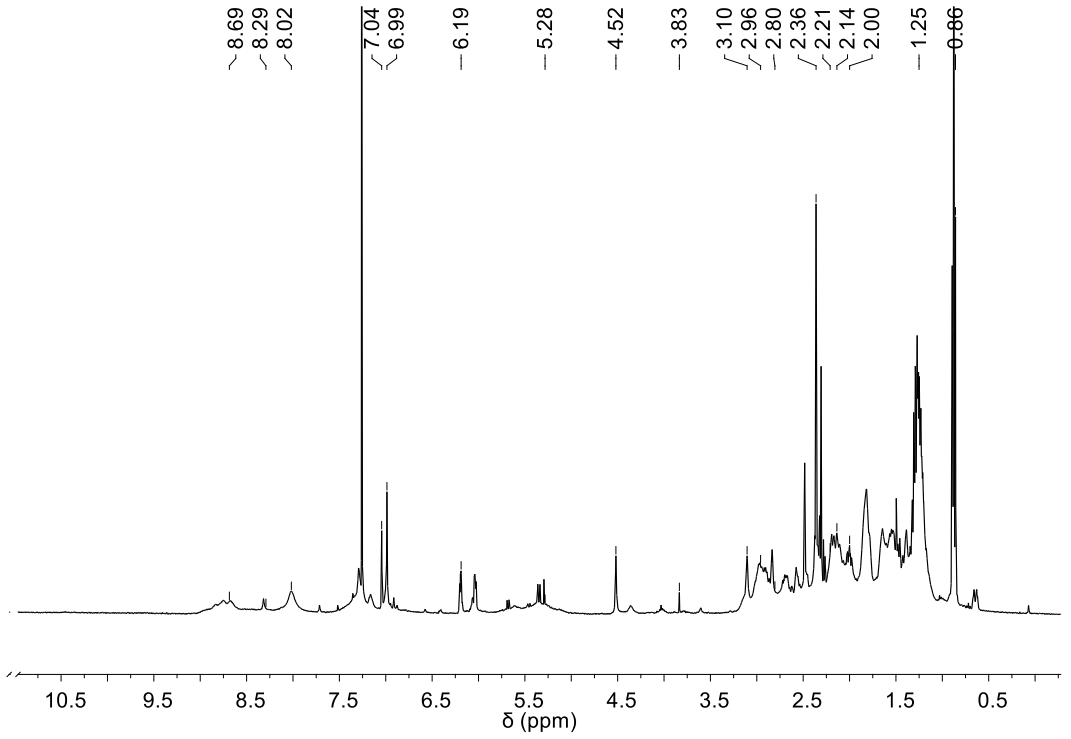


Figure S118. ^{1}H-NMR (400 MHz, $CDCl_3$) of poly(bicyclo[2.2.1]hept-5-ene-2-ylmethyl) cyclohexanamine) obtained by action of **5**.

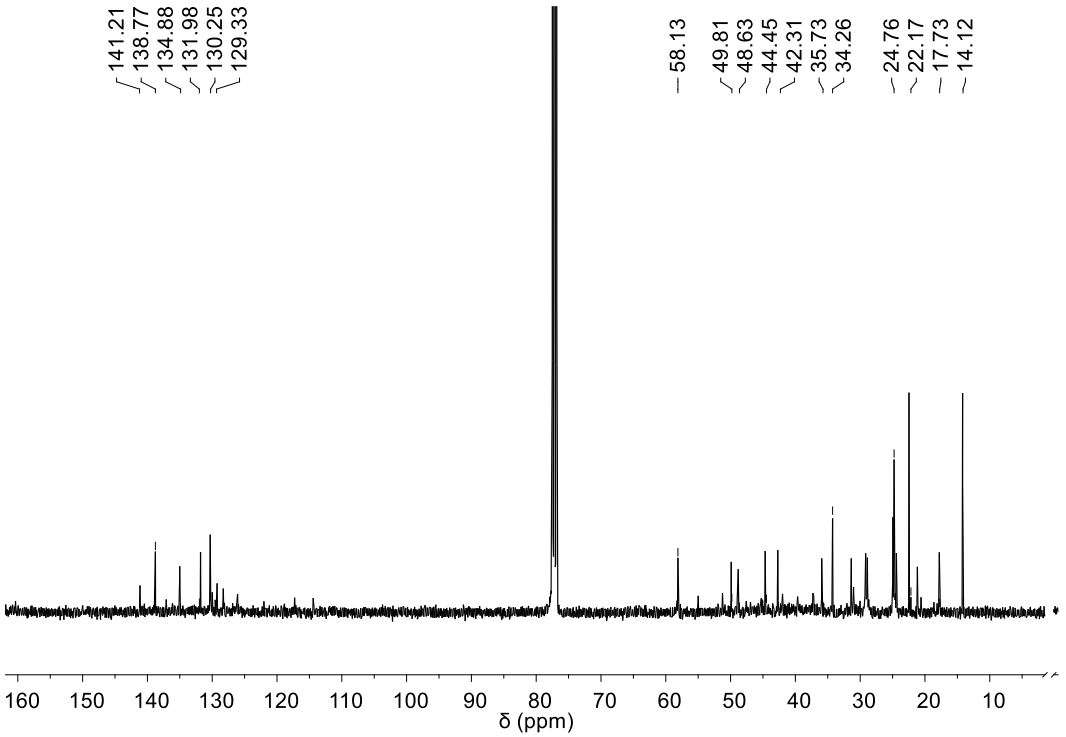


Figure S119. ^{13}C-NMR (101 MHz, $CDCl_3$) of poly (bicyclo[2.2.1]hept-5-ene-2-ylmethyl)cyclohexanamine) obtained by action of **5**.

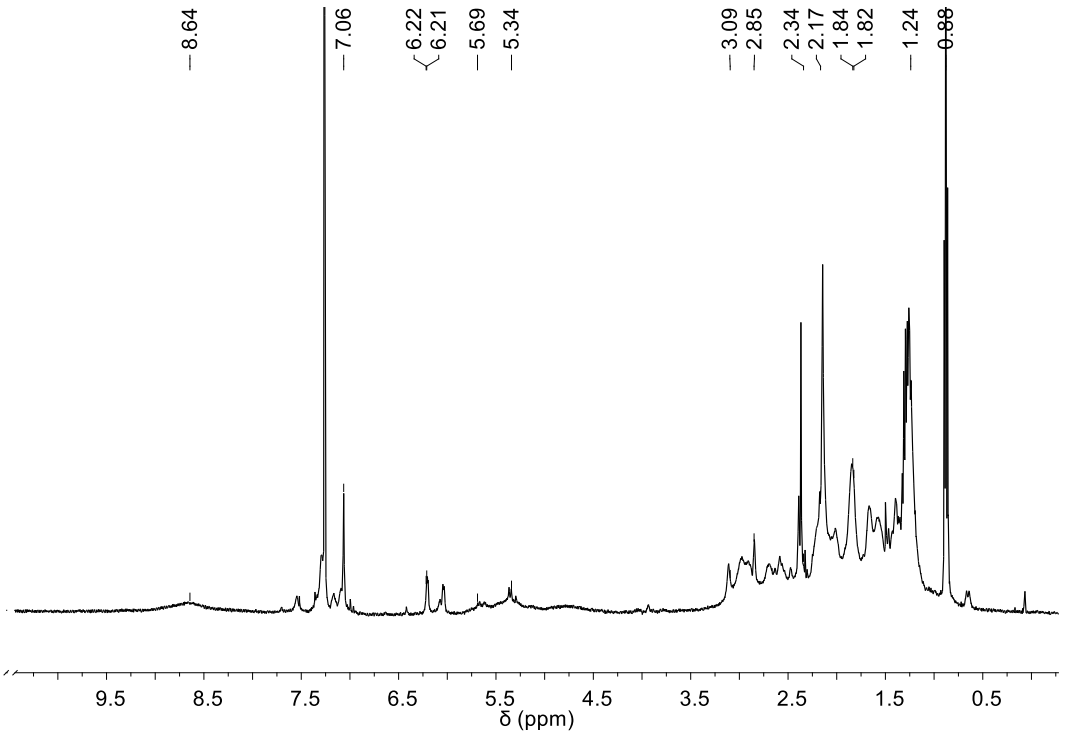


Figure S120. ^{1}H-NMR (400 MHz, $CDCl_3$) of poly(bicyclo[2.2.1]hept-5-ene-2-ylmethyl) cyclohexanamine) obtained by action of **6**.

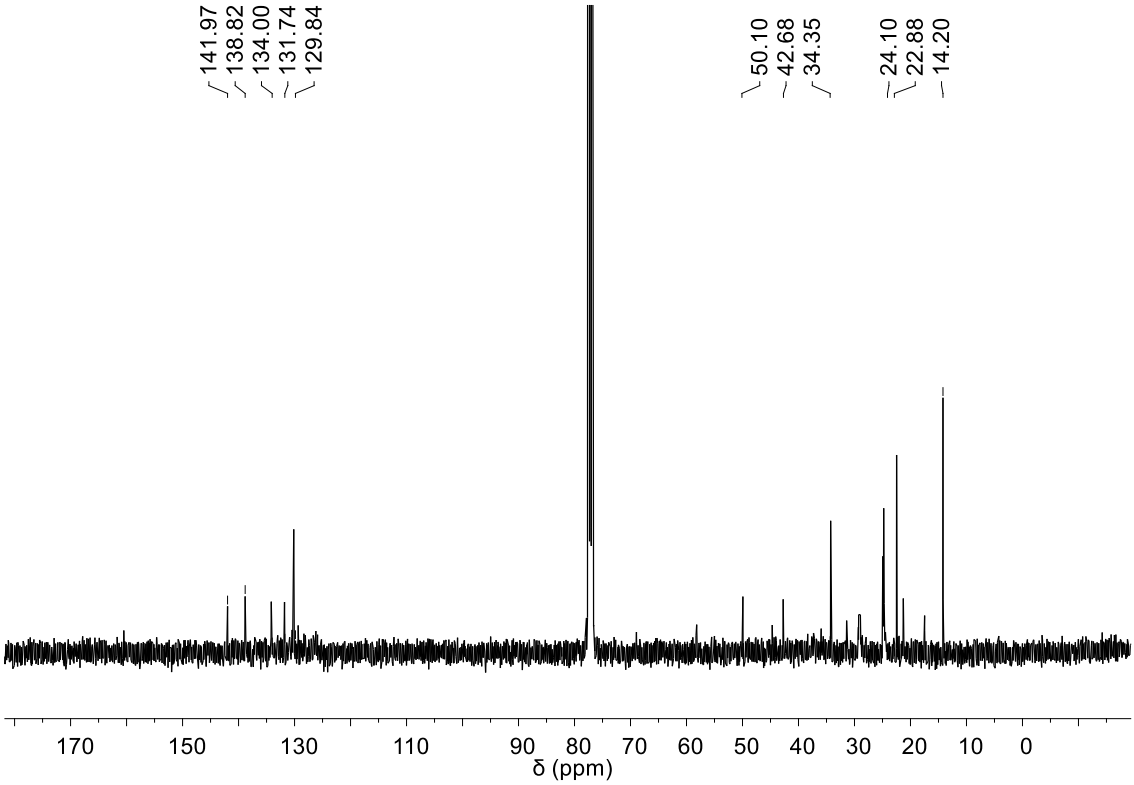


Figure S121. ^{13}C-NMR (101 MHz, $CDCl_3$) of poly(bicyclo[2.2.1]hept-5-ene-2-ylmethyl)cyclohexanamine) obtained by action of **6**.

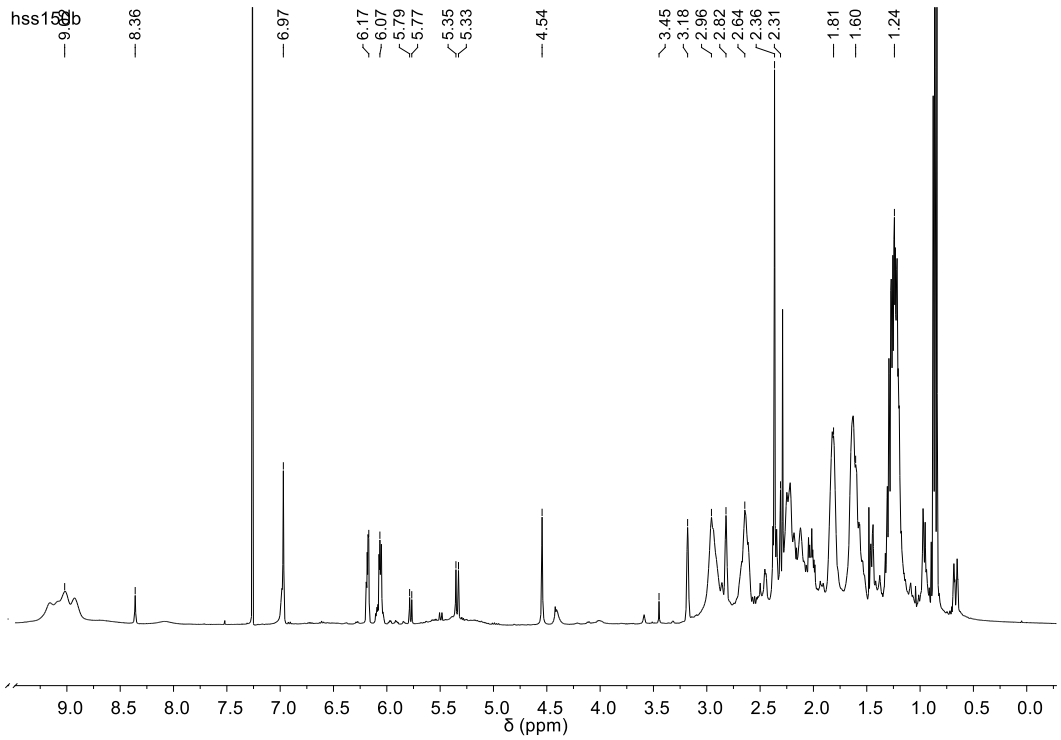


Figure S122. ^{1}H-NMR (400 MHz, $CDCl_3$) of poly(bicyclo[2.2.1]hept-5-ene-2-ylmethyl)cyclohexanamine) obtained by action of **7**.

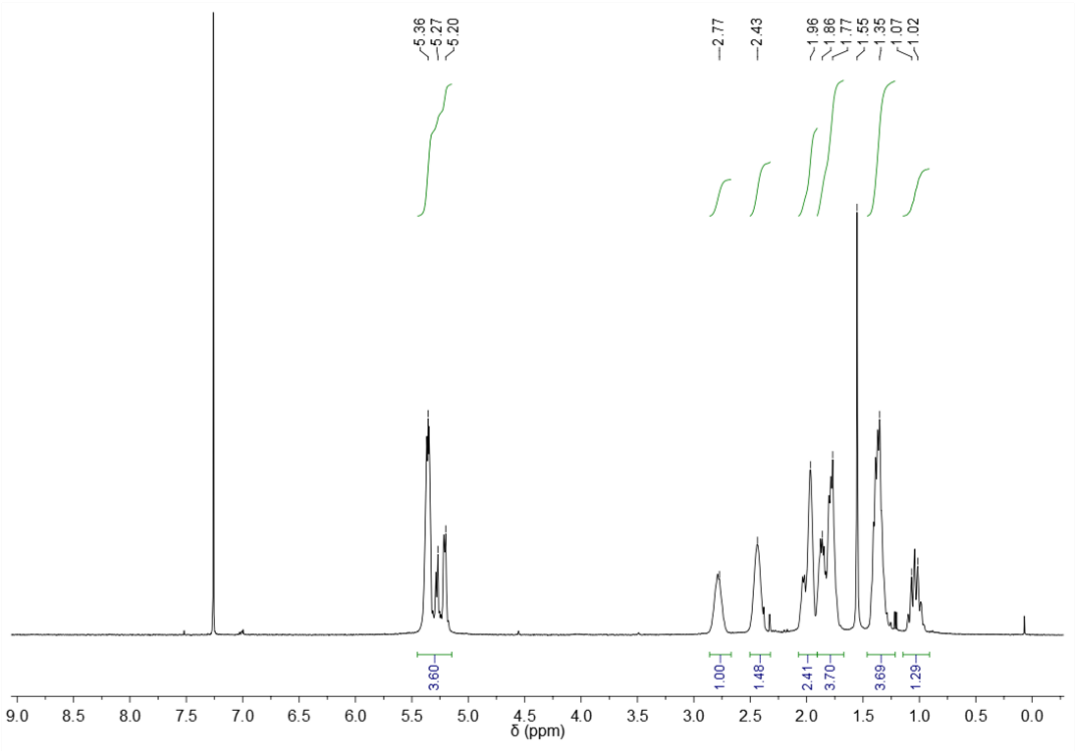


Figure S123. ^{1}H-NMR spectrum (400MHz, $CDCl_3$) of poly(NBE-co-CPE)$_n$ by action of **3**.

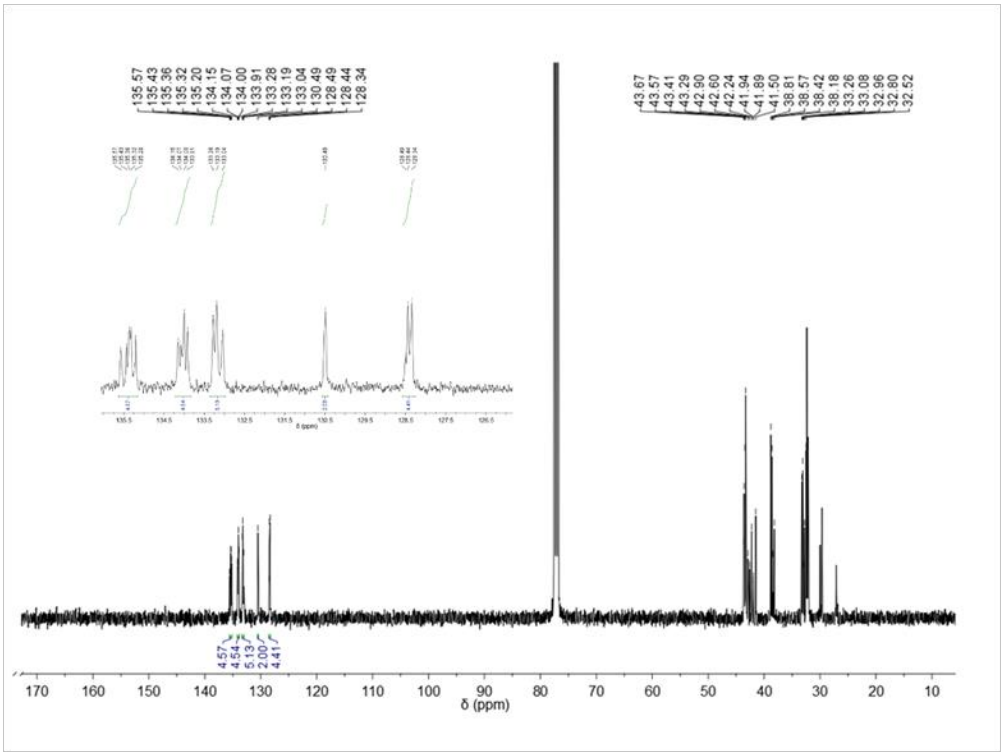


Figure S124. ^{13}C-NMR spectrum (101MHz, $CDCl_3$) of poly(NBE-co-CPE)$_n$ by action of **3**.

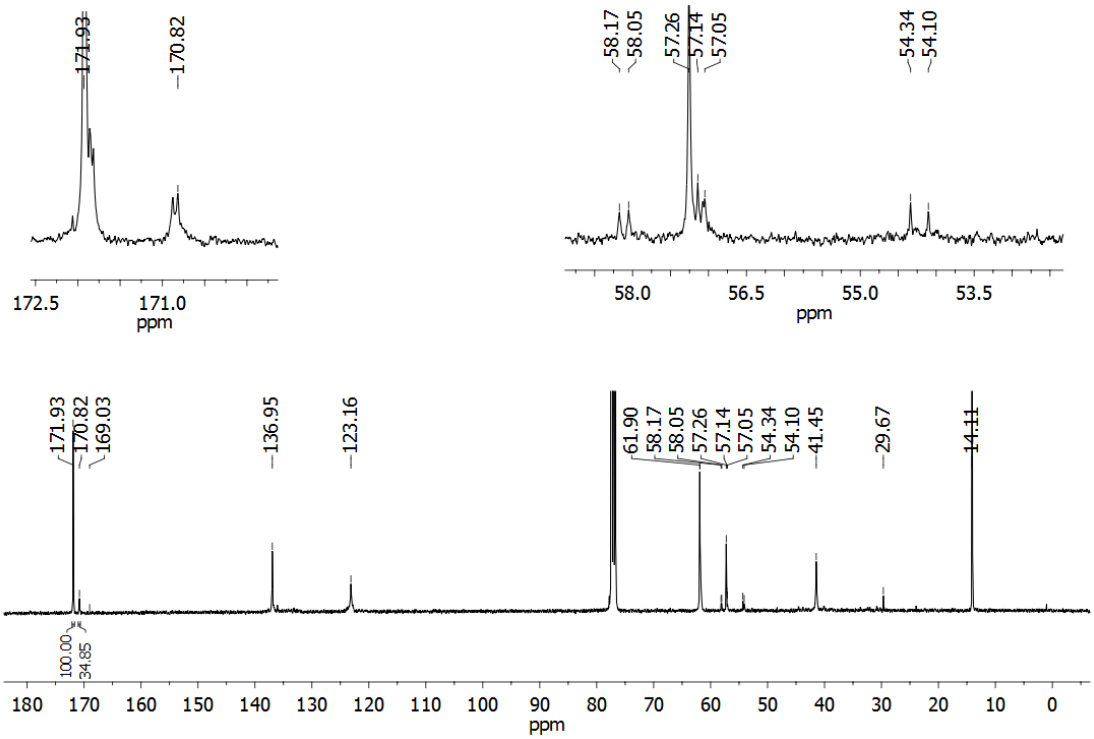


Figure S125. ^{13}C NMR (101 MHz, $CDCl_3$) of poly(**M7)** prepared by the action of **3**.

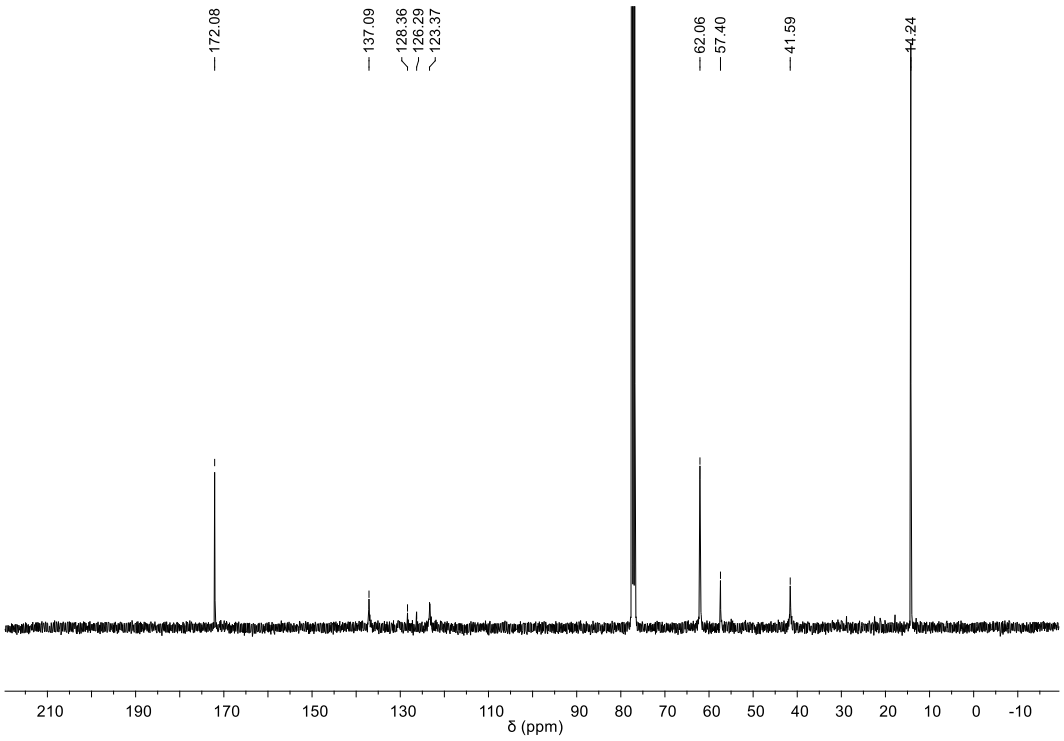


Figure S126. ^{13}C NMR (101 MHz, $CDCl_3$) of poly(**M7)** prepared by the action of **5**.

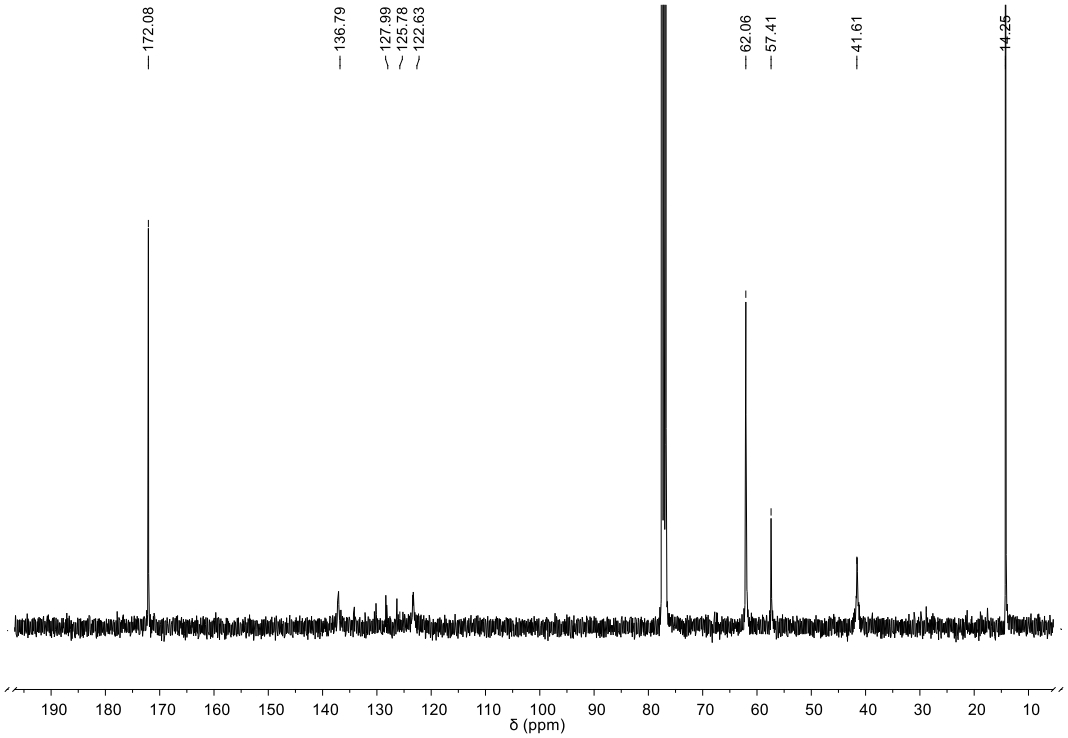


Figure S127. ^{13}C NMR (101 MHz, $CDCl_3$) of poly(**M7)** prepared by the action of **6**.

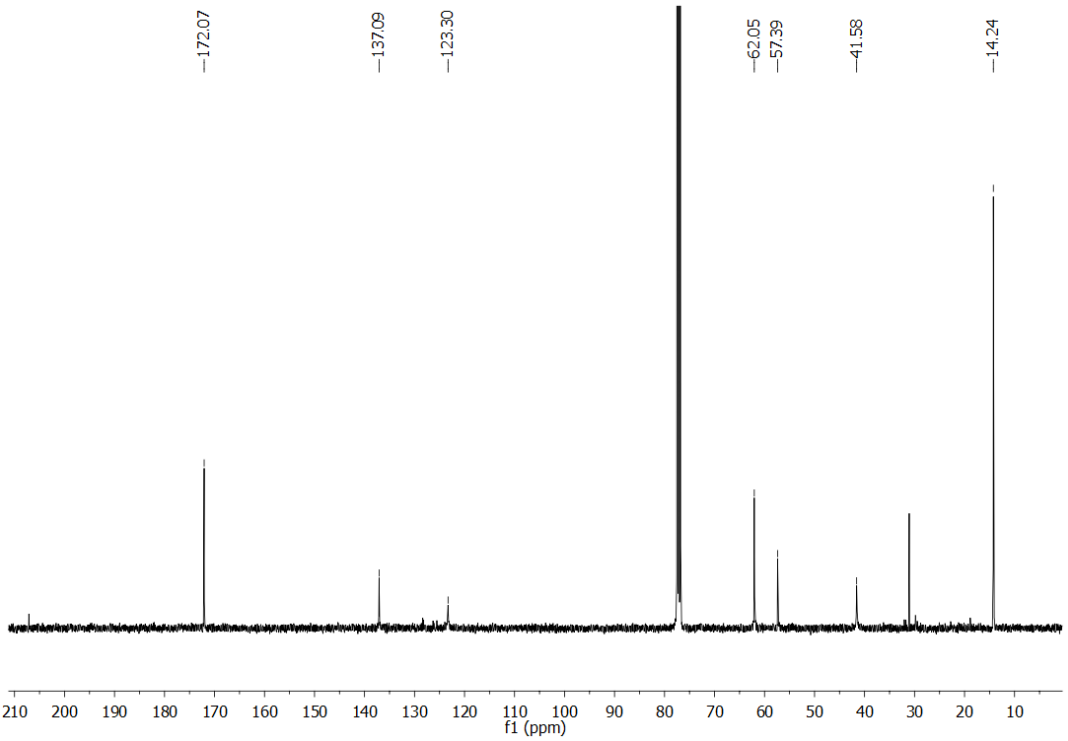


Figure S128. ^{13}C NMR (101 MHz, $CDCl_3$) of poly(**M7)** prepared by the action of **7**.

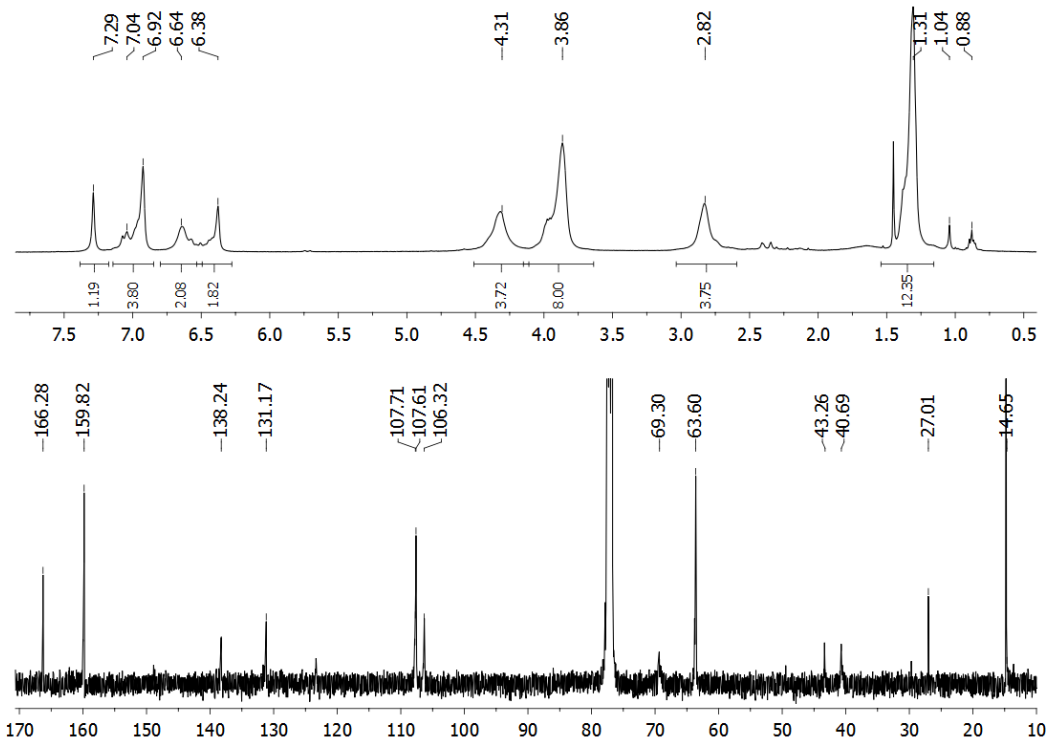


Figure S129. ^{13}C NMR (101 MHz, $CDCl_3$) of poly(**M8)** prepared by the action of **3**.

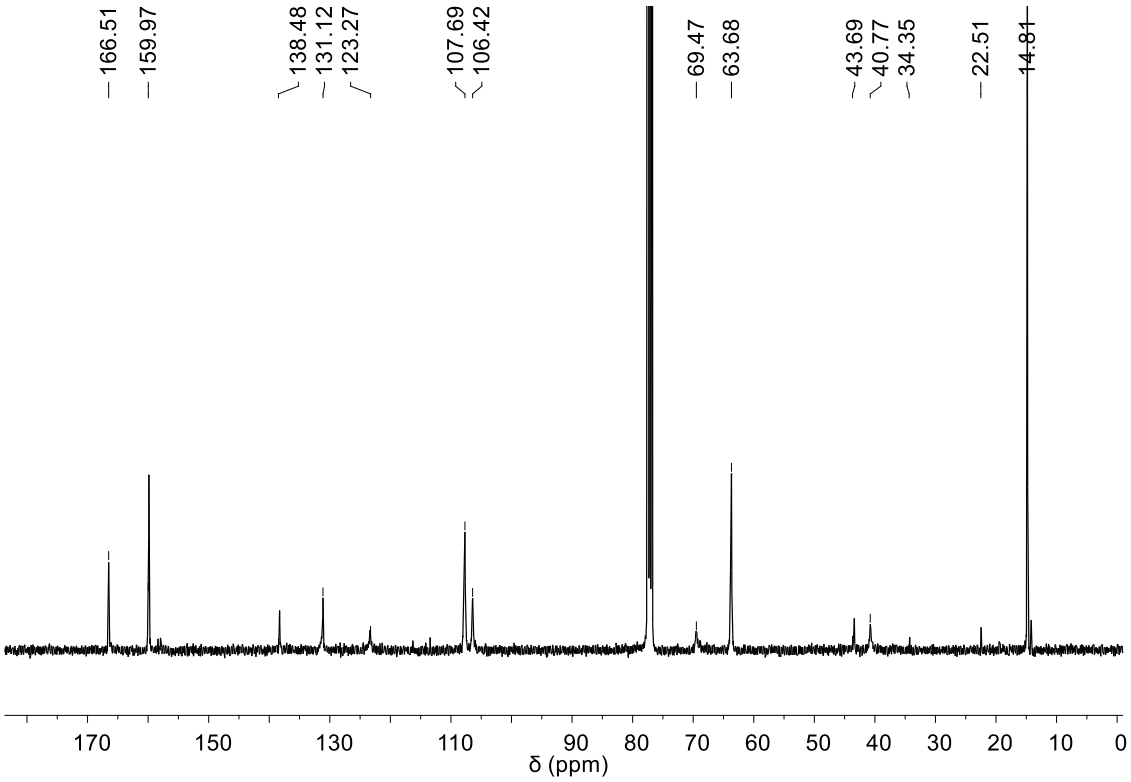


Figure S130. ^{13}C NMR (101 MHz, $CDCl_3$) of poly(**M8)** prepared by the action of **5**.

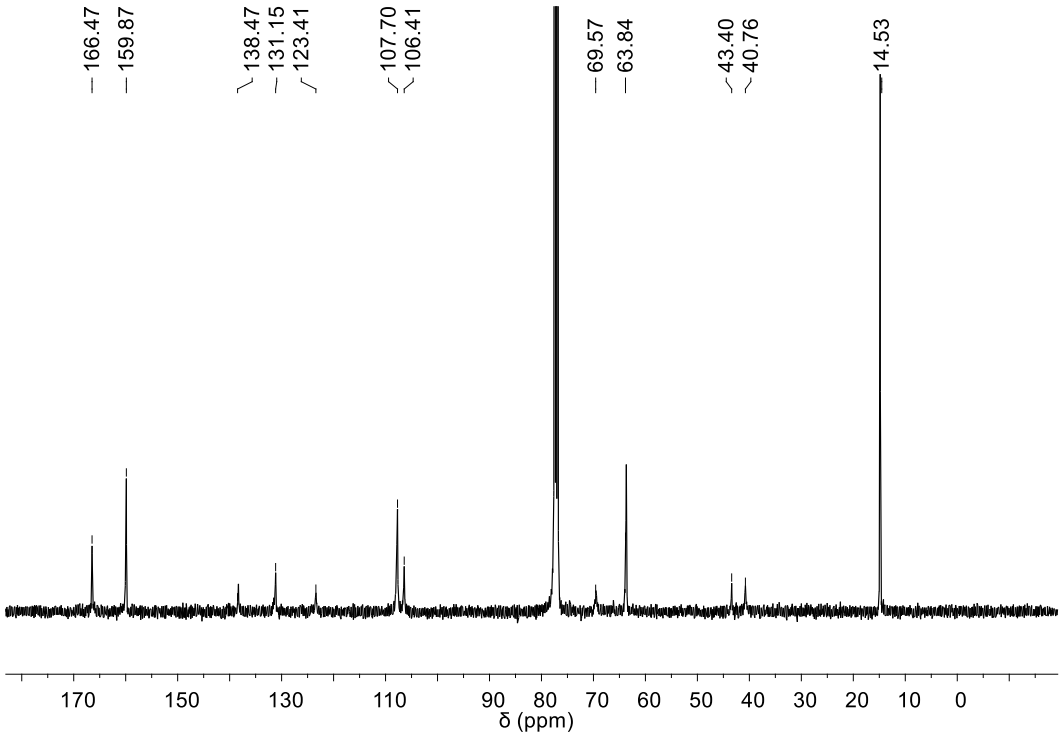


Figure S131. ^{13}C NMR (101 MHz, $CDCl_3$) of poly(**M8)** prepared by the action of **6**.

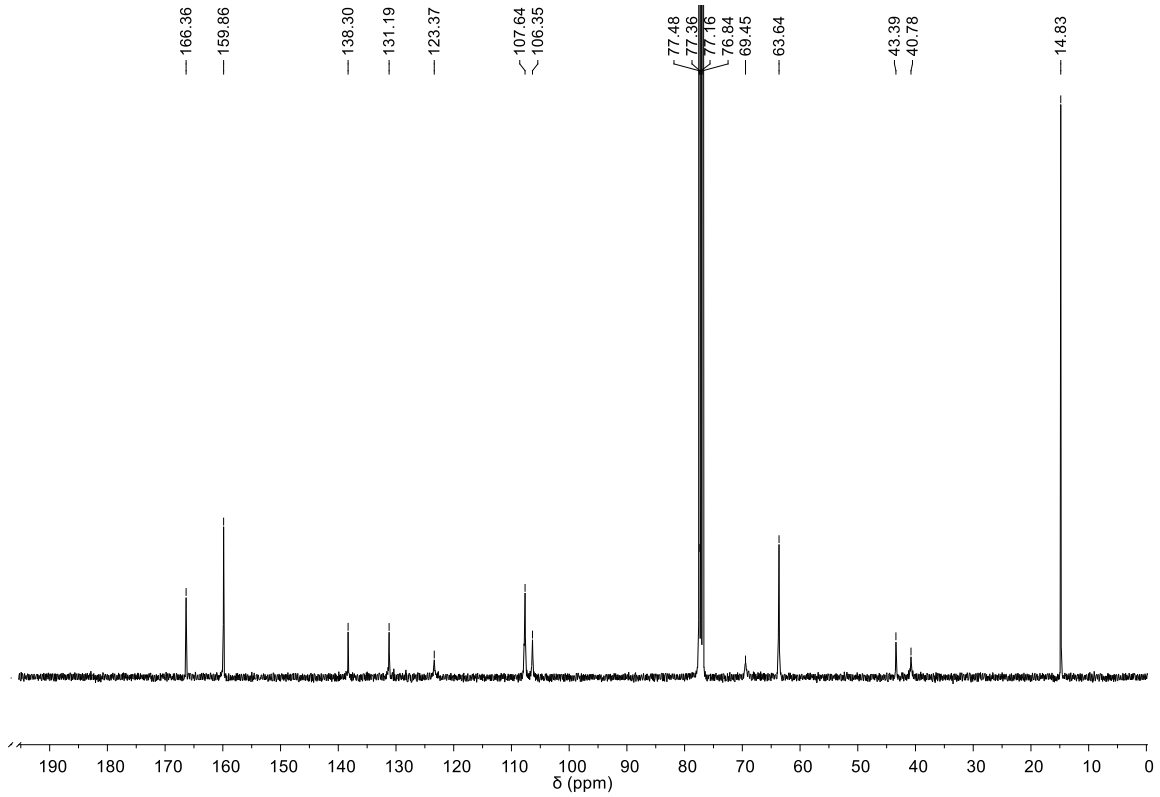


Figure S132. ^{13}C NMR (101 MHz, $CDCl_3$) of poly(**M8)** prepared by the action of **7**.

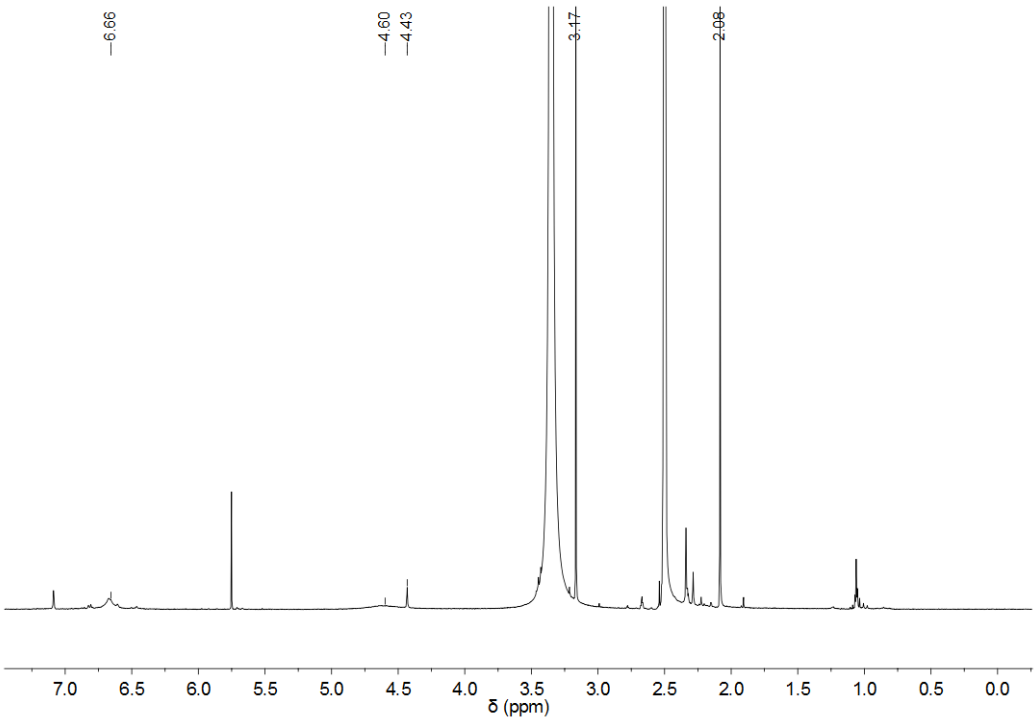


Figure S133. ^{1}H-NMR spectrum (400 MHz, DMSO-d_6) of poly(**M9**) obtained by the action of **3**.

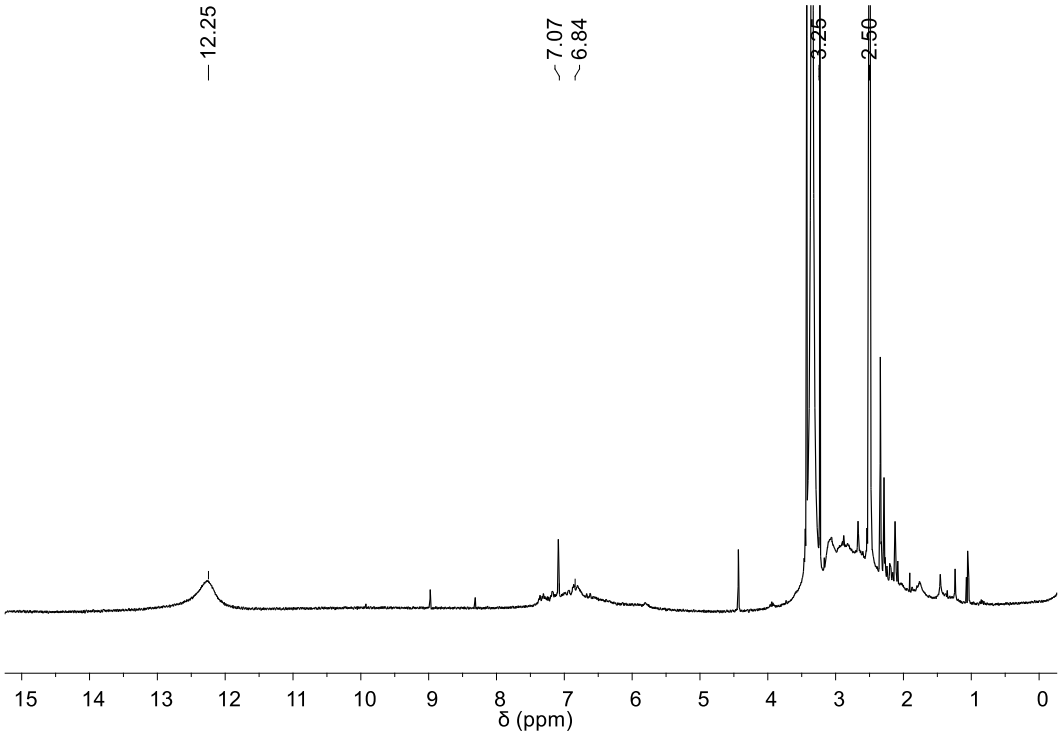


Figure S134. ^{1}H-NMR spectrum (400 MHz, DMSO-d_6) of poly(2-(prop-2-yn-1-yl)pent-4-ynoic acid) obtained by the action of **5**.

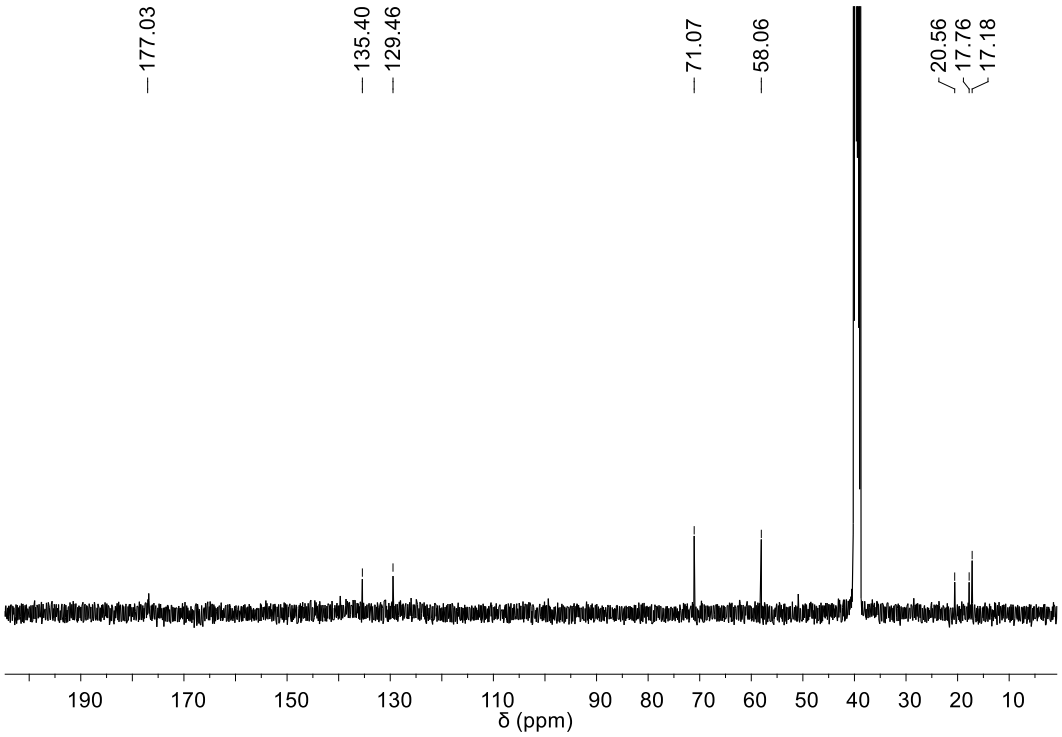


Figure S135. ^{13}C-NMR spectrum (101 MHz, DMSO-d_6) of poly(2-(prop-2-yn-1-yl)pent-4-ynoic acid) obtained by the action of **5**.

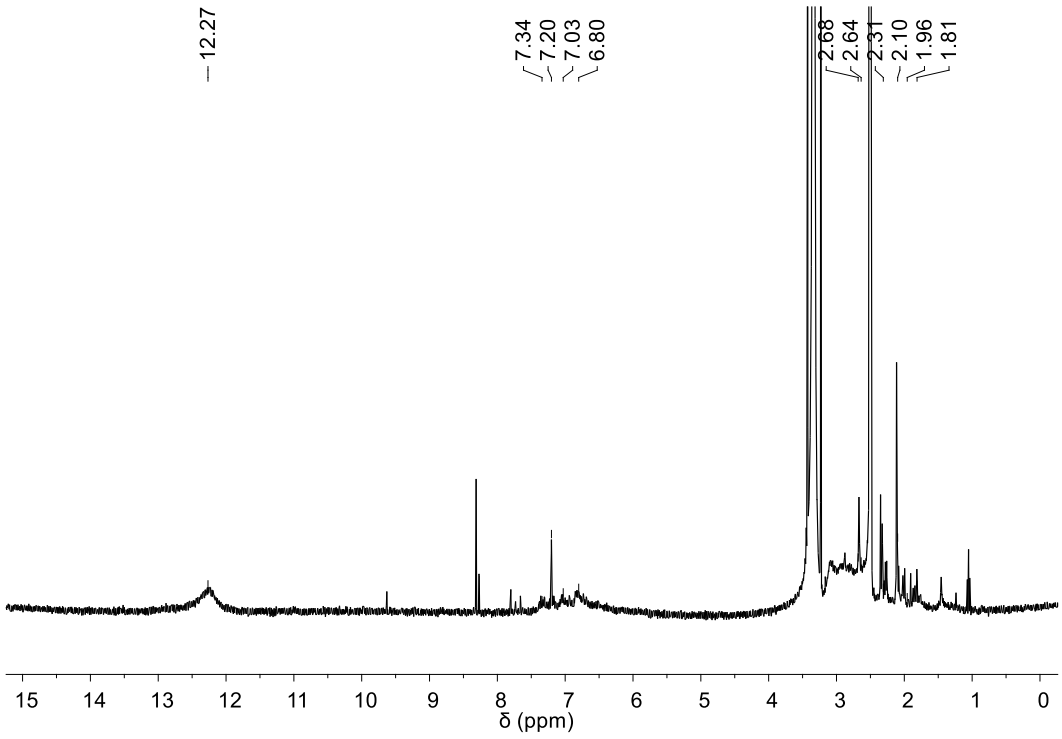


Figure S136. ^{1}H-NMR spectrum (400 MHz, DMSO- d_6) of poly(2-(prop-2-yn-1-yl)pent-4-ynoic acid) obtained by the action of **6**.

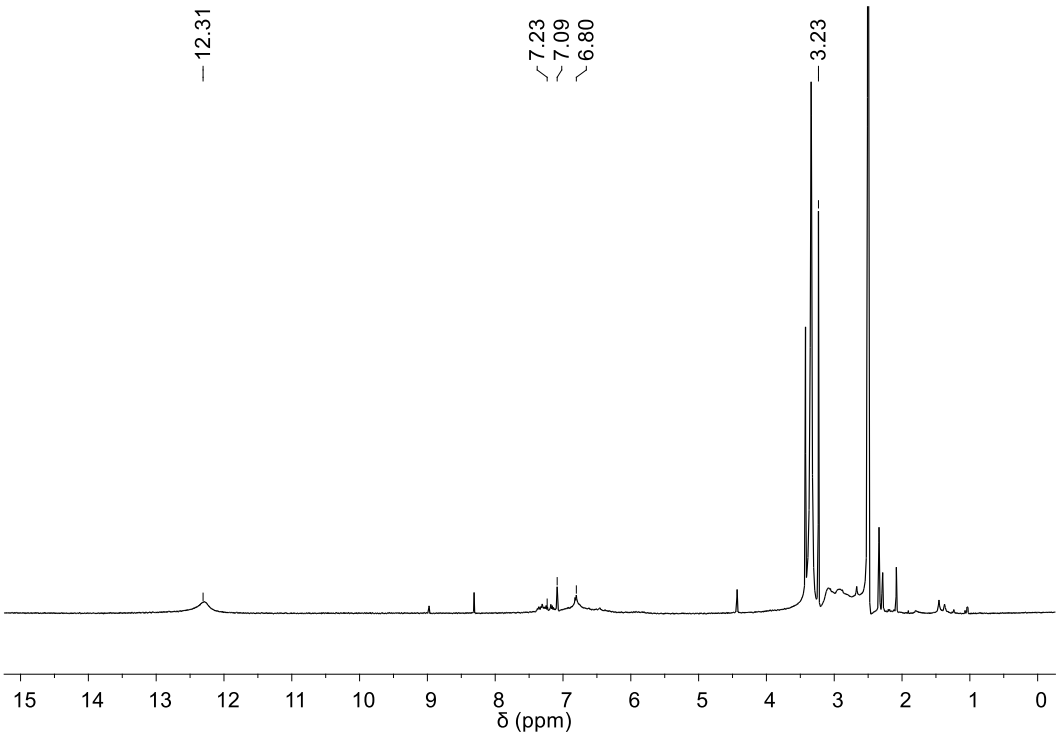


Figure S137. ^{1}H-NMR spectrum (400 MHz, DMSO-d_6) of poly(2-(prop-2-yn-1-yl)pent-4-ynoic acid) obtained by the action of **7**.

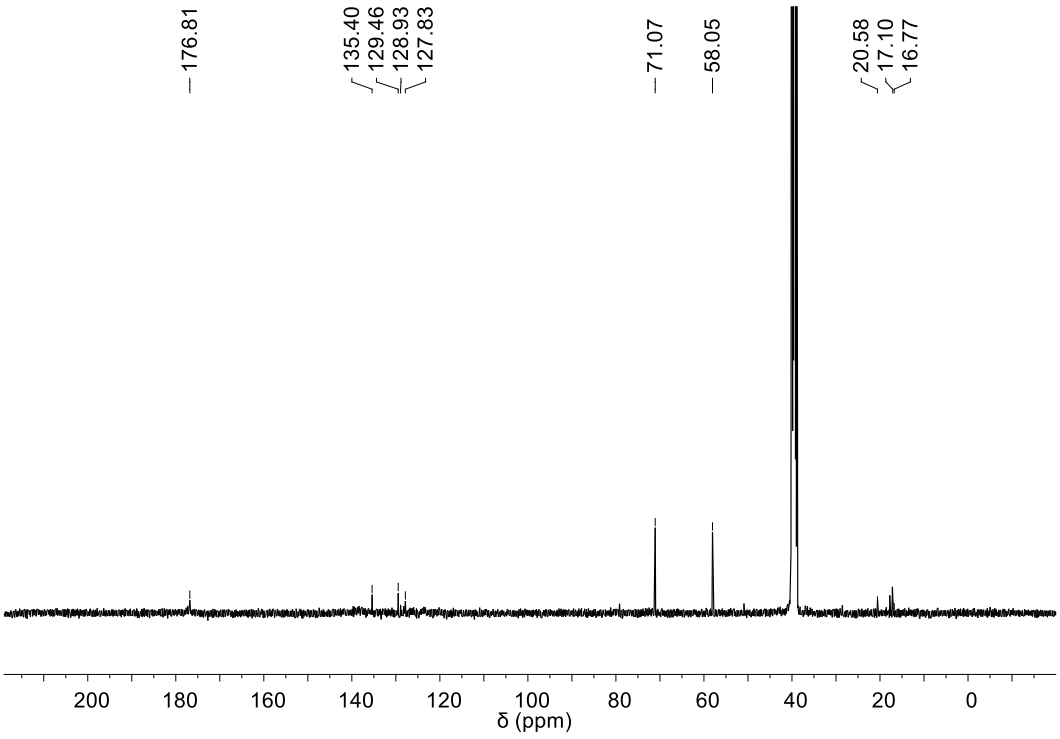


Figure S138. ^{13}C-NMR spectrum (101 MHz, DMSO-d_6) of poly(2-(prop-2-yn-1-yl)pent-4-ynoic acid) obtained by the action of **7**.

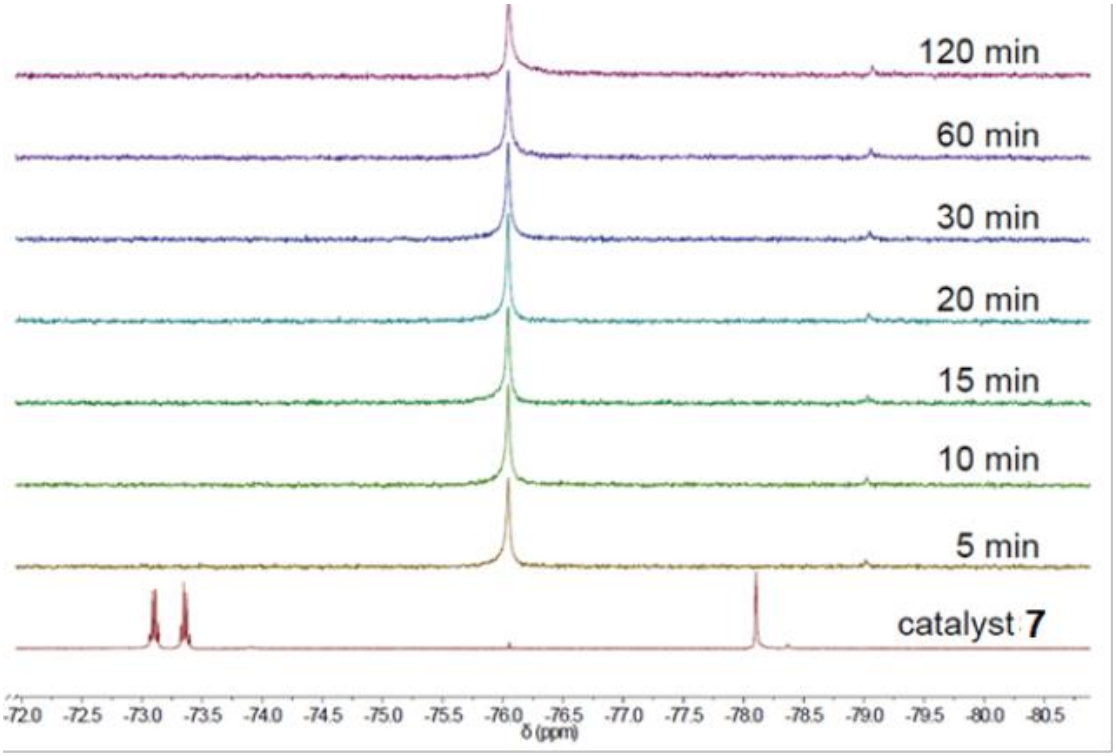


Figure S139. ^{19}F-NMR spectra (CD_2Cl_2) of **7** during the cyclopolymerization of 2,2-di(prop-2-yn-1-yl) propane-1,3-diol.

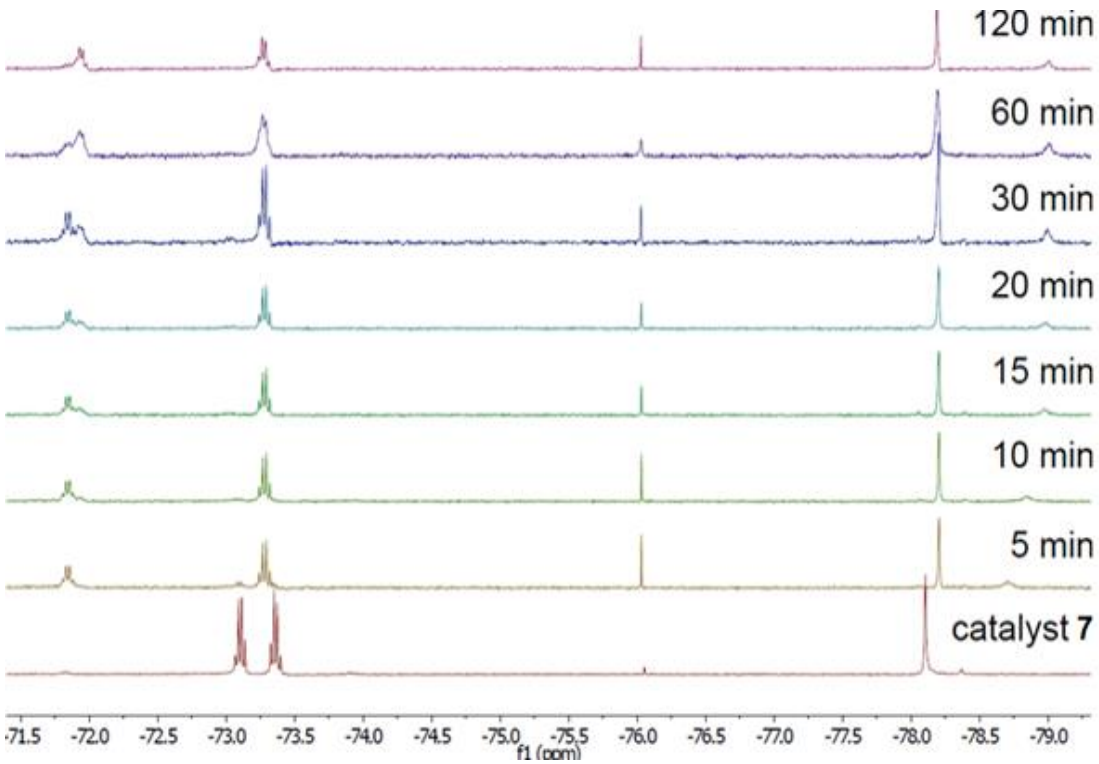


Figure S140. ^{19}F-NMR spectra (CD_2Cl_2) of **7** during the cyclopolymerization of DEDPM.

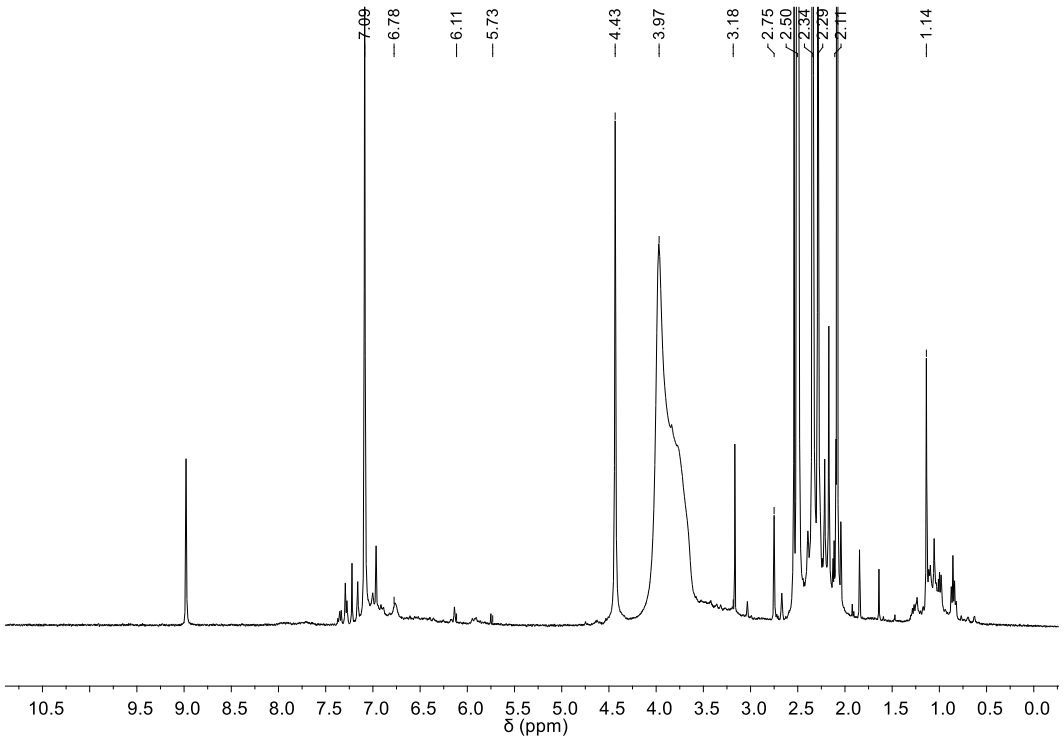


Figure S141. ^{1}H-NMR (400 MHz, DMSO-d_6) of poly(4,4-dicyano-1,7-heptadiyne) prepared by the action of **3**.

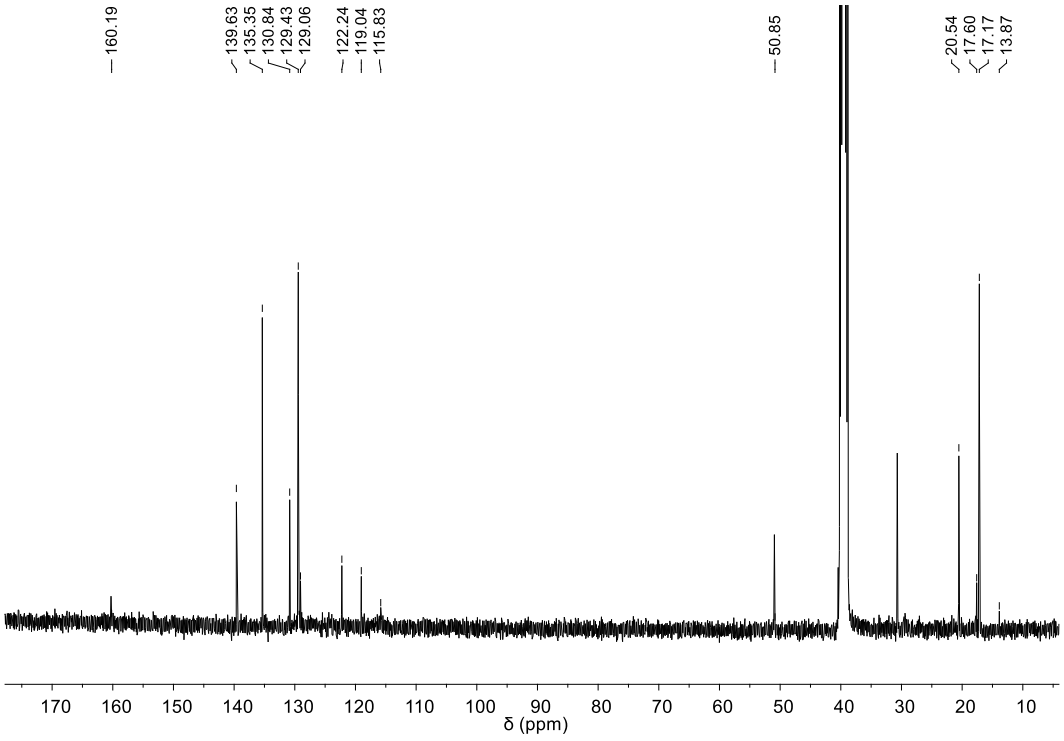


Figure S142. ^{13}C-NMR (101 MHz, DMSO-d_6) of poly(4,4-dicyano-1,7-heptadiyne) prepared by the action of **3**.

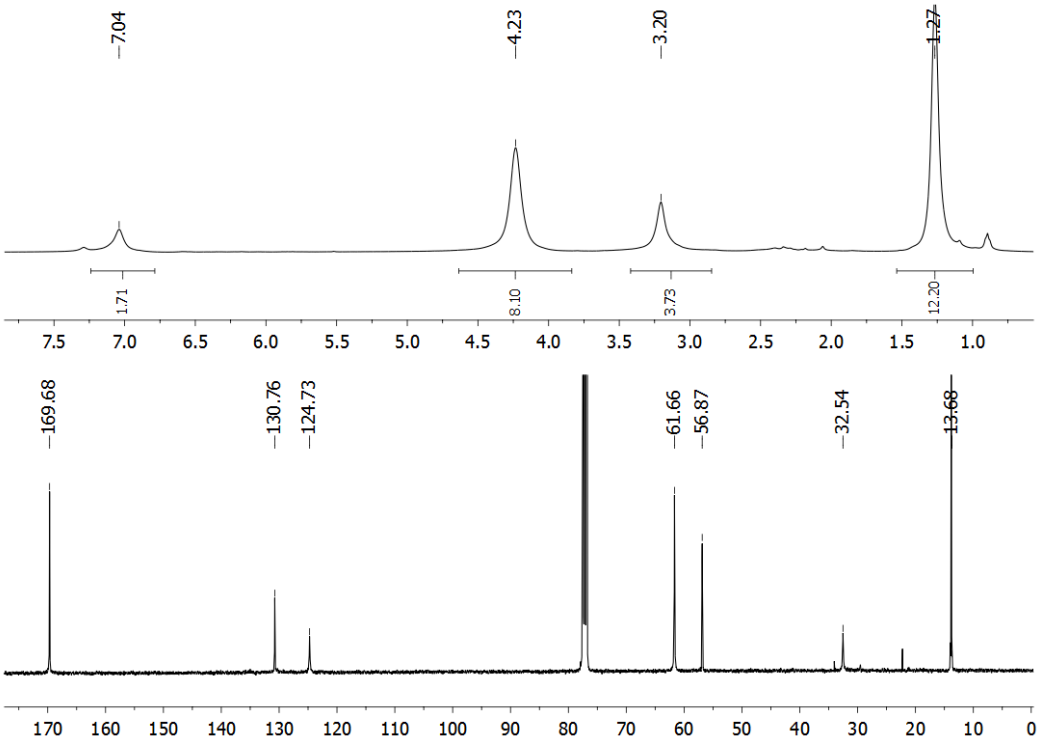


Figure S143. ^{1}H and ^{13}C NMR of poly**(**4,4,5,5-tetrakis(ethoxycarbonyl)-1,7-octadiyne**)** prepared by the action of **3**·($CDCl_3$).

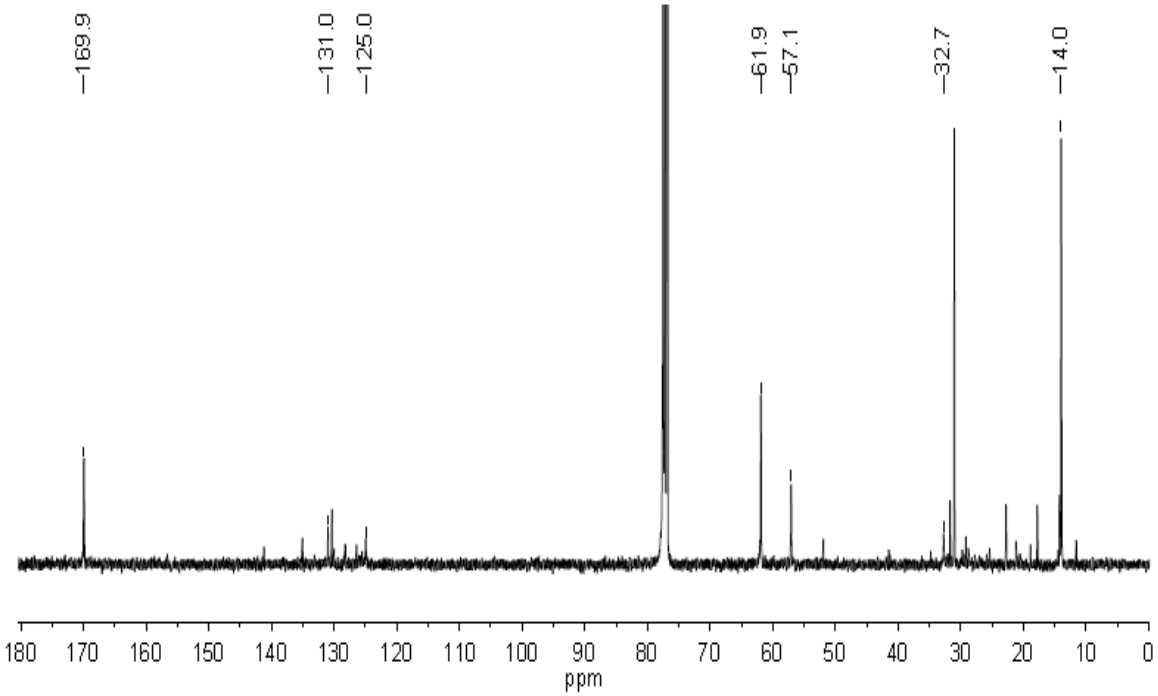


Figure S144. ^{13}C NMR·($CDCl_3$, 101 MHz) of poly**(**4,4,5,5-tetrakis(ethoxycarbonyl)-1,7-octadiyne**)** prepared by the action of **5**.

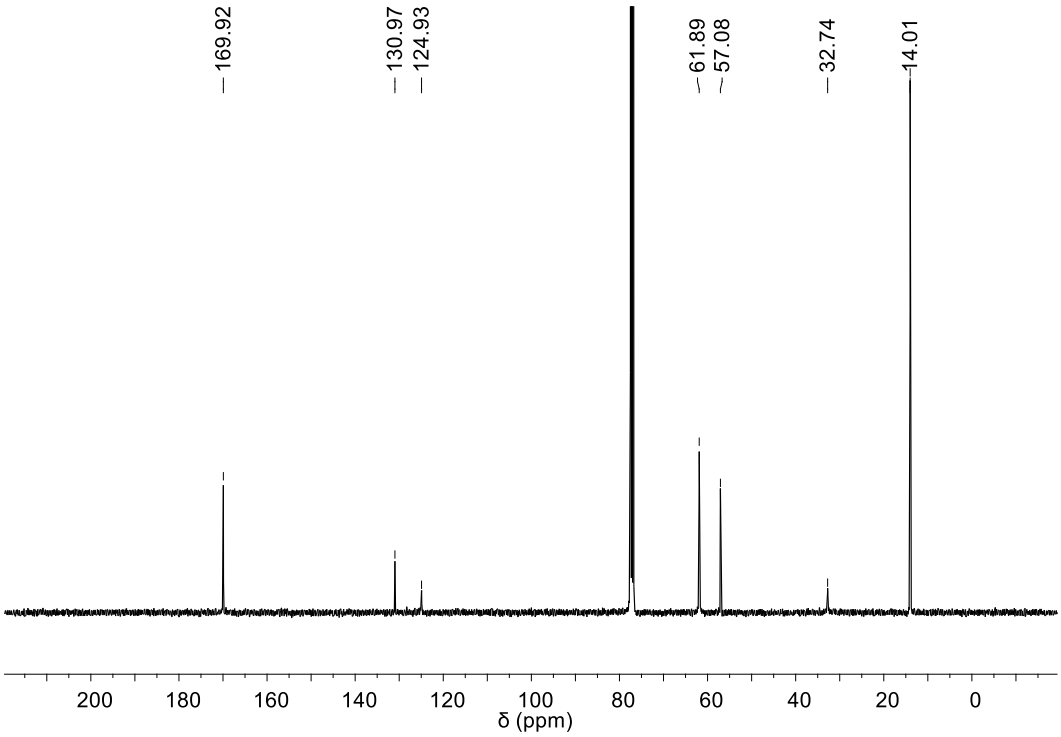


Figure S145. ^{13}C NMR (CDCl$_3$, 101 MHz) of poly**(**4,4,5,5-tetrakis(ethoxycarbonyl)-1,7-octadiyne**)** prepared by the action of **6**.

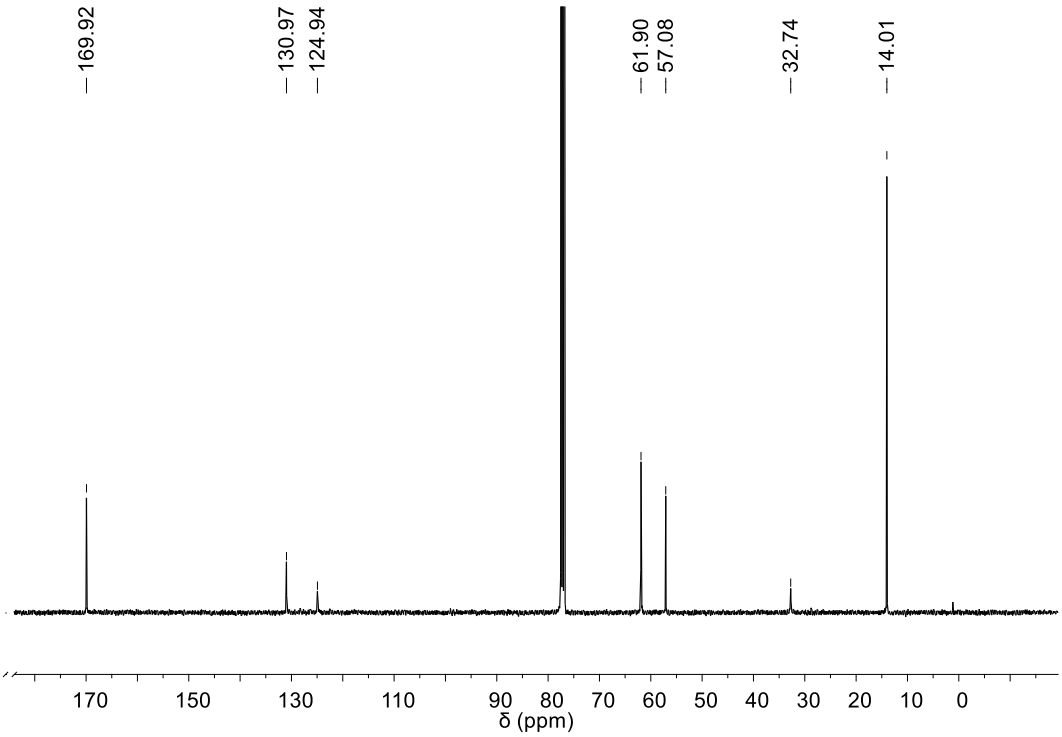


Figure S146. ^{13}C NMR (CDCl$_3$, 101 MHz) of poly**(**4,4,5,5-tetrakis(ethoxycarbonyl)-1,7-octadiyne**)** prepared by the action of **7**

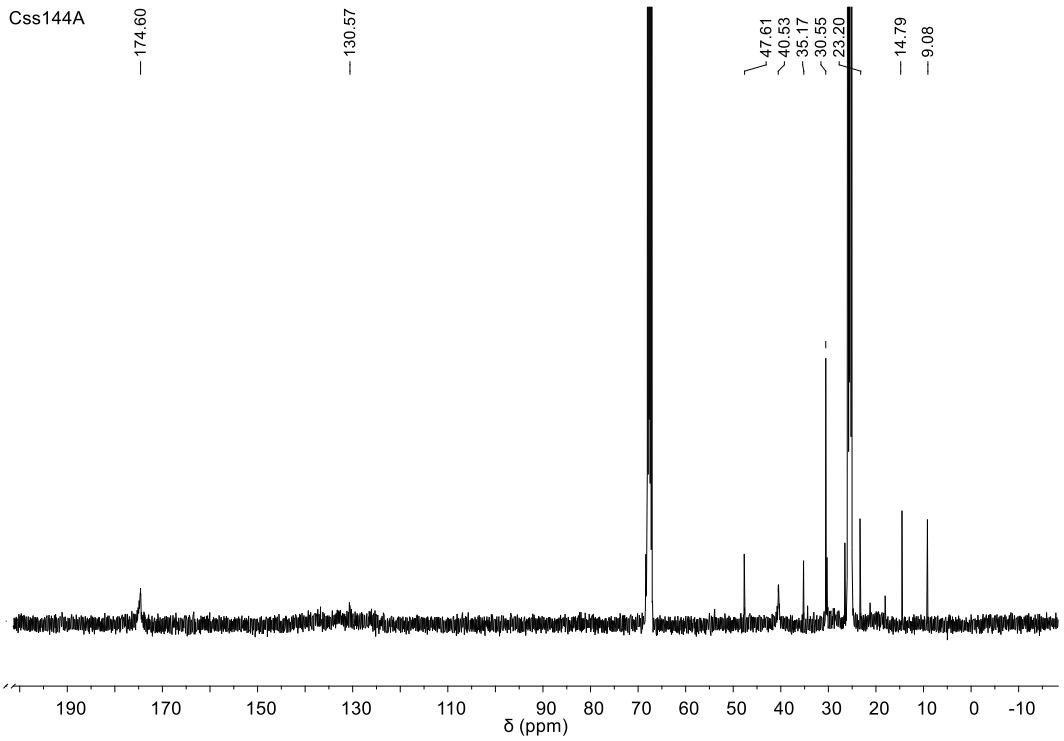


Figure S147. ^{13}C-NMR (101 MHz, THF-d_8) of poly(1,7-octadiyne-4,5-dicarboxylic acid) by action of **3**.

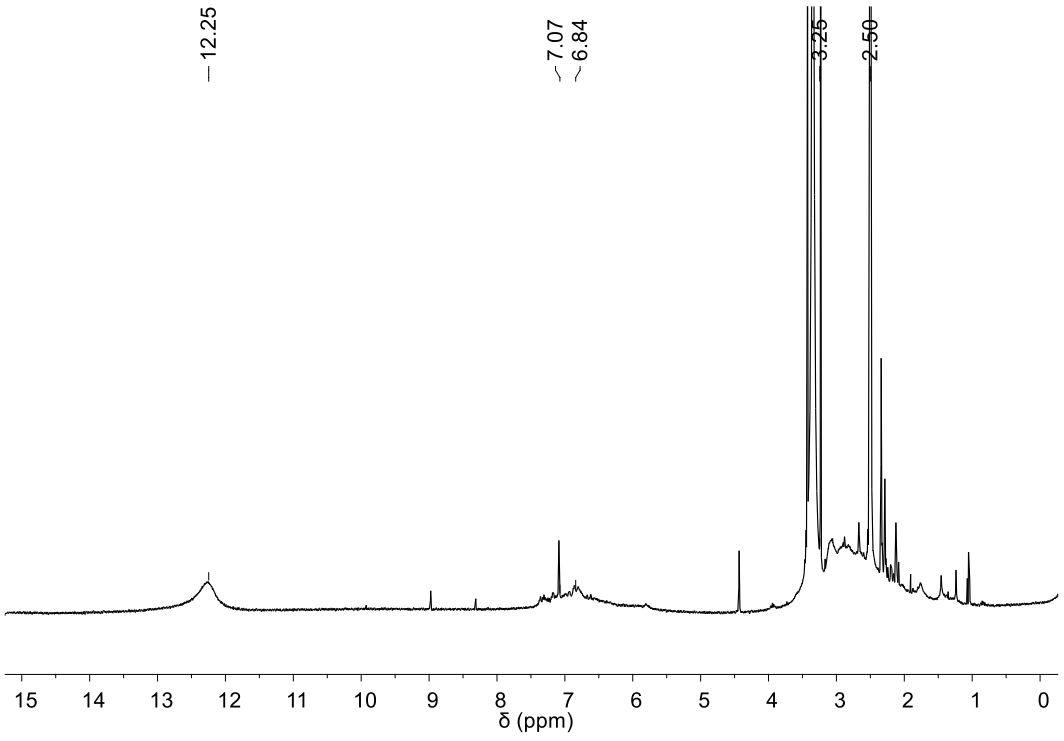


Figure S148. ^{1}H-NMR spectrum (400 MHz, DMSO-d_6) of poly-(2-(prop-2-yn-1-yl)pent-4-ynoic acid) obtained by the action of **3**.

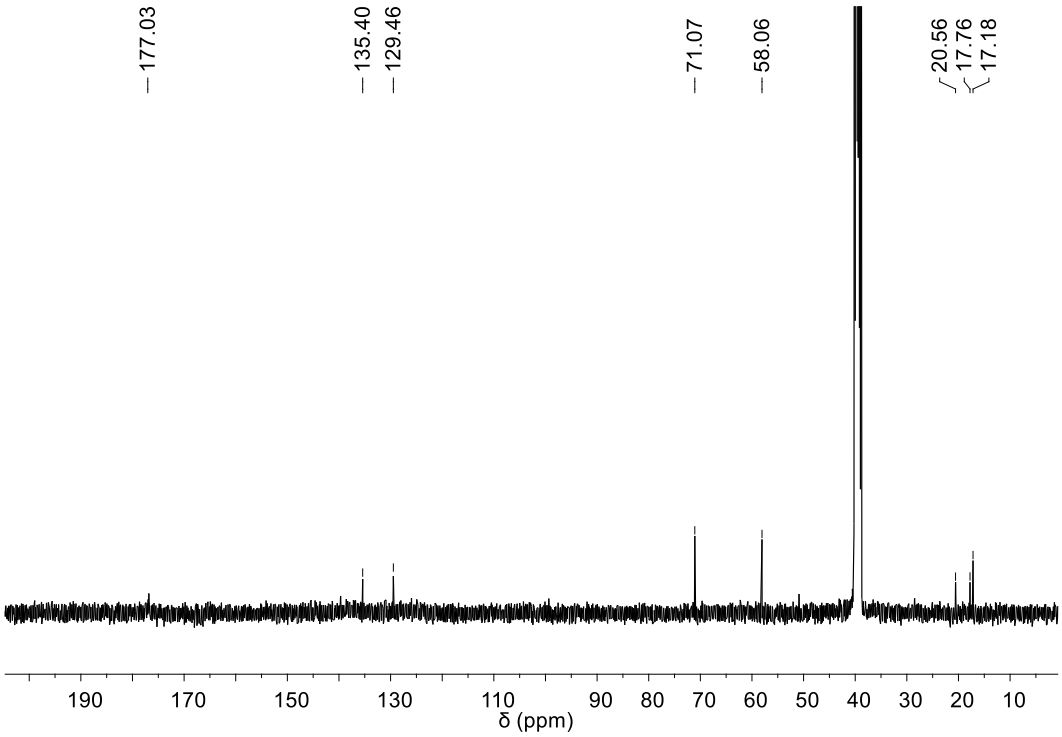


Figure S149. ^{13}C-NMR spectrum (101 MHz, DMSO-d_6) of poly-(2-(prop-2-yn-1-yl)pent-4-ynoic acid) obtained by the action of **3**.

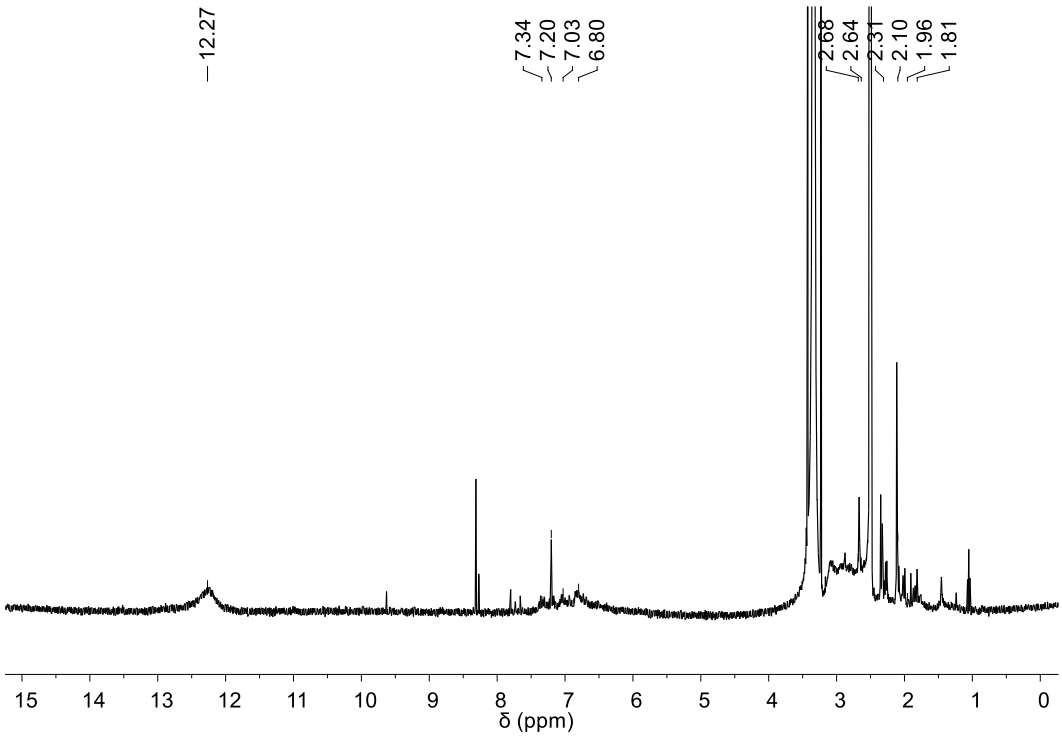


Figure S150. ^{1}H-NMR spectrum (400 MHz, DMSO-d_6) of poly(2-(prop-2-yn-1-yl)pent-4-ynoic acid) obtained by the action of **4**.

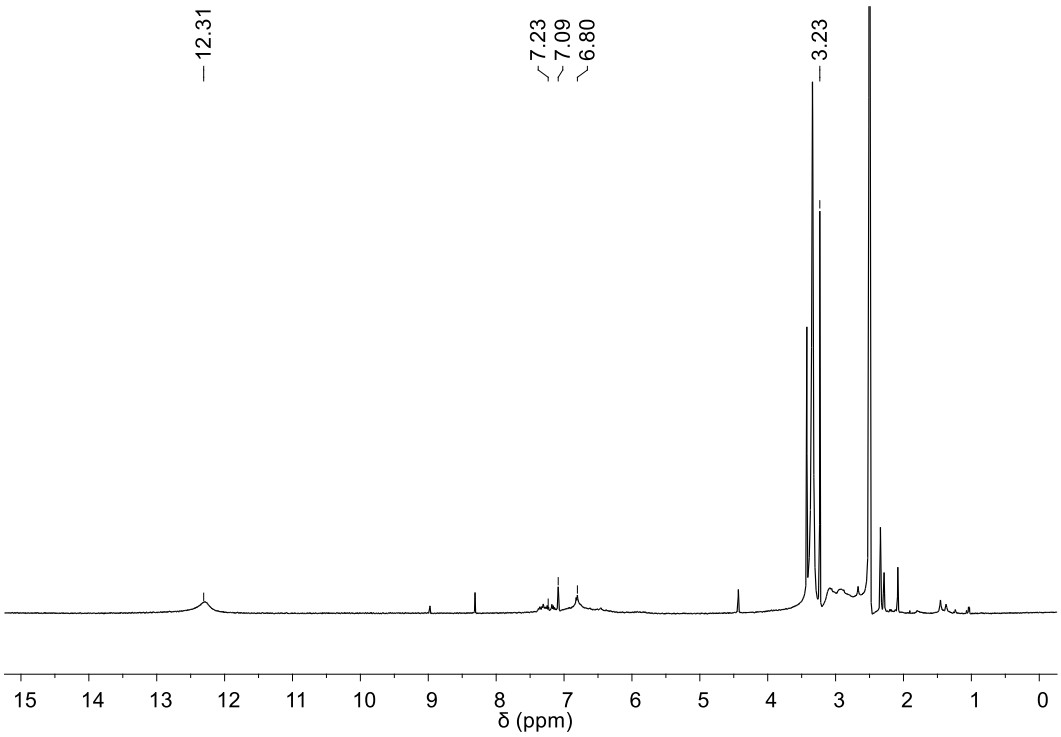


Figure S151. ^{1}H-NMR spectrum (400 MHz, DMSO-d_6) of poly(2-(prop-2-yn-1-yl)pent-4-ynoic acid) obtained by the action of **5**.

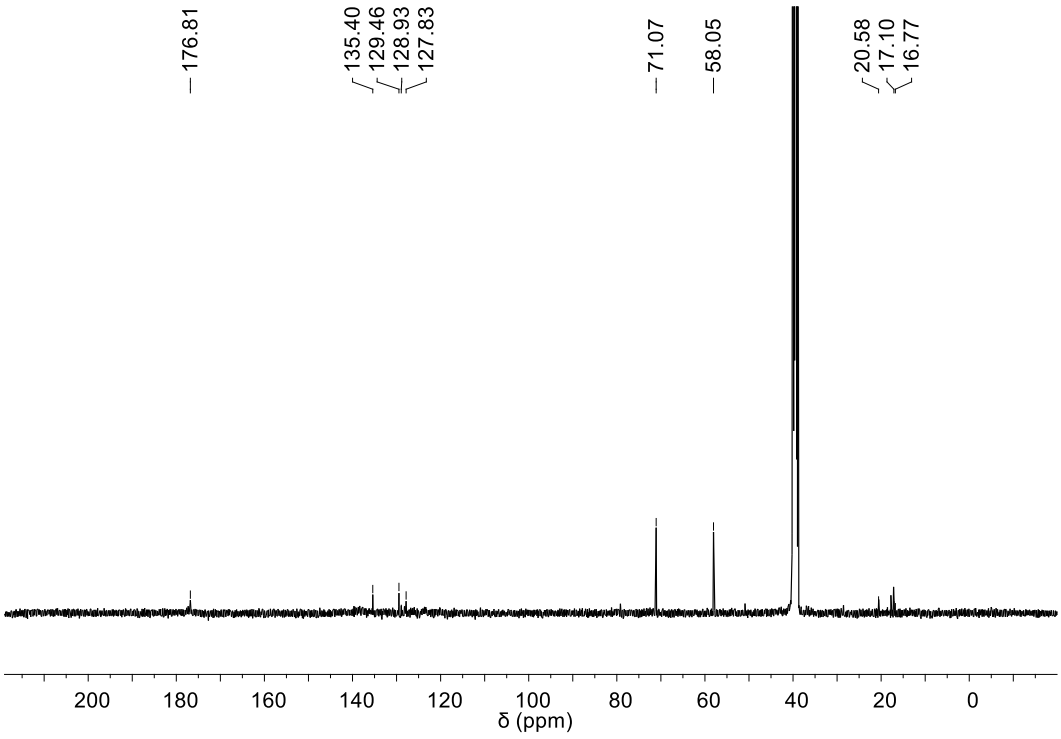


Figure S152. ^{13}C-NMR spectrum (101 MHz, DMSO-d_6) of poly(2-(prop-2-yn-1-yl)pent-4-ynoic acid) obtained by the action of **5**.

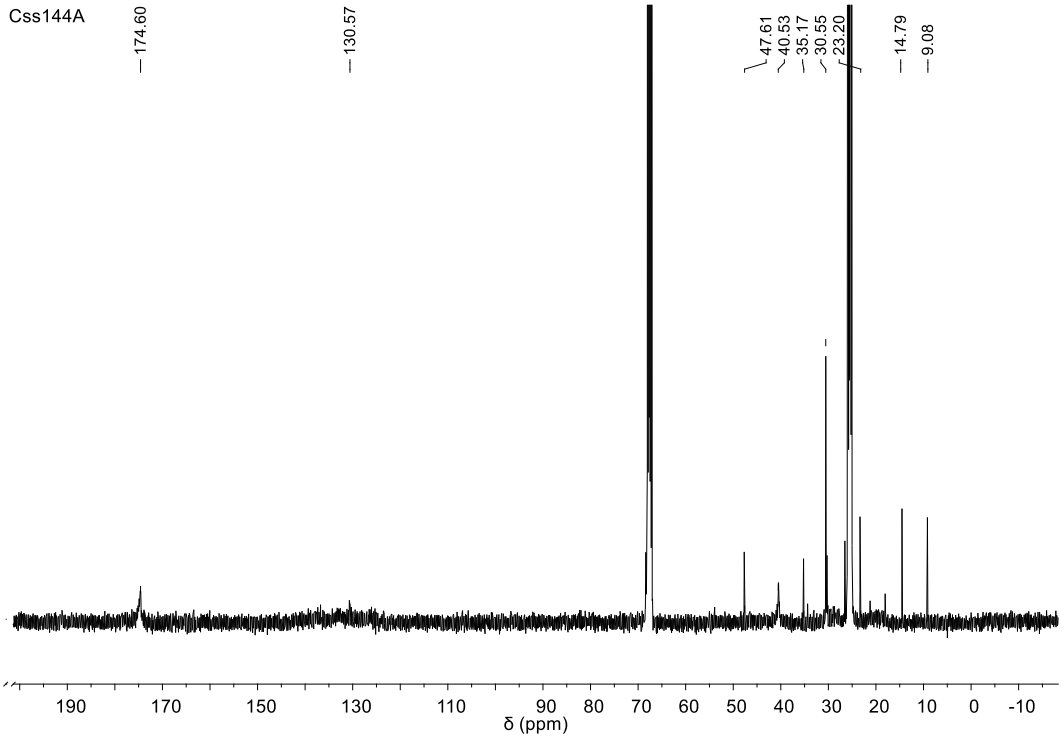


Figure S153. ^{13}C-NMR (101 MHz, THF-d_8) of poly(1,7-octadiyne-4,5-dicarboxylic acid) by action of **3**.

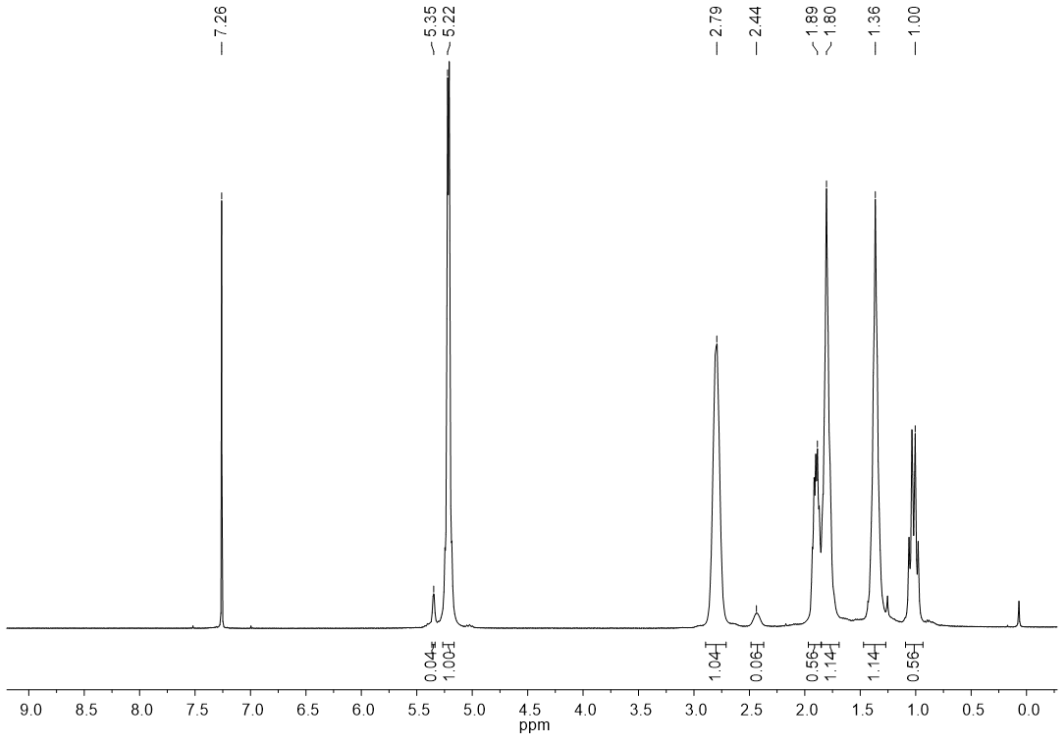


Figure S154. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of poly(norborn-2-ene) prepared by the action of **29**. σ_{cis} = 96%.

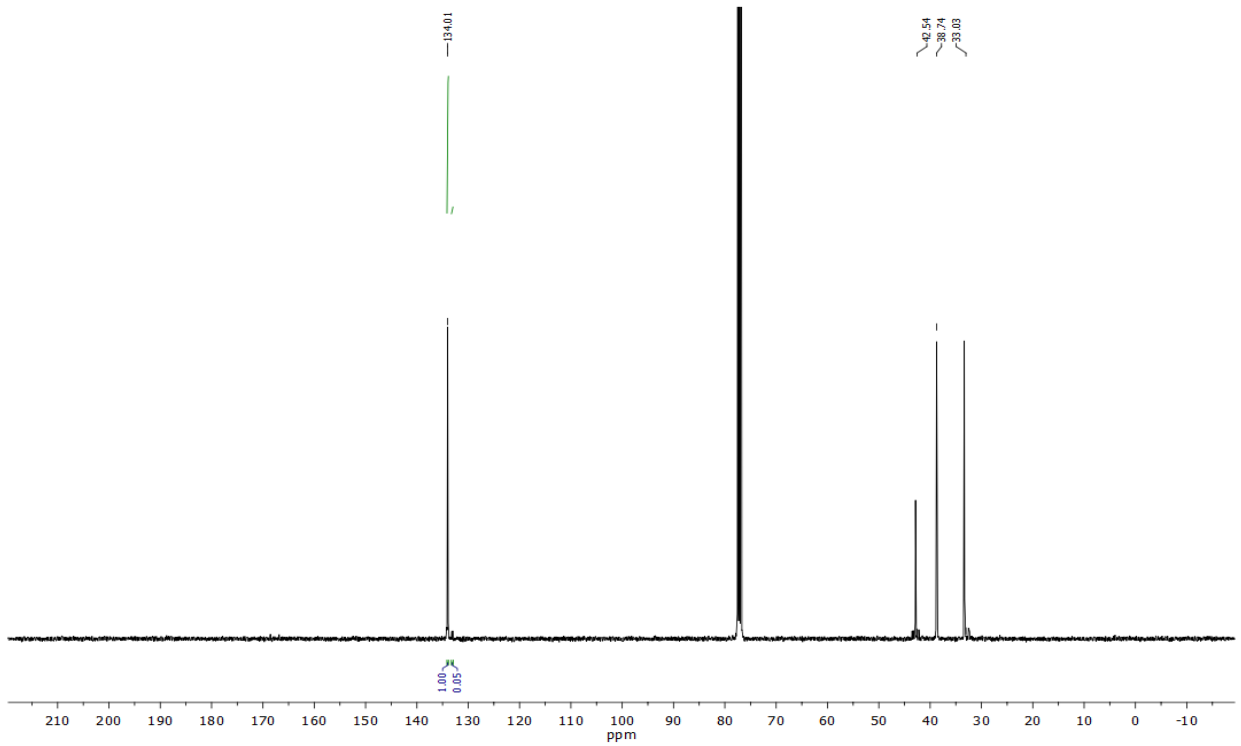


Figure S155. ^{13}C-NMR (101 MHz, $CDCl_3$) spectrum of poly(norborn-2-ene) prepared by the action of **29**.

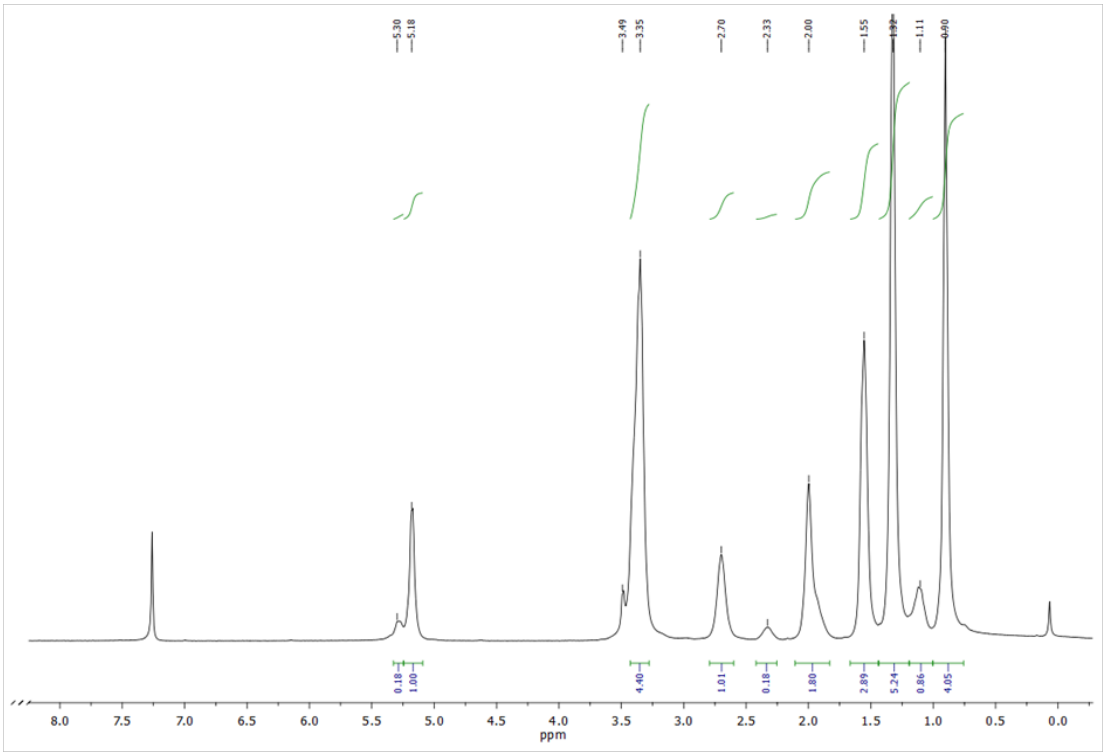


Figure S156. ^{1}H-NMR spectrum (400 MHz, $CDCl_3$) of poly(2,3-di(pentoxymethyl)-norborn-5-ene) obtained by the action of **29**. σ_{cis} = 85%.

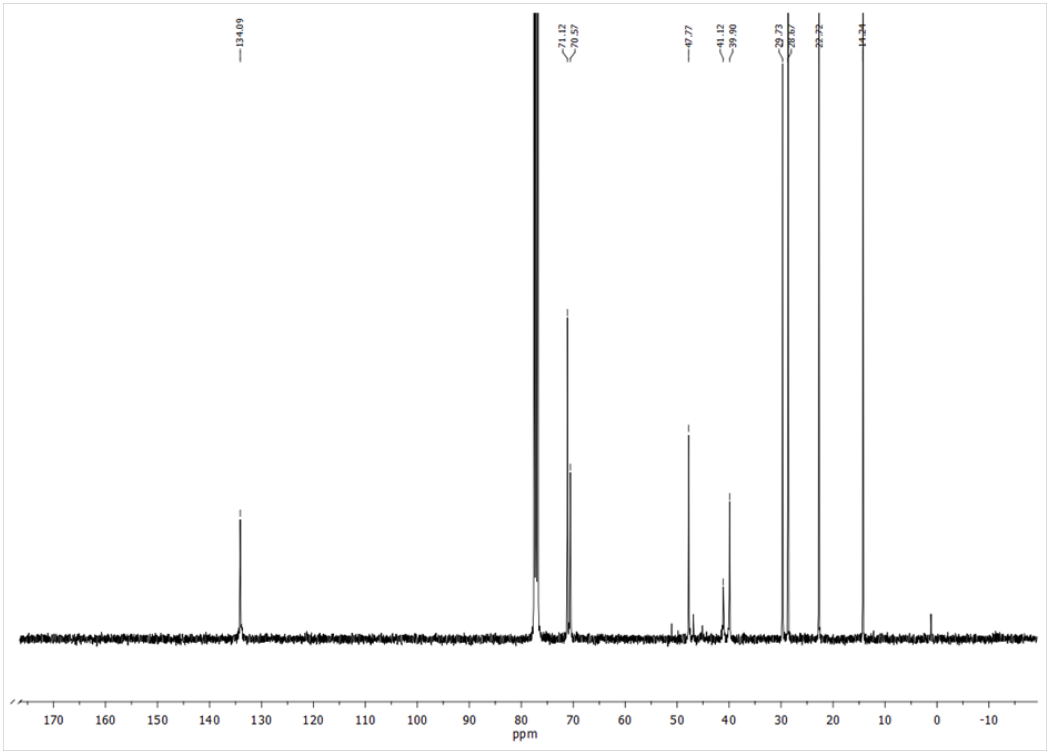


Figure S157. ^{13}C-NMR spectrum (101 MHz, $CDCl_3$) of poly(2,3-di(pentoxymethyl)-norborn-5-ene) obtained by the action of **29**.

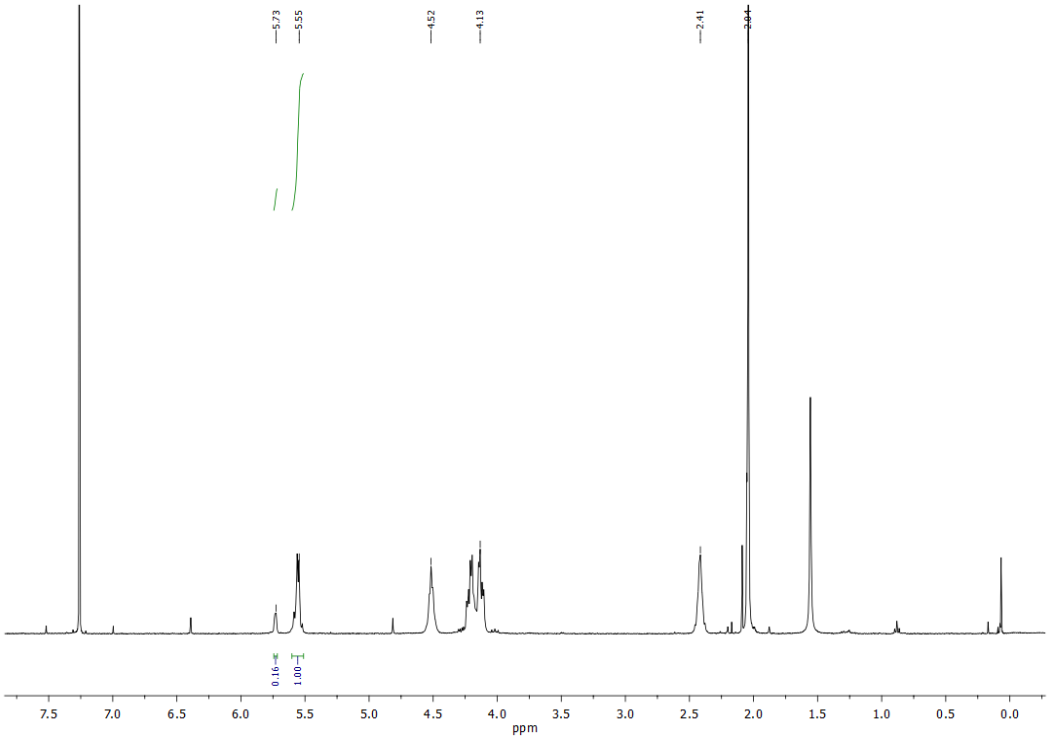


Figure S158. ^{1}H-NMR spectrum (101 MHz, $CDCl_3$) of poly(7-oxabicyclo[2.2.1]hept-5-ene-2,3-diylbis(methylene)diacetate) prepared by the action of **1**. σ_{cis} = 86%.

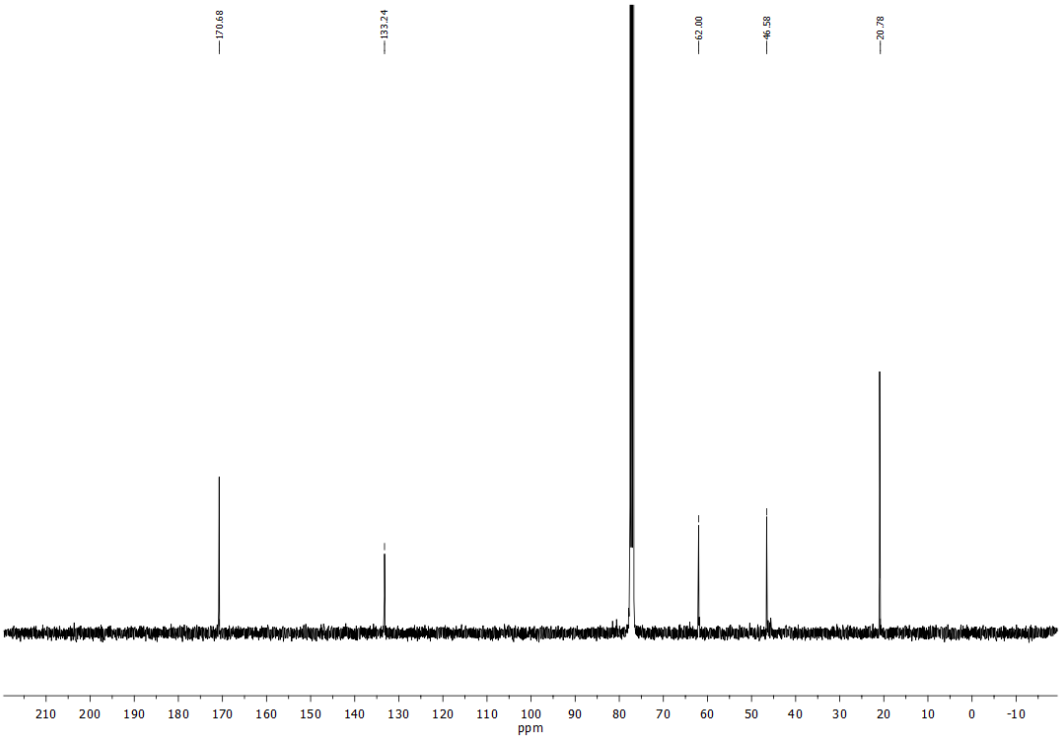


Figure S159. ^{13}C-NMR spectrum (101 MHz, $CDCl_3$) of poly(7-oxabicyclo[2.2.1]hept-5-ene-2,3-diylbis(methylene)diacetate) prepared by the action of **29**.

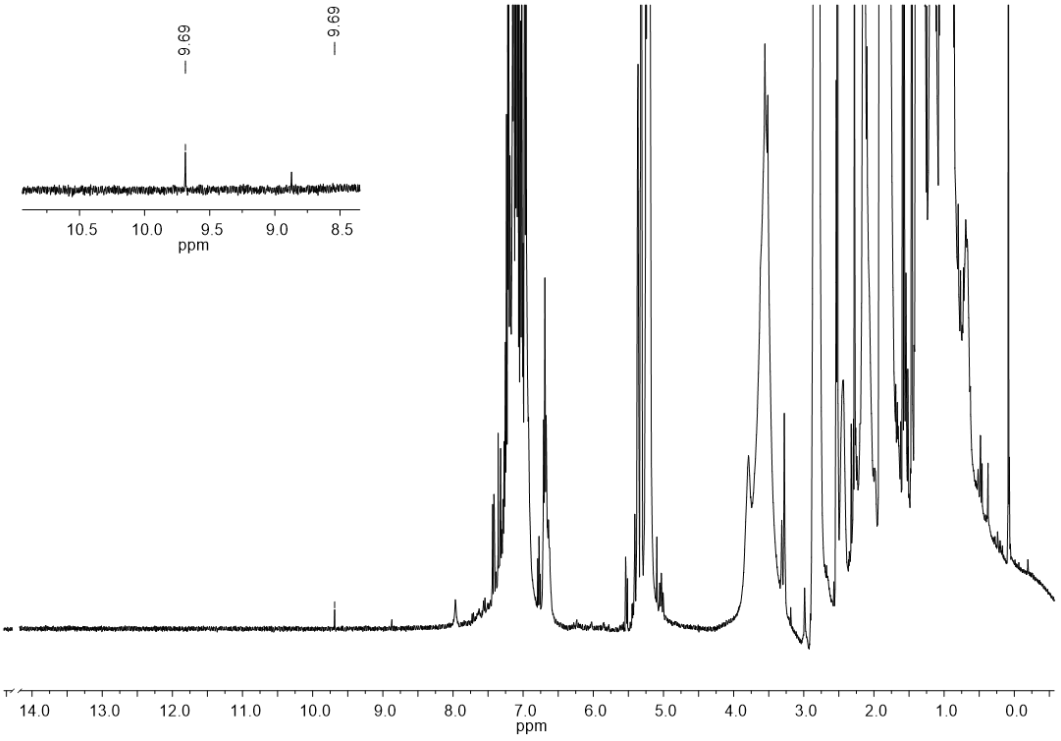


Figure S160. ^{1}H-NMR spectrum (400 MHz, CD_2Cl_2) of the reaction of norborn-2-ene with **29** after 5 h.

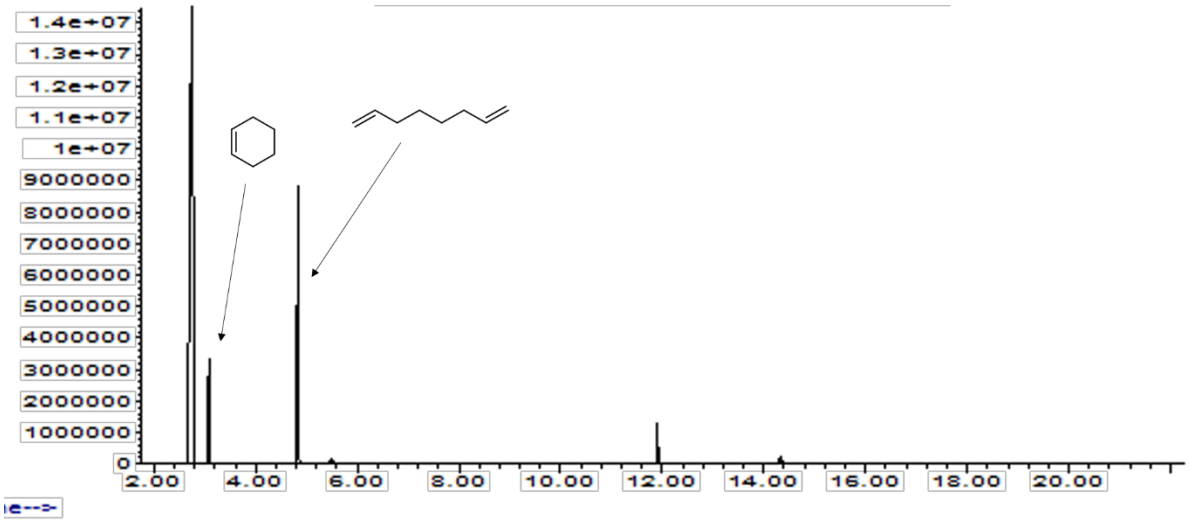


Figure S161. GC result of RCM of 1,7-octadiene by action of **14**

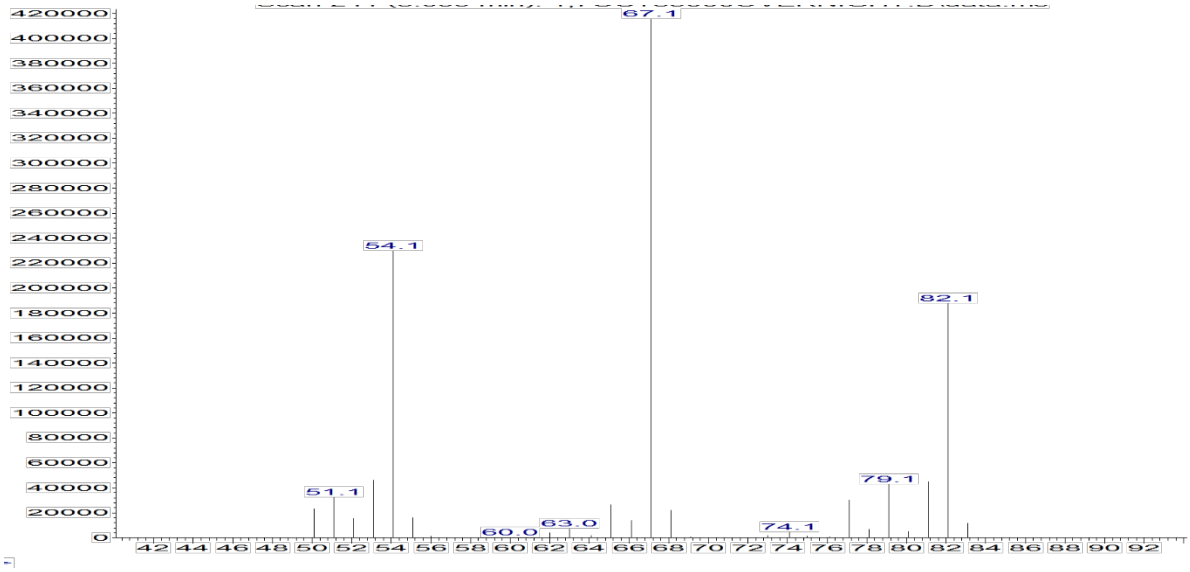


Figure S162. MS result of RCM of 1,7-octadiene by action of **14**.

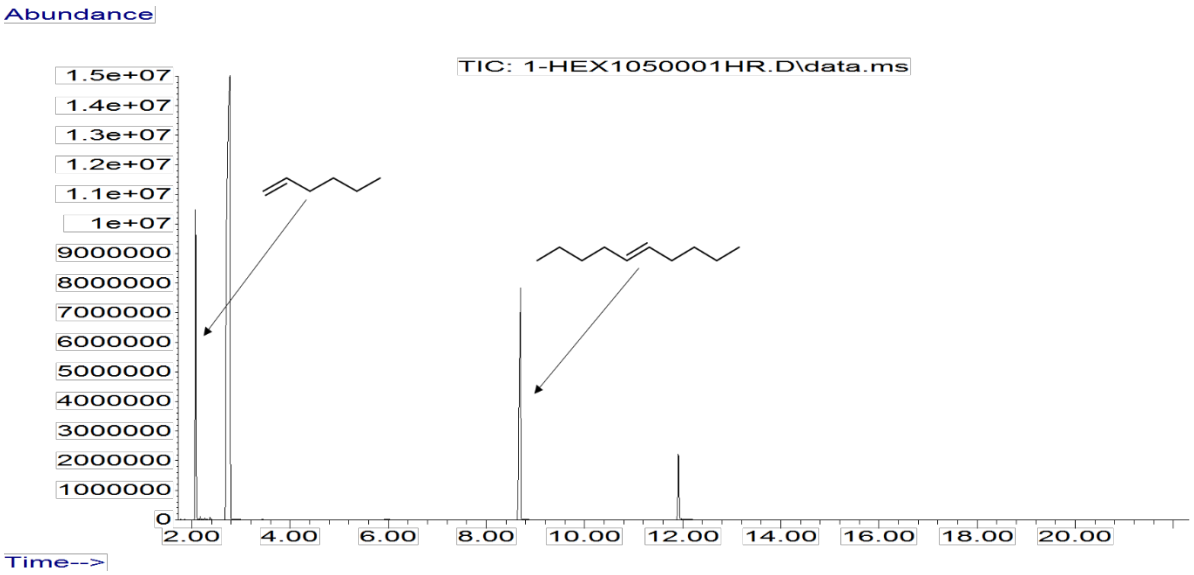


Figure S163. GC result of HM of 1-hexene by action of **14**.

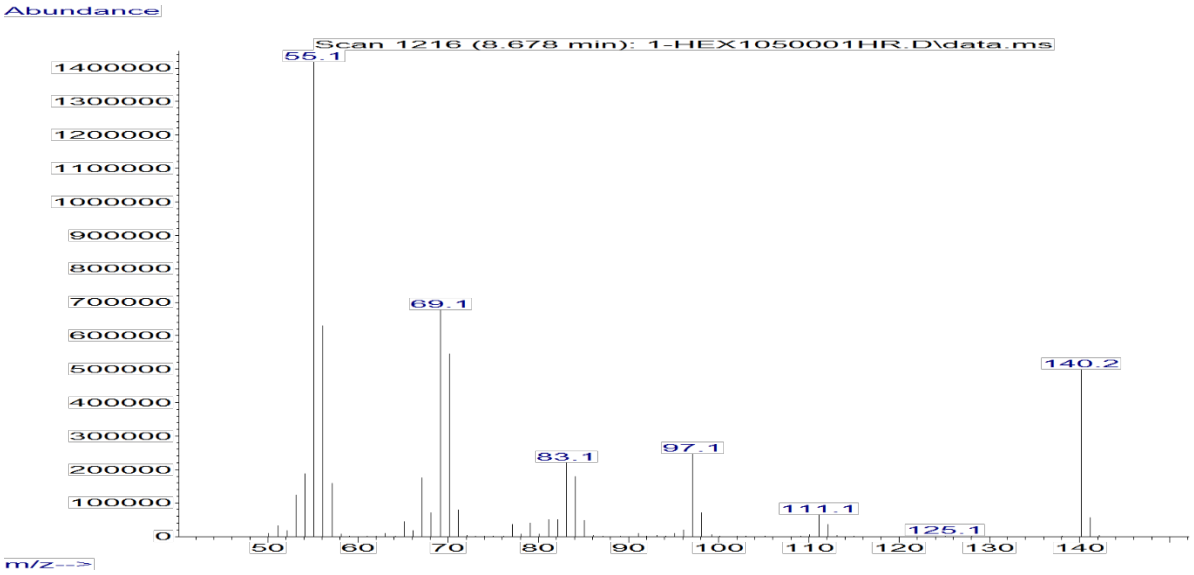


Figure S164. MS result of HM of 1-hexene by action of **14**.

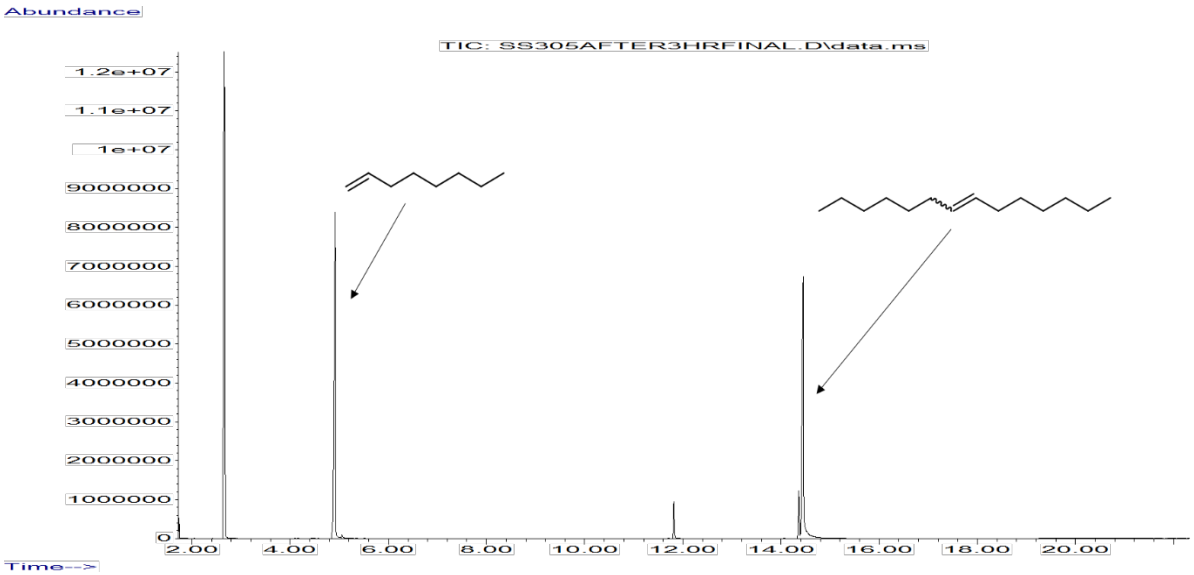


Figure S165. GC result of HM of 1-octene by action of **14**.

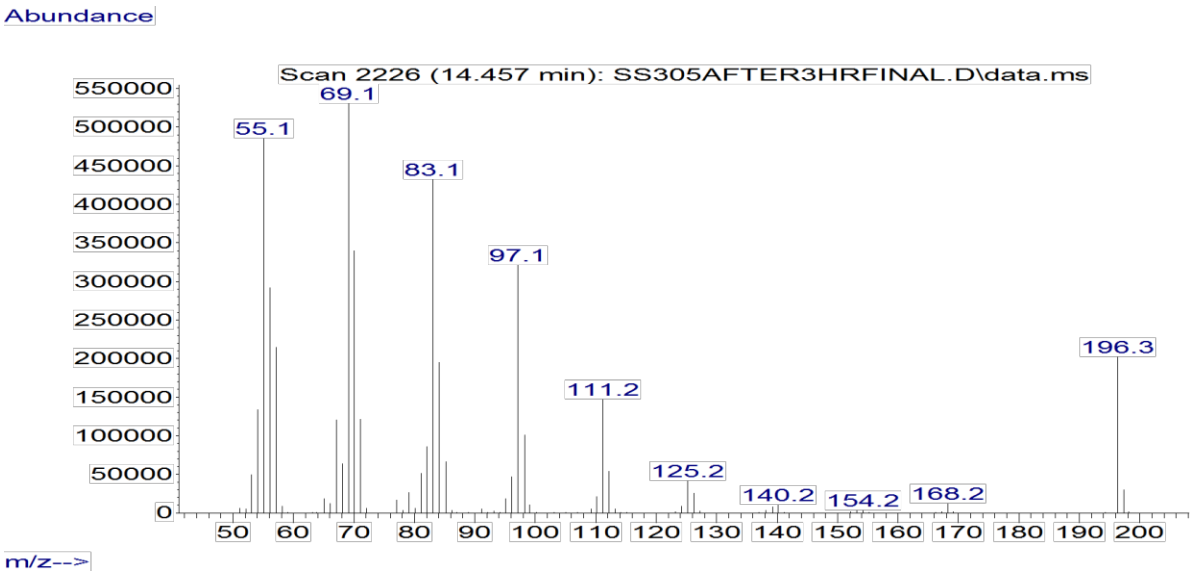


Figure S166. MS result of HM of 1-octene by action of **14.**

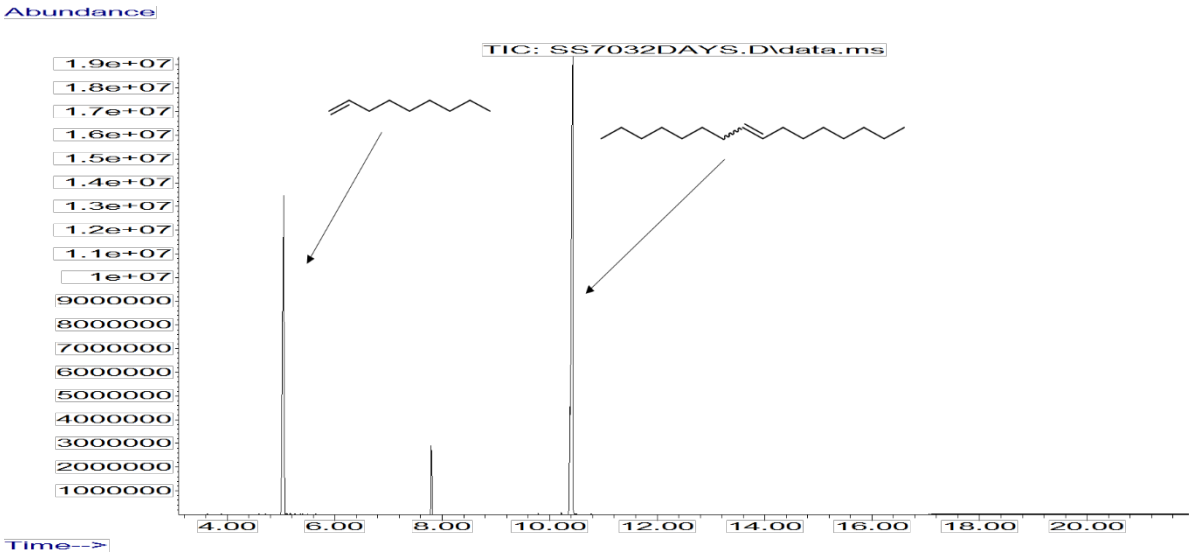


Figure S167. GC result of HM of 1-nonene by action of **15**.

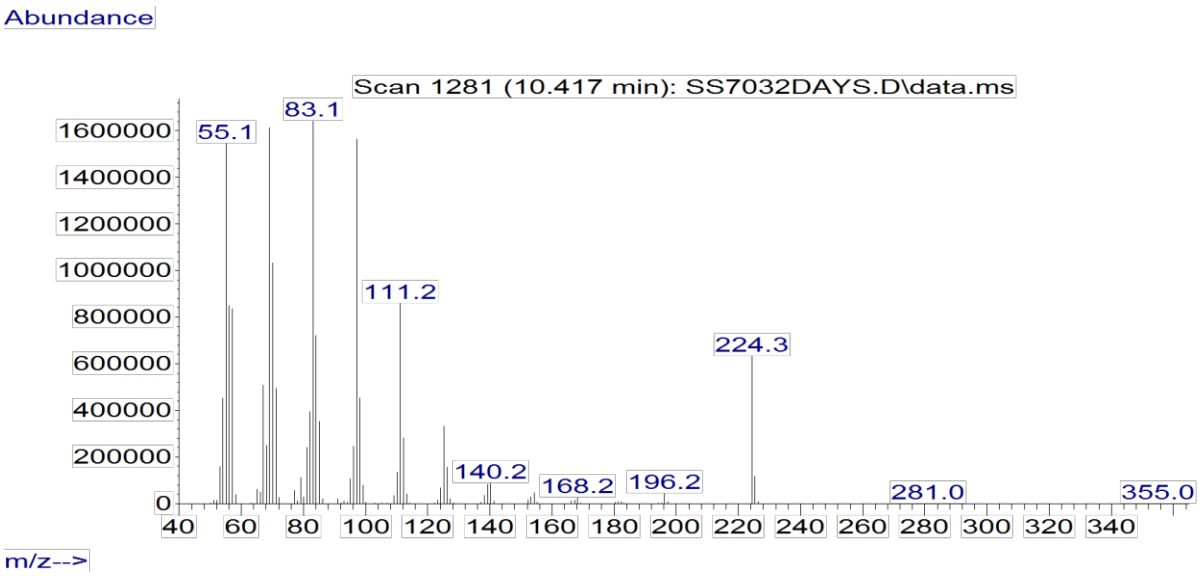


Figure S168. MS result of HM of 1-nonene by action of **15**.

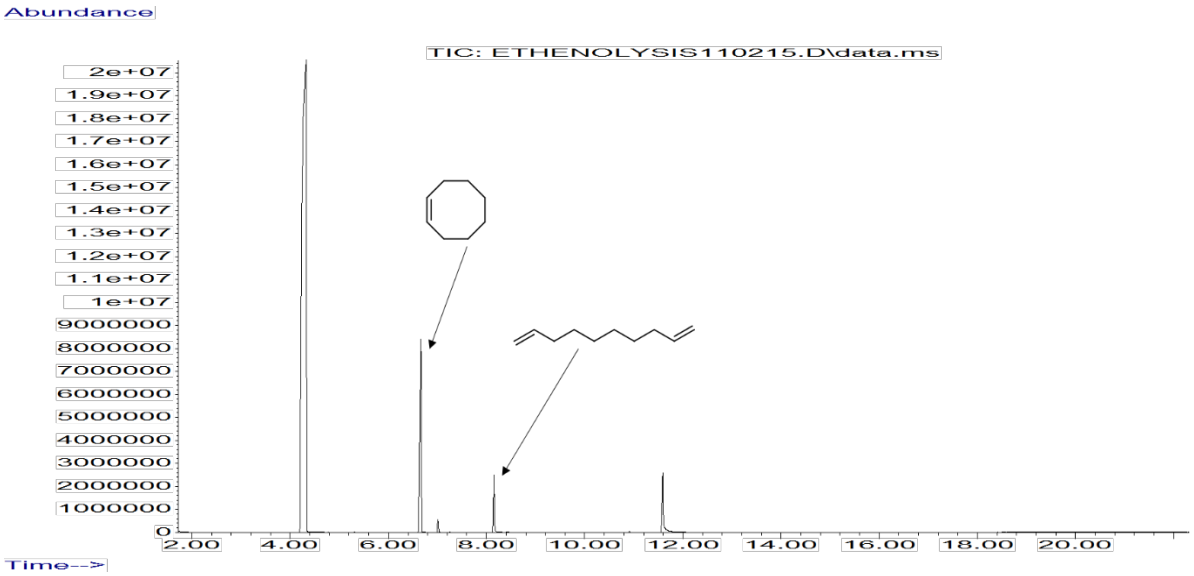


Figure S169. GC result of ethenolysis of *cis*-cyclooctene by action of **14**.

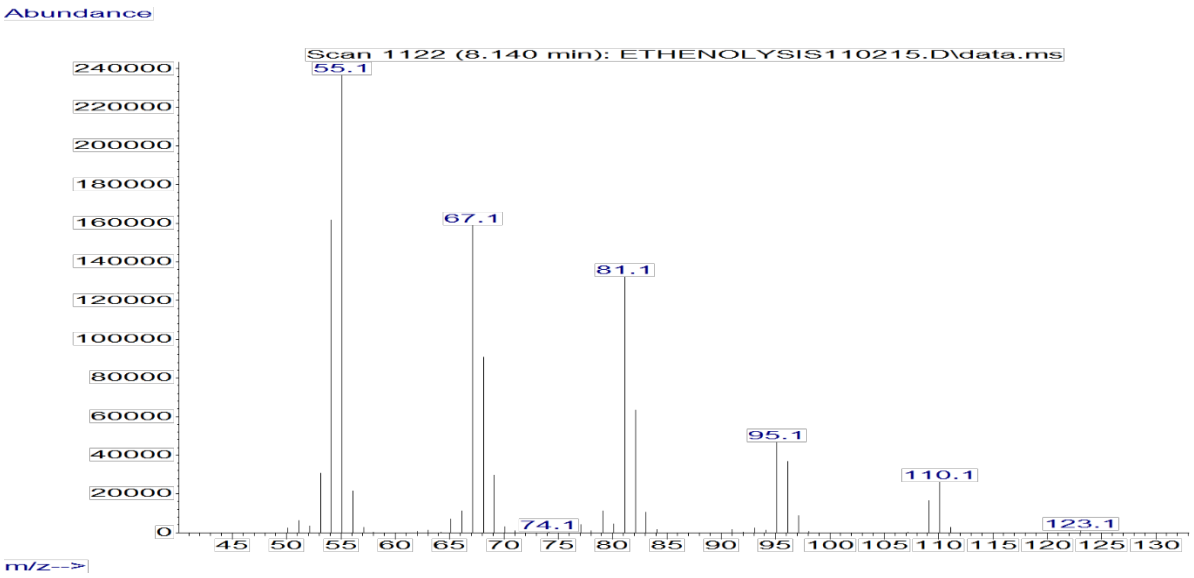
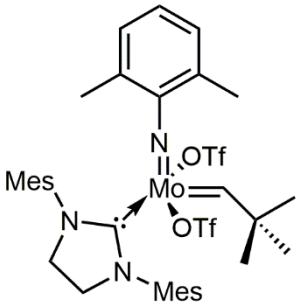


Figure S170. MS result of ethenolysis of *cis*-cyclooctene by action of **14**.

Appendix II

Complex 3


N
OTf
Mes
Mo
N
OTf
N
Mes

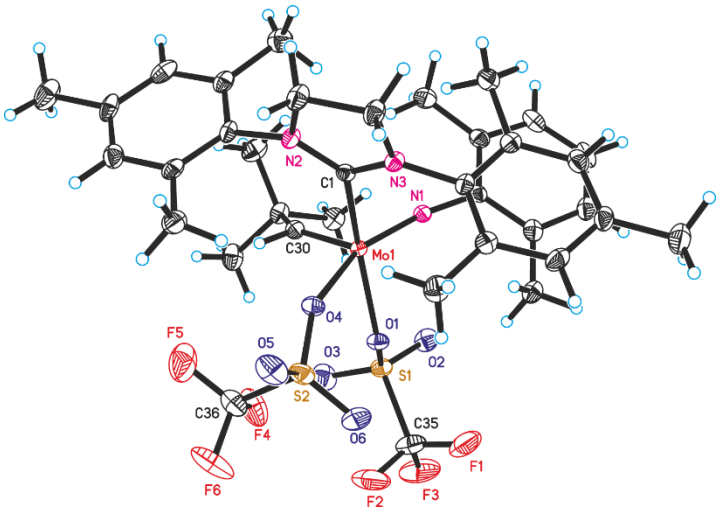

N2
C1
N3
N1
C30
Mo1
O4
O1
F5
O5
O3
O2
S1
S2
C36
F4
O6
C35
F1
F6
F2
F3

Table 3.1. Crystal data and structure refinement for **3**.

Empirical formula	$C_{36}H_{45}F_6MoN_3O_6S_2$
Formula weight	889.81
Temperature	110(2) K
Wavelength	0.71073 Å
Crystal system, space group	orthorhombic, *Pbca*
Unit cell dimensions	a = 18.2413(6) Å, α = 90°
	b = 21.1749(6) Å, β = 90°
	c = 22.1635(5) Å, γ= 90°
Volume	8560.8(4) $Å^3$
Z, Calculated density	8, 1.381 Mg/m^3
Absorption coefficient	0.474 mm^{-1}
F(000)	3664
Crystal size	0.27 x 0.22 x 0.15 mm
Theta range for data collection	1.74 to 28.31°
Limiting indices	-24<=h<=24, -28<=k<=28, -27<=l<=29
Reflections collected / unique	90580 / 10600 [R(int) = 0.0932]
Completeness to theta = 28.31	99.5 %
Absorption correction	Numerical
Max. and min. transmission	1.0000 and 0.8288
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10600 / 1 / 502
Goodness-of-fit on F^2	1.039
Final R indices [I>2σ(I)]	R1 = 0.0462, wR2 = 0.0886
R indices (all data)	R1 = 0.0807, wR2 = 0.0968
Largest diff. peak and hole	0.479 and -0.458 $e.Å^{-3}$

****

REMARK: Disordered solvent electron density (CH_2Cl_2) squeezed by PLATON

****

Table 3.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	3207(1)	1984(1)	4285(1)	12(1)
N(1)	3522(1)	2288(1)	4961(1)	14(1)
C(1)	2016(1)	1984(1)	4523(1)	14(1)
N(2)	1437(1)	2214(1)	4227(1)	16(1)
C(2)	965(2)	1597(1)	5014(1)	22(1)
N(3)	1766(1)	1619(1)	4974(1)	15(1)
C(3)	726(2)	1997(2)	4474(1)	23(1)
C(4)	1401(2)	2643(1)	3720(1)	16(1)
C(5)	1362(2)	3289(1)	3841(1)	19(1)
C(6)	1235(2)	3698(1)	3357(1)	24(1)
C(7)	1139(2)	3471(2)	2773(1)	23(1)
C(8)	1170(2)	2829(1)	2675(1)	23(1)
C(9)	1284(2)	2403(1)	3144(1)	19(1)
C(10)	1436(2)	3544(2)	4474(1)	27(1)
C(11)	992(2)	3925(2)	2259(1)	36(1)
C(12)	1236(2)	1703(1)	3018(1)	25(1)
C(13)	2182(2)	1310(1)	5444(1)	15(1)
C(14)	2312(2)	1644(1)	5978(1)	17(1)
C(15)	2659(2)	1330(1)	6446(1)	21(1)
C(16)	2852(2)	698(2)	6411(1)	22(1)
C(17)	2684(2)	374(1)	5880(1)	22(1)
C(18)	2340(2)	667(1)	5391(1)	18(1)
C(19)	2065(2)	2319(1)	6053(1)	22(1)
C(20)	3241(2)	373(2)	6929(1)	31(1)
C(21)	2146(2)	284(1)	4843(1)	25(1)
C(22)	3809(1)	2430(1)	5532(1)	14(1)
C(23)	3686(2)	3033(1)	5779(1)	19(1)
C(24)	3971(2)	3154(2)	6352(1)	24(1)
C(25)	4352(2)	2697(2)	6669(1)	24(1)
C(26)	4459(2)	2108(1)	6418(1)	22(1)
C(27)	4198(2)	1955(1)	5849(1)	19(1)
C(28)	3242(2)	3534(1)	5469(1)	26(1)
C(29)	4316(2)	1315(1)	5583(1)	22(1)
C(30)	3300(2)	2683(1)	3772(1)	17(1)
C(31)	3666(2)	3309(1)	3649(1)	19(1)
C(32)	4306(2)	3423(1)	4084(1)	23(1)
C(33)	3119(2)	3852(1)	3694(1)	28(1)
C(34)	3972(2)	3287(2)	3002(1)	28(1)
S(1)	4961(1)	1727(1)	3916(1)	20(1)
O(1)	4202(1)	1518(1)	4044(1)	18(1)
O(2)	5295(1)	2039(1)	4417(1)	27(1)
O(3)	5051(1)	2010(1)	3337(1)	33(1)
C(35)	5429(2)	969(2)	3866(2)	33(1)

F(1)	5348(1)	631(1)	4365(1)	49(1)
F(2)	5193(1)	631(1)	3402(1)	51(1)
F(3)	6149(1)	1072(1)	3788(1)	56(1)
S(2)	2930(1)	639(1)	3409(1)	22(1)
O(4)	2807(1)	1247(1)	3731(1)	19(1)
O(5)	2250(1)	340(1)	3265(1)	31(1)
O(6)	3510(1)	275(1)	3661(1)	33(1)
C(36)	3272(2)	924(2)	2682(1)	30(1)
F(4)	3901(1)	1223(1)	2739(1)	43(1)
F(5)	2796(1)	1310(1)	2425(1)	55(1)
F(6)	3375(1)	447(1)	2309(1)	59(1)

Table 3.3. Bond lengths [Å] and angles [°] for **3**.

Mo(1)-N(1)	1.729(2)
Mo(1)-C(30)	1.873(3)
Mo(1)-O(4)	2.1145(18)
Mo(1)-O(1)	2.1352(18)
Mo(1)-C(1)	2.235(3)
N(1)-C(22)	1.402(3)
C(1)-N(2)	1.335(3)
C(1)-N(3)	1.344(3)
N(2)-C(4)	1.446(3)
N(2)-C(3)	1.479(3)
C(2)-N(3)	1.465(4)
C(2)-C(3)	1.530(4)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
N(3)-C(13)	1.444(3)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(9)	1.391(4)
C(4)-C(5)	1.395(4)
C(5)-C(6)	1.399(4)
C(5)-C(10)	1.509(4)
C(6)-C(7)	1.391(4)
C(6)-H(6)	0.9500
C(7)-C(8)	1.378(4)
C(7)-C(11)	1.516(4)
C(8)-C(9)	1.390(4)
C(8)-H(8)	0.9500
C(9)-C(12)	1.510(4)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800

C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.397(4)
C(13)-C(18)	1.397(4)
C(14)-C(15)	1.385(4)
C(14)-C(19)	1.510(4)
C(15)-C(16)	1.386(4)
C(15)-H(15)	0.9500
C(16)-C(17)	1.397(4)
C(16)-C(20)	1.515(4)
C(17)-C(18)	1.397(4)
C(17)-H(17)	0.9500
C(18)-C(21)	1.504(4)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(23)	1.407(4)
C(22)-C(27)	1.418(4)
C(23)-C(24)	1.395(4)
C(23)-C(28)	1.502(4)
C(24)-C(25)	1.385(4)
C(24)-H(24)	0.9500
C(25)-C(26)	1.379(4)
C(25)-H(25)	0.9500
C(26)-C(27)	1.386(4)
C(26)-H(26)	0.9500
C(27)-C(29)	1.495(4)
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-C(31)	1.510(4)
C(30)-H(30)	0.952(17)
C(31)-C(33)	1.525(4)
C(31)-C(32)	1.534(4)
C(31)-C(34)	1.540(4)
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800

C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
S(1)-O(3)	1.427(2)
S(1)-O(2)	1.428(2)
S(1)-O(1)	1.480(2)
S(1)-C(35)	1.822(3)
C(35)-F(2)	1.325(4)
C(35)-F(1)	1.325(4)
C(35)-F(3)	1.343(4)
S(2)-O(6)	1.424(2)
S(2)-O(5)	1.427(2)
S(2)-O(4)	1.4906(19)
S(2)-C(36)	1.830(3)
C(36)-F(4)	1.317(4)
C(36)-F(6)	1.320(4)
C(36)-F(5)	1.321(4)

N(1)-Mo(1)-C(30)	101.61(11)
N(1)-Mo(1)-O(4)	153.17(9)
C(30)-Mo(1)-O(4)	105.17(10)
N(1)-Mo(1)-O(1)	96.08(9)
C(30)-Mo(1)-O(1)	97.82(10)
O(4)-Mo(1)-O(1)	78.86(7)
N(1)-Mo(1)-C(1)	96.84(10)
C(30)-Mo(1)-C(1)	103.36(11)
O(4)-Mo(1)-C(1)	78.59(9)
O(1)-Mo(1)-C(1)	152.35(9)
C(22)-N(1)-Mo(1)	170.5(2)
N(2)-C(1)-N(3)	107.9(2)
N(2)-C(1)-Mo(1)	130.79(19)
N(3)-C(1)-Mo(1)	120.27(19)
C(1)-N(2)-C(4)	130.2(2)
C(1)-N(2)-C(3)	113.5(2)
C(4)-N(2)-C(3)	116.3(2)
N(3)-C(2)-C(3)	102.7(2)
N(3)-C(2)-H(2A)	111.2
C(3)-C(2)-H(2A)	111.2
N(3)-C(2)-H(2B)	111.2
C(3)-C(2)-H(2B)	111.2
H(2A)-C(2)-H(2B)	109.1
C(1)-N(3)-C(13)	128.3(2)
C(1)-N(3)-C(2)	113.6(2)
C(13)-N(3)-C(2)	117.8(2)
N(2)-C(3)-C(2)	102.2(2)
N(2)-C(3)-H(3A)	111.3
C(2)-C(3)-H(3A)	111.3
N(2)-C(3)-H(3B)	111.3
C(2)-C(3)-H(3B)	111.3
H(3A)-C(3)-H(3B)	109.2

C(9)-C(4)-C(5)	121.8(2)
C(9)-C(4)-N(2)	119.4(2)
C(5)-C(4)-N(2)	118.0(2)
C(4)-C(5)-C(6)	117.9(2)
C(4)-C(5)-C(10)	121.7(2)
C(6)-C(5)-C(10)	120.4(3)
C(7)-C(6)-C(5)	121.4(3)
C(7)-C(6)-H(6)	119.3
C(5)-C(6)-H(6)	119.3
C(8)-C(7)-C(6)	118.8(3)
C(8)-C(7)-C(11)	121.0(3)
C(6)-C(7)-C(11)	120.2(3)
C(7)-C(8)-C(9)	121.9(3)
C(7)-C(8)-H(8)	119.0
C(9)-C(8)-H(8)	119.0
C(8)-C(9)-C(4)	118.2(3)
C(8)-C(9)-C(12)	119.4(2)
C(4)-C(9)-C(12)	122.4(2)
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(7)-C(11)-H(11A)	109.5
C(7)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(7)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(9)-C(12)-H(12A)	109.5
C(9)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(9)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(18)	121.8(2)
C(14)-C(13)-N(3)	118.1(2)
C(18)-C(13)-N(3)	119.3(2)
C(15)-C(14)-C(13)	118.0(3)
C(15)-C(14)-C(19)	120.5(2)
C(13)-C(14)-C(19)	121.4(2)
C(14)-C(15)-C(16)	122.5(3)
C(14)-C(15)-H(15)	118.8
C(16)-C(15)-H(15)	118.8
C(15)-C(16)-C(17)	117.8(3)
C(15)-C(16)-C(20)	121.0(3)
C(17)-C(16)-C(20)	121.1(3)
C(18)-C(17)-C(16)	122.2(3)
C(18)-C(17)-H(17)	118.9

C(16)-C(17)-H(17)	118.9
C(17)-C(18)-C(13)	117.5(2)
C(17)-C(18)-C(21)	119.5(3)
C(13)-C(18)-C(21)	123.0(2)
C(14)-C(19)-H(19A)	109.5
C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-H(20A)	109.5
C(16)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(16)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(1)-C(22)-C(23)	119.2(2)
N(1)-C(22)-C(27)	118.8(2)
C(23)-C(22)-C(27)	122.0(2)
C(24)-C(23)-C(22)	117.6(3)
C(24)-C(23)-C(28)	119.1(3)
C(22)-C(23)-C(28)	123.2(2)
C(25)-C(24)-C(23)	121.3(3)
C(25)-C(24)-H(24)	119.3
C(23)-C(24)-H(24)	119.3
C(26)-C(25)-C(24)	119.9(3)
C(26)-C(25)-H(25)	120.0
C(24)-C(25)-H(25)	120.0
C(25)-C(26)-C(27)	121.9(3)
C(25)-C(26)-H(26)	119.0
C(27)-C(26)-H(26)	119.0
C(26)-C(27)-C(22)	117.3(3)
C(26)-C(27)-C(29)	121.4(3)
C(22)-C(27)-C(29)	121.3(2)
C(23)-C(28)-H(28A)	109.5
C(23)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(23)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(27)-C(29)-H(29A)	109.5
C(27)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(27)-C(29)-H(29C)	109.5

H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(31)-C(30)-Mo(1)	147.5(2)
C(31)-C(30)-H(30)	113.5(18)
Mo(1)-C(30)-H(30)	98.1(18)
C(30)-C(31)-C(33)	111.1(2)
C(30)-C(31)-C(32)	111.2(2)
C(33)-C(31)-C(32)	109.8(2)
C(30)-C(31)-C(34)	107.6(2)
C(33)-C(31)-C(34)	108.8(2)
C(32)-C(31)-C(34)	108.3(2)
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(31)-C(33)-H(33A)	109.5
C(31)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(31)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(31)-C(34)-H(34A)	109.5
C(31)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(31)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
O(3)-S(1)-O(2)	117.20(14)
O(3)-S(1)-O(1)	113.90(12)
O(2)-S(1)-O(1)	112.91(12)
O(3)-S(1)-C(35)	105.11(15)
O(2)-S(1)-C(35)	104.72(14)
O(1)-S(1)-C(35)	100.71(14)
S(1)-O(1)-Mo(1)	134.76(12)
F(2)-C(35)-F(1)	108.7(3)
F(2)-C(35)-F(3)	107.8(3)
F(1)-C(35)-F(3)	107.7(3)
F(2)-C(35)-S(1)	111.8(2)
F(1)-C(35)-S(1)	111.9(2)
F(3)-C(35)-S(1)	108.9(2)
O(6)-S(2)-O(5)	119.54(14)
O(6)-S(2)-O(4)	113.07(12)
O(5)-S(2)-O(4)	111.09(13)
O(6)-S(2)-C(36)	105.70(15)
O(5)-S(2)-C(36)	104.24(14)
O(4)-S(2)-C(36)	100.81(13)
S(2)-O(4)-Mo(1)	149.81(13)
F(4)-C(36)-F(6)	107.8(3)

F(4)-C(36)-F(5)	108.5(3)
F(6)-C(36)-F(5)	107.3(3)
F(4)-C(36)-S(2)	111.8(2)
F(6)-C(36)-S(2)	110.3(2)
F(5)-C(36)-S(2)	111.1(2)

Symmetry transformations used to generate equivalent atoms:

Table 3.4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	11(1)	11(1)	13(1)	0(1)	0(1)	0(1)
N(1)	10(1)	16(1)	15(1)	-1(1)	0(1)	0(1)
C(1)	15(1)	12(1)	14(1)	-1(1)	1(1)	0(1)
N(2)	13(1)	19(1)	17(1)	5(1)	1(1)	1(1)
C(2)	15(2)	26(2)	23(1)	9(1)	0(1)	0(1)
N(3)	12(1)	16(1)	18(1)	3(1)	1(1)	0(1)
C(3)	14(1)	28(2)	25(1)	10(1)	1(1)	0(1)
C(4)	13(2)	19(2)	17(1)	7(1)	-1(1)	0(1)
C(5)	11(1)	22(2)	23(1)	4(1)	-1(1)	-1(1)
C(6)	13(2)	18(2)	40(2)	7(1)	-1(1)	-1(1)
C(7)	13(2)	31(2)	26(2)	14(1)	-3(1)	-3(1)
C(8)	19(2)	31(2)	19(1)	5(1)	0(1)	1(1)
C(9)	10(1)	22(2)	25(2)	3(1)	0(1)	2(1)
C(10)	22(2)	28(2)	30(2)	-4(1)	-2(1)	-1(1)
C(11)	28(2)	41(2)	38(2)	22(2)	2(2)	2(2)
C(12)	23(2)	24(2)	27(2)	-3(1)	-3(1)	3(1)
C(13)	10(1)	19(2)	17(1)	5(1)	1(1)	0(1)
C(14)	14(1)	17(2)	20(1)	3(1)	3(1)	-2(1)
C(15)	18(2)	26(2)	17(1)	1(1)	1(1)	-1(1)
C(16)	16(2)	30(2)	19(1)	8(1)	2(1)	3(1)
C(17)	22(2)	16(2)	28(2)	6(1)	2(1)	3(1)
C(18)	17(2)	17(2)	20(1)	4(1)	4(1)	-2(1)
C(19)	22(2)	25(2)	20(2)	-1(1)	1(1)	1(1)
C(20)	31(2)	36(2)	26(2)	8(1)	-5(1)	3(2)
C(21)	31(2)	17(2)	27(2)	1(1)	-2(1)	-3(1)
C(22)	11(1)	20(1)	12(1)	0(1)	1(1)	0(1)
C(23)	17(1)	22(1)	18(1)	-1(1)	3(1)	-1(1)
C(24)	26(2)	29(2)	18(1)	-5(1)	5(1)	-6(1)
C(25)	20(2)	41(2)	13(1)	0(1)	0(1)	-8(1)
C(26)	14(2)	32(2)	21(1)	7(1)	0(1)	0(1)
C(27)	13(1)	27(2)	19(1)	4(1)	3(1)	-3(1)
C(28)	30(2)	23(2)	25(2)	-5(1)	-1(1)	3(2)
C(29)	20(2)	21(2)	24(2)	5(1)	0(1)	1(1)
C(30)	13(2)	20(2)	18(1)	-1(1)	0(1)	0(1)
C(31)	18(2)	18(2)	21(1)	4(1)	-1(1)	-3(1)

C(32)	22(2)	19(2)	29(2)	2(1)	-1(1)	-5(1)
C(33)	25(2)	18(2)	40(2)	7(1)	1(1)	-1(1)
C(34)	27(2)	32(2)	25(2)	9(1)	1(1)	-6(2)
S(1)	14(1)	23(1)	24(1)	-1(1)	3(1)	2(1)
O(1)	14(1)	18(1)	22(1)	-4(1)	2(1)	1(1)
O(2)	20(1)	28(1)	33(1)	-3(1)	-5(1)	-1(1)
O(3)	30(1)	43(1)	26(1)	6(1)	9(1)	-2(1)
C(35)	26(2)	27(2)	46(2)	-6(2)	3(2)	9(2)
F(1)	53(2)	34(1)	60(1)	8(1)	2(1)	21(1)
F(2)	45(1)	47(1)	61(1)	-29(1)	2(1)	14(1)
F(3)	22(1)	58(2)	88(2)	-15(1)	10(1)	15(1)
S(2)	30(1)	16(1)	22(1)	-5(1)	3(1)	-2(1)
O(4)	20(1)	14(1)	21(1)	-4(1)	1(1)	-1(1)
O(5)	43(2)	18(1)	32(1)	-7(1)	2(1)	-13(1)
O(6)	43(2)	19(1)	37(1)	-1(1)	0(1)	9(1)
C(36)	31(2)	36(2)	23(2)	-6(1)	3(1)	-3(2)
F(4)	39(1)	64(2)	26(1)	1(1)	4(1)	-21(1)
F(5)	44(1)	88(2)	34(1)	24(1)	9(1)	13(1)
F(6)	76(2)	63(2)	40(1)	-30(1)	23(1)	-11(1)

Table 3.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **3**.

	x	y	z	U(eq)
H(2A)	789	1781	5398	26
H(2B)	783	1158	4978	26
H(3A)	453	1741	4175	27
H(3B)	419	2358	4602	27
H(6)	1215	4140	3428	28
H(8)	1112	2673	2276	27
H(10A)	1010	3415	4714	40
H(10B)	1461	4006	4460	40
H(10C)	1884	3378	4659	40
H(11A)	1449	4138	2146	53
H(11B)	630	4240	2386	53
H(11C)	803	3691	1911	53
H(12A)	724	1567	3045	37
H(12B)	1530	1473	3316	37
H(12C)	1424	1616	2613	37
H(15)	2770	1557	6804	25
H(17)	2808	-61	5850	26
H(19A)	1536	2329	6133	34
H(19B)	2170	2556	5683	34
H(19C)	2327	2512	6392	34
H(20A)	3761	491	6927	46
H(20B)	3196	-86	6883	46

H(20C)	3018	502	7311	46
H(21A)	2585	68	4694	37
H(21B)	1955	564	4528	37
H(21C)	1773	-29	4950	37
H(24)	3901	3559	6528	29
H(25)	4541	2788	7059	29
H(26)	4719	1798	6642	27
H(28A)	2846	3673	5736	39
H(28B)	3033	3362	5096	39
H(28C)	3558	3894	5372	39
H(29A)	4529	1035	5888	32
H(29B)	4651	1347	5239	32
H(29C)	3846	1142	5447	32
H(30)	3047(15)	2515(13)	3432(10)	24(8)
H(32A)	4128	3405	4501	35
H(32B)	4520	3840	4006	35
H(32C)	4680	3097	4023	35
H(33A)	2706	3772	3421	41
H(33B)	3360	4248	3581	41
H(33C)	2938	3884	4110	41
H(34A)	4350	2959	2975	42
H(34B)	4187	3698	2900	42
H(34C)	3575	3190	2719	42

Table 3.6. Torsion angles [°] for **3**.

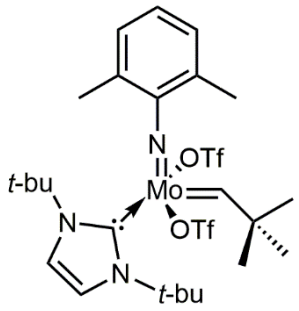
C(30)-Mo(1)-N(1)-C(22)	-153.3(11)
O(4)-Mo(1)-N(1)-C(22)	23.3(13)
O(1)-Mo(1)-N(1)-C(22)	-54.0(12)
C(1)-Mo(1)-N(1)-C(22)	101.5(12)
N(1)-Mo(1)-C(1)-N(2)	129.3(3)
C(30)-Mo(1)-C(1)-N(2)	25.6(3)
O(4)-Mo(1)-C(1)-N(2)	-77.5(2)
O(1)-Mo(1)-C(1)-N(2)	-113.4(3)
N(1)-Mo(1)-C(1)-N(3)	-63.8(2)
C(30)-Mo(1)-C(1)-N(3)	-167.5(2)
O(4)-Mo(1)-C(1)-N(3)	89.4(2)
O(1)-Mo(1)-C(1)-N(3)	53.5(3)
N(3)-C(1)-N(2)-C(4)	177.9(2)
Mo(1)-C(1)-N(2)-C(4)	-14.0(4)
N(3)-C(1)-N(2)-C(3)	-0.6(3)
Mo(1)-C(1)-N(2)-C(3)	167.5(2)
N(2)-C(1)-N(3)-C(13)	-174.8(2)
Mo(1)-C(1)-N(3)-C(13)	15.7(4)
N(2)-C(1)-N(3)-C(2)	-1.4(3)
Mo(1)-C(1)-N(3)-C(2)	-171.01(18)
C(3)-C(2)-N(3)-C(1)	2.7(3)
C(3)-C(2)-N(3)-C(13)	176.8(2)
C(1)-N(2)-C(3)-C(2)	2.2(3)

C(4)-N(2)-C(3)-C(2)	-176.5(2)
N(3)-C(2)-C(3)-N(2)	-2.7(3)
C(1)-N(2)-C(4)-C(9)	100.7(3)
C(3)-N(2)-C(4)-C(9)	-80.8(3)
C(1)-N(2)-C(4)-C(5)	-89.9(4)
C(3)-N(2)-C(4)-C(5)	88.6(3)
C(9)-C(4)-C(5)-C(6)	-3.0(4)
N(2)-C(4)-C(5)-C(6)	-172.1(2)
C(9)-C(4)-C(5)-C(10)	175.5(3)
N(2)-C(4)-C(5)-C(10)	6.4(4)
C(4)-C(5)-C(6)-C(7)	1.0(4)
C(10)-C(5)-C(6)-C(7)	-177.5(3)
C(5)-C(6)-C(7)-C(8)	-0.1(4)
C(5)-C(6)-C(7)-C(11)	179.2(3)
C(6)-C(7)-C(8)-C(9)	1.0(5)
C(11)-C(7)-C(8)-C(9)	-178.2(3)
C(7)-C(8)-C(9)-C(4)	-2.9(4)
C(7)-C(8)-C(9)-C(12)	173.8(3)
C(5)-C(4)-C(9)-C(8)	3.9(4)
N(2)-C(4)-C(9)-C(8)	172.9(3)
C(5)-C(4)-C(9)-C(12)	-172.7(3)
N(2)-C(4)-C(9)-C(12)	-3.7(4)
C(1)-N(3)-C(13)-C(14)	89.2(3)
C(2)-N(3)-C(13)-C(14)	-83.9(3)
C(1)-N(3)-C(13)-C(18)	-100.5(3)
C(2)-N(3)-C(13)-C(18)	86.4(3)
C(18)-C(13)-C(14)-C(15)	5.0(4)
N(3)-C(13)-C(14)-C(15)	175.0(2)
C(18)-C(13)-C(14)-C(19)	-173.3(3)
N(3)-C(13)-C(14)-C(19)	-3.3(4)
C(13)-C(14)-C(15)-C(16)	-2.7(4)
C(19)-C(14)-C(15)-C(16)	175.6(3)
C(14)-C(15)-C(16)-C(17)	0.0(4)
C(14)-C(15)-C(16)-C(20)	179.2(3)
C(15)-C(16)-C(17)-C(18)	0.6(4)
C(20)-C(16)-C(17)-C(18)	-178.6(3)
C(16)-C(17)-C(18)-C(13)	1.5(4)
C(16)-C(17)-C(18)-C(21)	-177.4(3)
C(14)-C(13)-C(18)-C(17)	-4.4(4)
N(3)-C(13)-C(18)-C(17)	-174.3(2)
C(14)-C(13)-C(18)-C(21)	174.5(3)
N(3)-C(13)-C(18)-C(21)	4.6(4)
Mo(1)-N(1)-C(22)-C(23)	-168.4(10)
Mo(1)-N(1)-C(22)-C(27)	9.8(13)
N(1)-C(22)-C(23)-C(24)	179.1(2)
C(27)-C(22)-C(23)-C(24)	0.9(4)
N(1)-C(22)-C(23)-C(28)	1.6(4)
C(27)-C(22)-C(23)-C(28)	-176.6(3)
C(22)-C(23)-C(24)-C(25)	-0.8(4)
C(28)-C(23)-C(24)-C(25)	176.7(3)

C(23)-C(24)-C(25)-C(26)	0.2(5)
C(24)-C(25)-C(26)-C(27)	0.4(4)
C(25)-C(26)-C(27)-C(22)	-0.3(4)
C(25)-C(26)-C(27)-C(29)	-179.9(3)
N(1)-C(22)-C(27)-C(26)	-178.5(2)
C(23)-C(22)-C(27)-C(26)	-0.4(4)
N(1)-C(22)-C(27)-C(29)	1.1(4)
C(23)-C(22)-C(27)-C(29)	179.3(3)
N(1)-Mo(1)-C(30)-C(31)	22.0(4)
O(4)-Mo(1)-C(30)-C(31)	-156.4(4)
O(1)-Mo(1)-C(30)-C(31)	-75.9(4)
C(1)-Mo(1)-C(30)-C(31)	122.0(4)
Mo(1)-C(30)-C(31)-C(33)	-112.4(4)
Mo(1)-C(30)-C(31)-C(32)	10.2(5)
Mo(1)-C(30)-C(31)-C(34)	128.6(3)
O(3)-S(1)-O(1)-Mo(1)	-76.08(18)
O(2)-S(1)-O(1)-Mo(1)	60.81(19)
C(35)-S(1)-O(1)-Mo(1)	171.96(16)
N(1)-Mo(1)-O(1)-S(1)	-61.96(17)
C(30)-Mo(1)-O(1)-S(1)	40.69(17)
O(4)-Mo(1)-O(1)-S(1)	144.70(16)
C(1)-Mo(1)-O(1)-S(1)	-179.44(15)
O(3)-S(1)-C(35)-F(2)	-53.6(3)
O(2)-S(1)-C(35)-F(2)	-177.7(2)
O(1)-S(1)-C(35)-F(2)	64.9(3)
O(3)-S(1)-C(35)-F(1)	-175.7(2)
O(2)-S(1)-C(35)-F(1)	60.2(3)
O(1)-S(1)-C(35)-F(1)	-57.2(3)
O(3)-S(1)-C(35)-F(3)	65.4(3)
O(2)-S(1)-C(35)-F(3)	-58.7(3)
O(1)-S(1)-C(35)-F(3)	-176.0(2)
O(6)-S(2)-O(4)-Mo(1)	23.8(3)
O(5)-S(2)-O(4)-Mo(1)	161.4(2)
C(36)-S(2)-O(4)-Mo(1)	-88.6(3)
N(1)-Mo(1)-O(4)-S(2)	-68.3(3)
C(30)-Mo(1)-O(4)-S(2)	108.3(2)
O(1)-Mo(1)-O(4)-S(2)	13.1(2)
C(1)-Mo(1)-O(4)-S(2)	-150.8(2)
O(6)-S(2)-C(36)-F(4)	-54.0(3)
O(5)-S(2)-C(36)-F(4)	179.2(2)
O(4)-S(2)-C(36)-F(4)	63.9(3)
O(6)-S(2)-C(36)-F(6)	65.9(3)
O(5)-S(2)-C(36)-F(6)	-61.0(3)
O(4)-S(2)-C(36)-F(6)	-176.2(2)
O(6)-S(2)-C(36)-F(5)	-175.3(2)
O(5)-S(2)-C(36)-F(5)	57.9(3)
O(4)-S(2)-C(36)-F(5)	-57.4(3)

Symmetry transformations used to generate equivalent atoms:

Complex 4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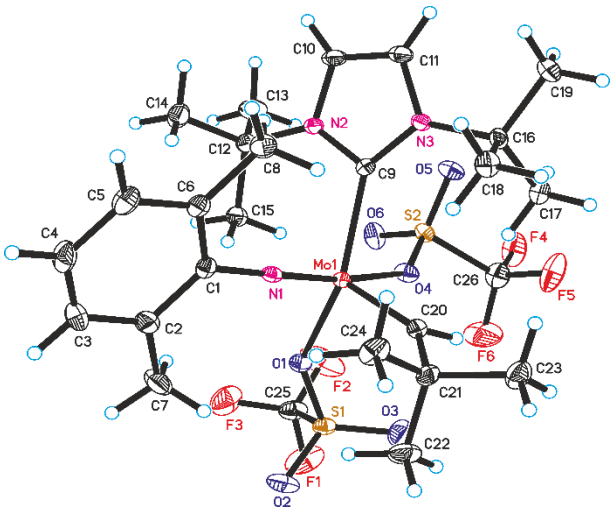
OTf
t-bu
Mo
N
OTf
N
t-bu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C11
C19
C14
C13
N2
N3
C16
C12
C8
C9
O5
C18
C6
C5
C15
O6
S2
C17
C4
F4
Mo1
C1
N1
O4
C26
F5
C20
C2
C3
C24
F6
O1
F2
C23
C25
C21
C7
F3
S1
O3
C22
F1
O2

Table 4.1. Crystal data and structure refinement for **4**.

Empirical formula	$C_{26}H_{39}F_6MoN_3O_6S_2$
Formula weight	763.66
Temperature	110(2) K
Wavelength	0.71073 Å
Crystal system, space group	tetragonal, $P42_1c$
Unit cell dimensions	a = 24.4986(11) Å, α = 90°
	b = 24.4986(11) Å, β = 90°
	c = 10.9368(7) Å, γ = 90°
Volume	6564.1(6) $Å^3$
Z, Calculated density	8, 1.545 Mg/m^3
Absorption coefficient	0.603 mm^{-1}
F(000)	3136
Crystal size	0.24 x 0.22 x 0.16 mm
Theta range for data collection	1.66 to 30.57°
Limiting indices	-35<=h<=34, -35<=k<=33, -15<=l<=15
Reflections collected / unique	106969 / 10062 [R(int) = 0.0574]
Completeness to theta = 30.57	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7349 and 0.7005
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10062 / 0 / 412
Goodness-of-fit on F^2	1.022
Final R indices [I>2σ(I)]	R1 = 0.0264, wR2 = 0.0524
R indices (all data)	R1 = 0.0345, wR2 = 0.0545
Absolute structure parameter	-0.036(16)
Largest diff. peak and hole	0.331 and -0.334 $e.Å^{-3}$

Table 4.1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	9834(1)	2471(1)	7649(1)	10(1)
S(1)	8516(1)	2263(1)	6811(1)	16(1)
N(1)	9934(1)	2220(1)	9110(1)	12(1)
O(1)	8973(1)	2450(1)	7597(1)	17(1)
F(1)	7662(1)	2807(1)	6106(1)	41(1)
C(1)	9980(1)	2075(1)	10334(2)	13(1)
S(2)	9778(1)	3495(1)	5414(1)	14(1)
N(2)	10589(1)	3435(1)	8395(1)	12(1)
O(2)	8162(1)	1892(1)	7432(1)	26(1)
F(2)	8397(1)	3290(1)	6204(2)	50(1)
C(2)	9501(1)	1927(1)	10962(2)	19(1)
N(3)	11106(1)	2943(1)	7214(1)	13(1)
F(3)	7977(1)	3058(1)	7832(1)	39(1)
O(3)	8677(1)	2132(1)	5596(1)	26(1)
C(3)	9554(1)	1779(1)	12183(2)	24(1)
O(4)	9694(1)	2959(1)	6012(1)	17(1)
F(4)	9612(1)	3786(1)	3172(1)	35(1)
C(4)	10057(1)	1775(1)	12752(2)	24(1)
O(5)	10337(1)	3657(1)	5366(1)	21(1)
F(5)	9963(1)	2989(1)	3359(1)	41(1)
C(5)	10522(1)	1921(1)	12124(2)	21(1)
C(6)	10497(1)	2077(1)	10900(2)	15(1)
O(6)	9391(1)	3898(1)	5787(1)	23(1)
F(6)	9114(1)	3116(1)	3750(1)	50(1)
C(7)	8958(1)	1929(1)	10330(2)	28(1)
C(8)	11002(1)	2244(1)	10221(2)	20(1)
C(9)	10590(1)	2971(1)	7689(2)	11(1)
C(10)	11099(1)	3673(1)	8381(2)	19(1)
C(11)	11417(1)	3370(1)	7650(2)	18(1)
C(12)	10140(1)	3715(1)	9101(2)	14(1)
C(13)	10125(1)	4311(1)	8692(2)	22(1)
C(14)	10276(1)	3674(1)	10462(2)	23(1)
C(15)	9578(1)	3472(1)	8870(2)	17(1)
C(16)	11339(1)	2530(1)	6328(2)	14(1)
C(17)	10982(1)	2486(1)	5192(2)	18(1)
C(18)	11404(1)	1987(1)	6983(2)	19(1)
C(19)	11905(1)	2718(1)	5905(2)	22(1)
C(20)	9969(1)	1813(1)	6806(2)	14(1)
C(21)	10008(1)	1201(1)	7034(2)	16(1)
C(22)	9420(1)	981(1)	6965(2)	26(1)
C(23)	10351(1)	934(1)	6018(2)	24(1)
C(24)	10249(1)	1050(1)	8281(2)	23(1)
C(25)	8121(1)	2894(1)	6726(2)	24(1)

C(26)	9603(1)	3332(1)	3839(2)	24(1)

Table 4.3. Bond lengths [Å] and angles [°] for **4**.

Mo(1)-N(1)	1.7298(14)
Mo(1)-C(20)	1.8869(18)
Mo(1)-O(1)	2.1107(11)
Mo(1)-O(4)	2.1798(12)
Mo(1)-C(9)	2.2212(16)
S(1)-O(3)	1.4236(15)
S(1)-O(2)	1.4272(13)
S(1)-O(1)	1.4850(12)
S(1)-C(25)	1.826(2)
N(1)-C(1)	1.390(2)
F(1)-C(25)	1.330(2)
C(1)-C(2)	1.407(3)
C(1)-C(6)	1.410(2)
S(2)-O(5)	1.4263(14)
S(2)-O(6)	1.4286(14)
S(2)-O(4)	1.4806(13)
S(2)-C(26)	1.820(2)
N(2)-C(9)	1.374(2)
N(2)-C(10)	1.381(2)
N(2)-C(12)	1.508(2)
F(2)-C(25)	1.313(2)
C(2)-C(3)	1.389(3)
C(2)-C(7)	1.499(3)
N(3)-C(9)	1.367(2)
N(3)-C(11)	1.380(2)
N(3)-C(16)	1.513(2)
F(3)-C(25)	1.323(2)
C(3)-C(4)	1.380(3)
C(3)-H(3)	0.9500
F(4)-C(26)	1.331(2)
C(4)-C(5)	1.378(3)
C(4)-H(4)	0.9500
F(5)-C(26)	1.327(2)
C(5)-C(6)	1.393(3)
C(5)-H(5)	0.9500
C(6)-C(8)	1.500(3)
F(6)-C(26)	1.313(3)
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(10)-C(11)	1.340(3)
C(10)-H(10)	0.9500

C(11)-H(11)	0.9500
C(12)-C(15)	1.522(3)
C(12)-C(13)	1.528(2)
C(12)-C(14)	1.529(3)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-C(18)	1.519(3)
C(16)-C(17)	1.523(2)
C(16)-C(19)	1.531(2)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-C(21)	1.523(3)
C(20)-H(20)	0.96(2)
C(21)-C(24)	1.530(3)
C(21)-C(23)	1.539(3)
C(21)-C(22)	1.541(3)
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800

N(1)-Mo(1)-C(20)	97.03(8)
N(1)-Mo(1)-O(1)	99.04(6)
C(20)-Mo(1)-O(1)	98.13(6)
N(1)-Mo(1)-O(4)	167.42(6)
C(20)-Mo(1)-O(4)	95.48(7)
O(1)-Mo(1)-O(4)	80.44(5)
N(1)-Mo(1)-C(9)	93.43(6)
C(20)-Mo(1)-C(9)	109.57(7)
O(1)-Mo(1)-C(9)	147.93(5)
O(4)-Mo(1)-C(9)	81.11(5)

O(3)-S(1)-O(2)	118.08(9)
O(3)-S(1)-O(1)	113.60(8)
O(2)-S(1)-O(1)	112.32(8)
O(3)-S(1)-C(25)	106.81(10)
O(2)-S(1)-C(25)	103.95(9)
O(1)-S(1)-C(25)	99.63(8)
C(1)-N(1)-Mo(1)	172.92(13)
S(1)-O(1)-Mo(1)	140.96(8)
N(1)-C(1)-C(2)	117.92(16)
N(1)-C(1)-C(6)	119.74(16)
C(2)-C(1)-C(6)	122.34(16)
O(5)-S(2)-O(6)	117.08(9)
O(5)-S(2)-O(4)	113.41(8)
O(6)-S(2)-O(4)	113.17(8)
O(5)-S(2)-C(26)	104.68(9)
O(6)-S(2)-C(26)	105.37(9)
O(4)-S(2)-C(26)	100.97(9)
C(9)-N(2)-C(10)	109.91(14)
C(9)-N(2)-C(12)	131.76(14)
C(10)-N(2)-C(12)	118.29(14)
C(3)-C(2)-C(1)	117.34(18)
C(3)-C(2)-C(7)	121.76(18)
C(1)-C(2)-C(7)	120.91(17)
C(9)-N(3)-C(11)	109.93(14)
C(9)-N(3)-C(16)	128.79(14)
C(11)-N(3)-C(16)	121.28(14)
C(4)-C(3)-C(2)	121.23(19)
C(4)-C(3)-H(3)	119.4
C(2)-C(3)-H(3)	119.4
S(2)-O(4)-Mo(1)	145.78(8)
C(5)-C(4)-C(3)	120.74(18)
C(5)-C(4)-H(4)	119.6
C(3)-C(4)-H(4)	119.6
C(4)-C(5)-C(6)	120.91(19)
C(4)-C(5)-H(5)	119.5
C(6)-C(5)-H(5)	119.5
C(5)-C(6)-C(1)	117.44(17)
C(5)-C(6)-C(8)	120.98(17)
C(1)-C(6)-C(8)	121.58(16)
C(2)-C(7)-H(7A)	109.5
C(2)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(2)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(6)-C(8)-H(8A)	109.5
C(6)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(6)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5

H(8B)-C(8)-H(8C)	109.5
N(3)-C(9)-N(2)	104.95(13)
N(3)-C(9)-Mo(1)	137.31(11)
N(2)-C(9)-Mo(1)	117.69(11)
C(11)-C(10)-N(2)	107.40(15)
C(11)-C(10)-H(10)	126.3
N(2)-C(10)-H(10)	126.3
C(10)-C(11)-N(3)	107.77(15)
C(10)-C(11)-H(11)	126.1
N(3)-C(11)-H(11)	126.1
N(2)-C(12)-C(15)	113.42(14)
N(2)-C(12)-C(13)	107.61(15)
C(15)-C(12)-C(13)	107.67(15)
N(2)-C(12)-C(14)	108.00(15)
C(15)-C(12)-C(14)	109.49(15)
C(13)-C(12)-C(14)	110.65(15)
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(12)-C(15)-H(15A)	109.5
C(12)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(12)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
N(3)-C(16)-C(18)	108.81(14)
N(3)-C(16)-C(17)	110.62(14)
C(18)-C(16)-C(17)	112.50(15)
N(3)-C(16)-C(19)	109.53(14)
C(18)-C(16)-C(19)	108.19(15)
C(17)-C(16)-C(19)	107.13(14)
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5

H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(16)-C(19)-H(19A)	109.5
C(16)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(16)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(21)-C(20)-Mo(1)	140.58(14)
C(21)-C(20)-H(20)	110.7(12)
Mo(1)-C(20)-H(20)	106.1(12)
C(20)-C(21)-C(24)	114.07(15)
C(20)-C(21)-C(23)	109.54(15)
C(24)-C(21)-C(23)	109.36(15)
C(20)-C(21)-C(22)	106.01(15)
C(24)-C(21)-C(22)	108.67(16)
C(23)-C(21)-C(22)	109.04(15)
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(21)-C(23)-H(23A)	109.5
C(21)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(21)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(21)-C(24)-H(24A)	109.5
C(21)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(21)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
F(2)-C(25)-F(3)	108.04(18)
F(2)-C(25)-F(1)	109.41(18)
F(3)-C(25)-F(1)	106.78(16)
F(2)-C(25)-S(1)	112.03(14)
F(3)-C(25)-S(1)	110.60(14)
F(1)-C(25)-S(1)	109.83(13)
F(6)-C(26)-F(5)	108.90(18)
F(6)-C(26)-F(4)	108.14(17)
F(5)-C(26)-F(4)	107.51(17)
F(6)-C(26)-S(2)	111.96(14)
F(5)-C(26)-S(2)	110.88(14)
F(4)-C(26)-S(2)	109.33(14)

Symmetry transformations used to generate equivalent atoms:

Table 4.4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	9(1)	10(1)	11(1)	1(1)	-1(1)	-1(1)
S(1)	12(1)	15(1)	21(1)	0(1)	-2(1)	-1(1)
N(1)	9(1)	12(1)	15(1)	0(1)	0(1)	-1(1)
O(1)	12(1)	21(1)	18(1)	-1(1)	-1(1)	-1(1)
F(1)	27(1)	36(1)	59(1)	-13(1)	-23(1)	14(1)
C(1)	18(1)	10(1)	12(1)	0(1)	0(1)	1(1)
S(2)	14(1)	14(1)	14(1)	4(1)	1(1)	1(1)
N(2)	11(1)	12(1)	13(1)	-1(1)	-1(1)	-1(1)
O(2)	19(1)	19(1)	42(1)	4(1)	1(1)	-6(1)
F(2)	34(1)	27(1)	90(1)	28(1)	9(1)	4(1)
C(2)	20(1)	19(1)	18(1)	2(1)	1(1)	-3(1)
N(3)	11(1)	13(1)	14(1)	-1(1)	1(1)	-1(1)
F(3)	36(1)	33(1)	49(1)	-18(1)	-1(1)	10(1)
O(3)	24(1)	34(1)	21(1)	-7(1)	-3(1)	3(1)
C(3)	27(1)	28(1)	17(1)	5(1)	6(1)	-3(1)
O(4)	17(1)	16(1)	17(1)	7(1)	-2(1)	-2(1)
F(4)	58(1)	29(1)	17(1)	9(1)	2(1)	11(1)
C(4)	36(1)	23(1)	12(1)	4(1)	0(1)	1(1)
O(5)	17(1)	21(1)	26(1)	6(1)	1(1)	-5(1)
F(5)	62(1)	35(1)	26(1)	-10(1)	-4(1)	22(1)
C(5)	26(1)	20(1)	17(1)	0(1)	-6(1)	4(1)
C(6)	18(1)	11(1)	16(1)	-2(1)	0(1)	1(1)
O(6)	26(1)	23(1)	21(1)	5(1)	5(1)	9(1)
F(6)	43(1)	75(1)	31(1)	11(1)	-21(1)	-25(1)
C(7)	17(1)	44(1)	24(1)	7(1)	3(1)	-8(1)
C(8)	15(1)	27(1)	18(1)	0(1)	-4(1)	1(1)
C(9)	13(1)	10(1)	11(1)	0(1)	-2(1)	0(1)
C(10)	14(1)	17(1)	24(1)	-5(1)	-1(1)	-5(1)
C(11)	13(1)	19(1)	23(1)	-3(1)	0(1)	-5(1)
C(12)	12(1)	13(1)	16(1)	-3(1)	0(1)	3(1)
C(13)	20(1)	12(1)	34(1)	-1(1)	-2(1)	-1(1)
C(14)	25(1)	27(1)	17(1)	-3(1)	-1(1)	0(1)
C(15)	15(1)	15(1)	21(1)	-3(1)	3(1)	2(1)
C(16)	13(1)	14(1)	14(1)	-2(1)	3(1)	2(1)
C(17)	21(1)	19(1)	15(1)	-2(1)	1(1)	2(1)
C(18)	22(1)	14(1)	20(1)	1(1)	1(1)	4(1)
C(19)	16(1)	27(1)	24(1)	-3(1)	6(1)	-1(1)
C(20)	14(1)	16(1)	13(1)	0(1)	1(1)	-2(1)
C(21)	19(1)	12(1)	17(1)	-3(1)	0(1)	-1(1)
C(22)	26(1)	15(1)	37(1)	-2(1)	-1(1)	-6(1)
C(23)	30(1)	18(1)	23(1)	-5(1)	2(1)	2(1)
C(24)	33(1)	13(1)	22(1)	2(1)	-4(1)	1(1)
C(25)	17(1)	20(1)	35(1)	-2(1)	-5(1)	-1(1)

C(26)	30(1)	22(1)	19(1)	5(1)	-2(1)	3(1)

Table 4.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **4**.

	x	y	z	U(eq)
H(3)	9238	1680	12634	29
H(4)	10082	1670	13586	29
H(5)	10865	1915	12530	25
H(7A)	8672	1828	10914	42
H(7B)	8964	1665	9656	42
H(7C)	8884	2295	10007	42
H(8A)	10983	2635	10031	30
H(8B)	11028	2035	9459	30
H(8C)	11323	2172	10728	30
H(10)	11206	3992	8811	22
H(11)	11790	3437	7465	22
H(13A)	10474	4486	8888	33
H(13B)	9829	4501	9119	33
H(13C)	10063	4328	7808	33
H(14A)	10271	3290	10713	34
H(14B)	10006	3878	10936	34
H(14C)	10640	3826	10609	34
H(15A)	9504	3469	7989	25
H(15B)	9301	3693	9286	25
H(15C)	9566	3098	9187	25
H(17A)	10610	2386	5432	27
H(17B)	11131	2206	4646	27
H(17C)	10976	2838	4767	27
H(18A)	11652	2032	7678	28
H(18B)	11554	1716	6416	28
H(18C)	11047	1864	7277	28
H(19A)	11874	3077	5517	33
H(19B)	12052	2455	5316	33
H(19C)	12149	2742	6612	33
H(20)	9893(8)	1886(8)	5963(18)	17(5)
H(22A)	9203	1139	7629	39
H(22B)	9424	583	7044	39
H(22C)	9258	1082	6176	39
H(23A)	10189	1017	5220	36
H(23B)	10357	537	6138	36
H(23C)	10724	1076	6048	36
H(24A)	10615	1207	8356	34
H(24B)	10270	652	8353	34
H(24C)	10014	1195	8930	34

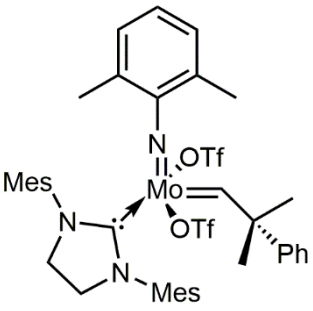
Table 4.6. Torsion angles [°] for **4**.

C(20)-Mo(1)-N(1)-C(1)	-162.8(11)
O(1)-Mo(1)-N(1)-C(1)	-63.3(11)
O(4)-Mo(1)-N(1)-C(1)	23.3(12)
C(9)-Mo(1)-N(1)-C(1)	87.0(11)
O(3)-S(1)-O(1)-Mo(1)	-14.57(16)
O(2)-S(1)-O(1)-Mo(1)	122.70(12)
C(25)-S(1)-O(1)-Mo(1)	-127.79(13)
N(1)-Mo(1)-O(1)-S(1)	-131.13(13)
C(20)-Mo(1)-O(1)-S(1)	-32.62(14)
O(4)-Mo(1)-O(1)-S(1)	61.60(12)
C(9)-Mo(1)-O(1)-S(1)	117.28(13)
Mo(1)-N(1)-C(1)-C(2)	68.9(11)
Mo(1)-N(1)-C(1)-C(6)	-111.6(10)
N(1)-C(1)-C(2)-C(3)	179.49(17)
C(6)-C(1)-C(2)-C(3)	0.0(3)
N(1)-C(1)-C(2)-C(7)	-0.4(3)
C(6)-C(1)-C(2)-C(7)	-179.83(18)
C(1)-C(2)-C(3)-C(4)	-0.4(3)
C(7)-C(2)-C(3)-C(4)	179.4(2)
O(5)-S(2)-O(4)-Mo(1)	54.95(17)
O(6)-S(2)-O(4)-Mo(1)	-81.50(15)
C(26)-S(2)-O(4)-Mo(1)	166.37(14)
N(1)-Mo(1)-O(4)-S(2)	32.4(3)
C(20)-Mo(1)-O(4)-S(2)	-141.59(15)
O(1)-Mo(1)-O(4)-S(2)	121.06(15)
C(9)-Mo(1)-O(4)-S(2)	-32.59(14)
C(2)-C(3)-C(4)-C(5)	0.4(3)
C(3)-C(4)-C(5)-C(6)	0.1(3)
C(4)-C(5)-C(6)-C(1)	-0.4(3)
C(4)-C(5)-C(6)-C(8)	179.00(18)
N(1)-C(1)-C(6)-C(5)	-179.05(16)
C(2)-C(1)-C(6)-C(5)	0.4(3)
N(1)-C(1)-C(6)-C(8)	1.5(3)
C(2)-C(1)-C(6)-C(8)	-179.04(18)
C(11)-N(3)-C(9)-N(2)	1.89(19)
C(16)-N(3)-C(9)-N(2)	-177.38(15)
C(11)-N(3)-C(9)-Mo(1)	-175.40(14)
C(16)-N(3)-C(9)-Mo(1)	5.3(3)
C(10)-N(2)-C(9)-N(3)	-2.06(19)
C(12)-N(2)-C(9)-N(3)	175.72(16)
C(10)-N(2)-C(9)-Mo(1)	175.87(12)
C(12)-N(2)-C(9)-Mo(1)	-6.4(2)
N(1)-Mo(1)-C(9)-N(3)	103.63(18)
C(20)-Mo(1)-C(9)-N(3)	4.9(2)
O(1)-Mo(1)-C(9)-N(3)	-143.29(15)
O(4)-Mo(1)-C(9)-N(3)	-87.77(18)
N(1)-Mo(1)-C(9)-N(2)	-73.41(13)
C(20)-Mo(1)-C(9)-N(2)	-172.12(12)

O(1)-Mo(1)-C(9)-N(2)	39.67(19)
O(4)-Mo(1)-C(9)-N(2)	95.19(12)
C(9)-N(2)-C(10)-C(11)	1.5(2)
C(12)-N(2)-C(10)-C(11)	-176.64(16)
N(2)-C(10)-C(11)-N(3)	-0.3(2)
C(9)-N(3)-C(11)-C(10)	-1.0(2)
C(16)-N(3)-C(11)-C(10)	178.29(16)
C(9)-N(2)-C(12)-C(15)	-7.7(3)
C(10)-N(2)-C(12)-C(15)	169.89(16)
C(9)-N(2)-C(12)-C(13)	-126.72(19)
C(10)-N(2)-C(12)-C(13)	50.9(2)
C(9)-N(2)-C(12)-C(14)	113.8(2)
C(10)-N(2)-C(12)-C(14)	-68.6(2)
C(9)-N(3)-C(16)-C(18)	-70.9(2)
C(11)-N(3)-C(16)-C(18)	109.94(18)
C(9)-N(3)-C(16)-C(17)	53.2(2)
C(11)-N(3)-C(16)-C(17)	-126.00(17)
C(9)-N(3)-C(16)-C(19)	171.05(17)
C(11)-N(3)-C(16)-C(19)	-8.1(2)
N(1)-Mo(1)-C(20)-C(21)	16.2(2)
O(1)-Mo(1)-C(20)-C(21)	-84.1(2)
O(4)-Mo(1)-C(20)-C(21)	-165.2(2)
C(9)-Mo(1)-C(20)-C(21)	112.4(2)
Mo(1)-C(20)-C(21)-C(24)	-34.7(3)
Mo(1)-C(20)-C(21)-C(23)	-157.61(17)
Mo(1)-C(20)-C(21)-C(22)	84.9(2)
O(3)-S(1)-C(25)-F(2)	-56.36(18)
O(2)-S(1)-C(25)-F(2)	178.06(15)
O(1)-S(1)-C(25)-F(2)	62.02(17)
O(3)-S(1)-C(25)-F(3)	-176.96(14)
O(2)-S(1)-C(25)-F(3)	57.47(16)
O(1)-S(1)-C(25)-F(3)	-58.57(15)
O(3)-S(1)-C(25)-F(1)	65.44(16)
O(2)-S(1)-C(25)-F(1)	-60.13(17)
O(1)-S(1)-C(25)-F(1)	-176.17(14)
O(5)-S(2)-C(26)-F(6)	172.99(14)
O(6)-S(2)-C(26)-F(6)	-62.96(17)
O(4)-S(2)-C(26)-F(6)	55.01(16)
O(5)-S(2)-C(26)-F(5)	51.15(17)
O(6)-S(2)-C(26)-F(5)	175.20(14)
O(4)-S(2)-C(26)-F(5)	-66.83(16)
O(5)-S(2)-C(26)-F(4)	-67.21(16)
O(6)-S(2)-C(26)-F(4)	56.84(16)
O(4)-S(2)-C(26)-F(4)	174.81(14)

Symmetry transformations used to generate equivalent atoms:

Complex 5


N
OTf
Mes
Mo
N
OTf
Ph
N
Mes

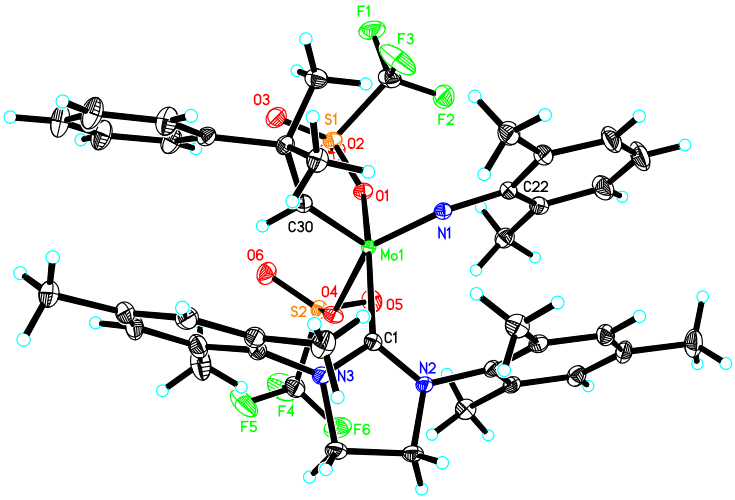

F1
F3
O3
S1
F2
O2
O1
C22
C30
N1
Mo1
O6
O4
S2
O5
C1
N2
N3
F4
F5
F6

Table 5.1. Crystal data and structure refinement for **5**.

Empirical formula	$C_{41}H_{47}F_6MoN_3O_6S_2$
Formula weight	951.88
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	monoclinic, $P2_1/n$
Unit cell dimensions	a = 10.8419(8) Å, α = 90°
	b = 18.1447(14) Å, β = 96.689(4)°
	c = 21.4766(16) Å, γ = 90°
Volume	4196.2(5) $Å^3$
Z, Calculated density	4, 1.507 Mg/m^3
Absorption coefficient	0.489 mm^{-1}
F(000)	1960
Crystal size	0.41 x 0.32 x 0.29 mm
Theta range for data collection	2.02 to 30.53°.
Limiting indices	-15<=h<=15, -25<=k<=25, -30<=l<=30
Reflections collected / unique	90595 / 12826 [R(int) = 0.0399]
Completeness to theta = 30.53	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7447 and 0.7123
Refinement method	full-matrix least-squares on F^2
Data / restraints / parameters	12826 / 0 / 542
Goodness-of-fit on F^2	1.027
Final R indices [I>2σ (I)]	R1 = 0.0295, wR2 = 0.0714
R indices (all data)	R1 = 0.0422, wR2 = 0.0754

Table 5.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	520(1)	4725(1)	2231(1)	9(1)
S(1)	-755(1)	3049(1)	1706(1)	15(1)
N(1)	-812(1)	5247(1)	2053(1)	12(1)
O(1)	-240(1)	3801(1)	1692(1)	15(1)
F(1)	-3065(1)	2620(1)	1519(1)	33(1)
C(1)	1880(1)	5621(1)	2503(1)	12(1)
S(2)	2308(1)	3753(1)	1366(1)	14(1)
N(2)	2059(1)	6173(1)	2110(1)	13(1)
F(2)	-2689(1)	3610(1)	1027(1)	29(1)
O(2)	-519(1)	2613(1)	1178(1)	25(1)
C(2)	3157(1)	6632(1)	2331(1)	17(1)
N(3)	2821(1)	5621(1)	2971(1)	14(1)
F(3)	-2794(1)	3649(1)	2017(1)	41(1)
O(3)	-570(1)	2714(1)	2316(1)	21(1)
C(3)	3791(1)	6171(1)	2868(1)	20(1)
O(4)	2104(1)	4364(1)	1810(1)	15(1)
F(4)	4262(1)	3375(1)	860(1)	40(1)
C(4)	1186(1)	6476(1)	1618(1)	13(1)
O(5)	1666(1)	3866(1)	755(1)	21(1)
F(5)	4673(1)	3792(1)	1791(1)	39(1)
C(5)	1347(1)	6357(1)	991(1)	14(1)
O(6)	2278(1)	3044(1)	1654(1)	22(1)
C(6)	566(2)	6728(1)	529(1)	18(1)
F(6)	4157(1)	4537(1)	1027(1)	43(1)
C(7)	-349(2)	7209(1)	681(1)	19(1)
C(8)	-486(1)	7314(1)	1315(1)	18(1)
C(9)	276(1)	6962(1)	1789(1)	15(1)
C(10)	2324(2)	5836(1)	803(1)	18(1)
C(11)	-1179(2)	7607(1)	178(1)	26(1)
C(12)	128(2)	7110(1)	2467(1)	20(1)
C(13)	2964(1)	5235(1)	3563(1)	16(1)
C(14)	3566(2)	4554(1)	3629(1)	20(1)
C(15)	3774(2)	4242(1)	4226(1)	23(1)
C(16)	3440(2)	4597(1)	4754(1)	21(1)
C(17)	2865(2)	5282(1)	4675(1)	20(1)
C(18)	2618(1)	5614(1)	4087(1)	16(1)
C(19)	4025(2)	4165(1)	3082(1)	31(1)
C(20)	3743(2)	4263(1)	5399(1)	28(1)
C(21)	2010(2)	6362(1)	4022(1)	22(1)
C(22)	-1785(1)	5598(1)	1689(1)	15(1)
C(23)	-1844(1)	5550(1)	1029(1)	17(1)
C(24)	-2790(2)	5929(1)	670(1)	26(1)

C(25)	-3638(2)	6350(1)	948(1)	33(1)
C(26)	-3573(2)	6391(1)	1596(1)	27(1)
C(27)	-2674(1)	6007(1)	1980(1)	18(1)
C(28)	-932(2)	5102(1)	709(1)	18(1)
C(29)	-2653(2)	6039(1)	2679(1)	20(1)
C(30)	412(1)	4367(1)	3040(1)	13(1)
C(31)	-367(1)	4295(1)	3581(1)	13(1)
C(32)	-1669(1)	4008(1)	3335(1)	19(1)
C(33)	-499(2)	5061(1)	3870(1)	17(1)
C(34)	242(1)	3742(1)	4059(1)	14(1)
C(35)	306(2)	3855(1)	4703(1)	21(1)
C(36)	864(2)	3339(1)	5126(1)	26(1)
C(37)	1376(2)	2705(1)	4910(1)	27(1)
C(38)	1301(2)	2582(1)	4269(1)	25(1)
C(39)	727(2)	3087(1)	3849(1)	20(1)
C(40)	-2422(2)	3245(1)	1561(1)	21(1)
C(41)	3949(2)	3884(1)	1261(1)	22(1)

Table 5.3. Bond lengths [Å] and angles [°] for **5**.

Mo(1)-N(1)	1.7318(12)
Mo(1)-C(30)	1.8704(14)
Mo(1)-O(4)	2.1360(10)
Mo(1)-O(1)	2.1479(10)
Mo(1)-C(1)	2.2266(14)
S(1)-O(2)	1.4309(12)
S(1)-O(3)	1.4368(12)
S(1)-O(1)	1.4749(11)
S(1)-C(40)	1.8326(17)
N(1)-C(22)	1.3919(19)
F(1)-C(40)	1.3291(19)
C(1)-N(2)	1.3384(18)
C(1)-N(3)	1.3464(19)
S(2)-O(5)	1.4263(12)
S(2)-O(6)	1.4291(12)
S(2)-O(4)	1.4954(11)
S(2)-C(41)	1.8345(16)
N(2)-C(4)	1.4423(19)
N(2)-C(2)	1.4858(19)
F(2)-C(40)	1.327(2)
C(2)-C(3)	1.522(2)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
N(3)-C(13)	1.4439(19)
N(3)-C(3)	1.4844(19)
F(3)-C(40)	1.322(2)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
F(4)-C(41)	1.332(2)

C(4)-C(5)	1.396(2)
C(4)-C(9)	1.403(2)
F(5)-C(41)	1.317(2)
C(5)-C(6)	1.400(2)
C(5)-C(10)	1.509(2)
C(6)-C(7)	1.387(2)
C(6)-H(6)	0.9500
F(6)-C(41)	1.316(2)
C(7)-C(8)	1.399(2)
C(7)-C(11)	1.507(2)
C(8)-C(9)	1.391(2)
C(8)-H(8)	0.9500
C(9)-C(12)	1.506(2)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.398(2)
C(13)-C(18)	1.406(2)
C(14)-C(15)	1.397(2)
C(14)-C(19)	1.503(2)
C(15)-C(16)	1.388(2)
C(15)-H(15)	0.9500
C(16)-C(17)	1.393(2)
C(16)-C(20)	1.511(2)
C(17)-C(18)	1.396(2)
C(17)-H(17)	0.9500
C(18)-C(21)	1.509(2)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(23)	1.415(2)
C(22)-C(27)	1.418(2)
C(23)-C(24)	1.391(2)
C(23)-C(28)	1.505(2)
C(24)-C(25)	1.384(3)
C(24)-H(24)	0.9500
C(25)-C(26)	1.387(3)
C(25)-H(25)	0.9500

C(26)-C(27)	1.388(2)
C(26)-H(26)	0.9500
C(27)-C(29)	1.501(2)
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-C(31)	1.5206(19)
C(30)-H(30)	0.9500
C(31)-C(34)	1.528(2)
C(31)-C(33)	1.536(2)
C(31)-C(32)	1.539(2)
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-C(35)	1.392(2)
C(34)-C(39)	1.396(2)
C(35)-C(36)	1.392(2)
C(35)-H(35)	0.9500
C(36)-C(37)	1.380(3)
C(36)-H(36)	0.9500
C(37)-C(38)	1.389(2)
C(37)-H(37)	0.9500
C(38)-C(39)	1.381(2)
C(38)-H(38)	0.9500
C(39)-H(39)	0.9500

N(1)-Mo(1)-C(30)	104.75(6)
N(1)-Mo(1)-O(4)	139.94(5)
C(30)-Mo(1)-O(4)	115.25(5)
N(1)-Mo(1)-O(1)	92.85(5)
C(30)-Mo(1)-O(1)	99.65(5)
O(4)-Mo(1)-O(1)	78.95(4)
N(1)-Mo(1)-C(1)	99.72(5)
C(30)-Mo(1)-C(1)	96.98(6)
O(4)-Mo(1)-C(1)	78.16(5)
O(1)-Mo(1)-C(1)	155.85(4)
O(2)-S(1)-O(3)	117.97(8)
O(2)-S(1)-O(1)	113.07(7)
O(3)-S(1)-O(1)	113.46(7)
O(2)-S(1)-C(40)	103.69(8)
O(3)-S(1)-C(40)	105.51(7)
O(1)-S(1)-C(40)	100.66(7)
C(22)-N(1)-Mo(1)	158.79(11)
S(1)-O(1)-Mo(1)	146.38(7)

N(2)-C(1)-N(3)	108.59(12)
N(2)-C(1)-Mo(1)	121.34(10)
N(3)-C(1)-Mo(1)	128.09(10)
O(5)-S(2)-O(6)	119.62(8)
O(5)-S(2)-O(4)	112.76(7)
O(6)-S(2)-O(4)	112.22(7)
O(5)-S(2)-C(41)	104.16(8)
O(6)-S(2)-C(41)	104.00(7)
O(4)-S(2)-C(41)	101.55(7)
C(1)-N(2)-C(4)	128.08(12)
C(1)-N(2)-C(2)	112.72(12)
C(4)-N(2)-C(2)	116.98(11)
N(2)-C(2)-C(3)	102.07(12)
N(2)-C(2)-H(2A)	111.4
C(3)-C(2)-H(2A)	111.4
N(2)-C(2)-H(2B)	111.4
C(3)-C(2)-H(2B)	111.4
H(2A)-C(2)-H(2B)	109.2
C(1)-N(3)-C(13)	130.64(12)
C(1)-N(3)-C(3)	112.17(12)
C(13)-N(3)-C(3)	116.87(12)
N(3)-C(3)-C(2)	102.53(12)
N(3)-C(3)-H(3A)	111.3
C(2)-C(3)-H(3A)	111.3
N(3)-C(3)-H(3B)	111.3
C(2)-C(3)-H(3B)	111.3
H(3A)-C(3)-H(3B)	109.2
S(2)-O(4)-Mo(1)	133.15(6)
C(5)-C(4)-C(9)	121.44(14)
C(5)-C(4)-N(2)	120.15(13)
C(9)-C(4)-N(2)	117.95(13)
C(4)-C(5)-C(6)	118.38(14)
C(4)-C(5)-C(10)	121.74(13)
C(6)-C(5)-C(10)	119.88(13)
C(7)-C(6)-C(5)	121.78(14)
C(7)-C(6)-H(6)	119.1
C(5)-C(6)-H(6)	119.1
C(6)-C(7)-C(8)	118.28(14)
C(6)-C(7)-C(11)	121.11(15)
C(8)-C(7)-C(11)	120.61(15)
C(9)-C(8)-C(7)	121.95(14)
C(9)-C(8)-H(8)	119.0
C(7)-C(8)-H(8)	119.0
C(8)-C(9)-C(4)	118.16(14)
C(8)-C(9)-C(12)	120.31(14)
C(4)-C(9)-C(12)	121.53(13)
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5

H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(7)-C(11)-H(11A)	109.5
C(7)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(7)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(9)-C(12)-H(12A)	109.5
C(9)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(9)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(18)	121.11(14)
C(14)-C(13)-N(3)	121.19(14)
C(18)-C(13)-N(3)	117.20(14)
C(15)-C(14)-C(13)	118.33(15)
C(15)-C(14)-C(19)	119.61(15)
C(13)-C(14)-C(19)	122.03(15)
C(16)-C(15)-C(14)	122.17(16)
C(16)-C(15)-H(15)	118.9
C(14)-C(15)-H(15)	118.9
C(15)-C(16)-C(17)	118.08(15)
C(15)-C(16)-C(20)	120.84(16)
C(17)-C(16)-C(20)	121.02(16)
C(16)-C(17)-C(18)	122.09(15)
C(16)-C(17)-H(17)	119.0
C(18)-C(17)-H(17)	119.0
C(17)-C(18)-C(13)	118.17(15)
C(17)-C(18)-C(21)	120.56(14)
C(13)-C(18)-C(21)	121.27(14)
C(14)-C(19)-H(19A)	109.5
C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-H(20A)	109.5
C(16)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(16)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5

N(1)-C(22)-C(23)	118.49(13)
N(1)-C(22)-C(27)	120.14(14)
C(23)-C(22)-C(27)	121.35(14)
C(24)-C(23)-C(22)	117.94(15)
C(24)-C(23)-C(28)	119.68(15)
C(22)-C(23)-C(28)	122.37(14)
C(25)-C(24)-C(23)	121.20(16)
C(25)-C(24)-H(24)	119.4
C(23)-C(24)-H(24)	119.4
C(24)-C(25)-C(26)	120.29(16)
C(24)-C(25)-H(25)	119.9
C(26)-C(25)-H(25)	119.9
C(25)-C(26)-C(27)	121.23(16)
C(25)-C(26)-H(26)	119.4
C(27)-C(26)-H(26)	119.4
C(26)-C(27)-C(22)	117.90(15)
C(26)-C(27)-C(29)	120.17(14)
C(22)-C(27)-C(29)	121.93(14)
C(23)-C(28)-H(28A)	109.5
C(23)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(23)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(27)-C(29)-H(29A)	109.5
C(27)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(27)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(31)-C(30)-Mo(1)	147.16(11)
C(31)-C(30)-H(30)	106.4
Mo(1)-C(30)-H(30)	106.4
C(30)-C(31)-C(34)	109.56(12)
C(30)-C(31)-C(33)	108.53(12)
C(34)-C(31)-C(33)	112.12(12)
C(30)-C(31)-C(32)	109.57(12)
C(34)-C(31)-C(32)	108.36(12)
C(33)-C(31)-C(32)	108.67(12)
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(31)-C(33)-H(33A)	109.5
C(31)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(31)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5

H(33B)-C(33)-H(33C)	109.5
C(35)-C(34)-C(39)	117.90(14)
C(35)-C(34)-C(31)	122.57(13)
C(39)-C(34)-C(31)	119.51(13)
C(34)-C(35)-C(36)	121.15(15)
C(34)-C(35)-H(35)	119.4
C(36)-C(35)-H(35)	119.4
C(37)-C(36)-C(35)	120.17(16)
C(37)-C(36)-H(36)	119.9
C(35)-C(36)-H(36)	119.9
C(36)-C(37)-C(38)	119.16(16)
C(36)-C(37)-H(37)	120.4
C(38)-C(37)-H(37)	120.4
C(39)-C(38)-C(37)	120.67(16)
C(39)-C(38)-H(38)	119.7
C(37)-C(38)-H(38)	119.7
C(38)-C(39)-C(34)	120.90(15)
C(38)-C(39)-H(39)	119.6
C(34)-C(39)-H(39)	119.6
F(3)-C(40)-F(2)	107.99(15)
F(3)-C(40)-F(1)	108.64(14)
F(2)-C(40)-F(1)	107.85(13)
F(3)-C(40)-S(1)	111.20(11)
F(2)-C(40)-S(1)	110.85(11)
F(1)-C(40)-S(1)	110.20(12)
F(6)-C(41)-F(5)	109.46(16)
F(6)-C(41)-F(4)	108.07(14)
F(5)-C(41)-F(4)	107.46(14)
F(6)-C(41)-S(2)	112.03(11)
F(5)-C(41)-S(2)	111.42(11)
F(4)-C(41)-S(2)	108.23(12)

Symmetry transformations used to generate equivalent atoms:

Table 5.4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **5**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	9(1)	8(1)	10(1)	0(1)	1(1)	0(1)
S(1)	16(1)	12(1)	16(1)	-2(1)	2(1)	-3(1)
N(1)	13(1)	10(1)	13(1)	-1(1)	1(1)	-1(1)
O(1)	15(1)	12(1)	16(1)	-2(1)	2(1)	-3(1)
F(1)	25(1)	38(1)	33(1)	9(1)	-4(1)	-18(1)
C(1)	12(1)	12(1)	13(1)	-2(1)	2(1)	1(1)
S(2)	15(1)	13(1)	15(1)	0(1)	4(1)	3(1)
N(2)	12(1)	12(1)	13(1)	1(1)	-1(1)	-3(1)
F(2)	26(1)	29(1)	29(1)	7(1)	-8(1)	-6(1)
O(2)	31(1)	19(1)	25(1)	-10(1)	7(1)	-5(1)

C(2)	15(1)	17(1)	18(1)	1(1)	-1(1)	-6(1)
N(3)	14(1)	15(1)	14(1)	2(1)	-2(1)	-3(1)
F(3)	18(1)	71(1)	34(1)	-24(1)	-1(1)	7(1)
O(3)	23(1)	20(1)	20(1)	4(1)	1(1)	-4(1)
C(3)	15(1)	24(1)	20(1)	5(1)	-4(1)	-8(1)
O(4)	12(1)	16(1)	17(1)	-4(1)	3(1)	0(1)
F(4)	29(1)	49(1)	44(1)	-15(1)	19(1)	10(1)
C(4)	14(1)	10(1)	14(1)	2(1)	-1(1)	-2(1)
O(5)	22(1)	26(1)	16(1)	-2(1)	2(1)	4(1)
F(5)	16(1)	68(1)	32(1)	1(1)	1(1)	7(1)
C(5)	15(1)	12(1)	15(1)	2(1)	1(1)	-3(1)
O(6)	26(1)	15(1)	28(1)	3(1)	6(1)	5(1)
C(6)	22(1)	16(1)	14(1)	1(1)	-1(1)	-2(1)
F(6)	23(1)	32(1)	76(1)	18(1)	22(1)	4(1)
C(7)	22(1)	12(1)	20(1)	3(1)	-5(1)	-1(1)
C(8)	17(1)	12(1)	25(1)	0(1)	-2(1)	1(1)
C(9)	15(1)	11(1)	18(1)	-1(1)	0(1)	-2(1)
C(10)	20(1)	18(1)	17(1)	-2(1)	4(1)	1(1)
C(11)	31(1)	20(1)	25(1)	4(1)	-9(1)	4(1)
C(12)	20(1)	20(1)	19(1)	-3(1)	4(1)	1(1)
C(13)	15(1)	16(1)	14(1)	2(1)	-4(1)	-4(1)
C(14)	19(1)	20(1)	20(1)	1(1)	-5(1)	1(1)
C(15)	22(1)	20(1)	25(1)	6(1)	-6(1)	2(1)
C(16)	17(1)	24(1)	19(1)	7(1)	-5(1)	-5(1)
C(17)	20(1)	23(1)	16(1)	1(1)	-2(1)	-5(1)
C(18)	17(1)	16(1)	16(1)	1(1)	-3(1)	-4(1)
C(19)	35(1)	31(1)	24(1)	-1(1)	-3(1)	15(1)
C(20)	25(1)	34(1)	23(1)	14(1)	-4(1)	-3(1)
C(21)	30(1)	16(1)	18(1)	-2(1)	-1(1)	-2(1)
C(22)	12(1)	14(1)	18(1)	3(1)	0(1)	0(1)
C(23)	14(1)	19(1)	17(1)	2(1)	1(1)	-2(1)
C(24)	20(1)	38(1)	20(1)	6(1)	-1(1)	4(1)
C(25)	22(1)	48(1)	28(1)	13(1)	-1(1)	14(1)
C(26)	18(1)	34(1)	30(1)	8(1)	6(1)	13(1)
C(27)	15(1)	18(1)	22(1)	3(1)	4(1)	3(1)
C(28)	21(1)	18(1)	16(1)	1(1)	2(1)	-1(1)
C(29)	20(1)	20(1)	22(1)	0(1)	6(1)	5(1)
C(30)	14(1)	12(1)	14(1)	-1(1)	1(1)	-1(1)
C(31)	15(1)	13(1)	12(1)	0(1)	2(1)	0(1)
C(32)	16(1)	22(1)	18(1)	-1(1)	2(1)	-2(1)
C(33)	21(1)	15(1)	16(1)	-1(1)	3(1)	2(1)
C(34)	16(1)	15(1)	12(1)	1(1)	2(1)	-2(1)
C(35)	29(1)	19(1)	14(1)	-1(1)	4(1)	5(1)
C(36)	39(1)	26(1)	13(1)	3(1)	2(1)	3(1)
C(37)	37(1)	23(1)	19(1)	6(1)	-1(1)	6(1)
C(38)	36(1)	17(1)	23(1)	2(1)	5(1)	7(1)
C(39)	28(1)	16(1)	15(1)	0(1)	3(1)	1(1)
C(40)	17(1)	27(1)	19(1)	-3(1)	-1(1)	-6(1)
C(41)	17(1)	24(1)	26(1)	2(1)	7(1)	7(1)

Table 5.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **5**.

	x	y	z	U(eq)
H(2A)	2906	7120	2480	20
H(2B)	3703	6701	1997	20
H(3A)	4548	5928	2749	24
H(3B)	4016	6475	3247	24
H(6)	664	6649	100	21
H(8)	-1118	7636	1424	22
H(10A)	3041	5837	1126	27
H(10B)	2587	5997	403	27
H(10C)	1979	5337	757	27
H(11A)	-861	7540	-227	39
H(11B)	-1193	8134	279	39
H(11C)	-2022	7407	156	39
H(12A)	-610	7415	2492	29
H(12B)	864	7370	2665	29
H(12C)	35	6642	2684	29
H(15)	4157	3771	4273	27
H(17)	2633	5532	5032	24
H(19A)	4865	3976	3206	46
H(19B)	4039	4510	2733	46
H(19C)	3469	3753	2952	46
H(20A)	3804	3727	5362	42
H(20B)	3085	4387	5657	42
H(20C)	4536	4461	5595	42
H(21A)	1707	6499	4418	32
H(21B)	1312	6346	3688	32
H(21C)	2617	6728	3916	32
H(24)	-2856	5898	226	31
H(25)	-4268	6612	694	39
H(26)	-4155	6688	1781	32
H(28A)	-1190	4584	694	27
H(28B)	-104	5145	944	27
H(28C)	-909	5286	281	27
H(29A)	-3238	6415	2789	30
H(29B)	-1814	6164	2870	30
H(29C)	-2892	5558	2835	30
H(30)	1176	4124	3167	16
H(32A)	-2062	4348	3018	28
H(32B)	-2176	3974	3683	28
H(32C)	-1597	3520	3148	28
H(33A)	308	5221	4080	26
H(33B)	-1102	5039	4175	26
H(33C)	-786	5413	3539	26
H(35)	-38	4291	4857	25
H(36)	893	3424	5564	31

H(37)	1775	2358	5197	32
H(38)	1649	2146	4116	30
H(39)	662	2987	3413	23

Table 5.6. Torsion angles [º] for **5**.

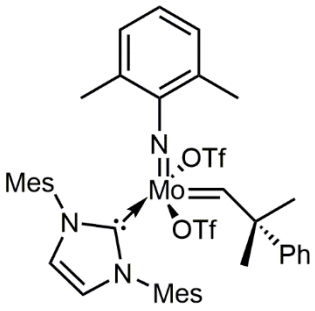
C(30)-Mo(1)-N(1)-C(22)	-155.3(3)
O(4)-Mo(1)-N(1)-C(22)	21.6(3)
O(1)-Mo(1)-N(1)-C(22)	-54.6(3)
C(1)-Mo(1)-N(1)-C(22)	104.8(3)
O(2)-S(1)-O(1)-Mo(1)	-149.97(11)
O(3)-S(1)-O(1)-Mo(1)	-12.19(14)
C(40)-S(1)-O(1)-Mo(1)	100.03(12)
N(1)-Mo(1)-O(1)-S(1)	-106.87(12)
C(30)-Mo(1)-O(1)-S(1)	-1.38(13)
O(4)-Mo(1)-O(1)-S(1)	112.68(12)
C(1)-Mo(1)-O(1)-S(1)	131.50(13)
N(1)-Mo(1)-C(1)-N(2)	-57.09(12)
C(30)-Mo(1)-C(1)-N(2)	-163.43(11)
O(4)-Mo(1)-C(1)-N(2)	82.15(11)
O(1)-Mo(1)-C(1)-N(2)	63.27(17)
N(1)-Mo(1)-C(1)-N(3)	140.84(13)
C(30)-Mo(1)-C(1)-N(3)	34.50(13)
O(4)-Mo(1)-C(1)-N(3)	-79.92(13)
O(1)-Mo(1)-C(1)-N(3)	-98.80(16)
N(3)-C(1)-N(2)-C(4)	-166.54(13)
Mo(1)-C(1)-N(2)-C(4)	28.27(19)
N(3)-C(1)-N(2)-C(2)	-4.16(17)
Mo(1)-C(1)-N(2)-C(2)	-169.35(10)
C(1)-N(2)-C(2)-C(3)	11.39(16)
C(4)-N(2)-C(2)-C(3)	175.88(12)
N(2)-C(1)-N(3)-C(13)	167.64(14)
Mo(1)-C(1)-N(3)-C(13)	-28.5(2)
N(2)-C(1)-N(3)-C(3)	-5.50(17)
Mo(1)-C(1)-N(3)-C(3)	158.39(11)
C(1)-N(3)-C(3)-C(2)	12.22(17)
C(13)-N(3)-C(3)-C(2)	-161.96(13)
N(2)-C(2)-C(3)-N(3)	-13.10(15)
O(5)-S(2)-O(4)-Mo(1)	68.17(11)
O(6)-S(2)-O(4)-Mo(1)	-70.46(11)
C(41)-S(2)-O(4)-Mo(1)	179.05(9)
N(1)-Mo(1)-O(4)-S(2)	-80.43(12)
C(30)-Mo(1)-O(4)-S(2)	96.30(10)
O(1)-Mo(1)-O(4)-S(2)	0.75(9)
C(1)-Mo(1)-O(4)-S(2)	-171.50(10)
C(1)-N(2)-C(4)-C(5)	-109.59(17)
C(2)-N(2)-C(4)-C(5)	88.67(16)
C(1)-N(2)-C(4)-C(9)	78.08(19)
C(2)-N(2)-C(4)-C(9)	-83.66(16)

C(9)-C(4)-C(5)-C(6)	-0.8(2)
N(2)-C(4)-C(5)-C(6)	-172.84(13)
C(9)-C(4)-C(5)-C(10)	179.92(14)
N(2)-C(4)-C(5)-C(10)	7.9(2)
C(4)-C(5)-C(6)-C(7)	0.4(2)
C(10)-C(5)-C(6)-C(7)	179.68(14)
C(5)-C(6)-C(7)-C(8)	-0.5(2)
C(5)-C(6)-C(7)-C(11)	179.72(15)
C(6)-C(7)-C(8)-C(9)	1.0(2)
C(11)-C(7)-C(8)-C(9)	-179.17(15)
C(7)-C(8)-C(9)-C(4)	-1.4(2)
C(7)-C(8)-C(9)-C(12)	177.83(14)
C(5)-C(4)-C(9)-C(8)	1.3(2)
N(2)-C(4)-C(9)-C(8)	173.52(13)
C(5)-C(4)-C(9)-C(12)	-177.95(14)
N(2)-C(4)-C(9)-C(12)	-5.7(2)
C(1)-N(3)-C(13)-C(14)	93.8(2)
C(3)-N(3)-C(13)-C(14)	-93.34(18)
C(1)-N(3)-C(13)-C(18)	-94.21(19)
C(3)-N(3)-C(13)-C(18)	78.67(17)
C(18)-C(13)-C(14)-C(15)	2.5(2)
N(3)-C(13)-C(14)-C(15)	174.19(14)
C(18)-C(13)-C(14)-C(19)	-175.60(16)
N(3)-C(13)-C(14)-C(19)	-3.9(2)
C(13)-C(14)-C(15)-C(16)	-2.2(2)
C(19)-C(14)-C(15)-C(16)	175.98(17)
C(14)-C(15)-C(16)-C(17)	0.9(2)
C(14)-C(15)-C(16)-C(20)	-176.56(16)
C(15)-C(16)-C(17)-C(18)	0.1(2)
C(20)-C(16)-C(17)-C(18)	177.56(15)
C(16)-C(17)-C(18)-C(13)	0.2(2)
C(16)-C(17)-C(18)-C(21)	-179.05(15)
C(14)-C(13)-C(18)-C(17)	-1.6(2)
N(3)-C(13)-C(18)-C(17)	-173.57(13)
C(14)-C(13)-C(18)-C(21)	177.70(15)
N(3)-C(13)-C(18)-C(21)	5.7(2)
Mo(1)-N(1)-C(22)-C(23)	-0.8(4)
Mo(1)-N(1)-C(22)-C(27)	-179.3(2)
N(1)-C(22)-C(23)-C(24)	-177.35(14)
C(27)-C(22)-C(23)-C(24)	1.2(2)
N(1)-C(22)-C(23)-C(28)	3.2(2)
C(27)-C(22)-C(23)-C(28)	-178.27(14)
C(22)-C(23)-C(24)-C(25)	1.0(3)
C(28)-C(23)-C(24)-C(25)	-179.50(17)
C(23)-C(24)-C(25)-C(26)	-1.2(3)
C(24)-C(25)-C(26)-C(27)	-0.8(3)
C(25)-C(26)-C(27)-C(22)	2.9(3)
C(25)-C(26)-C(27)-C(29)	-177.75(18)
N(1)-C(22)-C(27)-C(26)	175.41(15)
C(23)-C(22)-C(27)-C(26)	-3.1(2)

N(1)-C(22)-C(27)-C(29)	-3.9(2)
C(23)-C(22)-C(27)-C(29)	177.55(15)
N(1)-Mo(1)-C(30)-C(31)	6.3(2)
O(4)-Mo(1)-C(30)-C(31)	-171.50(18)
O(1)-Mo(1)-C(30)-C(31)	-89.2(2)
C(1)-Mo(1)-C(30)-C(31)	108.3(2)
Mo(1)-C(30)-C(31)-C(34)	168.75(16)
Mo(1)-C(30)-C(31)-C(33)	-68.5(2)
Mo(1)-C(30)-C(31)-C(32)	50.0(2)
C(30)-C(31)-C(34)-C(35)	139.05(15)
C(33)-C(31)-C(34)-C(35)	18.5(2)
C(32)-C(31)-C(34)-C(35)	-101.46(17)
C(30)-C(31)-C(34)-C(39)	-42.69(18)
C(33)-C(31)-C(34)-C(39)	-163.26(14)
C(32)-C(31)-C(34)-C(39)	76.81(17)
C(39)-C(34)-C(35)-C(36)	1.6(2)
C(31)-C(34)-C(35)-C(36)	179.86(15)
C(34)-C(35)-C(36)-C(37)	0.5(3)
C(35)-C(36)-C(37)-C(38)	-1.5(3)
C(36)-C(37)-C(38)-C(39)	0.3(3)
C(37)-C(38)-C(39)-C(34)	1.9(3)
C(35)-C(34)-C(39)-C(38)	-2.8(2)
C(31)-C(34)-C(39)-C(38)	178.89(15)
O(2)-S(1)-C(40)-F(3)	179.70(12)
O(3)-S(1)-C(40)-F(3)	55.05(14)
O(1)-S(1)-C(40)-F(3)	-63.16(14)
O(2)-S(1)-C(40)-F(2)	-60.16(13)
O(3)-S(1)-C(40)-F(2)	175.19(11)
O(1)-S(1)-C(40)-F(2)	56.99(13)
O(2)-S(1)-C(40)-F(1)	59.16(13)
O(3)-S(1)-C(40)-F(1)	-65.49(13)
O(1)-S(1)-C(40)-F(1)	176.31(11)
O(5)-S(2)-C(41)-F(6)	57.29(15)
O(6)-S(2)-C(41)-F(6)	-176.67(13)
O(4)-S(2)-C(41)-F(6)	-60.01(14)
O(5)-S(2)-C(41)-F(5)	-179.70(12)
O(6)-S(2)-C(41)-F(5)	-53.67(14)
O(4)-S(2)-C(41)-F(5)	62.99(14)
O(5)-S(2)-C(41)-F(4)	-61.76(13)
O(6)-S(2)-C(41)-F(4)	64.27(13)
O(4)-S(2)-C(41)-F(4)	-179.07(12)

Symmetry transformations used to generate equivalent atoms:

Complex 6


N
OTf
Mes
Mo
N
OTf
Ph
N
Mes

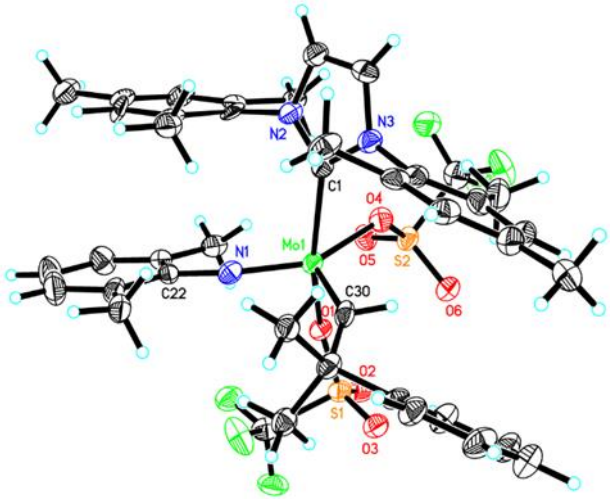

N2
N3
C1
O4
Mo1
N1
O5
S2
C22
C30
O6
O1
O2
S1
O3

Table 6.1. Crystal data and structure refinement for **6**.

Empirical formula	$C_{41}H_{45}F_6MoN_3O_6S_2$
Formula weight	949.86
Temperature	100(2) K
Wavelength	0.71073Å
Crystal system, space group	Monoclinic, $P2_1/n$
Unit cell dimensions	a = 10.7422(12) Å, α= 90º
	b = 18.1658(16) Å, β= 96.218(7)º
	c = 21.495(2) Å, γ = 90º
Volume	4169.9(7) A^3
Z, Calculated density	4, 1.513 Mg/m^3
Absorption coefficient	0.492 mm^{-1}
F(000)	1952
Crystal size	0.18 x 0.18 x 0.16 mm
Theta range for data collection	1.47 to 25.00º
Limiting indices	-12<=h<=12, -21<=k<=21, -24<=l<=25
Reflections collected / unique	20363 / 7303 [R(int) = 0.0820]
Completeness to theta =	25.00 99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7454 and 0.5679
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7303 / 0 / 542
Goodness-of-fit on F^2	1.059
Final R indices [I>2σ(I)]	R1 = 0.0671, wR2 = 0.1626
R indices (all data)	R1 = 0.1322, wR2 = 0.1828
Largest diff. peak and hole	1.751 and -0.961 $e.Å^{-3}$

Table 6.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **6**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	5523(1)	4714(1)	2224(1)	21(1)
N(1)	4152(5)	5209(3)	2047(3)	23(1)
C(1)	6831(7)	5627(4)	2509(3)	24(2)
N(2)	7001(5)	6214(3)	2133(3)	25(1)
C(2)	8053(7)	6614(4)	2369(3)	28(2)
N(3)	7790(5)	5670(3)	2972(3)	25(1)
C(3)	8525(7)	6276(4)	2889(3)	27(2)
C(4)	6157(7)	6507(3)	1630(3)	24(2)
C(5)	6304(6)	6378(4)	1008(3)	24(2)
C(6)	5533(7)	6729(4)	549(4)	31(2)
C(7)	4586(7)	7208(4)	698(3)	28(2)
C(8)	4457(7)	7309(4)	1319(4)	32(2)
C(9)	5194(7)	6981(4)	1802(4)	26(2)
C(10)	7311(7)	5853(4)	825(3)	27(2)
C(11)	3755(8)	7588(4)	187(4)	37(2)
C(12)	5053(7)	7131(4)	2476(4)	32(2)
C(13)	7988(6)	5264(4)	3554(3)	26(2)
C(14)	7615(7)	5620(4)	4087(3)	25(2)
C(15)	7869(7)	5265(4)	4659(3)	30(2)
C(16)	8462(7)	4578(4)	4722(4)	33(2)
C(17)	8797(7)	4255(4)	4184(4)	36(2)
C(18)	8621(6)	4587(4)	3601(3)	29(2)
C(19)	7000(8)	6366(4)	4045(3)	31(2)
C(20)	8764(7)	4228(5)	5350(4)	38(2)
C(21)	9077(8)	4231(5)	3045(4)	41(2)
C(22)	3168(6)	5545(4)	1673(3)	23(2)
C(23)	3135(7)	5496(4)	1022(3)	27(2)
C(24)	2158(7)	5837(5)	654(4)	36(2)
C(25)	1239(8)	6218(5)	929(4)	47(2)
C(26)	1283(8)	6268(5)	1568(4)	43(2)
C(27)	2217(7)	5930(4)	1966(3)	27(2)
C(28)	4108(7)	5070(4)	708(3)	30(2)
C(29)	2219(7)	5977(4)	2653(4)	32(2)
C(30)	5408(7)	4362(4)	3035(3)	25(2)
C(31)	4609(7)	4286(4)	3568(3)	25(2)
C(32)	3288(7)	4016(4)	3321(3)	29(2)
C(33)	4487(7)	5061(4)	3852(3)	27(2)
C(34)	5195(7)	3739(4)	4052(3)	23(2)
C(35)	5315(7)	3861(4)	4689(4)	31(2)
C(36)	5878(8)	3341(4)	5105(4)	36(2)
C(37)	6326(8)	2679(4)	4880(4)	37(2)
C(38)	6207(8)	2555(4)	4245(4)	35(2)
C(39)	5640(8)	3072(4)	3840(4)	32(2)

S(1)	4291(2)	3022(1)	1711(1)	26(1)
O(1)	4785(4)	3779(2)	1691(2)	25(1)
O(2)	4549(5)	2578(3)	1188(2)	34(1)
O(3)	4456(5)	2701(3)	2319(2)	30(1)
C(40)	2606(7)	3213(4)	1553(3)	30(2)
F(1)	1976(4)	2573(3)	1503(2)	40(1)
F(2)	2211(4)	3596(3)	2010(2)	47(1)
F(3)	2352(4)	3573(2)	1026(2)	40(1)
S(2)	7346(2)	3762(1)	1349(1)	26(1)
O(4)	7125(5)	4371(3)	1793(2)	28(1)
O(5)	6698(5)	3866(3)	746(2)	30(1)
O(6)	7338(5)	3056(3)	1639(3)	34(1)
C(41)	8984(7)	3915(5)	1236(4)	34(2)
F(4)	9335(4)	3409(3)	833(2)	48(1)
F(5)	9179(4)	4567(3)	993(3)	49(1)
F(6)	9731(4)	3841(3)	1761(2)	50(1)

Table 6.3. Bond lengths [Å] and angles [°] for **6**.

Mo(1)-N(1)	1.732(6)
Mo(1)-C(30)	1.873(7)
Mo(1)-O(4)	2.135(5)
Mo(1)-O(1)	2.153(5)
Mo(1)-C(1)	2.217(7)
N(1)-C(22)	1.397(9)
C(1)-N(3)	1.355(9)
C(1)-N(2)	1.362(9)
N(2)-C(2)	1.392(9)
N(2)-C(4)	1.435(9)
C(2)-C(3)	1.327(10)
C(2)-H(2)	0.9500
N(3)-C(3)	1.378(9)
N(3)-C(13)	1.447(9)
C(3)-H(3)	0.9500
C(4)-C(5)	1.383(10)
C(4)-C(9)	1.426(10)
C(5)-C(6)	1.375(10)
C(5)-C(10)	1.525(10)
C(6)-C(7)	1.402(11)
C(6)-H(6)	0.9500
C(7)-C(8)	1.369(11)
C(7)-C(11)	1.506(10)
C(8)-C(9)	1.371(10)
C(8)-H(8)	0.9500
C(9)-C(12)	1.497(11)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800

C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(18)	1.404(10)
C(13)-C(14)	1.410(10)
C(14)-C(15)	1.389(10)
C(14)-C(19)	1.506(10)
C(15)-C(16)	1.401(11)
C(15)-H(15)	0.9500
C(16)-C(17)	1.380(11)
C(16)-C(20)	1.495(11)
C(17)-C(18)	1.386(10)
C(17)-H(17)	0.9500
C(18)-C(21)	1.486(11)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(23)	1.400(10)
C(22)-C(27)	1.438(10)
C(23)-C(24)	1.389(10)
C(23)-C(28)	1.516(11)
C(24)-C(25)	1.389(12)
C(24)-H(24)	0.9500
C(25)-C(26)	1.372(12)
C(25)-H(25)	0.9500
C(26)-C(27)	1.388(10)
C(26)-H(26)	0.9500
C(27)-C(29)	1.478(10)
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-C(31)	1.510(10)
C(30)-H(30)	0.9500
C(31)-C(34)	1.525(9)
C(31)-C(32)	1.541(10)
C(31)-C(33)	1.545(10)
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800

C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-C(35)	1.380(10)
C(34)-C(39)	1.397(10)
C(35)-C(36)	1.393(10)
C(35)-H(35)	0.9500
C(36)-C(37)	1.399(11)
C(36)-H(36)	0.9500
C(37)-C(38)	1.376(11)
C(37)-H(37)	0.9500
C(38)-C(39)	1.377(10)
C(38)-H(38)	0.9500
C(39)-H(39)	0.9500
S(1)-O(3)	1.425(5)
S(1)-O(2)	1.435(5)
S(1)-O(1)	1.477(5)
S(1)-C(40)	1.838(8)
C(40)-F(2)	1.312(9)
C(40)-F(3)	1.312(8)
C(40)-F(1)	1.344(8)
S(2)-O(5)	1.416(5)
S(2)-O(6)	1.426(5)
S(2)-O(4)	1.495(5)
S(2)-C(41)	1.824(8)
C(41)-F(5)	1.321(9)
C(41)-F(6)	1.318(9)
C(41)-F(4)	1.345(9)

N(1)-Mo(1)-C(30)	104.0(3)
N(1)-Mo(1)-O(4)	139.6(2)
C(30)-Mo(1)-O(4)	116.2(3)
N(1)-Mo(1)-O(1)	92.1(2)
C(30)-Mo(1)-O(1)	99.7(2)
O(4)-Mo(1)-O(1)	78.80(18)
N(1)-Mo(1)-C(1)	99.9(3)
C(30)-Mo(1)-C(1)	95.8(3)
O(4)-Mo(1)-C(1)	79.7(2)
O(1)-Mo(1)-C(1)	157.5(2)
C(22)-N(1)-Mo(1)	157.8(5)
N(3)-C(1)-N(2)	104.6(6)
N(3)-C(1)-Mo(1)	130.9(5)
N(2)-C(1)-Mo(1)	122.9(5)
C(1)-N(2)-C(2)	110.3(6)
C(1)-N(2)-C(4)	128.5(6)
C(2)-N(2)-C(4)	120.1(5)
C(3)-C(2)-N(2)	106.7(6)
C(3)-C(2)-H(2)	126.7
N(2)-C(2)-H(2)	126.7
C(1)-N(3)-C(3)	110.5(6)

C(1)-N(3)-C(13)	129.4(6)
C(3)-N(3)-C(13)	119.1(6)
C(2)-C(3)-N(3)	107.9(6)
C(2)-C(3)-H(3)	126.1
N(3)-C(3)-H(3)	126.1
C(5)-C(4)-C(9)	121.0(6)
C(5)-C(4)-N(2)	122.4(6)
C(9)-C(4)-N(2)	116.5(6)
C(6)-C(5)-C(4)	119.6(7)
C(6)-C(5)-C(10)	119.5(7)
C(4)-C(5)-C(10)	120.9(6)
C(5)-C(6)-C(7)	121.2(7)
C(5)-C(6)-H(6)	119.4
C(7)-C(6)-H(6)	119.4
C(8)-C(7)-C(6)	117.3(7)
C(8)-C(7)-C(11)	122.3(7)
C(6)-C(7)-C(11)	120.3(7)
C(7)-C(8)-C(9)	124.7(7)
C(7)-C(8)-H(8)	117.7
C(9)-C(8)-H(8)	117.7
C(8)-C(9)-C(4)	116.2(7)
C(8)-C(9)-C(12)	122.9(7)
C(4)-C(9)-C(12)	120.9(6)
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(7)-C(11)-H(11A)	109.5
C(7)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(7)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(9)-C(12)-H(12A)	109.5
C(9)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(9)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(18)-C(13)-C(14)	121.5(6)
C(18)-C(13)-N(3)	122.1(7)
C(14)-C(13)-N(3)	116.2(6)
C(15)-C(14)-C(13)	117.4(7)
C(15)-C(14)-C(19)	120.9(7)
C(13)-C(14)-C(19)	121.7(6)
C(14)-C(15)-C(16)	122.9(7)
C(14)-C(15)-H(15)	118.5
C(16)-C(15)-H(15)	118.5

C(17)-C(16)-C(15)	117.0(7)
C(17)-C(16)-C(20)	121.8(7)
C(15)-C(16)-C(20)	121.2(7)
C(16)-C(17)-C(18)	123.4(7)
C(16)-C(17)-H(17)	118.3
C(18)-C(17)-H(17)	118.3
C(17)-C(18)-C(13)	117.6(7)
C(17)-C(18)-C(21)	120.8(7)
C(13)-C(18)-C(21)	121.6(7)
C(14)-C(19)-H(19A)	109.5
C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-H(20A)	109.5
C(16)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(16)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(23)-C(22)-N(1)	118.8(6)
C(23)-C(22)-C(27)	121.8(6)
N(1)-C(22)-C(27)	119.4(6)
C(24)-C(23)-C(22)	118.4(7)
C(24)-C(23)-C(28)	119.3(7)
C(22)-C(23)-C(28)	122.2(6)
C(25)-C(24)-C(23)	120.5(7)
C(25)-C(24)-H(24)	119.7
C(23)-C(24)-H(24)	119.7
C(26)-C(25)-C(24)	120.7(7)
C(26)-C(25)-H(25)	119.7
C(24)-C(25)-H(25)	119.7
C(25)-C(26)-C(27)	122.1(8)
C(25)-C(26)-H(26)	119.0
C(27)-C(26)-H(26)	119.0
C(26)-C(27)-C(22)	116.5(7)
C(26)-C(27)-C(29)	120.7(7)
C(22)-C(27)-C(29)	122.8(6)
C(23)-C(28)-H(28A)	109.5
C(23)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(23)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5

H(28B)-C(28)-H(28C)	109.5
C(27)-C(29)-H(29A)	109.5
C(27)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(27)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(31)-C(30)-Mo(1)	146.9(5)
C(31)-C(30)-H(30)	106.6
Mo(1)-C(30)-H(30)	106.6
C(30)-C(31)-C(34)	110.5(6)
C(30)-C(31)-C(32)	110.2(6)
C(34)-C(31)-C(32)	108.9(6)
C(30)-C(31)-C(33)	107.2(6)
C(34)-C(31)-C(33)	111.7(6)
C(32)-C(31)-C(33)	108.2(6)
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(31)-C(33)-H(33A)	109.5
C(31)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(31)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(35)-C(34)-C(39)	117.7(6)
C(35)-C(34)-C(31)	124.1(6)
C(39)-C(34)-C(31)	118.3(6)
C(34)-C(35)-C(36)	121.0(7)
C(34)-C(35)-H(35)	119.5
C(36)-C(35)-H(35)	119.5
C(35)-C(36)-C(37)	120.3(7)
C(35)-C(36)-H(36)	119.9
C(37)-C(36)-H(36)	119.9
C(38)-C(37)-C(36)	119.0(7)
C(38)-C(37)-H(37)	120.5
C(36)-C(37)-H(37)	120.5
C(39)-C(38)-C(37)	120.2(7)
C(39)-C(38)-H(38)	119.9
C(37)-C(38)-H(38)	119.9
C(38)-C(39)-C(34)	121.9(7)
C(38)-C(39)-H(39)	119.0
C(34)-C(39)-H(39)	119.0
O(3)-S(1)-O(2)	118.3(3)
O(3)-S(1)-O(1)	113.5(3)
O(2)-S(1)-O(1)	113.6(3)
O(3)-S(1)-C(40)	105.6(3)

O(2)-S(1)-C(40)	103.4(3)
O(1)-S(1)-C(40)	99.7(3)
S(1)-O(1)-Mo(1)	146.4(3)
F(2)-C(40)-F(3)	109.1(6)
F(2)-C(40)-F(1)	108.5(6)
F(3)-C(40)-F(1)	107.9(6)
F(2)-C(40)-S(1)	110.7(5)
F(3)-C(40)-S(1)	111.3(5)
F(1)-C(40)-S(1)	109.2(5)
O(5)-S(2)-O(6)	119.5(3)
O(5)-S(2)-O(4)	112.9(3)
O(6)-S(2)-O(4)	112.2(3)
O(5)-S(2)-C(41)	104.1(3)
O(6)-S(2)-C(41)	104.3(3)
O(4)-S(2)-C(41)	101.2(3)
S(2)-O(4)-Mo(1)	133.1(3)
F(5)-C(41)-F(6)	108.8(7)
F(5)-C(41)-F(4)	106.9(6)
F(6)-C(41)-F(4)	107.1(6)
F(5)-C(41)-S(2)	112.7(5)
F(6)-C(41)-S(2)	112.2(5)
F(4)-C(41)-S(2)	108.9(5)

Symmetry transformations used to generate equivalent atoms:

Table 6.4. Anisotropic displacement parameters ($Å^2$x 10^3) for **6**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11}+ ... +2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	23(1)	15(1)	25(1)	0(1)	0(1)	0(1)
N(1)	30(3)	19(3)	21(3)	-2(2)	2(2)	-1(3)
C(1)	25(4)	21(4)	24(4)	3(3)	2(3)	2(3)
N(2)	28(3)	19(3)	27(3)	3(2)	3(3)	-1(3)
C(2)	30(4)	22(4)	31(4)	2(3)	-1(3)	-2(3)
N(3)	27(3)	20(3)	26(3)	0(3)	0(3)	-1(3)
C(3)	23(4)	28(4)	30(4)	-4(3)	2(3)	-6(3)
C(4)	32(4)	7(3)	30(4)	1(3)	-2(3)	-6(3)
C(5)	21(3)	18(4)	33(4)	2(3)	6(3)	-8(3)
C(6)	44(5)	21(4)	25(4)	-1(3)	-3(3)	-6(4)
C(7)	33(4)	17(4)	33(4)	2(3)	4(3)	-4(3)
C(8)	33(4)	12(4)	50(5)	0(3)	0(4)	10(3)
C(9)	25(4)	16(3)	36(4)	2(3)	4(3)	-10(3)
C(10)	30(4)	23(4)	30(4)	-1(3)	5(3)	-2(3)
C(11)	43(5)	28(4)	38(5)	4(4)	-7(4)	-3(4)
C(12)	30(4)	26(4)	41(5)	-2(3)	7(3)	-3(3)
C(13)	27(4)	21(4)	28(4)	0(3)	-7(3)	-7(3)
C(14)	25(4)	26(4)	24(4)	0(3)	-3(3)	-11(3)
C(15)	34(4)	31(4)	26(4)	0(3)	1(3)	-10(4)
C(16)	30(4)	29(4)	38(4)	6(4)	-4(3)	-2(3)

C(17)	34(4)	28(4)	42(5)	8(4)	-9(4)	-2(4)
C(18)	23(4)	29(4)	32(4)	-3(3)	-6(3)	-2(3)
C(19)	47(5)	20(4)	25(4)	-1(3)	-4(3)	-7(3)
C(20)	25(4)	42(5)	48(5)	9(4)	3(4)	1(4)
C(21)	38(5)	37(5)	47(5)	3(4)	-3(4)	10(4)
C(22)	18(3)	16(3)	34(4)	-3(3)	0(3)	-2(3)
C(23)	22(4)	24(4)	35(4)	6(3)	2(3)	-2(3)
C(24)	32(4)	48(5)	27(4)	7(4)	-1(3)	2(4)
C(25)	35(5)	67(6)	39(5)	15(5)	-2(4)	18(5)
C(26)	32(4)	48(5)	48(5)	10(4)	5(4)	15(4)
C(27)	30(4)	20(4)	33(4)	4(3)	7(3)	6(3)
C(28)	33(4)	28(4)	29(4)	2(3)	2(3)	-6(3)
C(29)	29(4)	28(4)	39(5)	5(3)	8(3)	8(3)
C(30)	26(4)	17(4)	31(4)	-3(3)	-2(3)	7(3)
C(31)	31(4)	19(4)	25(4)	0(3)	-1(3)	1(3)
C(32)	32(4)	27(4)	26(4)	2(3)	-3(3)	1(3)
C(33)	27(4)	23(4)	31(4)	-1(3)	0(3)	2(3)
C(34)	30(4)	12(3)	28(4)	0(3)	7(3)	-3(3)
C(35)	36(4)	17(4)	39(5)	0(3)	2(4)	1(3)
C(36)	49(5)	35(5)	23(4)	8(3)	1(4)	-4(4)
C(37)	46(5)	28(4)	35(5)	6(4)	2(4)	7(4)
C(38)	41(5)	21(4)	42(5)	6(4)	5(4)	6(4)
C(39)	44(5)	22(4)	29(4)	1(3)	2(3)	2(4)
S(1)	27(1)	21(1)	31(1)	-2(1)	1(1)	-4(1)
O(1)	26(3)	17(2)	32(3)	-2(2)	3(2)	-1(2)
O(2)	40(3)	23(3)	40(3)	-9(2)	9(3)	-11(2)
O(3)	32(3)	25(3)	33(3)	3(2)	2(2)	-2(2)
C(40)	35(4)	29(4)	25(4)	-2(3)	3(3)	-6(4)
F(1)	32(2)	41(3)	46(3)	4(2)	0(2)	-16(2)
F(2)	27(2)	67(3)	45(3)	-20(3)	0(2)	8(2)
F(3)	39(3)	35(3)	42(3)	8(2)	-8(2)	-8(2)
S(2)	29(1)	21(1)	29(1)	-2(1)	2(1)	3(1)
O(4)	28(3)	23(3)	31(3)	-6(2)	-1(2)	0(2)
O(5)	27(3)	32(3)	31(3)	-4(2)	3(2)	4(2)
O(6)	34(3)	23(3)	45(3)	5(2)	2(2)	2(2)
C(41)	35(4)	36(5)	32(4)	-3(4)	9(4)	5(4)
F(4)	37(3)	48(3)	62(3)	-16(3)	17(2)	8(2)
F(5)	36(3)	36(3)	79(4)	12(3)	17(3)	1(2)
F(6)	26(2)	75(4)	48(3)	1(3)	1(2)	10(2)

Table 6.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **6**.

	x	y	z	U(eq)
H(2)	8370	7045	2192	34
H(3)	9243	6426	3156	33
H(6)	5644	6645	122	37
H(8)	3811	7628	1423	38

H(10A)	7043	5344	880	41
H(10B)	8095	5943	1092	41
H(10C)	7442	5935	386	41
H(11A)	2880	7451	216	56
H(11B)	3994	7437	-221	56
H(11C)	3848	8122	234	56
H(12A)	4334	7457	2504	48
H(12B)	5814	7369	2674	48
H(12C)	4918	6667	2690	48
H(15)	7630	5498	5023	36
H(17)	9167	3779	4214	43
H(19A)	6712	6490	4450	47
H(19B)	6283	6356	3722	47
H(19C)	7604	6736	3937	47
H(20A)	8855	3696	5300	57
H(20B)	8087	4328	5609	57
H(20C)	9549	4433	5553	57
H(21A)	9952	4083	3147	62
H(21B)	9014	4580	2696	62
H(21C)	8565	3796	2928	62
H(24)	2118	5810	211	43
H(25)	573	6447	673	57
H(26)	655	6543	1744	51
H(28A)	4920	5105	962	45
H(28B)	4177	5277	292	45
H(28C)	3857	4552	667	45
H(29A)	1570	6324	2753	48
H(29B)	3039	6150	2840	48
H(29C)	2048	5490	2820	48
H(30)	6186	4133	3168	30
H(32A)	2910	4360	3003	43
H(32B)	2768	3989	3667	43
H(32C)	3346	3527	3134	43
H(33A)	5306	5221	4051	41
H(33B)	3890	5044	4166	41
H(33C)	4188	5408	3520	41
H(35)	5008	4306	4847	37
H(36)	5959	3435	5542	43
H(37)	6707	2322	5162	44
H(38)	6516	2111	4086	42
H(39)	5548	2972	3404	38

Table 6.6. Torsion angles [°] for **6**.

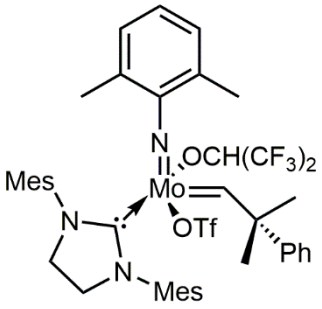
C(30)-Mo(1)-N(1)-C(22)	-157.2(13)
O(4)-Mo(1)-N(1)-C(22)	18.5(15)
O(1)-Mo(1)-N(1)-C(22)	-56.6(13)
C(1)-Mo(1)-N(1)-C(22)	104.2(13)
N(1)-Mo(1)-C(1)-N(3)	141.2(7)
C(30)-Mo(1)-C(1)-N(3)	35.9(7)
O(4)-Mo(1)-C(1)-N(3)	-79.8(7)
O(1)-Mo(1)-C(1)-N(3)	-97.6(8)
N(1)-Mo(1)-C(1)-N(2)	-55.9(6)
C(30)-Mo(1)-C(1)-N(2)	-161.2(6)
O(4)-Mo(1)-C(1)-N(2)	83.1(6)
O(1)-Mo(1)-C(1)-N(2)	65.3(9)
N(3)-C(1)-N(2)-C(2)	-0.5(8)
Mo(1)-C(1)-N(2)-C(2)	-167.2(5)
N(3)-C(1)-N(2)-C(4)	-168.9(7)
Mo(1)-C(1)-N(2)-C(4)	24.4(10)
C(1)-N(2)-C(2)-C(3)	-0.1(9)
C(4)-N(2)-C(2)-C(3)	169.4(7)
N(2)-C(1)-N(3)-C(3)	0.9(8)
Mo(1)-C(1)-N(3)-C(3)	166.2(5)
N(2)-C(1)-N(3)-C(13)	169.4(7)
Mo(1)-C(1)-N(3)-C(13)	-25.4(11)
N(2)-C(2)-C(3)-N(3)	0.7(8)
C(1)-N(3)-C(3)-C(2)	-1.1(9)
C(13)-N(3)-C(3)-C(2)	-170.9(7)
C(1)-N(2)-C(4)-C(5)	-102.7(9)
C(2)-N(2)-C(4)-C(5)	90.0(8)
C(1)-N(2)-C(4)-C(9)	81.2(9)
C(2)-N(2)-C(4)-C(9)	-86.2(8)
C(9)-C(4)-C(5)-C(6)	1.9(10)
N(2)-C(4)-C(5)-C(6)	-174.1(6)
C(9)-C(4)-C(5)-C(10)	-178.2(6)
N(2)-C(4)-C(5)-C(10)	5.8(10)
C(4)-C(5)-C(6)-C(7)	-1.0(10)
C(10)-C(5)-C(6)-C(7)	179.2(6)
C(5)-C(6)-C(7)-C(8)	-0.3(11)
C(5)-C(6)-C(7)-C(11)	179.8(7)
C(6)-C(7)-C(8)-C(9)	0.7(11)
C(11)-C(7)-C(8)-C(9)	-179.5(7)
C(7)-C(8)-C(9)-C(4)	0.2(11)
C(7)-C(8)-C(9)-C(12)	177.4(7)
C(5)-C(4)-C(9)-C(8)	-1.5(10)
N(2)-C(4)-C(9)-C(8)	174.7(6)
C(5)-C(4)-C(9)-C(12)	-178.8(6)
N(2)-C(4)-C(9)-C(12)	-2.6(9)
C(1)-N(3)-C(13)-C(18)	89.0(10)
C(3)-N(3)-C(13)-C(18)	-103.4(8)
C(1)-N(3)-C(13)-C(14)	-96.9(9)

C(3)-N(3)-C(13)-C(14)	70.8(8)
C(18)-C(13)-C(14)-C(15)	-1.7(10)
N(3)-C(13)-C(14)-C(15)	-175.8(6)
C(18)-C(13)-C(14)-C(19)	176.6(7)
N(3)-C(13)-C(14)-C(19)	2.4(10)
C(13)-C(14)-C(15)-C(16)	-0.5(11)
C(19)-C(14)-C(15)-C(16)	-178.7(7)
C(14)-C(15)-C(16)-C(17)	0.0(11)
C(14)-C(15)-C(16)-C(20)	177.5(7)
C(15)-C(16)-C(17)-C(18)	2.7(11)
C(20)-C(16)-C(17)-C(18)	-174.8(7)
C(16)-C(17)-C(18)-C(13)	-4.7(11)
C(16)-C(17)-C(18)-C(21)	176.0(7)
C(14)-C(13)-C(18)-C(17)	4.1(10)
N(3)-C(13)-C(18)-C(17)	177.9(6)
C(14)-C(13)-C(18)-C(21)	-176.6(7)
N(3)-C(13)-C(18)-C(21)	-2.7(10)
Mo(1)-N(1)-C(22)-C(23)	0.7(17)
Mo(1)-N(1)-C(22)-C(27)	-179.4(10)
N(1)-C(22)-C(23)-C(24)	-179.5(6)
C(27)-C(22)-C(23)-C(24)	0.7(10)
N(1)-C(22)-C(23)-C(28)	2.0(10)
C(27)-C(22)-C(23)-C(28)	-177.9(6)
C(22)-C(23)-C(24)-C(25)	0.1(12)
C(28)-C(23)-C(24)-C(25)	178.7(8)
C(23)-C(24)-C(25)-C(26)	0.4(14)
C(24)-C(25)-C(26)-C(27)	-1.6(14)
C(25)-C(26)-C(27)-C(22)	2.3(12)
C(25)-C(26)-C(27)-C(29)	-178.4(8)
C(23)-C(22)-C(27)-C(26)	-1.8(10)
N(1)-C(22)-C(27)-C(26)	178.3(7)
C(23)-C(22)-C(27)-C(29)	178.8(7)
N(1)-C(22)-C(27)-C(29)	-1.0(10)
N(1)-Mo(1)-C(30)-C(31)	6.4(10)
O(4)-Mo(1)-C(30)-C(31)	-170.5(8)
O(1)-Mo(1)-C(30)-C(31)	-88.3(9)
C(1)-Mo(1)-C(30)-C(31)	108.1(9)
Mo(1)-C(30)-C(31)-C(34)	167.4(7)
Mo(1)-C(30)-C(31)-C(32)	47.0(11)
Mo(1)-C(30)-C(31)-C(33)	-70.6(10)
C(30)-C(31)-C(34)-C(35)	134.4(7)
C(32)-C(31)-C(34)-C(35)	-104.4(8)
C(33)-C(31)-C(34)-C(35)	15.1(10)
C(30)-C(31)-C(34)-C(39)	-45.7(9)
C(32)-C(31)-C(34)-C(39)	75.5(8)
C(33)-C(31)-C(34)-C(39)	-165.0(7)
C(39)-C(34)-C(35)-C(36)	1.1(11)
C(31)-C(34)-C(35)-C(36)	-179.0(7)
C(34)-C(35)-C(36)-C(37)	-0.5(12)
C(35)-C(36)-C(37)-C(38)	0.4(13)

C(36)-C(37)-C(38)-C(39)	-0.8(13)
C(37)-C(38)-C(39)-C(34)	1.4(13)
C(35)-C(34)-C(39)-C(38)	-1.5(12)
C(31)-C(34)-C(39)-C(38)	178.5(7)
O(3)-S(1)-O(1)-Mo(1)	-10.4(7)
O(2)-S(1)-O(1)-Mo(1)	-149.4(5)
C(40)-S(1)-O(1)-Mo(1)	101.4(6)
N(1)-Mo(1)-O(1)-S(1)	-106.7(6)
C(30)-Mo(1)-O(1)-S(1)	-2.2(6)
O(4)-Mo(1)-O(1)-S(1)	112.9(6)
C(1)-Mo(1)-O(1)-S(1)	130.8(6)
O(3)-S(1)-C(40)-F(2)	52.6(6)
O(2)-S(1)-C(40)-F(2)	177.5(5)
O(1)-S(1)-C(40)-F(2)	-65.3(6)
O(3)-S(1)-C(40)-F(3)	174.2(5)
O(2)-S(1)-C(40)-F(3)	-60.9(6)
O(1)-S(1)-C(40)-F(3)	56.3(6)
O(3)-S(1)-C(40)-F(1)	-66.8(5)
O(2)-S(1)-C(40)-F(1)	58.1(6)
O(1)-S(1)-C(40)-F(1)	175.3(5)
O(5)-S(2)-O(4)-Mo(1)	68.4(5)
O(6)-S(2)-O(4)-Mo(1)	-70.2(5)
C(41)-S(2)-O(4)-Mo(1)	179.1(4)
N(1)-Mo(1)-O(4)-S(2)	-79.2(5)
C(30)-Mo(1)-O(4)-S(2)	96.1(5)
O(1)-Mo(1)-O(4)-S(2)	0.7(4)
C(1)-Mo(1)-O(4)-S(2)	-172.4(5)
O(5)-S(2)-C(41)-F(5)	56.6(6)
O(6)-S(2)-C(41)-F(5)	-177.3(5)
O(4)-S(2)-C(41)-F(5)	-60.7(6)
O(5)-S(2)-C(41)-F(6)	179.9(6)
O(6)-S(2)-C(41)-F(6)	-54.1(6)
O(4)-S(2)-C(41)-F(6)	62.5(6)
O(5)-S(2)-C(41)-F(4)	-61.8(6)
O(6)-S(2)-C(41)-F(4)	64.3(6)
O(4)-S(2)-C(41)-F(4)	-179.1(5)

Symmetry transformations used to generate equivalent atoms

Complex 7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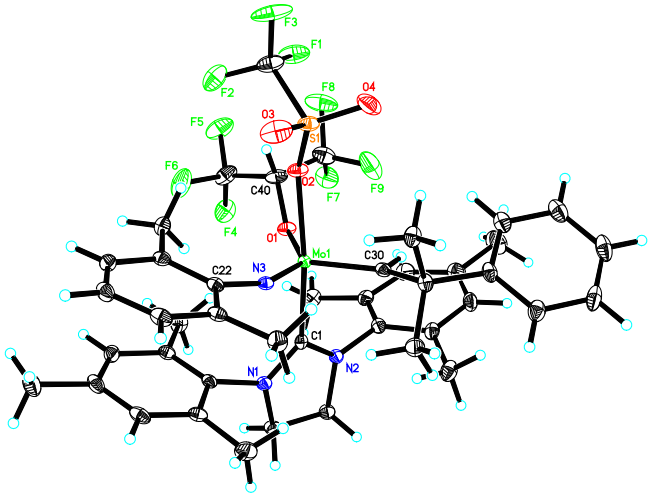
Mes
N
OTf
Ph
N
Mes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O3
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F5
F6
O2
C40
F7
F9
F4
O1
Mo1
C30
C22
N3
C1
N1
N2

Table 7.1. Crystal data and structure refinement for **7**.

Empirical formula	$C_{44}H_{50}Cl_2F_9MoN_3O_4S$
Formula weight	1054.77
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	triclinic, *P* -1
Unit cell dimensions	a = 10.8028(6) Å, α = 85.488(3)°
	b = 11.1926(7) Å, β = 88.695(3)°
	c = 21.5761(13) Å, γ = 61.342(3)°
Volume	2281.8(2) $Å^3$
Z, Calculated density	2, 1.535 Mg/m^3
Absorption coefficient	0.533 mm^{-1}
F(000)	1080
Crystal size	0.31 x 0.23 x 0.22 mm
Theta range for data collection	1.89 to 28.41°.
Limiting indice	-14<=h<=14, -14<=k<=14, -28<=l<=28
Reflections collected / unique	40639 / 11373 [R(int) = 0.0396]
Completeness to theta =	28.41 99.3 %
Absorption correctionequivalents	semi-empirical from
Max. and min. transmission	0.7457 and 0.7109
Refinement method	full-matrix least-squares on F^2
Data / restraints / parameters	11373 / 0 / 595
Goodness-of-fit on F^2	1.056
Final R indices [I>2σ(I)]	R1 = 0.0328, wR2 = 0.0726
R indices (all data)	R1 = 0.0461, wR2 = 0.0763
Largest diff. peak and hole	0.719 and -0.459 $e.Å^{-3}$

Table 7.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **7**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	2045(1)	8292(1)	2547(1)	9(1)
S(1)	-1571(1)	9451(1)	2389(1)	17(1)
O(1)	1776(1)	10144(1)	2708(1)	14(1)
F(1)	-2813(1)	12024(1)	2637(1)	32(1)
N(1)	5308(2)	7196(2)	2217(1)	12(1)
C(1)	4338(2)	7669(2)	2663(1)	11(1)
O(2)	-247(1)	9506(1)	2446(1)	16(1)
F(2)	-2360(2)	11683(1)	1670(1)	41(1)
N(2)	5000(2)	7634(2)	3190(1)	12(1)
C(2)	6743(2)	6870(2)	2433(1)	18(1)
N(3)	2147(2)	7403(2)	1900(1)	11(1)
O(3)	-1631(2)	8784(2)	1863(1)	31(1)
C(3)	6549(2)	6995(2)	3129(1)	16(1)
F(3)	-4080(1)	11480(1)	2095(1)	44(1)
F(4)	1983(1)	12513(1)	2435(1)	29(1)
O(4)	-2083(2)	9154(2)	2966(1)	34(1)
C(4)	4411(2)	8121(2)	3782(1)	14(1)
F(5)	-261(2)	13740(1)	2361(1)	36(1)
C(5)	4335(2)	7215(2)	4246(1)	16(1)
F(6)	855(2)	12244(1)	1704(1)	37(1)
C(6)	3778(2)	7724(2)	4818(1)	23(1)
F(7)	1070(1)	12231(1)	3621(1)	31(1)
C(7)	3381(2)	9055(2)	4941(1)	25(1)
F(8)	-1103(1)	12870(2)	3404(1)	42(1)
C(8)	3570(2)	9892(2)	4483(1)	22(1)
F(9)	275(2)	10789(2)	3742(1)	43(1)
C(9)	4091(2)	9447(2)	3898(1)	16(1)
C(10)	4908(2)	5733(2)	4153(1)	21(1)
C(11)	2757(3)	9584(3)	5560(1)	40(1)
C(12)	4339(2)	10360(2)	3420(1)	21(1)
C(13)	5060(2)	7367(2)	1557(1)	12(1)
C(14)	5391(2)	6218(2)	1236(1)	15(1)
C(15)	5236(2)	6386(2)	593(1)	18(1)
C(16)	4779(2)	7651(2)	265(1)	18(1)
C(17)	4502(2)	8762(2)	600(1)	17(1)
C(18)	4642(2)	8648(2)	1246(1)	14(1)
C(19)	5947(2)	4830(2)	1576(1)	22(1)
C(20)	4598(2)	7813(3)	-432(1)	26(1)
C(21)	4372(2)	9865(2)	1589(1)	19(1)
C(22)	1947(2)	7268(2)	1275(1)	12(1)
C(23)	2179(2)	6006(2)	1074(1)	14(1)
C(24)	2026(2)	5921(2)	443(1)	17(1)
C(25)	1667(2)	7037(2)	17(1)	18(1)

C(26)	1415(2)	8274(2)	222(1)	16(1)
C(27)	1525(2)	8427(2)	848(1)	14(1)
C(28)	2549(2)	4772(2)	1515(1)	19(1)
C(29)	1157(2)	9796(2)	1063(1)	17(1)
C(30)	2028(2)	7130(2)	3234(1)	13(1)
C(31)	1930(2)	5826(2)	3391(1)	14(1)
C(32)	3225(2)	4598(2)	3138(1)	19(1)
C(33)	583(2)	5987(2)	3066(1)	17(1)
C(34)	1745(2)	5614(2)	4093(1)	16(1)
C(35)	776(2)	6713(2)	4410(1)	21(1)
C(36)	538(2)	6555(2)	5040(1)	25(1)
C(37)	1258(2)	5283(3)	5361(1)	26(1)
C(38)	2208(2)	4179(2)	5052(1)	25(1)
C(39)	2455(2)	4338(2)	4422(1)	20(1)
C(40)	597(2)	11416(2)	2709(1)	19(1)
C(41)	809(2)	12479(2)	2309(1)	24(1)
C(42)	213(2)	11833(2)	3372(1)	27(1)
C(43)	-2778(2)	11256(2)	2187(1)	25(1)
C(1X)	1626(2)	2743(2)	9306(1)	27(1)
Cl(1X)	1805(1)	2574(1)	10126(1)	26(1)
Cl(2X)	989(1)	4452(1)	9009(1)	34(1)

Table 7.3. Bond lengths [Å] and angles [°] for **7**.

Mo(1)-N(3)	1.7469(15)
Mo(1)-C(30)	1.8995(19)
Mo(1)-O(1)	2.0088(13)
Mo(1)-O(2)	2.1850(13)
Mo(1)-C(1)	2.2425(18)
S(1)-O(3)	1.4263(16)
S(1)-O(4)	1.4295(16)
S(1)-O(2)	1.4691(13)
S(1)-C(43)	1.826(2)
O(1)-C(40)	1.382(2)
F(1)-C(43)	1.333(2)
N(1)-C(1)	1.345(2)
N(1)-C(13)	1.435(2)
N(1)-C(2)	1.490(2)
C(1)-N(2)	1.344(2)
F(2)-C(43)	1.334(3)
N(2)-C(4)	1.442(2)
N(2)-C(3)	1.479(2)
C(2)-C(3)	1.519(3)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
N(3)-C(22)	1.403(2)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
F(3)-C(43)	1.322(2)

F(4)-C(41)	1.322(3)
C(4)-C(9)	1.395(3)
C(4)-C(5)	1.397(3)
F(5)-C(41)	1.340(2)
C(5)-C(6)	1.399(3)
C(5)-C(10)	1.495(3)
F(6)-C(41)	1.347(2)
C(6)-C(7)	1.385(3)
C(6)-H(6)	0.9500
F(7)-C(42)	1.341(3)
C(7)-C(8)	1.387(3)
C(7)-C(11)	1.513(3)
F(8)-C(42)	1.341(3)
C(8)-C(9)	1.399(3)
C(8)-H(8)	0.9500
F(9)-C(42)	1.338(3)
C(9)-C(12)	1.504(3)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(18)	1.397(3)
C(13)-C(14)	1.397(3)
C(14)-C(15)	1.389(3)
C(14)-C(19)	1.502(3)
C(15)-C(16)	1.392(3)
C(15)-H(15)	0.9500
C(16)-C(17)	1.390(3)
C(16)-C(20)	1.507(3)
C(17)-C(18)	1.393(3)
C(17)-H(17)	0.9500
C(18)-C(21)	1.503(3)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(23)	1.414(3)
C(22)-C(27)	1.416(3)
C(23)-C(24)	1.392(3)
C(23)-C(28)	1.501(3)

C(24)-C(25)	1.388(3)
C(24)-H(24)	0.9500
C(25)-C(26)	1.384(3)
C(25)-H(25)	0.9500
C(26)-C(27)	1.390(2)
C(26)-H(26)	0.9500
C(27)-C(29)	1.496(3)
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-C(31)	1.525(3)
C(30)-H(30)	0.96(2)
C(31)-C(34)	1.538(2)
C(31)-C(32)	1.543(3)
C(31)-C(33)	1.554(3)
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-C(35)	1.394(3)
C(34)-C(39)	1.396(3)
C(35)-C(36)	1.390(3)
C(35)-H(35)	0.9500
C(36)-C(37)	1.386(3)
C(36)-H(36)	0.9500
C(37)-C(38)	1.381(3)
C(37)-H(37)	0.9500
C(38)-C(39)	1.393(3)
C(38)-H(38)	0.9500
C(39)-H(39)	0.9500
C(40)-C(41)	1.518(3)
C(40)-C(42)	1.527(3)
C(40)-H(40)	0.98(2)
C(1X)-Cl(2X)	1.763(2)
C(1X)-Cl(1X)	1.769(2)
C(1X)-H(1X1)	0.9900
C(1X)-H(1X2)	0.9900

N(3)-Mo(1)-C(30)	104.04(8)
N(3)-Mo(1)-O(1)	137.24(6)
C(30)-Mo(1)-O(1)	118.40(7)
N(3)-Mo(1)-O(2)	91.87(6)
C(30)-Mo(1)-O(2)	95.73(6)
O(1)-Mo(1)-O(2)	79.59(5)
N(3)-Mo(1)-C(1)	99.16(6)

C(30)-Mo(1)-C(1)	94.40(7)
O(1)-Mo(1)-C(1)	83.33(6)
O(2)-Mo(1)-C(1)	162.76(6)
O(3)-S(1)-O(4)	117.83(11)
O(3)-S(1)-O(2)	113.70(9)
O(4)-S(1)-O(2)	114.21(10)
O(3)-S(1)-C(43)	104.32(10)
O(4)-S(1)-C(43)	104.26(10)
O(2)-S(1)-C(43)	99.59(9)
C(40)-O(1)-Mo(1)	132.80(12)
C(1)-N(1)-C(13)	127.32(15)
C(1)-N(1)-C(2)	112.82(15)
C(13)-N(1)-C(2)	116.86(14)
N(2)-C(1)-N(1)	107.94(15)
N(2)-C(1)-Mo(1)	126.82(12)
N(1)-C(1)-Mo(1)	125.17(13)
S(1)-O(2)-Mo(1)	144.90(8)
C(1)-N(2)-C(4)	129.17(15)
C(1)-N(2)-C(3)	113.08(14)
C(4)-N(2)-C(3)	117.75(14)
N(1)-C(2)-C(3)	102.22(14)
N(1)-C(2)-H(2A)	111.3
C(3)-C(2)-H(2A)	111.3
N(1)-C(2)-H(2B)	111.3
C(3)-C(2)-H(2B)	111.3
H(2A)-C(2)-H(2B)	109.2
C(22)-N(3)-Mo(1)	155.44(13)
N(2)-C(3)-C(2)	102.61(14)
N(2)-C(3)-H(3A)	111.2
C(2)-C(3)-H(3A)	111.2
N(2)-C(3)-H(3B)	111.2
C(2)-C(3)-H(3B)	111.2
H(3A)-C(3)-H(3B)	109.2
C(9)-C(4)-C(5)	121.89(17)
C(9)-C(4)-N(2)	118.24(16)
C(5)-C(4)-N(2)	119.43(17)
C(4)-C(5)-C(6)	117.59(19)
C(4)-C(5)-C(10)	121.64(18)
C(6)-C(5)-C(10)	120.66(18)
C(7)-C(6)-C(5)	122.1(2)
C(7)-C(6)-H(6)	118.9
C(5)-C(6)-H(6)	118.9
C(6)-C(7)-C(8)	118.36(19)
C(6)-C(7)-C(11)	120.9(2)
C(8)-C(7)-C(11)	120.7(2)
C(7)-C(8)-C(9)	121.9(2)
C(7)-C(8)-H(8)	119.0
C(9)-C(8)-H(8)	119.0
C(4)-C(9)-C(8)	117.77(19)
C(4)-C(9)-C(12)	121.54(17)

C(8)-C(9)-C(12)	120.66(19)
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(7)-C(11)-H(11A)	109.5
C(7)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(7)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(9)-C(12)-H(12A)	109.5
C(9)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(9)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(18)-C(13)-C(14)	121.62(17)
C(18)-C(13)-N(1)	119.09(16)
C(14)-C(13)-N(1)	118.91(17)
C(15)-C(14)-C(13)	118.22(18)
C(15)-C(14)-C(19)	120.92(17)
C(13)-C(14)-C(19)	120.83(17)
C(14)-C(15)-C(16)	122.01(18)
C(14)-C(15)-H(15)	119.0
C(16)-C(15)-H(15)	119.0
C(17)-C(16)-C(15)	117.98(18)
C(17)-C(16)-C(20)	121.0(2)
C(15)-C(16)-C(20)	121.06(19)
C(16)-C(17)-C(18)	122.26(19)
C(16)-C(17)-H(17)	118.9
C(18)-C(17)-H(17)	118.9
C(17)-C(18)-C(13)	117.84(17)
C(17)-C(18)-C(21)	120.62(18)
C(13)-C(18)-C(21)	121.54(17)
C(14)-C(19)-H(19A)	109.5
C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-H(20A)	109.5
C(16)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(16)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(18)-C(21)-H(21A)	109.5

C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(3)-C(22)-C(23)	120.99(17)
N(3)-C(22)-C(27)	118.15(16)
C(23)-C(22)-C(27)	120.86(17)
C(24)-C(23)-C(22)	118.24(18)
C(24)-C(23)-C(28)	119.03(17)
C(22)-C(23)-C(28)	122.71(17)
C(25)-C(24)-C(23)	121.32(18)
C(25)-C(24)-H(24)	119.3
C(23)-C(24)-H(24)	119.3
C(26)-C(25)-C(24)	119.81(17)
C(26)-C(25)-H(25)	120.1
C(24)-C(25)-H(25)	120.1
C(25)-C(26)-C(27)	121.44(19)
C(25)-C(26)-H(26)	119.3
C(27)-C(26)-H(26)	119.3
C(26)-C(27)-C(22)	118.25(17)
C(26)-C(27)-C(29)	120.48(18)
C(22)-C(27)-C(29)	121.24(16)
C(23)-C(28)-H(28A)	109.5
C(23)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(23)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(27)-C(29)-H(29A)	109.5
C(27)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(27)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(31)-C(30)-Mo(1)	141.66(13)
C(31)-C(30)-H(30)	115.5(13)
Mo(1)-C(30)-H(30)	102.3(13)
C(30)-C(31)-C(34)	111.12(15)
C(30)-C(31)-C(32)	109.93(15)
C(34)-C(31)-C(32)	112.59(16)
C(30)-C(31)-C(33)	108.17(15)
C(34)-C(31)-C(33)	106.46(15)
C(32)-C(31)-C(33)	108.39(15)
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5

C(31)-C(33)-H(33A)	109.5
C(31)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(31)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(35)-C(34)-C(39)	118.14(18)
C(35)-C(34)-C(31)	119.35(18)
C(39)-C(34)-C(31)	122.40(17)
C(36)-C(35)-C(34)	121.2(2)
C(36)-C(35)-H(35)	119.4
C(34)-C(35)-H(35)	119.4
C(37)-C(36)-C(35)	119.9(2)
C(37)-C(36)-H(36)	120.0
C(35)-C(36)-H(36)	120.0
C(38)-C(37)-C(36)	119.60(19)
C(38)-C(37)-H(37)	120.2
C(36)-C(37)-H(37)	120.2
C(37)-C(38)-C(39)	120.5(2)
C(37)-C(38)-H(38)	119.7
C(39)-C(38)-H(38)	119.7
C(38)-C(39)-C(34)	120.6(2)
C(38)-C(39)-H(39)	119.7
C(34)-C(39)-H(39)	119.7
O(1)-C(40)-C(41)	111.20(17)
O(1)-C(40)-C(42)	110.75(17)
C(41)-C(40)-C(42)	111.30(17)
O(1)-C(40)-H(40)	114.8(14)
C(41)-C(40)-H(40)	99.5(14)
C(42)-C(40)-H(40)	108.9(14)
F(4)-C(41)-F(5)	106.96(17)
F(4)-C(41)-F(6)	106.57(18)
F(5)-C(41)-F(6)	106.37(17)
F(4)-C(41)-C(40)	114.37(18)
F(5)-C(41)-C(40)	111.72(19)
F(6)-C(41)-C(40)	110.41(17)
F(9)-C(42)-F(8)	106.88(18)
F(9)-C(42)-F(7)	107.47(19)
F(8)-C(42)-F(7)	106.70(18)
F(9)-C(42)-C(40)	110.29(18)
F(8)-C(42)-C(40)	111.97(19)
F(7)-C(42)-C(40)	113.22(18)
F(3)-C(43)-F(1)	107.66(17)
F(3)-C(43)-F(2)	108.42(19)
F(1)-C(43)-F(2)	107.66(18)
F(3)-C(43)-S(1)	111.58(15)
F(1)-C(43)-S(1)	111.30(15)
F(2)-C(43)-S(1)	110.07(15)
Cl(2X)-C(1X)-Cl(1X)	111.50(12)
Cl(2X)-C(1X)-H(1X1)	109.3

Cl(1X)-C(1X)-H(1X1)	109.3
Cl(2X)-C(1X)-H(1X2)	109.3
Cl(1X)-C(1X)-H(1X2)	109.3
H(1X1)-C(1X)-H(1X2)	108.0

Symmetry transformations used to generate equivalent atoms:

Table 7.4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **7**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	9(1)	10(1)	9(1)	-1(1)	0(1)	-5(1)
S(1)	11(1)	13(1)	27(1)	-2(1)	0(1)	-6(1)
O(1)	12(1)	11(1)	20(1)	-4(1)	-1(1)	-5(1)
F(1)	22(1)	20(1)	51(1)	-14(1)	-5(1)	-4(1)
N(1)	10(1)	14(1)	13(1)	-1(1)	-1(1)	-6(1)
C(1)	14(1)	8(1)	11(1)	0(1)	0(1)	-8(1)
O(2)	10(1)	12(1)	26(1)	-2(1)	-1(1)	-5(1)
F(2)	42(1)	26(1)	41(1)	14(1)	-7(1)	-8(1)
N(2)	11(1)	15(1)	11(1)	-1(1)	-1(1)	-7(1)
C(2)	10(1)	24(1)	19(1)	-4(1)	0(1)	-7(1)
N(3)	8(1)	12(1)	14(1)	-1(1)	0(1)	-5(1)
O(3)	26(1)	24(1)	43(1)	-13(1)	-9(1)	-11(1)
C(3)	10(1)	22(1)	16(1)	1(1)	-2(1)	-8(1)
F(3)	14(1)	26(1)	89(1)	-9(1)	-18(1)	-5(1)
F(4)	35(1)	23(1)	34(1)	3(1)	-4(1)	-20(1)
O(4)	25(1)	25(1)	46(1)	1(1)	17(1)	-11(1)
C(4)	12(1)	20(1)	12(1)	0(1)	-2(1)	-9(1)
F(5)	36(1)	13(1)	50(1)	-3(1)	-11(1)	-4(1)
C(5)	14(1)	22(1)	14(1)	3(1)	-4(1)	-11(1)
F(6)	61(1)	26(1)	23(1)	0(1)	-10(1)	-19(1)
C(6)	20(1)	34(1)	13(1)	5(1)	-1(1)	-13(1)
F(7)	32(1)	36(1)	27(1)	-13(1)	2(1)	-17(1)
C(7)	23(1)	36(1)	13(1)	-5(1)	-1(1)	-10(1)
F(8)	23(1)	39(1)	59(1)	-28(1)	10(1)	-8(1)
C(8)	22(1)	24(1)	18(1)	-6(1)	-2(1)	-9(1)
F(9)	54(1)	41(1)	38(1)	-11(1)	23(1)	-27(1)
C(9)	14(1)	20(1)	14(1)	-1(1)	-4(1)	-7(1)
C(10)	23(1)	23(1)	22(1)	5(1)	-5(1)	-16(1)
C(11)	43(2)	52(2)	19(1)	-10(1)	8(1)	-16(1)
C(12)	23(1)	19(1)	23(1)	-1(1)	-2(1)	-12(1)
C(13)	8(1)	17(1)	13(1)	-2(1)	1(1)	-7(1)
C(14)	10(1)	15(1)	20(1)	-4(1)	2(1)	-6(1)
C(15)	14(1)	23(1)	18(1)	-11(1)	4(1)	-10(1)
C(16)	14(1)	31(1)	14(1)	-5(1)	3(1)	-13(1)
C(17)	14(1)	22(1)	16(1)	3(1)	0(1)	-9(1)
C(18)	11(1)	16(1)	17(1)	-3(1)	2(1)	-7(1)

C(19)	23(1)	16(1)	27(1)	-5(1)	3(1)	-8(1)
C(20)	25(1)	43(1)	15(1)	-4(1)	2(1)	-19(1)
C(21)	24(1)	15(1)	20(1)	0(1)	0(1)	-12(1)
C(22)	10(1)	14(1)	14(1)	-3(1)	1(1)	-7(1)
C(23)	10(1)	16(1)	17(1)	-4(1)	2(1)	-7(1)
C(24)	15(1)	20(1)	19(1)	-8(1)	3(1)	-9(1)
C(25)	16(1)	27(1)	12(1)	-5(1)	1(1)	-10(1)
C(26)	14(1)	20(1)	14(1)	0(1)	-1(1)	-7(1)
C(27)	10(1)	16(1)	16(1)	-3(1)	1(1)	-6(1)
C(28)	23(1)	16(1)	18(1)	-4(1)	2(1)	-10(1)
C(29)	19(1)	16(1)	16(1)	1(1)	-2(1)	-9(1)
C(30)	10(1)	16(1)	13(1)	-2(1)	0(1)	-6(1)
C(31)	17(1)	16(1)	13(1)	-1(1)	1(1)	-10(1)
C(32)	21(1)	16(1)	19(1)	-3(1)	2(1)	-8(1)
C(33)	21(1)	19(1)	17(1)	1(1)	-2(1)	-14(1)
C(34)	18(1)	22(1)	14(1)	0(1)	1(1)	-15(1)
C(35)	22(1)	24(1)	18(1)	-1(1)	3(1)	-14(1)
C(36)	27(1)	36(1)	18(1)	-5(1)	5(1)	-19(1)
C(37)	31(1)	45(2)	13(1)	3(1)	-2(1)	-28(1)
C(38)	28(1)	34(1)	20(1)	13(1)	-10(1)	-22(1)
C(39)	21(1)	23(1)	20(1)	4(1)	-3(1)	-15(1)
C(40)	14(1)	14(1)	29(1)	-7(1)	-3(1)	-4(1)
C(41)	28(1)	13(1)	27(1)	-3(1)	-9(1)	-6(1)
C(42)	22(1)	25(1)	33(1)	-10(1)	6(1)	-10(1)
C(43)	16(1)	19(1)	39(1)	-5(1)	-6(1)	-7(1)
C(1X)	21(1)	28(1)	26(1)	-7(1)	3(1)	-6(1)
Cl(1X)	26(1)	30(1)	25(1)	3(1)	-2(1)	-17(1)
Cl(2X)	23(1)	42(1)	34(1)	13(1)	-2(1)	-16(1)

Table 7.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **7**.

	x	y	z	U(eq)
H(2A)	7029	7530	2240	22
H(2B)	7454	5934	2342	22
H(3A)	7026	6088	3363	20
H(3B)	6917	7581	3278	20
H(6)	3668	7138	5131	27
H(8)	3340	10794	4570	26
H(10A)	4924	5611	3708	32
H(10B)	4307	5399	4364	32
H(10C)	5869	5217	4327	32
H(11A)	2869	10382	5629	60
H(11B)	3247	8868	5894	60
H(11C)	1752	9845	5559	60
H(12A)	5352	9968	3344	31
H(12B)	3986	11266	3574	31

H(12C)	3841	10441	3033	31
H(15)	5448	5613	369	21
H(17)	4207	9628	382	21
H(19A)	6951	4463	1674	33
H(19B)	5826	4217	1312	33
H(19C)	5426	4904	1961	33
H(20A)	4066	8785	-570	39
H(20B)	4082	7347	-555	39
H(20C)	5527	7411	-625	39
H(21A)	3705	9973	1924	29
H(21B)	3974	10686	1301	29
H(21C)	5261	9728	1767	29
H(24)	2170	5082	301	20
H(25)	1594	6952	-413	21
H(26)	1163	9035	-73	19
H(28A)	2518	4057	1292	28
H(28B)	1870	5019	1853	28
H(28C)	3500	4434	1687	28
H(29A)	1135	10405	706	25
H(29B)	1867	9695	1367	25
H(29C)	228	10184	1256	25
H(30)	1940(20)	7650(20)	3581(10)	22(6)
H(32A)	3418	4854	2716	28
H(32B)	3032	3829	3128	28
H(32C)	4046	4332	3408	28
H(33A)	-252	6748	3230	26
H(33B)	522	5143	3147	26
H(33C)	631	6171	2617	26
H(35)	269	7586	4192	25
H(36)	-118	7319	5249	30
H(37)	1100	5171	5792	31
H(38)	2696	3304	5270	30
H(39)	3113	3571	4215	24
H(40)	-240(20)	11500(20)	2499(11)	28(6)
H(1X1)	2554	2165	9123	33
H(1X2)	968	2418	9184	33

Table 7.6. Torsion angles [°] for **7**.

N(3)-Mo(1)-O(1)-C(40)	79.88(18)
C(30)-Mo(1)-O(1)-C(40)	-92.43(18)
O(2)-Mo(1)-O(1)-C(40)	-1.51(16)
C(1)-Mo(1)-O(1)-C(40)	176.17(17)
C(13)-N(1)-C(1)-N(2)	-162.65(17)
C(2)-N(1)-C(1)-N(2)	-3.1(2)
C(13)-N(1)-C(1)-Mo(1)	20.3(3)
C(2)-N(1)-C(1)-Mo(1)	179.85(13)
N(3)-Mo(1)-C(1)-N(2)	-155.54(15)
C(30)-Mo(1)-C(1)-N(2)	-50.54(16)

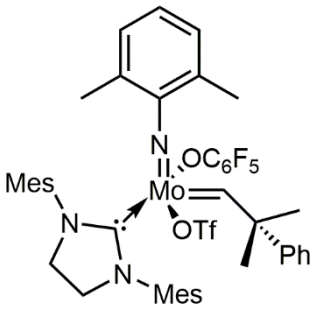
O(1)-Mo(1)-C(1)-N(2)	67.58(16)
O(2)-Mo(1)-C(1)-N(2)	75.3(3)
N(3)-Mo(1)-C(1)-N(1)	20.99(16)
C(30)-Mo(1)-C(1)-N(1)	125.99(16)
O(1)-Mo(1)-C(1)-N(1)	-115.89(15)
O(2)-Mo(1)-C(1)-N(1)	-108.2(2)
O(3)-S(1)-O(2)-Mo(1)	-59.52(17)
O(4)-S(1)-O(2)-Mo(1)	79.63(17)
C(43)-S(1)-O(2)-Mo(1)	-169.89(15)
N(3)-Mo(1)-O(2)-S(1)	53.19(16)
C(30)-Mo(1)-O(2)-S(1)	-51.13(16)
O(1)-Mo(1)-O(2)-S(1)	-169.00(16)
C(1)-Mo(1)-O(2)-S(1)	-176.81(15)
N(1)-C(1)-N(2)-C(4)	175.10(17)
Mo(1)-C(1)-N(2)-C(4)	-7.9(3)
N(1)-C(1)-N(2)-C(3)	-5.0(2)
Mo(1)-C(1)-N(2)-C(3)	172.03(13)
C(1)-N(1)-C(2)-C(3)	9.2(2)
C(13)-N(1)-C(2)-C(3)	171.12(16)
C(30)-Mo(1)-N(3)-C(22)	153.7(3)
O(1)-Mo(1)-N(3)-C(22)	-19.3(3)
O(2)-Mo(1)-N(3)-C(22)	57.4(3)
C(1)-Mo(1)-N(3)-C(22)	-109.3(3)
C(1)-N(2)-C(3)-C(2)	10.4(2)
C(4)-N(2)-C(3)-C(2)	-169.63(16)
N(1)-C(2)-C(3)-N(2)	-10.87(19)
C(1)-N(2)-C(4)-C(9)	-92.7(2)
C(3)-N(2)-C(4)-C(9)	87.4(2)
C(1)-N(2)-C(4)-C(5)	94.8(2)
C(3)-N(2)-C(4)-C(5)	-85.1(2)
C(9)-C(4)-C(5)-C(6)	6.8(3)
N(2)-C(4)-C(5)-C(6)	178.98(16)
C(9)-C(4)-C(5)-C(10)	-169.47(18)
N(2)-C(4)-C(5)-C(10)	2.7(3)
C(4)-C(5)-C(6)-C(7)	-3.4(3)
C(10)-C(5)-C(6)-C(7)	172.85(19)
C(5)-C(6)-C(7)-C(8)	-1.2(3)
C(5)-C(6)-C(7)-C(11)	178.9(2)
C(6)-C(7)-C(8)-C(9)	2.7(3)
C(11)-C(7)-C(8)-C(9)	-177.4(2)
C(5)-C(4)-C(9)-C(8)	-5.3(3)
N(2)-C(4)-C(9)-C(8)	-177.63(16)
C(5)-C(4)-C(9)-C(12)	172.65(18)
N(2)-C(4)-C(9)-C(12)	0.4(3)
C(7)-C(8)-C(9)-C(4)	0.4(3)
C(7)-C(8)-C(9)-C(12)	-177.56(19)
C(1)-N(1)-C(13)-C(18)	72.7(2)
C(2)-N(1)-C(13)-C(18)	-86.2(2)
C(1)-N(1)-C(13)-C(14)	-114.3(2)
C(2)-N(1)-C(13)-C(14)	86.9(2)

C(18)-C(13)-C(14)-C(15)	-2.8(3)
N(1)-C(13)-C(14)-C(15)	-175.69(16)
C(18)-C(13)-C(14)-C(19)	175.16(17)
N(1)-C(13)-C(14)-C(19)	2.3(3)
C(13)-C(14)-C(15)-C(16)	0.7(3)
C(19)-C(14)-C(15)-C(16)	-177.28(18)
C(14)-C(15)-C(16)-C(17)	1.2(3)
C(14)-C(15)-C(16)-C(20)	-179.07(18)
C(15)-C(16)-C(17)-C(18)	-1.2(3)
C(20)-C(16)-C(17)-C(18)	179.13(18)
C(16)-C(17)-C(18)-C(13)	-0.8(3)
C(16)-C(17)-C(18)-C(21)	178.25(18)
C(14)-C(13)-C(18)-C(17)	2.9(3)
N(1)-C(13)-C(18)-C(17)	175.73(16)
C(14)-C(13)-C(18)-C(21)	-176.18(17)
N(1)-C(13)-C(18)-C(21)	-3.3(3)
Mo(1)-N(3)-C(22)-C(23)	-169.7(2)
Mo(1)-N(3)-C(22)-C(27)	11.1(4)
N(3)-C(22)-C(23)-C(24)	-177.08(16)
C(27)-C(22)-C(23)-C(24)	2.1(3)
N(3)-C(22)-C(23)-C(28)	4.3(3)
C(27)-C(22)-C(23)-C(28)	-176.51(17)
C(22)-C(23)-C(24)-C(25)	0.5(3)
C(28)-C(23)-C(24)-C(25)	179.17(17)
C(23)-C(24)-C(25)-C(26)	-1.8(3)
C(24)-C(25)-C(26)-C(27)	0.5(3)
C(25)-C(26)-C(27)-C(22)	2.0(3)
C(25)-C(26)-C(27)-C(29)	-176.00(17)
N(3)-C(22)-C(27)-C(26)	175.86(16)
C(23)-C(22)-C(27)-C(26)	-3.3(3)
N(3)-C(22)-C(27)-C(29)	-6.1(3)
C(23)-C(22)-C(27)-C(29)	174.67(17)
N(3)-Mo(1)-C(30)-C(31)	-8.2(2)
O(1)-Mo(1)-C(30)-C(31)	166.45(19)
O(2)-Mo(1)-C(30)-C(31)	85.2(2)
C(1)-Mo(1)-C(30)-C(31)	-108.8(2)
Mo(1)-C(30)-C(31)-C(34)	-170.69(17)
Mo(1)-C(30)-C(31)-C(32)	64.0(3)
Mo(1)-C(30)-C(31)-C(33)	-54.2(3)
C(30)-C(31)-C(34)-C(35)	45.4(2)
C(32)-C(31)-C(34)-C(35)	169.18(17)
C(33)-C(31)-C(34)-C(35)	-72.2(2)
C(30)-C(31)-C(34)-C(39)	-138.43(18)
C(32)-C(31)-C(34)-C(39)	-14.6(3)
C(33)-C(31)-C(34)-C(39)	104.0(2)
C(39)-C(34)-C(35)-C(36)	1.2(3)
C(31)-C(34)-C(35)-C(36)	177.57(18)
C(34)-C(35)-C(36)-C(37)	-0.8(3)
C(35)-C(36)-C(37)-C(38)	-0.1(3)
C(36)-C(37)-C(38)-C(39)	0.6(3)

C(37)-C(38)-C(39)-C(34)	-0.1(3)
C(35)-C(34)-C(39)-C(38)	-0.7(3)
C(31)-C(34)-C(39)-C(38)	-176.97(18)
Mo(1)-O(1)-C(40)-C(41)	-128.96(15)
Mo(1)-O(1)-C(40)-C(42)	106.74(18)
O(1)-C(40)-C(41)-F(4)	-51.4(2)
C(42)-C(40)-C(41)-F(4)	72.6(2)
O(1)-C(40)-C(41)-F(5)	-173.08(16)
C(42)-C(40)-C(41)-F(5)	-49.1(2)
O(1)-C(40)-C(41)-F(6)	68.8(2)
C(42)-C(40)-C(41)-F(6)	-167.25(17)
O(1)-C(40)-C(42)-F(9)	-44.9(2)
C(41)-C(40)-C(42)-F(9)	-169.16(18)
O(1)-C(40)-C(42)-F(8)	-163.79(17)
C(41)-C(40)-C(42)-F(8)	72.0(2)
O(1)-C(40)-C(42)-F(7)	75.5(2)
C(41)-C(40)-C(42)-F(7)	-48.7(2)
O(3)-S(1)-C(43)-F(3)	61.00(19)
O(4)-S(1)-C(43)-F(3)	-63.20(19)
O(2)-S(1)-C(43)-F(3)	178.63(16)
O(3)-S(1)-C(43)-F(1)	-178.71(15)
O(4)-S(1)-C(43)-F(1)	57.09(17)
O(2)-S(1)-C(43)-F(1)	-61.07(16)
O(3)-S(1)-C(43)-F(2)	-59.42(17)
O(4)-S(1)-C(43)-F(2)	176.38(15)
O(2)-S(1)-C(43)-F(2)	58.21(16)

Symmetry transformations used to generate equivalent atoms:

Complex 10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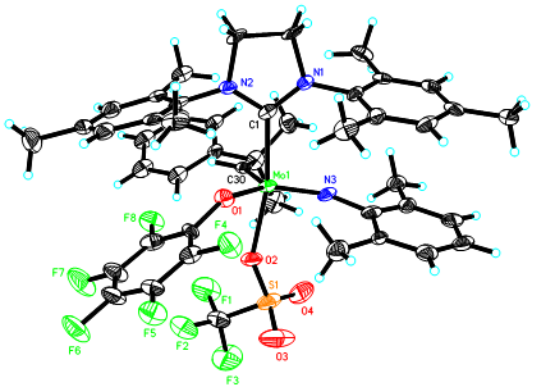
OC6F5
Mes
Mo
N
OTf
Ph
N
Mes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C1
C30
Mo1
N3
O1
F8
F4
O2
F7
S1
F1
O4
F5
F2
O3
F6
F3

Table 10.1. Crystal data and structure refinement for **10**.

Empirical formula	$C_{46}H_{47}F_8MoN_3O_4S$
Formula weight	985.87
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Unit cell dimensions	a = 10.4991(6) Å, α = 90°
	b = 19.8661(11) Å, β = 90°
	c = 21.2905(12) Å, γ = 90°
Volume	4440.7(4) $Å^3$
Z, Calculated density	4, 1.475 mg/m^3
Absorption coefficient	0.423 mm^{-1}
F(000)	2024
Crystal size	0.20 x 0.12 x 0.09 mm
Theta range for data collection	1.91 to 26.39 °
Limiting indices	-10<=h<=13, -24<=k<=24, -26<=l<=26
Reflections collected / unique	33262 / 9083 [R(int) = 0.0782]
Completeness to theta = 26.39	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7430 and 0.6823
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9083 / 0 / 577
Goodness-of-fit on F^2	1.051
Final R indices [I>2σ(I)]	R1 = 0.0654, wR2 = 0.1343
R indices (all data)	R1 = 0.1074, wR2 = 0.1465
Absolute structure parameter	-0.04(5)
Largest diff. peak and hole	2.669 and -1.174 $e.Å^{-3}$

Table 10.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **10**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	9818(1)	6421(1)	7509(1)	20(1)
S(1)	7699(2)	7757(1)	7500(1)	41(1)
N(1)	12044(5)	5419(3)	8003(3)	19(1)
O(1)	10835(4)	6833(2)	6833(2)	25(1)
C(1)	11383(5)	5660(2)	7512(4)	19(1)
F(1)	6087(5)	7144(3)	6759(3)	68(2)
N(2)	11801(5)	5360(3)	6993(3)	21(1)
O(2)	8662(4)	7280(2)	7260(2)	33(1)
C(2)	13010(7)	4914(4)	7821(4)	28(2)
F(2)	7106(5)	7944(3)	6325(2)	65(1)
N(3)	9747(5)	6590(2)	8316(2)	23(1)
C(3)	12858(7)	4882(4)	7110(4)	26(2)
O(3)	8150(5)	8424(2)	7498(4)	73(2)
F(3)	5597(4)	8179(3)	6974(3)	74(2)
F(4)	12411(4)	7920(2)	6712(2)	42(1)
C(4)	12082(6)	5654(3)	8641(3)	21(1)
O(4)	7001(6)	7507(3)	8035(3)	58(2)
F(5)	12234(4)	8749(2)	5707(2)	40(1)
C(5)	11590(6)	5269(3)	9115(3)	19(1)
F(6)	10451(5)	8518(2)	4818(2)	58(1)
C(6)	11750(6)	5491(3)	9734(3)	23(2)
F(7)	8760(5)	7474(2)	4957(2)	64(2)
C(7)	12407(6)	6074(4)	9875(3)	26(2)
F(8)	8953(4)	6651(2)	5949(2)	39(1)
C(8)	12917(6)	6442(4)	9383(3)	29(2)
C(9)	12809(7)	6244(3)	8762(3)	26(2)
C(10)	10905(6)	4613(3)	8996(3)	29(2)
C(11)	12600(7)	6310(4)	10541(3)	35(2)
C(12)	13501(7)	6621(4)	8254(3)	34(2)
C(13)	11373(6)	5436(3)	6354(3)	22(2)
C(14)	10418(6)	5014(3)	6137(3)	26(2)
C(15)	10033(7)	5085(3)	5506(3)	33(2)
C(16)	10660(8)	5534(4)	5105(3)	41(2)
C(17)	11639(7)	5909(4)	5339(4)	36(2)
C(18)	12041(7)	5877(3)	5964(3)	30(2)
C(19)	9844(7)	4481(3)	6542(3)	32(2)
C(20)	10241(9)	5586(5)	4423(4)	66(3)
C(21)	13162(7)	6264(4)	6179(4)	35(2)
C(22)	9965(6)	6982(3)	8856(3)	26(2)
C(23)	9448(6)	6775(3)	9439(3)	27(2)
C(24)	9785(7)	7147(4)	9973(4)	40(2)
C(25)	10590(6)	7705(4)	9923(4)	34(2)

C(26)	11029(7)	7912(4)	9344(4)	33(2)
C(27)	10728(7)	7569(3)	8798(3)	30(2)
C(28)	8579(7)	6182(3)	9475(3)	31(2)
C(29)	11174(7)	7820(4)	8172(3)	38(2)
C(30)	8563(6)	5759(3)	7321(3)	20(2)
C(31)	7491(6)	5348(3)	7601(4)	29(2)
C(32)	6549(6)	5847(4)	7896(3)	34(2)
C(33)	8024(7)	4877(4)	8113(3)	34(2)
C(34)	6798(6)	4964(3)	7081(3)	24(2)
C(35)	6352(6)	4301(3)	7163(3)	27(2)
C(36)	5714(6)	3987(3)	6684(3)	28(2)
C(37)	5505(7)	4300(4)	6122(4)	38(2)
C(38)	5919(6)	4946(4)	6034(4)	35(2)
C(39)	6550(6)	5274(3)	6507(3)	27(2)
C(40)	10690(6)	7268(3)	6354(3)	21(2)
C(41)	11500(6)	7808(3)	6275(3)	25(2)
C(42)	11441(6)	8229(3)	5767(3)	27(2)
C(43)	10529(7)	8104(4)	5313(4)	37(2)
C(44)	9707(8)	7580(3)	5384(4)	40(2)
C(45)	9793(7)	7175(3)	5892(4)	32(2)
C(46)	6569(10)	7748(4)	6853(4)	51(2)

Table 10.3. Bond lengths [Å] and angles [°] for **10**.

Mo(1)-N(3)	1.751(5)
Mo(1)-C(30)	1.905(6)
Mo(1)-O(1)	1.971(4)
Mo(1)-O(2)	2.161(4)
Mo(1)-C(1)	2.232(5)
S(1)-O(3)	1.408(5)
S(1)-O(4)	1.443(7)
S(1)-O(2)	1.476(5)
S(1)-C(46)	1.817(9)
N(1)-C(1)	1.343(9)
N(1)-C(4)	1.436(8)
N(1)-C(2)	1.477(9)
O(1)-C(40)	1.345(7)
C(1)-N(2)	1.330(9)
F(1)-C(46)	1.318(10)
N(2)-C(13)	1.441(9)
N(2)-C(3)	1.482(9)
C(2)-C(3)	1.524(9)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
F(2)-C(46)	1.317(10)
N(3)-C(22)	1.407(8)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900

F(3)-C(46)	1.357(10)
F(4)-C(41)	1.354(7)
C(4)-C(5)	1.368(9)
C(4)-C(9)	1.422(10)
F(5)-C(42)	1.333(7)
C(5)-C(6)	1.402(9)
C(5)-C(10)	1.509(9)
F(6)-C(43)	1.339(8)
C(6)-C(7)	1.380(9)
C(6)-H(6)	0.9500
F(7)-C(44)	1.364(8)
C(7)-C(8)	1.384(9)
C(7)-C(11)	1.508(9)
F(8)-C(45)	1.369(8)
C(8)-C(9)	1.384(9)
C(8)-H(8)	0.9500
C(9)-C(12)	1.504(9)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.386(9)
C(13)-C(18)	1.397(9)
C(14)-C(15)	1.410(9)
C(14)-C(19)	1.493(9)
C(15)-C(16)	1.400(11)
C(15)-H(15)	0.9500
C(16)-C(17)	1.365(11)
C(16)-C(20)	1.521(10)
C(17)-C(18)	1.398(10)
C(17)-H(17)	0.9500
C(18)-C(21)	1.477(10)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(23)	1.416(10)
C(22)-C(27)	1.420(10)
C(23)-C(24)	1.402(10)
C(23)-C(28)	1.491(10)

C(24)-C(25)	1.399(10)
C(24)-H(24)	0.9500
C(25)-C(26)	1.378(11)
C(25)-H(25)	0.9500
C(26)-C(27)	1.384(10)
C(26)-H(26)	0.9500
C(27)-C(29)	1.499(10)
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-C(31)	1.511(9)
C(30)-H(30)	0.9500
C(31)-C(34)	1.528(10)
C(31)-C(32)	1.535(10)
C(31)-C(33)	1.543(10)
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-C(39)	1.394(10)
C(34)-C(35)	1.408(9)
C(35)-C(36)	1.370(9)
C(35)-H(35)	0.9500
C(36)-C(37)	1.366(10)
C(36)-H(36)	0.9500
C(37)-C(38)	1.368(10)
C(37)-H(37)	0.9500
C(38)-C(39)	1.370(9)
C(38)-H(38)	0.9500
C(39)-H(39)	0.9500
C(40)-C(45)	1.375(10)
C(40)-C(41)	1.379(9)
C(41)-C(42)	1.369(9)
C(42)-C(43)	1.383(10)
C(43)-C(44)	1.361(10)
C(44)-C(45)	1.352(10)

N(3)-Mo(1)-C(30)	108.0(3)
N(3)-Mo(1)-O(1)	131.2(2)
C(30)-Mo(1)-O(1)	120.6(2)
N(3)-Mo(1)-O(2)	93.8(2)
C(30)-Mo(1)-O(2)	96.1(2)
O(1)-Mo(1)-O(2)	78.25(18)
N(3)-Mo(1)-C(1)	99.1(3)
C(30)-Mo(1)-C(1)	92.4(2)

O(1)-Mo(1)-C(1)	83.4(2)
O(2)-Mo(1)-C(1)	161.6(2)
O(3)-S(1)-O(4)	119.8(5)
O(3)-S(1)-O(2)	111.8(4)
O(4)-S(1)-O(2)	113.6(3)
O(3)-S(1)-C(46)	103.2(4)
O(4)-S(1)-C(46)	105.3(4)
O(2)-S(1)-C(46)	100.3(4)
C(1)-N(1)-C(4)	129.3(6)
C(1)-N(1)-C(2)	113.1(6)
C(4)-N(1)-C(2)	116.7(6)
C(40)-O(1)-Mo(1)	139.4(4)
N(2)-C(1)-N(1)	108.4(4)
N(2)-C(1)-Mo(1)	122.9(5)
N(1)-C(1)-Mo(1)	128.6(5)
C(1)-N(2)-C(13)	129.4(6)
C(1)-N(2)-C(3)	113.3(6)
C(13)-N(2)-C(3)	117.4(5)
S(1)-O(2)-Mo(1)	143.7(3)
N(1)-C(2)-C(3)	102.5(7)
N(1)-C(2)-H(2A)	111.3
C(3)-C(2)-H(2A)	111.3
N(1)-C(2)-H(2B)	111.3
C(3)-C(2)-H(2B)	111.3
H(2A)-C(2)-H(2B)	109.2
C(22)-N(3)-Mo(1)	154.2(5)
N(2)-C(3)-C(2)	102.6(6)
N(2)-C(3)-H(3A)	111.2
C(2)-C(3)-H(3A)	111.2
N(2)-C(3)-H(3B)	111.2
C(2)-C(3)-H(3B)	111.2
H(3A)-C(3)-H(3B)	109.2
C(5)-C(4)-C(9)	122.0(6)
C(5)-C(4)-N(1)	120.3(6)
C(9)-C(4)-N(1)	117.1(6)
C(4)-C(5)-C(6)	118.2(6)
C(4)-C(5)-C(10)	122.6(6)
C(6)-C(5)-C(10)	119.2(6)
C(7)-C(6)-C(5)	121.9(6)
C(7)-C(6)-H(6)	119.1
C(5)-C(6)-H(6)	119.1
C(6)-C(7)-C(8)	118.2(6)
C(6)-C(7)-C(11)	122.1(6)
C(8)-C(7)-C(11)	119.7(7)
C(9)-C(8)-C(7)	122.7(7)
C(9)-C(8)-H(8)	118.7
C(7)-C(8)-H(8)	118.7
C(8)-C(9)-C(4)	116.9(7)
C(8)-C(9)-C(12)	120.4(6)
C(4)-C(9)-C(12)	122.6(6)

C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(7)-C(11)-H(11A)	109.5
C(7)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(7)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(9)-C(12)-H(12A)	109.5
C(9)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(9)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(18)	123.0(7)
C(14)-C(13)-N(2)	118.5(6)
C(18)-C(13)-N(2)	118.1(6)
C(13)-C(14)-C(15)	117.7(6)
C(13)-C(14)-C(19)	122.0(6)
C(15)-C(14)-C(19)	120.3(6)
C(16)-C(15)-C(14)	120.7(7)
C(16)-C(15)-H(15)	119.6
C(14)-C(15)-H(15)	119.6
C(17)-C(16)-C(15)	118.6(7)
C(17)-C(16)-C(20)	122.0(8)
C(15)-C(16)-C(20)	119.4(8)
C(16)-C(17)-C(18)	123.4(7)
C(16)-C(17)-H(17)	118.3
C(18)-C(17)-H(17)	118.3
C(13)-C(18)-C(17)	116.3(7)
C(13)-C(18)-C(21)	122.9(7)
C(17)-C(18)-C(21)	120.7(7)
C(14)-C(19)-H(19A)	109.5
C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-H(20A)	109.5
C(16)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(16)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5

H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(3)-C(22)-C(23)	119.6(6)
N(3)-C(22)-C(27)	118.4(6)
C(23)-C(22)-C(27)	122.0(6)
C(24)-C(23)-C(22)	117.5(7)
C(24)-C(23)-C(28)	121.9(7)
C(22)-C(23)-C(28)	120.6(6)
C(25)-C(24)-C(23)	120.5(7)
C(25)-C(24)-H(24)	119.7
C(23)-C(24)-H(24)	119.7
C(26)-C(25)-C(24)	120.5(7)
C(26)-C(25)-H(25)	119.8
C(24)-C(25)-H(25)	119.8
C(25)-C(26)-C(27)	121.8(7)
C(25)-C(26)-H(26)	119.1
C(27)-C(26)-H(26)	119.1
C(26)-C(27)-C(22)	117.5(7)
C(26)-C(27)-C(29)	120.8(7)
C(22)-C(27)-C(29)	121.7(6)
C(23)-C(28)-H(28A)	109.5
C(23)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(23)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(27)-C(29)-H(29A)	109.5
C(27)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(27)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(31)-C(30)-Mo(1)	143.6(5)
C(31)-C(30)-H(30)	108.2
Mo(1)-C(30)-H(30)	108.2
C(30)-C(31)-C(34)	109.8(6)
C(30)-C(31)-C(32)	107.0(5)
C(34)-C(31)-C(32)	108.2(5)
C(30)-C(31)-C(33)	109.6(5)
C(34)-C(31)-C(33)	112.4(6)
C(32)-C(31)-C(33)	109.6(6)
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(31)-C(33)-H(33A)	109.5

C(31)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(31)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(39)-C(34)-C(35)	117.3(6)
C(39)-C(34)-C(31)	120.2(6)
C(35)-C(34)-C(31)	122.4(6)
C(36)-C(35)-C(34)	119.8(7)
C(36)-C(35)-H(35)	120.1
C(34)-C(35)-H(35)	120.1
C(37)-C(36)-C(35)	121.6(7)
C(37)-C(36)-H(36)	119.2
C(35)-C(36)-H(36)	119.2
C(36)-C(37)-C(38)	119.6(7)
C(36)-C(37)-H(37)	120.2
C(38)-C(37)-H(37)	120.2
C(37)-C(38)-C(39)	120.0(8)
C(37)-C(38)-H(38)	120.0
C(39)-C(38)-H(38)	120.0
C(38)-C(39)-C(34)	121.6(7)
C(38)-C(39)-H(39)	119.2
C(34)-C(39)-H(39)	119.2
O(1)-C(40)-C(45)	122.3(6)
O(1)-C(40)-C(41)	121.5(6)
C(45)-C(40)-C(41)	116.1(6)
F(4)-C(41)-C(42)	118.3(6)
F(4)-C(41)-C(40)	118.7(6)
C(42)-C(41)-C(40)	123.0(6)
F(5)-C(42)-C(41)	121.4(6)
F(5)-C(42)-C(43)	120.3(6)
C(41)-C(42)-C(43)	118.3(7)
F(6)-C(43)-C(44)	121.2(7)
F(6)-C(43)-C(42)	118.8(6)
C(44)-C(43)-C(42)	119.9(7)
C(45)-C(44)-C(43)	120.2(7)
C(45)-C(44)-F(7)	119.4(7)
C(43)-C(44)-F(7)	120.4(6)
C(44)-C(45)-F(8)	118.7(7)
C(44)-C(45)-C(40)	122.6(7)
F(8)-C(45)-C(40)	118.7(6)
F(2)-C(46)-F(1)	107.7(7)
F(2)-C(46)-F(3)	107.3(7)
F(1)-C(46)-F(3)	108.3(8)
F(2)-C(46)-S(1)	111.4(7)
F(1)-C(46)-S(1)	112.0(6)
F(3)-C(46)-S(1)	109.9(6)

Symmetry transformations used to generate equivalent atoms:

Table 10.4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **10**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2}\ U^{11} + ... + 2\ h\ k\ a^*\ b^* U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	19(1)	13(1)	29(1)	0(1)	6(1)	2(1)
S(1)	32(1)	31(1)	61(1)	-17(1)	-10(2)	15(1)
N(1)	16(3)	19(3)	23(3)	-4(3)	3(3)	3(2)
O(1)	27(3)	20(2)	28(3)	7(2)	6(2)	-4(2)
C(1)	14(3)	15(2)	27(3)	-4(4)	6(4)	-5(2)
F(1)	67(4)	49(3)	87(4)	0(3)	-34(3)	-8(3)
N(2)	19(3)	19(3)	24(3)	2(3)	6(3)	6(2)
O(2)	32(3)	24(2)	41(3)	-4(2)	-4(2)	14(2)
C(2)	22(4)	28(4)	34(5)	-11(4)	6(3)	16(3)
F(2)	69(3)	59(3)	65(4)	15(3)	-14(3)	18(3)
N(3)	18(3)	20(3)	32(3)	-8(2)	2(2)	7(2)
C(3)	22(4)	28(4)	29(5)	-7(3)	15(3)	11(3)
O(3)	66(3)	30(3)	122(5)	-8(5)	-36(5)	12(2)
F(3)	41(3)	89(4)	92(4)	-15(3)	-9(3)	37(3)
F(4)	49(3)	37(3)	42(3)	4(2)	-11(2)	-13(2)
C(4)	17(3)	22(3)	24(4)	-8(3)	2(3)	5(3)
O(4)	60(4)	59(4)	55(4)	-16(3)	13(3)	24(3)
F(5)	35(2)	31(2)	52(3)	7(2)	0(2)	-11(2)
C(5)	12(3)	16(3)	30(4)	5(3)	3(3)	5(2)
F(6)	83(3)	40(3)	51(3)	25(2)	-21(2)	-13(3)
C(6)	24(4)	18(3)	28(4)	11(3)	5(3)	4(3)
F(7)	77(4)	52(3)	61(3)	18(3)	-42(3)	-18(3)
C(7)	15(3)	33(4)	29(4)	7(3)	4(3)	16(3)
F(8)	34(2)	30(2)	53(3)	2(2)	-12(2)	-8(2)
C(8)	24(3)	20(3)	42(4)	-12(3)	-2(3)	1(3)
C(9)	25(4)	23(4)	29(4)	-4(3)	-3(3)	3(3)
C(10)	24(4)	18(3)	43(5)	11(3)	-5(3)	-5(3)
C(11)	38(4)	31(4)	37(4)	-3(3)	-10(3)	15(3)
C(12)	27(4)	34(4)	42(4)	-1(3)	11(3)	-3(3)
C(13)	16(3)	14(3)	34(4)	-9(3)	4(3)	5(3)
C(14)	31(4)	17(3)	30(4)	-6(3)	0(3)	11(3)
C(15)	27(4)	35(4)	38(4)	-11(3)	-7(3)	12(3)
C(16)	54(5)	43(5)	26(4)	1(4)	4(4)	33(4)
C(17)	37(5)	35(4)	34(5)	3(4)	15(4)	17(4)
C(18)	31(4)	24(4)	34(4)	4(3)	18(3)	18(3)
C(19)	28(4)	26(3)	41(4)	-6(3)	5(3)	3(3)
C(20)	72(6)	94(8)	32(5)	3(5)	-7(5)	44(6)
C(21)	22(4)	28(4)	55(5)	7(4)	21(4)	5(3)
C(22)	13(4)	20(3)	44(4)	-9(3)	-11(3)	7(3)
C(23)	22(4)	27(4)	32(4)	-7(3)	-7(3)	8(3)
C(24)	41(4)	38(4)	40(4)	-2(3)	0(4)	28(4)
C(25)	28(4)	25(4)	49(5)	-11(4)	-8(3)	11(3)
C(26)	25(4)	27(4)	48(5)	-4(4)	-15(4)	8(3)
C(27)	39(4)	21(4)	31(4)	-11(3)	-17(3)	15(3)
C(28)	28(4)	31(4)	35(4)	-2(3)	4(3)	8(3)

C(29)	35(4)	34(4)	45(5)	-9(4)	-8(4)	1(3)
C(30)	18(3)	17(3)	24(4)	-1(2)	-2(2)	7(2)
C(31)	20(3)	33(3)	35(5)	-6(4)	0(3)	-9(3)
C(32)	22(4)	41(4)	39(4)	-6(3)	2(3)	-14(3)
C(33)	31(4)	42(5)	30(4)	3(3)	2(3)	-1(3)
C(34)	26(4)	25(4)	22(4)	1(3)	14(3)	1(3)
C(35)	21(3)	25(4)	36(4)	-9(3)	5(3)	1(3)
C(36)	18(3)	22(4)	46(5)	-5(3)	-9(3)	-7(3)
C(37)	27(4)	37(4)	50(5)	-15(4)	-2(3)	-2(3)
C(38)	21(4)	37(4)	47(5)	-15(4)	-5(3)	-1(3)
C(39)	17(3)	26(4)	38(4)	-7(3)	4(3)	-8(3)
C(40)	17(3)	26(4)	19(4)	8(3)	4(3)	9(3)
C(41)	19(3)	21(3)	37(4)	-5(3)	1(3)	-3(3)
C(42)	24(4)	20(4)	37(4)	8(3)	2(3)	2(3)
C(43)	45(5)	24(4)	43(5)	12(4)	-10(4)	3(3)
C(44)	44(5)	28(4)	47(5)	5(3)	-27(4)	0(4)
C(45)	34(4)	15(3)	47(5)	0(3)	4(4)	-5(3)
C(46)	77(7)	28(4)	47(6)	8(4)	-7(5)	11(5)

Table 10.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **10**.

	x	y	z	U(eq)
H(2A)	12833	4472	8017	34
H(2B)	13877	5062	7940	34
H(3A)	13647	5027	6894	32
H(3B)	12633	4422	6970	32
H(6)	11396	5234	10067	28
H(8)	13358	6848	9476	34
H(10A)	10765	4558	8543	43
H(10B)	10083	4617	9213	43
H(10C)	11423	4239	9153	43
H(11A)	12112	6724	10611	53
H(11B)	13506	6399	10613	53
H(11C)	12306	5961	10833	53
H(12A)	12944	6669	7887	51
H(12B)	14270	6373	8134	51
H(12C)	13740	7068	8409	51
H(15)	9340	4826	5352	40
H(17)	12070	6208	5063	43
H(19A)	8934	4439	6446	48
H(19B)	9952	4602	6985	48
H(19C)	10269	4050	6460	48
H(20A)	9875	6032	4346	99
H(20B)	9600	5240	4335	99
H(20C)	10979	5519	4148	99
H(21A)	13008	6433	6604	53
H(21B)	13307	6644	5894	53

H(21C)	13913	5971	6180	53
H(24)	9465	7018	10373	48
H(25)	10836	7944	10290	40
H(26)	11553	8301	9319	40
H(28A)	7905	6228	9160	47
H(28B)	8197	6160	9895	47
H(28C)	9064	5770	9395	47
H(29A)	10468	8044	7955	57
H(29B)	11472	7439	7918	57
H(29C)	11873	8140	8232	57
H(30)	8639	5643	6890	23
H(32A)	7010	6156	8173	51
H(32B)	5911	5599	8140	51
H(32C)	6125	6104	7563	51
H(33A)	8530	4520	7916	52
H(33B)	7317	4675	8348	52
H(33C)	8564	5135	8401	52
H(35)	6493	4072	7549	33
H(36)	5411	3541	6744	34
H(37)	5073	4069	5794	45
H(38)	5770	5166	5645	42
H(39)	6825	5724	6442	32

Table 10.6. Torsion angles [°] for **10**.

N(3)-Mo(1)-O(1)-C(40)	-103.6(7)
C(30)-Mo(1)-O(1)-C(40)	71.2(7)
O(2)-Mo(1)-O(1)-C(40)	-18.9(6)
C(1)-Mo(1)-O(1)-C(40)	160.1(7)
C(4)-N(1)-C(1)-N(2)	169.5(6)
C(2)-N(1)-C(1)-N(2)	0.5(7)
C(4)-N(1)-C(1)-Mo(1)	-11.3(9)
C(2)-N(1)-C(1)-Mo(1)	179.7(5)
N(3)-Mo(1)-C(1)-N(2)	179.3(5)
C(30)-Mo(1)-C(1)-N(2)	70.6(5)
O(1)-Mo(1)-C(1)-N(2)	-49.9(5)
O(2)-Mo(1)-C(1)-N(2)	-46.9(9)
N(3)-Mo(1)-C(1)-N(1)	0.2(5)
C(30)-Mo(1)-C(1)-N(1)	-108.6(5)
O(1)-Mo(1)-C(1)-N(1)	130.9(5)
O(2)-Mo(1)-C(1)-N(1)	134.0(7)
N(1)-C(1)-N(2)-C(13)	178.3(7)
Mo(1)-C(1)-N(2)-C(13)	-1.0(9)
N(1)-C(1)-N(2)-C(3)	-1.6(7)
Mo(1)-C(1)-N(2)-C(3)	179.1(4)
O(3)-S(1)-O(2)-Mo(1)	117.7(6)
O(4)-S(1)-O(2)-Mo(1)	-21.7(7)
C(46)-S(1)-O(2)-Mo(1)	-133.5(5)
N(3)-Mo(1)-O(2)-S(1)	-22.9(5)

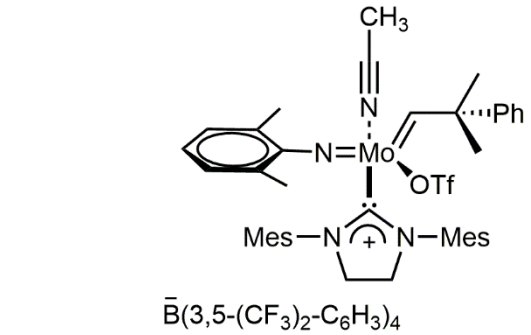
C(30)-Mo(1)-O(2)-S(1)	85.8(5)
O(1)-Mo(1)-O(2)-S(1)	-154.2(5)
C(1)-Mo(1)-O(2)-S(1)	-157.3(6)
C(1)-N(1)-C(2)-C(3)	0.8(9)
C(4)-N(1)-C(2)-C(3)	-169.7(6)
C(30)-Mo(1)-N(3)-C(22)	-159.6(10)
O(1)-Mo(1)-N(3)-C(22)	15.7(11)
O(2)-Mo(1)-N(3)-C(22)	-62.0(10)
C(1)-Mo(1)-N(3)-C(22)	104.8(10)
C(1)-N(2)-C(3)-C(2)	2.0(8)
C(13)-N(2)-C(3)-C(2)	-177.9(6)
N(1)-C(2)-C(3)-N(2)	-1.5(9)
C(1)-N(1)-C(4)-C(5)	112.8(7)
C(2)-N(1)-C(4)-C(5)	-78.6(8)
C(1)-N(1)-C(4)-C(9)	-76.2(8)
C(2)-N(1)-C(4)-C(9)	92.4(7)
C(9)-C(4)-C(5)-C(6)	3.9(9)
N(1)-C(4)-C(5)-C(6)	174.4(6)
C(9)-C(4)-C(5)-C(10)	-175.1(6)
N(1)-C(4)-C(5)-C(10)	-4.5(9)
C(4)-C(5)-C(6)-C(7)	-1.4(9)
C(10)-C(5)-C(6)-C(7)	177.6(6)
C(5)-C(6)-C(7)-C(8)	-0.1(9)
C(5)-C(6)-C(7)-C(11)	-179.0(6)
C(6)-C(7)-C(8)-C(9)	-1.0(10)
C(11)-C(7)-C(8)-C(9)	178.0(6)
C(7)-C(8)-C(9)-C(4)	3.3(10)
C(7)-C(8)-C(9)-C(12)	-173.3(6)
C(5)-C(4)-C(9)-C(8)	-4.8(9)
N(1)-C(4)-C(9)-C(8)	-175.7(6)
C(5)-C(4)-C(9)-C(12)	171.7(6)
N(1)-C(4)-C(9)-C(12)	0.9(9)
C(1)-N(2)-C(13)-C(14)	-90.6(8)
C(3)-N(2)-C(13)-C(14)	89.3(7)
C(1)-N(2)-C(13)-C(18)	96.8(8)
C(3)-N(2)-C(13)-C(18)	-83.3(7)
C(18)-C(13)-C(14)-C(15)	-6.3(9)
N(2)-C(13)-C(14)-C(15)	-178.5(5)
C(18)-C(13)-C(14)-C(19)	171.2(6)
N(2)-C(13)-C(14)-C(19)	-1.0(9)
C(13)-C(14)-C(15)-C(16)	4.5(10)
C(19)-C(14)-C(15)-C(16)	-173.1(6)
C(14)-C(15)-C(16)-C(17)	-1.1(10)
C(14)-C(15)-C(16)-C(20)	178.5(6)
C(15)-C(16)-C(17)-C(18)	-0.9(11)
C(20)-C(16)-C(17)-C(18)	179.5(7)
C(14)-C(13)-C(18)-C(17)	4.4(9)
N(2)-C(13)-C(18)-C(17)	176.6(5)
C(14)-C(13)-C(18)-C(21)	-172.1(6)
N(2)-C(13)-C(18)-C(21)	0.1(9)

C(16)-C(17)-C(18)-C(13)	-0.6(10)
C(16)-C(17)-C(18)-C(21)	176.0(7)
Mo(1)-N(3)-C(22)-C(23)	173.4(8)
Mo(1)-N(3)-C(22)-C(27)	-8.0(13)
N(3)-C(22)-C(23)-C(24)	174.3(6)
C(27)-C(22)-C(23)-C(24)	-4.2(9)
N(3)-C(22)-C(23)-C(28)	-5.6(9)
C(27)-C(22)-C(23)-C(28)	175.9(6)
C(22)-C(23)-C(24)-C(25)	0.8(9)
C(28)-C(23)-C(24)-C(25)	-179.2(6)
C(23)-C(24)-C(25)-C(26)	2.2(10)
C(24)-C(25)-C(26)-C(27)	-2.0(10)
C(25)-C(26)-C(27)-C(22)	-1.3(10)
C(25)-C(26)-C(27)-C(29)	177.5(6)
N(3)-C(22)-C(27)-C(26)	-174.1(6)
C(23)-C(22)-C(27)-C(26)	4.5(9)
N(3)-C(22)-C(27)-C(29)	7.1(9)
C(23)-C(22)-C(27)-C(29)	-174.4(6)
N(3)-Mo(1)-C(30)-C(31)	4.0(8)
O(1)-Mo(1)-C(30)-C(31)	-171.8(7)
O(2)-Mo(1)-C(30)-C(31)	-91.9(8)
C(1)-Mo(1)-C(30)-C(31)	104.4(8)
Mo(1)-C(30)-C(31)-C(34)	172.6(6)
Mo(1)-C(30)-C(31)-C(32)	55.4(10)
Mo(1)-C(30)-C(31)-C(33)	-63.4(9)
C(30)-C(31)-C(34)-C(39)	-40.8(8)
C(32)-C(31)-C(34)-C(39)	75.7(8)
C(33)-C(31)-C(34)-C(39)	-163.1(6)
C(30)-C(31)-C(34)-C(35)	141.1(6)
C(32)-C(31)-C(34)-C(35)	-102.4(7)
C(33)-C(31)-C(34)-C(35)	18.8(9)
C(39)-C(34)-C(35)-C(36)	0.6(9)
C(31)-C(34)-C(35)-C(36)	178.7(6)
C(34)-C(35)-C(36)-C(37)	0.5(10)
C(35)-C(36)-C(37)-C(38)	-1.1(11)
C(36)-C(37)-C(38)-C(39)	0.5(10)
C(37)-C(38)-C(39)-C(34)	0.7(10)
C(35)-C(34)-C(39)-C(38)	-1.2(9)
C(31)-C(34)-C(39)-C(38)	-179.4(6)
Mo(1)-O(1)-C(40)-C(45)	-55.7(9)
Mo(1)-O(1)-C(40)-C(41)	129.2(6)
O(1)-C(40)-C(41)-F(4)	-4.0(9)
C(45)-C(40)-C(41)-F(4)	-179.4(6)
O(1)-C(40)-C(41)-C(42)	174.8(6)
C(45)-C(40)-C(41)-C(42)	-0.6(10)
F(4)-C(41)-C(42)-F(5)	-1.7(10)
C(40)-C(41)-C(42)-F(5)	179.5(6)
F(4)-C(41)-C(42)-C(43)	178.6(6)
C(40)-C(41)-C(42)-C(43)	-0.2(10)
F(5)-C(42)-C(43)-F(6)	-0.6(10)

C(41)-C(42)-C(43)-F(6)	179.1(6)
F(5)-C(42)-C(43)-C(44)	-178.7(7)
C(41)-C(42)-C(43)-C(44)	1.0(11)
F(6)-C(43)-C(44)-C(45)	-179.1(7)
C(42)-C(43)-C(44)-C(45)	-1.0(12)
F(6)-C(43)-C(44)-F(7)	-1.5(12)
C(42)-C(43)-C(44)-F(7)	176.5(7)
C(43)-C(44)-C(45)-F(8)	-179.8(7)
F(7)-C(44)-C(45)-F(8)	2.6(11)
C(43)-C(44)-C(45)-C(40)	0.2(12)
F(7)-C(44)-C(45)-C(40)	-177.4(7)
O(1)-C(40)-C(45)-C(44)	-174.7(7)
C(41)-C(40)-C(45)-C(44)	0.6(11)
O(1)-C(40)-C(45)-F(8)	5.3(10)
C(41)-C(40)-C(45)-F(8)	-179.4(6)
O(3)-S(1)-C(46)-F(2)	56.0(7)
O(4)-S(1)-C(46)-F(2)	-177.7(5)
O(2)-S(1)-C(46)-F(2)	-59.6(6)
O(3)-S(1)-C(46)-F(1)	176.7(7)
O(4)-S(1)-C(46)-F(1)	-57.0(8)
O(2)-S(1)-C(46)-F(1)	61.2(7)
O(3)-S(1)-C(46)-F(3)	-62.9(7)
O(4)-S(1)-C(46)-F(3)	63.5(7)
O(2)-S(1)-C(46)-F(3)	-178.4(6)

Symmetry transformations used to generate equivalent atoms:

Complex 14


CH3
N
Ph
N=Mo
OTf
Mes—N
N—Mes
B̄(3,5-(CF3)2-C6H3)4

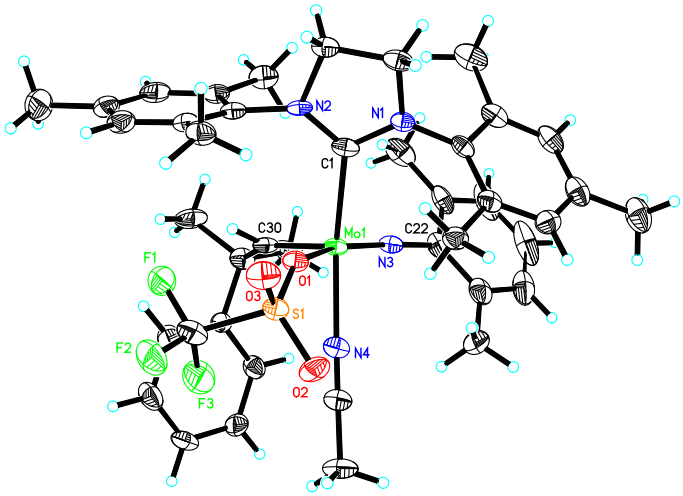

N2
N1
C1
C30
Mo1
C22
N3
F1
O1
O3
S1
N4
F2
O2
F3

Table 14.1. Crystal data and structure refinement for **14**.

Empirical formula	$C_{74}H_{62}BF_{27}MoN_4O_3S$
Formula weight	1707.09
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	triclinic, *P* -1
Unit cell dimensions	a = 12.8425(13) Å, α = 64.388(3)°
	b = 18.420(2) Å, β = 71.487(4)°
	c = 18.727(2) Å, γ = 72.459(4)°
Volume	3717.5(7) A^3
Z, Calculated density	2, 1.525 Mg/m^3
Absorption coefficient	0.323 mm^{-1}
F(000)	1728
Crystal size	0.14 x 0.11 x 0.11 mm
Theta range for data collection	1.70 to 26.37°.
Limiting indices	-13<=h<=16, -23<=k<=22, -23<=l<=23
Reflections collected / unique	57163 / 14995 [R(int) = 0.0707]
Completeness to theta = 26.37	98.6 %
Absorption correction	numerical
Max. and min. transmission	0.9951 and 0.9083
Refinement method	full-matrix least-squares on F^2
Data / restraints / parameters	14995 / 26 / 1020
Goodness-of-fit on F2	1.044
Final R indices [I>2σ(I)]	R1 = 0.0622, wR2 = 0.1461
R indices (all data)	R1 = 0.1232, wR2 = 0.1634
Largest diff. peak and hole	1.979 and -0.822 $e.Å^{-3}$

Table 14.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **14**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	7418(1)	195(1)	2535(1)	19(1)
N(1)	5156(3)	-336(2)	2838(2)	20(1)
C(1)	6161(4)	-614(3)	3031(3)	21(1)
N(2)	6163(3)	-1333(2)	3654(2)	19(1)
C(2)	4342(4)	-860(3)	3433(3)	26(1)
N(3)	7336(3)	583(2)	1528(2)	22(1)
C(3)	5080(4)	-1596(3)	3926(3)	26(1)
C(4)	4818(3)	390(3)	2185(3)	23(1)
C(5)	4601(4)	303(3)	1540(3)	26(1)
C(6)	4268(4)	1017(3)	909(3)	31(1)
C(7)	4128(4)	1793(3)	905(3)	32(1)
C(8)	4320(4)	1856(3)	1556(3)	28(1)
C(9)	4659(3)	1175(3)	2209(3)	23(1)
C(10)	4662(4)	-530(3)	1534(3)	39(1)
C(11)	3751(5)	2556(4)	211(3)	46(1)
C(12)	4863(4)	1280(3)	2899(3)	26(1)
C(13)	7107(4)	-1915(3)	3952(3)	22(1)
C(14)	7813(4)	-2394(3)	3504(3)	23(1)
C(15)	8667(4)	-2994(3)	3836(3)	31(1)
C(16)	8855(4)	-3136(3)	4580(3)	31(1)
C(17)	8114(4)	-2665(3)	5013(3)	31(1)
C(18)	7222(4)	-2072(3)	4722(3)	23(1)
C(19)	7635(4)	-2283(3)	2704(3)	31(1)
C(20)	9805(5)	-3797(3)	4922(3)	45(1)
C(21)	6381(4)	-1653(3)	5271(3)	29(1)
C(22)	7167(4)	981(3)	734(3)	29(1)
C(23)	6979(4)	1849(3)	377(3)	36(1)
C(24)	6811(4)	2196(4)	-409(3)	50(2)
C(25)	6809(4)	1724(5)	-826(3)	60(2)
C(26)	6997(4)	890(4)	-469(3)	48(2)
C(27)	7173(4)	496(3)	308(3)	32(1)
C(28)	6999(5)	2348(3)	805(4)	46(2)
C(29)	7361(4)	-416(3)	680(3)	42(1)
C(30)	8798(4)	-537(3)	2517(3)	24(1)
C(31)	9926(4)	-740(3)	1996(3)	27(1)
C(32)	9866(4)	-473(3)	1115(3)	37(1)
C(33)	10408(4)	-1673(3)	2322(3)	38(1)
C(34)	10632(3)	-264(3)	2101(3)	22(1)
C(35)	10876(4)	471(3)	1512(3)	29(1)
C(36)	11465(4)	917(3)	1629(3)	33(1)
C(37)	11822(4)	635(3)	2336(3)	32(1)
C(38)	11567(4)	-90(3)	2928(3)	39(1)
C(39)	10991(4)	-537(3)	2812(3)	33(1)
S(1)	6975(1)	487(1)	4346(1)	24(1)

O(1)	6992(2)	138(2)	3755(2)	22(1)
O(2)	6986(3)	1344(2)	3989(2)	32(1)
O(3)	6203(3)	195(2)	5093(2)	32(1)
C(40)	8368(4)	-23(3)	4582(3)	36(1)
F(1)	8629(2)	-800(2)	4624(2)	46(1)
F(2)	8405(3)	-41(2)	5283(2)	53(1)
F(3)	9150(2)	367(2)	4016(2)	55(1)
N(4)	8166(3)	1183(2)	2369(2)	25(1)
C(41)	8465(4)	1711(3)	2348(3)	28(1)
C(42)	8840(5)	2398(3)	2319(3)	41(1)
B(1)	8166(4)	-5005(3)	2620(3)	22(1)
C(43)	8786(4)	-5929(3)	3140(3)	22(1)
C(44)	9867(4)	-6273(3)	2810(3)	23(1)
C(45)	10406(4)	-7063(3)	3202(3)	25(1)
C(46)	9860(4)	-7558(3)	3949(3)	28(1)
C(47)	8787(4)	-7248(3)	4281(3)	26(1)
C(48)	8258(4)	-6444(3)	3883(3)	23(1)
C(49)	11558(4)	-7364(3)	2814(3)	31(1)
F(4)	11604(2)	-7377(2)	2085(2)	40(1)
F(5)	11998(2)	-8129(2)	3251(2)	41(1)
F(6)	12274(2)	-6896(2)	2666(2)	53(1)
C(50)	8204(5)	-7757(3)	5092(3)	38(1)
F(7)	7090(3)	-7603(2)	5185(2)	50(1)
F(8)	8400(3)	-7647(2)	5698(2)	50(1)
F(9)	8532(3)	-8566(2)	5239(2)	64(1)
C(51)	9067(3)	-4393(2)	2173(2)	19(1)
C(52)	9979(4)	-4504(3)	2498(3)	22(1)
C(53)	10724(4)	-3979(3)	2140(3)	24(1)
C(54)	10601(4)	-3298(3)	1440(3)	24(1)
C(55)	9698(4)	-3151(3)	1115(2)	21(1)
C(56)	8944(3)	-3689(3)	1480(2)	21(1)
C(57)	11693(4)	-4142(3)	2505(3)	31(1)
F(10)	11878(4)	-4867(3)	3061(3)	104(2)
F(11)	12656(3)	-4093(3)	1969(2)	95(2)
F(12)	11621(4)	-3620(3)	2815(4)	139(3)
C(58)	9550(4)	-2439(3)	347(3)	28(1)
F(13)	10048(3)	-1836(2)	217(2)	44(1)
F(14)	9988(3)	-2644(2)	-312(2)	50(1)
F(15)	8475(2)	-2101(2)	326(2)	44(1)
C(59)	7147(3)	-4581(2)	3189(2)	19(1)
C(60)	7196(4)	-4630(2)	3948(3)	22(1)
C(61)	6319(4)	-4241(3)	4403(3)	25(1)
C(62)	5367(4)	-3767(3)	4115(3)	29(1)
C(63)	5321(4)	-3681(3)	3355(3)	27(1)
C(64)	6189(4)	-4077(3)	2900(3)	23(1)
C(65)	6363(4)	-4322(3)	5227(3)	35(1)
F(16)	6150(3)	-3594(2)	5291(2)	50(1)
F(17)	5604(3)	-4725(2)	5815(2)	69(1)
F(18)	7368(3)	-4695(2)	5404(2)	67(1)
C(66)	4304(5)	-3177(4)	3027(4)	49(2)

F(19)	4115(3)	-2414(2)	2926(3)	84(1)
F(20)	4138(3)	-3317(2)	2473(3)	79(1)
F(21)	3328(3)	-3401(3)	3613(3)	106(2)
C(67)	7678(3)	-5171(3)	2004(3)	23(1)
C(68)	6748(4)	-5549(3)	2314(3)	31(1)
C(69)	6299(4)	-5740(3)	1846(3)	38(1)
C(70)	6773(4)	-5539(4)	1012(3)	46(2)
C(71)	7706(4)	-5181(3)	695(3)	38(1)
C(72)	8151(4)	-5012(3)	1180(3)	30(1)
C(73)	5332(5)	-6166(4)	2223(4)	59(2)
F(22)	4583(3)	-5924(3)	2766(2)	81(1)
F(23)	4810(4)	-6102(4)	1691(3)	125(2)
F(24)	5659(4)	-6959(3)	2539(4)	126(2)
C(74)	8219(5)	-4975(5)	-194(4)	62(2)
F(25)	8656(5)	-4315(3)	-536(3)	111(2)
F(26)	9148(5)	-5498(3)	-308(3)	118(2)
F(27)	7516(6)	-4629(5)	-686(4)	93(2)
F(27A)	7883(8)	-5408(6)	-469(5)	63(2)

Table 14.3. Bond lengths [Å] and angles [°] for **14**.

Mo(1)-N(3)	1.730(3)
Mo(1)-C(30)	1.876(4)
Mo(1)-O(1)	2.136(3)
Mo(1)-N(4)	2.170(4)
Mo(1)-C(1)	2.233(4)
N(1)-C(1)	1.341(5)
N(1)-C(4)	1.431(6)
N(1)-C(2)	1.484(5)
C(1)-N(2)	1.334(5)
N(2)-C(13)	1.435(6)
N(2)-C(3)	1.474(5)
C(2)-C(3)	1.513(6)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
N(3)-C(22)	1.400(5)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.404(6)
C(4)-C(9)	1.416(6)
C(5)-C(6)	1.395(7)
C(5)-C(10)	1.517(7)
C(6)-C(7)	1.383(7)
C(6)-H(6)	0.9500
C(7)-C(8)	1.375(6)
C(7)-C(11)	1.520(7)
C(8)-C(9)	1.393(6)
C(8)-H(8)	0.9500
C(9)-C(12)	1.497(6)

C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(18)	1.391(6)
C(13)-C(14)	1.407(6)
C(14)-C(15)	1.384(6)
C(14)-C(19)	1.505(6)
C(15)-C(16)	1.389(7)
C(15)-H(15)	0.9500
C(16)-C(17)	1.393(6)
C(16)-C(20)	1.519(7)
C(17)-C(18)	1.389(6)
C(17)-H(17)	0.9500
C(18)-C(21)	1.515(6)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(23)	1.417(7)
C(22)-C(27)	1.430(7)
C(23)-C(24)	1.388(7)
C(23)-C(28)	1.466(7)
C(24)-C(25)	1.399(9)
C(24)-H(24)	0.9500
C(25)-C(26)	1.362(9)
C(25)-H(25)	0.9500
C(26)-C(27)	1.376(7)
C(26)-H(26)	0.9500
C(27)-C(29)	1.489(7)
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-C(31)	1.510(6)
C(30)-H(30)	0.9500
C(31)-C(32)	1.525(7)
C(31)-C(34)	1.540(6)

C(31)-C(33)	1.549(7)
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-C(35)	1.376(6)
C(34)-C(39)	1.382(6)
C(35)-C(36)	1.389(6)
C(35)-H(35)	0.9500
C(36)-C(37)	1.372(7)
C(36)-H(36)	0.9500
C(37)-C(38)	1.368(7)
C(37)-H(37)	0.9500
C(38)-C(39)	1.378(7)
C(38)-H(38)	0.9500
C(39)-H(39)	0.9500
S(1)-O(3)	1.421(3)
S(1)-O(2)	1.426(3)
S(1)-O(1)	1.495(3)
S(1)-C(40)	1.847(5)
C(40)-F(2)	1.314(5)
C(40)-F(3)	1.323(6)
C(40)-F(1)	1.341(6)
N(4)-C(41)	1.131(5)
C(41)-C(42)	1.459(6)
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
B(1)-C(51)	1.633(6)
B(1)-C(59)	1.636(6)
B(1)-C(67)	1.640(7)
B(1)-C(43)	1.650(7)
C(43)-C(48)	1.394(6)
C(43)-C(44)	1.405(6)
C(44)-C(45)	1.389(6)
C(44)-H(44)	0.9500
C(45)-C(46)	1.393(6)
C(45)-C(49)	1.481(6)
C(46)-C(47)	1.379(6)
C(46)-H(46)	0.9500
C(47)-C(48)	1.404(6)
C(47)-C(50)	1.489(7)
C(48)-H(48)	0.9500
C(49)-F(6)	1.333(5)
C(49)-F(5)	1.337(5)
C(49)-F(4)	1.359(5)
C(50)-F(7)	1.341(6)
C(50)-F(8)	1.342(6)

C(50)-F(9)	1.347(6)
C(51)-C(56)	1.394(6)
C(51)-C(52)	1.408(6)
C(52)-C(53)	1.375(6)
C(52)-H(52)	0.9500
C(53)-C(54)	1.381(6)
C(53)-C(57)	1.499(6)
C(54)-C(55)	1.381(6)
C(54)-H(54)	0.9500
C(55)-C(56)	1.400(6)
C(55)-C(58)	1.489(6)
C(56)-H(56)	0.9500
C(57)-F(12)	1.290(6)
C(57)-F(10)	1.299(6)
C(57)-F(11)	1.322(6)
C(58)-F(15)	1.338(5)
C(58)-F(13)	1.341(5)
C(58)-F(14)	1.348(5)
C(59)-C(64)	1.402(6)
C(59)-C(60)	1.407(6)
C(60)-C(61)	1.393(6)
C(60)-H(60)	0.9500
C(61)-C(62)	1.384(6)
C(61)-C(65)	1.501(6)
C(62)-C(63)	1.381(6)
C(62)-H(62)	0.9500
C(63)-C(64)	1.395(6)
C(63)-C(66)	1.494(7)
C(64)-H(64)	0.9500
C(65)-F(17)	1.327(6)
C(65)-F(16)	1.338(5)
C(65)-F(18)	1.338(6)
C(66)-F(20)	1.261(6)
C(66)-F(19)	1.291(6)
C(66)-F(21)	1.411(7)
C(67)-C(72)	1.399(6)
C(67)-C(68)	1.400(6)
C(68)-C(69)	1.389(6)
C(68)-H(68)	0.9500
C(69)-C(70)	1.407(7)
C(69)-C(73)	1.487(8)
C(70)-C(71)	1.381(7)
C(70)-H(70)	0.9500
C(71)-C(72)	1.390(6)
C(71)-C(74)	1.502(8)
C(72)-H(72)	0.9500
C(73)-F(22)	1.291(7)
C(73)-F(24)	1.304(8)
C(73)-F(23)	1.316(7)
C(74)-F(25)	1.309(8)

C(74)-F(26)	1.311(7)
C(74)-F(27)	1.320(7)
C(74)-F(27A)	1.336(7)
N(3)-Mo(1)-C(30)	101.25(18)
N(3)-Mo(1)-O(1)	156.83(14)
C(30)-Mo(1)-O(1)	101.16(16)
N(3)-Mo(1)-N(4)	93.16(15)
C(30)-Mo(1)-N(4)	92.64(16)
O(1)-Mo(1)-N(4)	80.00(12)
N(3)-Mo(1)-C(1)	97.64(16)
C(30)-Mo(1)-C(1)	103.84(17)
O(1)-Mo(1)-C(1)	82.62(13)
N(4)-Mo(1)-C(1)	158.04(14)
C(1)-N(1)-C(4)	127.6(4)
C(1)-N(1)-C(2)	111.4(4)
C(4)-N(1)-C(2)	120.8(3)
N(2)-C(1)-N(1)	109.6(4)
N(2)-C(1)-Mo(1)	127.6(3)
N(1)-C(1)-Mo(1)	121.3(3)
C(1)-N(2)-C(13)	128.0(3)
C(1)-N(2)-C(3)	112.0(3)
C(13)-N(2)-C(3)	118.6(3)
N(1)-C(2)-C(3)	102.6(3)
N(1)-C(2)-H(2A)	111.2
C(3)-C(2)-H(2A)	111.2
N(1)-C(2)-H(2B)	111.2
C(3)-C(2)-H(2B)	111.2
H(2A)-C(2)-H(2B)	109.2
C(22)-N(3)-Mo(1)	172.6(3)
N(2)-C(3)-C(2)	103.1(3)
N(2)-C(3)-H(3A)	111.1
C(2)-C(3)-H(3A)	111.1
N(2)-C(3)-H(3B)	111.1
C(2)-C(3)-H(3B)	111.1
H(3A)-C(3)-H(3B)	109.1
C(5)-C(4)-C(9)	121.0(4)
C(5)-C(4)-N(1)	118.3(4)
C(9)-C(4)-N(1)	120.6(4)
C(6)-C(5)-C(4)	117.6(4)
C(6)-C(5)-C(10)	120.1(4)
C(4)-C(5)-C(10)	122.2(4)
C(7)-C(6)-C(5)	122.8(4)
C(7)-C(6)-H(6)	118.6
C(5)-C(6)-H(6)	118.6
C(8)-C(7)-C(6)	118.1(4)
C(8)-C(7)-C(11)	120.7(5)
C(6)-C(7)-C(11)	121.2(4)
C(7)-C(8)-C(9)	122.8(4)
C(7)-C(8)-H(8)	118.6

C(9)-C(8)-H(8)	118.6
C(8)-C(9)-C(4)	117.6(4)
C(8)-C(9)-C(12)	120.6(4)
C(4)-C(9)-C(12)	121.8(4)
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(7)-C(11)-H(11A)	109.5
C(7)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(7)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(9)-C(12)-H(12A)	109.5
C(9)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(9)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(18)-C(13)-C(14)	121.0(4)
C(18)-C(13)-N(2)	119.5(4)
C(14)-C(13)-N(2)	118.9(4)
C(15)-C(14)-C(13)	117.7(4)
C(15)-C(14)-C(19)	120.6(4)
C(13)-C(14)-C(19)	121.7(4)
C(14)-C(15)-C(16)	123.1(4)
C(14)-C(15)-H(15)	118.5
C(16)-C(15)-H(15)	118.5
C(15)-C(16)-C(17)	117.2(4)
C(15)-C(16)-C(20)	121.6(4)
C(17)-C(16)-C(20)	121.2(5)
C(18)-C(17)-C(16)	122.2(4)
C(18)-C(17)-H(17)	118.9
C(16)-C(17)-H(17)	118.9
C(17)-C(18)-C(13)	118.6(4)
C(17)-C(18)-C(21)	118.8(4)
C(13)-C(18)-C(21)	122.6(4)
C(14)-C(19)-H(19A)	109.5
C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-H(20A)	109.5
C(16)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(16)-C(20)-H(20C)	109.5

H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(3)-C(22)-C(23)	119.6(4)
N(3)-C(22)-C(27)	118.7(4)
C(23)-C(22)-C(27)	121.6(4)
C(24)-C(23)-C(22)	116.0(5)
C(24)-C(23)-C(28)	122.1(5)
C(22)-C(23)-C(28)	121.8(4)
C(23)-C(24)-C(25)	122.5(6)
C(23)-C(24)-H(24)	118.7
C(25)-C(24)-H(24)	118.7
C(26)-C(25)-C(24)	120.2(5)
C(26)-C(25)-H(25)	119.9
C(24)-C(25)-H(25)	119.9
C(25)-C(26)-C(27)	121.1(6)
C(25)-C(26)-H(26)	119.5
C(27)-C(26)-H(26)	119.5
C(26)-C(27)-C(22)	118.6(5)
C(26)-C(27)-C(29)	119.4(5)
C(22)-C(27)-C(29)	122.1(4)
C(23)-C(28)-H(28A)	109.5
C(23)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(23)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(27)-C(29)-H(29A)	109.5
C(27)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(27)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(31)-C(30)-Mo(1)	145.2(4)
C(31)-C(30)-H(30)	107.4
Mo(1)-C(30)-H(30)	107.4
C(30)-C(31)-C(32)	111.9(4)
C(30)-C(31)-C(34)	102.0(3)
C(32)-C(31)-C(34)	112.8(4)
C(30)-C(31)-C(33)	111.0(4)
C(32)-C(31)-C(33)	108.6(4)
C(34)-C(31)-C(33)	110.4(4)
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5

C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(31)-C(33)-H(33A)	109.5
C(31)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(31)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(35)-C(34)-C(39)	117.4(4)
C(35)-C(34)-C(31)	121.5(4)
C(39)-C(34)-C(31)	121.0(4)
C(34)-C(35)-C(36)	121.1(4)
C(34)-C(35)-H(35)	119.4
C(36)-C(35)-H(35)	119.4
C(37)-C(36)-C(35)	120.8(4)
C(37)-C(36)-H(36)	119.6
C(35)-C(36)-H(36)	119.6
C(38)-C(37)-C(36)	118.3(4)
C(38)-C(37)-H(37)	120.9
C(36)-C(37)-H(37)	120.9
C(37)-C(38)-C(39)	121.1(5)
C(37)-C(38)-H(38)	119.4
C(39)-C(38)-H(38)	119.4
C(38)-C(39)-C(34)	121.3(4)
C(38)-C(39)-H(39)	119.4
C(34)-C(39)-H(39)	119.4
O(3)-S(1)-O(2)	117.88(19)
O(3)-S(1)-O(1)	112.38(18)
O(2)-S(1)-O(1)	113.38(18)
O(3)-S(1)-C(40)	104.9(2)
O(2)-S(1)-C(40)	105.6(2)
O(1)-S(1)-C(40)	100.40(19)
S(1)-O(1)-Mo(1)	149.35(19)
F(2)-C(40)-F(3)	108.2(4)
F(2)-C(40)-F(1)	107.5(4)
F(3)-C(40)-F(1)	107.9(4)
F(2)-C(40)-S(1)	111.2(3)
F(3)-C(40)-S(1)	110.7(4)
F(1)-C(40)-S(1)	111.2(3)
C(41)-N(4)-Mo(1)	172.6(4)
N(4)-C(41)-C(42)	179.4(6)
C(41)-C(42)-H(42A)	109.5
C(41)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(41)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(51)-B(1)-C(59)	105.7(3)
C(51)-B(1)-C(67)	115.0(4)

C(59)-B(1)-C(67)	110.4(4)
C(51)-B(1)-C(43)	109.5(4)
C(59)-B(1)-C(43)	113.3(4)
C(67)-B(1)-C(43)	103.2(3)
C(48)-C(43)-C(44)	115.7(4)
C(48)-C(43)-B(1)	123.5(4)
C(44)-C(43)-B(1)	120.6(4)
C(45)-C(44)-C(43)	123.1(4)
C(45)-C(44)-H(44)	118.5
C(43)-C(44)-H(44)	118.5
C(44)-C(45)-C(46)	119.8(4)
C(44)-C(45)-C(49)	119.1(4)
C(46)-C(45)-C(49)	121.1(4)
C(47)-C(46)-C(45)	118.7(4)
C(47)-C(46)-H(46)	120.6
C(45)-C(46)-H(46)	120.6
C(46)-C(47)-C(48)	120.8(4)
C(46)-C(47)-C(50)	119.5(4)
C(48)-C(47)-C(50)	119.6(4)
C(43)-C(48)-C(47)	121.9(4)
C(43)-C(48)-H(48)	119.1
C(47)-C(48)-H(48)	119.1
F(6)-C(49)-F(5)	106.4(4)
F(6)-C(49)-F(4)	105.7(4)
F(5)-C(49)-F(4)	105.5(3)
F(6)-C(49)-C(45)	112.8(4)
F(5)-C(49)-C(45)	113.8(4)
F(4)-C(49)-C(45)	112.0(4)
F(7)-C(50)-F(8)	106.7(4)
F(7)-C(50)-F(9)	105.4(4)
F(8)-C(50)-F(9)	106.2(4)
F(7)-C(50)-C(47)	113.4(4)
F(8)-C(50)-C(47)	112.1(4)
F(9)-C(50)-C(47)	112.4(4)
C(56)-C(51)-C(52)	115.1(4)
C(56)-C(51)-B(1)	122.5(4)
C(52)-C(51)-B(1)	122.2(4)
C(53)-C(52)-C(51)	122.6(4)
C(53)-C(52)-H(52)	118.7
C(51)-C(52)-H(52)	118.7
C(52)-C(53)-C(54)	121.2(4)
C(52)-C(53)-C(57)	120.1(4)
C(54)-C(53)-C(57)	118.7(4)
C(55)-C(54)-C(53)	118.1(4)
C(55)-C(54)-H(54)	120.9
C(53)-C(54)-H(54)	120.9
C(54)-C(55)-C(56)	120.6(4)
C(54)-C(55)-C(58)	120.1(4)
C(56)-C(55)-C(58)	119.3(4)
C(51)-C(56)-C(55)	122.4(4)

C(51)-C(56)-H(56)	118.8
C(55)-C(56)-H(56)	118.8
F(12)-C(57)-F(10)	106.8(5)
F(12)-C(57)-F(11)	103.3(5)
F(10)-C(57)-F(11)	103.8(4)
F(12)-C(57)-C(53)	113.8(4)
F(10)-C(57)-C(53)	114.9(4)
F(11)-C(57)-C(53)	113.0(4)
F(15)-C(58)-F(13)	106.5(4)
F(15)-C(58)-F(14)	105.8(4)
F(13)-C(58)-F(14)	105.7(4)
F(15)-C(58)-C(55)	113.0(4)
F(13)-C(58)-C(55)	112.6(4)
F(14)-C(58)-C(55)	112.6(4)
C(64)-C(59)-C(60)	115.7(4)
C(64)-C(59)-B(1)	120.3(4)
C(60)-C(59)-B(1)	123.9(4)
C(61)-C(60)-C(59)	121.9(4)
C(61)-C(60)-H(60)	119.0
C(59)-C(60)-H(60)	119.0
C(62)-C(61)-C(60)	121.2(4)
C(62)-C(61)-C(65)	117.3(4)
C(60)-C(61)-C(65)	121.5(4)
C(63)-C(62)-C(61)	117.9(4)
C(63)-C(62)-H(62)	121.1
C(61)-C(62)-H(62)	121.1
C(62)-C(63)-C(64)	121.3(4)
C(62)-C(63)-C(66)	119.3(4)
C(64)-C(63)-C(66)	119.4(4)
C(63)-C(64)-C(59)	121.9(4)
C(63)-C(64)-H(64)	119.0
C(59)-C(64)-H(64)	119.0
F(17)-C(65)-F(16)	105.1(4)
F(17)-C(65)-F(18)	108.2(4)
F(16)-C(65)-F(18)	105.4(4)
F(17)-C(65)-C(61)	112.6(4)
F(16)-C(65)-C(61)	112.3(4)
F(18)-C(65)-C(61)	112.8(4)
F(20)-C(66)-F(19)	115.6(5)
F(20)-C(66)-F(21)	97.8(5)
F(19)-C(66)-F(21)	99.2(5)
F(20)-C(66)-C(63)	116.6(4)
F(19)-C(66)-C(63)	114.2(5)
F(21)-C(66)-C(63)	110.3(5)
C(72)-C(67)-C(68)	114.8(4)
C(72)-C(67)-B(1)	125.7(4)
C(68)-C(67)-B(1)	119.4(4)
C(69)-C(68)-C(67)	123.5(4)
C(69)-C(68)-H(68)	118.2
C(67)-C(68)-H(68)	118.2

C(68)-C(69)-C(70)	119.8(5)
C(68)-C(69)-C(73)	120.5(5)
C(70)-C(69)-C(73)	119.7(5)
C(71)-C(70)-C(69)	117.8(5)
C(71)-C(70)-H(70)	121.1
C(69)-C(70)-H(70)	121.1
C(70)-C(71)-C(72)	121.1(5)
C(70)-C(71)-C(74)	117.8(5)
C(72)-C(71)-C(74)	121.1(5)
C(71)-C(72)-C(67)	122.8(4)
C(71)-C(72)-H(72)	118.6
C(67)-C(72)-H(72)	118.6
F(22)-C(73)-F(24)	109.0(6)
F(22)-C(73)-F(23)	106.8(6)
F(24)-C(73)-F(23)	101.2(6)
F(22)-C(73)-C(69)	114.6(5)
F(24)-C(73)-C(69)	111.3(6)
F(23)-C(73)-C(69)	113.1(6)
F(25)-C(74)-F(26)	97.2(5)
F(25)-C(74)-F(27)	90.1(7)
F(26)-C(74)-F(27)	124.0(6)
F(25)-C(74)-F(27A)	134.6(7)
F(26)-C(74)-F(27A)	79.5(6)
F(27)-C(74)-F(27A)	57.9(5)
F(25)-C(74)-C(71)	113.7(5)
F(26)-C(74)-C(71)	110.9(6)
F(27)-C(74)-C(71)	116.3(6)
F(27A)-C(74)-C(71)	109.6(6)

Table 14.4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **14**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11}+ ... +2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	22(1)	21(1)	21(1)	-12(1)	-1(1)	-8(1)
N(1)	23(2)	23(2)	19(2)	-12(2)	-2(2)	-8(2)
C(1)	25(2)	27(3)	20(2)	-19(2)	3(2)	-10(2)
N(2)	23(2)	18(2)	21(2)	-11(2)	1(2)	-10(2)
C(2)	26(3)	36(3)	23(3)	-16(2)	4(2)	-16(2)
N(3)	25(2)	24(2)	23(2)	-10(2)	-2(2)	-12(2)
C(3)	29(3)	27(3)	25(3)	-11(2)	-2(2)	-13(2)
C(4)	13(2)	32(3)	24(2)	-14(2)	-1(2)	-6(2)
C(5)	20(2)	40(3)	26(3)	-21(2)	1(2)	-8(2)
C(6)	22(3)	52(3)	26(3)	-20(3)	-3(2)	-8(2)
C(7)	21(2)	49(3)	23(3)	-12(2)	-2(2)	-8(2)
C(8)	21(2)	28(3)	33(3)	-13(2)	1(2)	-6(2)
C(9)	13(2)	29(3)	27(3)	-15(2)	3(2)	-5(2)
C(10)	46(3)	59(4)	30(3)	-29(3)	-5(2)	-18(3)
C(11)	37(3)	63(4)	31(3)	-8(3)	-13(2)	-8(3)

C(12)	26(3)	26(3)	31(3)	-14(2)	-6(2)	-5(2)
C(13)	26(2)	20(2)	23(2)	-10(2)	0(2)	-11(2)
C(14)	28(3)	22(2)	23(2)	-12(2)	0(2)	-9(2)
C(15)	32(3)	25(3)	41(3)	-22(2)	1(2)	-9(2)
C(16)	35(3)	20(2)	42(3)	-12(2)	-11(2)	-5(2)
C(17)	41(3)	26(3)	31(3)	-14(2)	-8(2)	-11(2)
C(18)	28(3)	20(2)	24(3)	-8(2)	-3(2)	-11(2)
C(19)	35(3)	33(3)	29(3)	-19(2)	2(2)	-10(2)
C(20)	42(3)	35(3)	57(4)	-19(3)	-19(3)	4(3)
C(21)	35(3)	32(3)	28(3)	-17(2)	-5(2)	-11(2)
C(22)	22(2)	39(3)	20(3)	-7(2)	-2(2)	-9(2)
C(23)	19(3)	43(3)	35(3)	-4(3)	-4(2)	-12(2)
C(24)	24(3)	57(4)	38(3)	12(3)	-6(2)	-11(3)
C(25)	23(3)	116(6)	17(3)	-9(4)	-2(2)	-5(3)
C(26)	25(3)	90(5)	26(3)	-28(3)	-4(2)	0(3)
C(27)	17(2)	53(3)	26(3)	-19(2)	-4(2)	-3(2)
C(28)	45(3)	26(3)	60(4)	1(3)	-22(3)	-13(2)
C(29)	36(3)	60(4)	50(3)	-43(3)	-9(3)	-5(3)
C(30)	25(2)	21(2)	31(3)	-12(2)	-2(2)	-12(2)
C(31)	20(2)	30(3)	30(3)	-16(2)	2(2)	-7(2)
C(32)	26(3)	58(4)	42(3)	-35(3)	6(2)	-18(2)
C(33)	31(3)	30(3)	56(4)	-27(3)	7(2)	-11(2)
C(34)	15(2)	21(2)	30(3)	-14(2)	-3(2)	0(2)
C(35)	30(3)	35(3)	22(3)	-6(2)	-7(2)	-11(2)
C(36)	29(3)	26(3)	37(3)	-1(2)	-8(2)	-11(2)
C(37)	27(3)	36(3)	43(3)	-23(3)	-7(2)	-11(2)
C(38)	39(3)	54(4)	26(3)	-4(3)	-13(2)	-20(3)
C(39)	30(3)	34(3)	27(3)	2(2)	-8(2)	-15(2)
S(1)	29(1)	25(1)	24(1)	-15(1)	-6(1)	-5(1)
O(1)	26(2)	24(2)	22(2)	-14(1)	-3(1)	-7(1)
O(2)	44(2)	21(2)	36(2)	-17(2)	-7(2)	-4(2)
O(3)	38(2)	36(2)	26(2)	-20(2)	1(2)	-11(2)
C(40)	38(3)	40(3)	41(3)	-20(3)	-11(3)	-12(3)
F(1)	47(2)	31(2)	70(2)	-22(2)	-30(2)	5(1)
F(2)	69(2)	55(2)	53(2)	-25(2)	-36(2)	-6(2)
F(3)	33(2)	56(2)	70(2)	-11(2)	-15(2)	-14(2)
N(4)	22(2)	30(2)	28(2)	-17(2)	0(2)	-8(2)
C(41)	30(3)	32(3)	27(3)	-14(2)	-1(2)	-13(2)
C(42)	53(3)	38(3)	43(3)	-21(3)	-4(3)	-24(3)
B(1)	25(3)	20(3)	21(3)	-11(2)	-1(2)	-3(2)
C(43)	25(2)	22(2)	23(2)	-11(2)	-6(2)	-5(2)
C(44)	25(2)	18(2)	25(2)	-7(2)	-2(2)	-8(2)
C(45)	22(2)	23(2)	32(3)	-14(2)	-4(2)	-5(2)
C(46)	30(3)	18(2)	37(3)	-10(2)	-14(2)	2(2)
C(47)	32(3)	21(2)	24(3)	-6(2)	-5(2)	-8(2)
C(48)	21(2)	23(2)	24(3)	-11(2)	-2(2)	-3(2)
C(49)	29(3)	29(3)	42(3)	-22(2)	-9(2)	0(2)
F(4)	33(2)	45(2)	37(2)	-22(1)	-6(1)	8(1)
F(5)	38(2)	35(2)	48(2)	-21(1)	-18(1)	14(1)
F(6)	24(2)	52(2)	95(3)	-48(2)	4(2)	-10(1)

C(50)	49(4)	23(3)	36(3)	-6(2)	-7(3)	-7(2)
F(7)	47(2)	45(2)	44(2)	-2(2)	2(2)	-26(2)
F(8)	66(2)	51(2)	30(2)	-12(2)	-7(2)	-16(2)
F(9)	101(3)	20(2)	47(2)	-4(2)	6(2)	-12(2)
C(51)	21(2)	19(2)	18(2)	-11(2)	0(2)	-2(2)
C(52)	26(2)	17(2)	20(2)	-7(2)	-6(2)	-1(2)
C(53)	31(3)	22(2)	23(3)	-11(2)	-4(2)	-8(2)
C(54)	25(2)	23(2)	24(3)	-12(2)	4(2)	-12(2)
C(55)	25(2)	17(2)	18(2)	-8(2)	-1(2)	-6(2)
C(56)	20(2)	22(2)	22(2)	-12(2)	-2(2)	-1(2)
C(57)	30(3)	30(3)	38(3)	-13(2)	-8(2)	-10(2)
F(10)	103(3)	90(3)	114(4)	37(3)	-89(3)	-57(3)
F(11)	39(2)	157(4)	62(3)	-7(3)	-18(2)	-29(2)
F(12)	100(4)	147(4)	280(7)	-168(5)	-136(4)	60(3)
C(58)	34(3)	23(3)	25(3)	-8(2)	-2(2)	-9(2)
F(13)	62(2)	26(2)	41(2)	2(1)	-17(2)	-21(1)
F(14)	86(2)	38(2)	21(2)	-10(1)	-7(2)	-11(2)
F(15)	42(2)	30(2)	44(2)	5(1)	-19(1)	-5(1)
C(59)	24(2)	15(2)	20(2)	-6(2)	-3(2)	-10(2)
C(60)	26(2)	15(2)	23(2)	-5(2)	-8(2)	-6(2)
C(61)	34(3)	21(2)	24(3)	-9(2)	-2(2)	-14(2)
C(62)	28(3)	26(3)	36(3)	-19(2)	-3(2)	-5(2)
C(63)	27(3)	23(2)	35(3)	-13(2)	-11(2)	0(2)
C(64)	28(2)	19(2)	25(2)	-11(2)	-7(2)	-3(2)
C(65)	45(3)	30(3)	29(3)	-11(2)	-1(2)	-13(2)
F(16)	89(3)	41(2)	35(2)	-22(2)	-7(2)	-28(2)
F(17)	121(3)	75(2)	25(2)	-13(2)	12(2)	-77(2)
F(18)	79(3)	81(3)	50(2)	-31(2)	-37(2)	9(2)
C(66)	36(3)	56(4)	72(4)	-51(4)	-20(3)	15(3)
F(19)	90(3)	29(2)	159(4)	-30(2)	-95(3)	16(2)
F(20)	79(3)	71(3)	123(3)	-57(3)	-77(3)	27(2)
F(21)	46(3)	111(4)	147(4)	-47(3)	-22(3)	3(2)
C(67)	19(2)	17(2)	31(3)	-12(2)	0(2)	-4(2)
C(68)	30(3)	32(3)	35(3)	-20(2)	0(2)	-9(2)
C(69)	33(3)	47(3)	52(3)	-38(3)	3(2)	-13(2)
C(70)	39(3)	69(4)	57(4)	-50(3)	-11(3)	-4(3)
C(71)	30(3)	57(3)	40(3)	-38(3)	1(2)	-7(3)
C(72)	24(3)	37(3)	38(3)	-27(2)	0(2)	-5(2)
C(73)	56(4)	75(5)	73(5)	-46(4)	-6(4)	-30(4)
F(22)	57(2)	132(4)	90(3)	-80(3)	27(2)	-55(2)
F(23)	99(4)	240(7)	103(4)	-91(4)	4(3)	-109(4)
F(24)	88(3)	52(3)	213(6)	-31(3)	3(4)	-44(3)
C(74)	42(4)	111(6)	68(5)	-70(5)	2(3)	-24(4)
F(25)	162(3)	107(3)	57(2)	-40(2)	0(2)	-27(3)
F(26)	118(3)	97(3)	97(3)	-54(2)	40(2)	-4(2)
F(27)	81(3)	128(4)	62(3)	-20(3)	-33(3)	-16(3)
F(27A)	84(4)	82(4)	53(4)	-51(3)	-2(3)	-29(3)

Table 14.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **14**.

	x	y	z	U(eq)
H(2A)	3957	-1020	3157	32
H(2B)	3777	-577	3778	32
H(3A)	4782	-1722	4515	31
H(3B)	5149	-2086	3809	31
H(6)	4131	968	464	38
H(8)	4216	2387	1561	34
H(10A)	3925	-683	1780	59
H(10B)	5207	-940	1846	59
H(10C)	4895	-505	974	59
H(11A)	2942	2745	362	69
H(11B)	3925	2426	-274	69
H(11C)	4142	2988	99	69
H(12A)	5626	1373	2764	39
H(12B)	4769	784	3388	39
H(12C)	4327	1752	2998	39
H(15)	9147	-3324	3540	37
H(17)	8222	-2751	5525	37
H(19A)	7848	-1769	2289	46
H(19B)	6844	-2263	2756	46
H(19C)	8095	-2744	2546	46
H(20A)	9601	-4336	5140	67
H(20B)	9944	-3701	5356	67
H(20C)	10483	-3779	4490	67
H(21A)	5789	-1973	5598	44
H(21B)	6052	-1101	4940	44
H(21C)	6758	-1616	5631	44
H(24)	6692	2776	-673	60
H(25)	6677	1986	-1360	72
H(26)	7007	575	-762	57
H(28A)	6739	2928	497	69
H(28B)	7765	2268	857	69
H(28C)	6507	2182	1345	69
H(29A)	6929	-616	478	63
H(29B)	7120	-592	1271	63
H(29C)	8159	-642	534	63
H(30)	8780	-942	3048	29
H(32A)	9462	-825	1077	55
H(32B)	10625	-521	780	55
H(32C)	9471	98	923	55
H(33A)	10381	-1864	2903	56
H(33B)	11185	-1778	2031	56
H(33C)	9962	-1966	2238	56
H(35)	10637	677	1017	35
H(36)	11623	1423	1213	40
H(37)	12236	935	2413	38

H(38)	11790	-287	3427	47
H(39)	10838	-1044	3229	40
H(42A)	8525	2908	1920	61
H(42B)	9658	2311	2164	61
H(42C)	8588	2438	2855	61
H(44)	10247	-5949	2295	28
H(46)	10220	-8099	4224	34
H(48)	7519	-6245	4126	27
H(52)	10083	-4960	2985	26
H(54)	11124	-2941	1189	28
H(56)	8326	-3571	1246	25
H(60)	7847	-4937	4157	26
H(62)	4765	-3509	4430	34
H(64)	6130	-4003	2378	28
H(68)	6405	-5681	2873	37
H(70)	6462	-5645	678	56
H(72)	8805	-4779	942	36

Table 14.6. Torsion angles [°] for **14**.

C(4)-N(1)-C(1)-N(2)	-176.8(4)
C(2)-N(1)-C(1)-N(2)	6.7(4)
C(4)-N(1)-C(1)-Mo(1)	16.1(5)
C(2)-N(1)-C(1)-Mo(1)	-160.4(3)
N(3)-Mo(1)-C(1)-N(2)	147.0(3)
C(30)-Mo(1)-C(1)-N(2)	43.3(4)
O(1)-Mo(1)-C(1)-N(2)	-56.4(3)
N(4)-Mo(1)-C(1)-N(2)	-94.3(5)
N(3)-Mo(1)-C(1)-N(1)	-48.4(3)
C(30)-Mo(1)-C(1)-N(1)	-152.0(3)
O(1)-Mo(1)-C(1)-N(1)	108.2(3)
N(4)-Mo(1)-C(1)-N(1)	70.4(5)
N(1)-C(1)-N(2)-C(13)	166.9(4)
Mo(1)-C(1)-N(2)-C(13)	-27.0(6)
N(1)-C(1)-N(2)-C(3)	0.6(4)
Mo(1)-C(1)-N(2)-C(3)	166.7(3)
C(1)-N(1)-C(2)-C(3)	-10.8(4)
C(4)-N(1)-C(2)-C(3)	172.5(3)
C(30)-Mo(1)-N(3)-C(22)	-161(2)
O(1)-Mo(1)-N(3)-C(22)	4(3)
N(4)-Mo(1)-N(3)-C(22)	-68(2)
C(1)-Mo(1)-N(3)-C(22)	93(2)
C(1)-N(2)-C(3)-C(2)	-7.2(4)
C(13)-N(2)-C(3)-C(2)	-174.9(3)
N(1)-C(2)-C(3)-N(2)	10.1(4)
C(1)-N(1)-C(4)-C(5)	111.1(5)
C(2)-N(1)-C(4)-C(5)	-72.7(5)
C(1)-N(1)-C(4)-C(9)	-71.8(6)
C(2)-N(1)-C(4)-C(9)	104.4(5)

C(9)-C(4)-C(5)-C(6)	2.6(6)
N(1)-C(4)-C(5)-C(6)	179.7(4)
C(9)-C(4)-C(5)-C(10)	-174.4(4)
N(1)-C(4)-C(5)-C(10)	2.7(6)
C(4)-C(5)-C(6)-C(7)	-1.2(7)
C(10)-C(5)-C(6)-C(7)	175.8(4)
C(5)-C(6)-C(7)-C(8)	-0.5(7)
C(5)-C(6)-C(7)-C(11)	-179.3(4)
C(6)-C(7)-C(8)-C(9)	0.8(7)
C(11)-C(7)-C(8)-C(9)	179.6(4)
C(7)-C(8)-C(9)-C(4)	0.6(6)
C(7)-C(8)-C(9)-C(12)	179.6(4)
C(5)-C(4)-C(9)-C(8)	-2.4(6)
N(1)-C(4)-C(9)-C(8)	-179.4(4)
C(5)-C(4)-C(9)-C(12)	178.7(4)
N(1)-C(4)-C(9)-C(12)	1.6(6)
C(1)-N(2)-C(13)-C(18)	114.6(5)
C(3)-N(2)-C(13)-C(18)	-79.9(5)
C(1)-N(2)-C(13)-C(14)	-74.0(5)
C(3)-N(2)-C(13)-C(14)	91.5(5)
C(18)-C(13)-C(14)-C(15)	-3.9(6)
N(2)-C(13)-C(14)-C(15)	-175.2(4)
C(18)-C(13)-C(14)-C(19)	174.3(4)
N(2)-C(13)-C(14)-C(19)	3.1(6)
C(13)-C(14)-C(15)-C(16)	-0.3(7)
C(19)-C(14)-C(15)-C(16)	-178.5(4)
C(14)-C(15)-C(16)-C(17)	2.3(7)
C(14)-C(15)-C(16)-C(20)	-179.6(4)
C(15)-C(16)-C(17)-C(18)	-0.2(7)
C(20)-C(16)-C(17)-C(18)	-178.3(4)
C(16)-C(17)-C(18)-C(13)	-3.8(7)
C(16)-C(17)-C(18)-C(21)	173.2(4)
C(14)-C(13)-C(18)-C(17)	5.9(6)
N(2)-C(13)-C(18)-C(17)	177.1(4)
C(14)-C(13)-C(18)-C(21)	-171.0(4)
N(2)-C(13)-C(18)-C(21)	0.2(6)
Mo(1)-N(3)-C(22)-C(23)	37(3)
Mo(1)-N(3)-C(22)-C(27)	-142(2)
N(3)-C(22)-C(23)-C(24)	-179.5(4)
C(27)-C(22)-C(23)-C(24)	-0.5(7)
N(3)-C(22)-C(23)-C(28)	2.4(7)
C(27)-C(22)-C(23)-C(28)	-178.5(5)
C(22)-C(23)-C(24)-C(25)	0.8(7)
C(28)-C(23)-C(24)-C(25)	178.9(5)
C(23)-C(24)-C(25)-C(26)	-1.2(8)
C(24)-C(25)-C(26)-C(27)	1.1(8)
C(25)-C(26)-C(27)-C(22)	-0.7(7)
C(25)-C(26)-C(27)-C(29)	179.2(5)
N(3)-C(22)-C(27)-C(26)	179.5(4)
C(23)-C(22)-C(27)-C(26)	0.4(7)

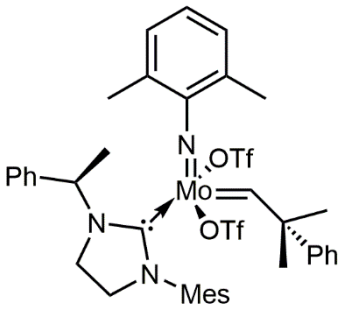
N(3)-C(22)-C(27)-C(29)	-0.5(7)
C(23)-C(22)-C(27)-C(29)	-179.6(4)
N(3)-Mo(1)-C(30)-C(31)	24.6(6)
O(1)-Mo(1)-C(30)-C(31)	-149.4(5)
N(4)-Mo(1)-C(30)-C(31)	-69.1(5)
C(1)-Mo(1)-C(30)-C(31)	125.5(5)
Mo(1)-C(30)-C(31)-C(32)	-30.9(7)
Mo(1)-C(30)-C(31)-C(34)	90.0(6)
Mo(1)-C(30)-C(31)-C(33)	-152.4(5)
C(30)-C(31)-C(34)-C(35)	-101.9(5)
C(32)-C(31)-C(34)-C(35)	18.4(6)
C(33)-C(31)-C(34)-C(35)	140.1(4)
C(30)-C(31)-C(34)-C(39)	74.4(5)
C(32)-C(31)-C(34)-C(39)	-165.3(4)
C(33)-C(31)-C(34)-C(39)	-43.6(5)
C(39)-C(34)-C(35)-C(36)	0.3(7)
C(31)-C(34)-C(35)-C(36)	176.7(4)
C(34)-C(35)-C(36)-C(37)	0.1(7)
C(35)-C(36)-C(37)-C(38)	-1.0(7)
C(36)-C(37)-C(38)-C(39)	1.6(8)
C(37)-C(38)-C(39)-C(34)	-1.3(8)
C(35)-C(34)-C(39)-C(38)	0.3(7)
C(31)-C(34)-C(39)-C(38)	-176.2(4)
O(3)-S(1)-O(1)-Mo(1)	162.2(3)
O(2)-S(1)-O(1)-Mo(1)	25.4(4)
C(40)-S(1)-O(1)-Mo(1)	-86.8(4)
N(3)-Mo(1)-O(1)-S(1)	-68.7(5)
C(30)-Mo(1)-O(1)-S(1)	96.4(4)
N(4)-Mo(1)-O(1)-S(1)	5.6(4)
C(1)-Mo(1)-O(1)-S(1)	-160.9(4)
O(3)-S(1)-C(40)-F(2)	-41.2(4)
O(2)-S(1)-C(40)-F(2)	84.0(4)
O(1)-S(1)-C(40)-F(2)	-157.9(3)
O(3)-S(1)-C(40)-F(3)	-161.5(3)
O(2)-S(1)-C(40)-F(3)	-36.3(4)
O(1)-S(1)-C(40)-F(3)	81.8(4)
O(3)-S(1)-C(40)-F(1)	78.6(4)
O(2)-S(1)-C(40)-F(1)	-156.2(3)
O(1)-S(1)-C(40)-F(1)	-38.1(4)
N(3)-Mo(1)-N(4)-C(41)	126(3)
C(30)-Mo(1)-N(4)-C(41)	-133(3)
O(1)-Mo(1)-N(4)-C(41)	-32(3)
C(1)-Mo(1)-N(4)-C(41)	6(3)
Mo(1)-N(4)-C(41)-C(42)	-67(50)
C(51)-B(1)-C(43)-C(48)	144.0(4)
C(59)-B(1)-C(43)-C(48)	26.4(6)
C(67)-B(1)-C(43)-C(48)	-93.1(5)
C(51)-B(1)-C(43)-C(44)	-42.1(5)
C(59)-B(1)-C(43)-C(44)	-159.7(4)
C(67)-B(1)-C(43)-C(44)	80.9(5)

C(48)-C(43)-C(44)-C(45)	-2.2(6)
B(1)-C(43)-C(44)-C(45)	-176.6(4)
C(43)-C(44)-C(45)-C(46)	1.5(7)
C(43)-C(44)-C(45)-C(49)	-178.6(4)
C(44)-C(45)-C(46)-C(47)	0.2(7)
C(49)-C(45)-C(46)-C(47)	-179.7(4)
C(45)-C(46)-C(47)-C(48)	-1.0(7)
C(45)-C(46)-C(47)-C(50)	-177.9(4)
C(44)-C(43)-C(48)-C(47)	1.3(6)
B(1)-C(43)-C(48)-C(47)	175.5(4)
C(46)-C(47)-C(48)-C(43)	0.3(7)
C(50)-C(47)-C(48)-C(43)	177.1(4)
C(44)-C(45)-C(49)-F(6)	57.8(6)
C(46)-C(45)-C(49)-F(6)	-122.3(5)
C(44)-C(45)-C(49)-F(5)	179.2(4)
C(46)-C(45)-C(49)-F(5)	-0.9(6)
C(44)-C(45)-C(49)-F(4)	-61.3(5)
C(46)-C(45)-C(49)-F(4)	118.7(5)
C(46)-C(47)-C(50)-F(7)	-149.9(4)
C(48)-C(47)-C(50)-F(7)	33.2(6)
C(46)-C(47)-C(50)-F(8)	89.2(5)
C(48)-C(47)-C(50)-F(8)	-87.7(5)
C(46)-C(47)-C(50)-F(9)	-30.4(7)
C(48)-C(47)-C(50)-F(9)	152.7(4)
C(59)-B(1)-C(51)-C(56)	-81.8(5)
C(67)-B(1)-C(51)-C(56)	40.3(5)
C(43)-B(1)-C(51)-C(56)	155.9(4)
C(59)-B(1)-C(51)-C(52)	93.1(5)
C(67)-B(1)-C(51)-C(52)	-144.9(4)
C(43)-B(1)-C(51)-C(52)	-29.2(5)
C(56)-C(51)-C(52)-C(53)	-2.9(6)
B(1)-C(51)-C(52)-C(53)	-178.1(4)
C(51)-C(52)-C(53)-C(54)	1.2(7)
C(51)-C(52)-C(53)-C(57)	-178.6(4)
C(52)-C(53)-C(54)-C(55)	0.9(6)
C(57)-C(53)-C(54)-C(55)	-179.3(4)
C(53)-C(54)-C(55)-C(56)	-1.3(6)
C(53)-C(54)-C(55)-C(58)	-178.0(4)
C(52)-C(51)-C(56)-C(55)	2.5(6)
B(1)-C(51)-C(56)-C(55)	177.7(4)
C(54)-C(55)-C(56)-C(51)	-0.5(6)
C(58)-C(55)-C(56)-C(51)	176.3(4)
C(52)-C(53)-C(57)-F(12)	-110.9(6)
C(54)-C(53)-C(57)-F(12)	69.3(7)
C(52)-C(53)-C(57)-F(10)	12.7(7)
C(54)-C(53)-C(57)-F(10)	-167.1(5)
C(52)-C(53)-C(57)-F(11)	131.6(5)
C(54)-C(53)-C(57)-F(11)	-48.2(6)
C(54)-C(55)-C(58)-F(15)	-145.7(4)
C(56)-C(55)-C(58)-F(15)	37.5(5)

C(54)-C(55)-C(58)-F(13)	-25.0(6)
C(56)-C(55)-C(58)-F(13)	158.2(4)
C(54)-C(55)-C(58)-F(14)	94.5(5)
C(56)-C(55)-C(58)-F(14)	-82.3(5)
C(51)-B(1)-C(59)-C(64)	95.4(4)
C(67)-B(1)-C(59)-C(64)	-29.6(5)
C(43)-B(1)-C(59)-C(64)	-144.8(4)
C(51)-B(1)-C(59)-C(60)	-79.0(5)
C(67)-B(1)-C(59)-C(60)	156.0(4)
C(43)-B(1)-C(59)-C(60)	40.8(6)
C(64)-C(59)-C(60)-C(61)	3.7(6)
B(1)-C(59)-C(60)-C(61)	178.3(4)
C(59)-C(60)-C(61)-C(62)	-1.9(6)
C(59)-C(60)-C(61)-C(65)	177.8(4)
C(60)-C(61)-C(62)-C(63)	-1.0(6)
C(65)-C(61)-C(62)-C(63)	179.4(4)
C(61)-C(62)-C(63)-C(64)	1.8(7)
C(61)-C(62)-C(63)-C(66)	179.6(4)
C(62)-C(63)-C(64)-C(59)	0.1(7)
C(66)-C(63)-C(64)-C(59)	-177.7(4)
C(60)-C(59)-C(64)-C(63)	-2.8(6)
B(1)-C(59)-C(64)-C(63)	-177.6(4)
C(62)-C(61)-C(65)-F(17)	65.9(6)
C(60)-C(61)-C(65)-F(17)	-113.8(5)
C(62)-C(61)-C(65)-F(16)	-52.4(6)
C(60)-C(61)-C(65)-F(16)	127.9(5)
C(62)-C(61)-C(65)-F(18)	-171.4(4)
C(60)-C(61)-C(65)-F(18)	9.0(6)
C(62)-C(63)-C(66)-F(20)	-158.5(5)
C(64)-C(63)-C(66)-F(20)	19.4(8)
C(62)-C(63)-C(66)-F(19)	62.6(7)
C(64)-C(63)-C(66)-F(19)	-119.6(5)
C(62)-C(63)-C(66)-F(21)	-48.1(6)
C(64)-C(63)-C(66)-F(21)	129.7(5)
C(51)-B(1)-C(67)-C(72)	16.7(6)
C(59)-B(1)-C(67)-C(72)	136.2(4)
C(43)-B(1)-C(67)-C(72)	-102.4(5)
C(51)-B(1)-C(67)-C(68)	-167.5(4)
C(59)-B(1)-C(67)-C(68)	-48.0(5)
C(43)-B(1)-C(67)-C(68)	73.4(5)
C(72)-C(67)-C(68)-C(69)	-1.4(7)
B(1)-C(67)-C(68)-C(69)	-177.7(4)
C(67)-C(68)-C(69)-C(70)	-1.2(8)
C(67)-C(68)-C(69)-C(73)	178.0(5)
C(68)-C(69)-C(70)-C(71)	2.4(8)
C(73)-C(69)-C(70)-C(71)	-176.8(5)
C(69)-C(70)-C(71)-C(72)	-1.1(8)
C(69)-C(70)-C(71)-C(74)	179.3(5)
C(70)-C(71)-C(72)-C(67)	-1.6(8)
C(74)-C(71)-C(72)-C(67)	177.9(5)

C(68)-C(67)-C(72)-C(71)	2.8(7)
B(1)-C(67)-C(72)-C(71)	178.8(4)
C(68)-C(69)-C(73)-F(22)	39.3(9)
C(70)-C(69)-C(73)-F(22)	-141.5(6)
C(68)-C(69)-C(73)-F(24)	-84.8(7)
C(70)-C(69)-C(73)-F(24)	94.4(7)
C(68)-C(69)-C(73)-F(23)	162.1(6)
C(70)-C(69)-C(73)-F(23)	-18.7(9)
C(70)-C(71)-C(74)-F(25)	146.5(6)
C(72)-C(71)-C(74)-F(25)	-33.1(8)
C(70)-C(71)-C(74)-F(26)	-105.2(6)
C(72)-C(71)-C(74)-F(26)	75.3(7)
C(70)-C(71)-C(74)-F(27)	43.8(9)
C(72)-C(71)-C(74)-F(27)	-135.8(7)
C(70)-C(71)-C(74)-F(27A)	-19.3(9)
C(72)-C(71)-C(74)-F(27A)	161.1(7)

Complex 18



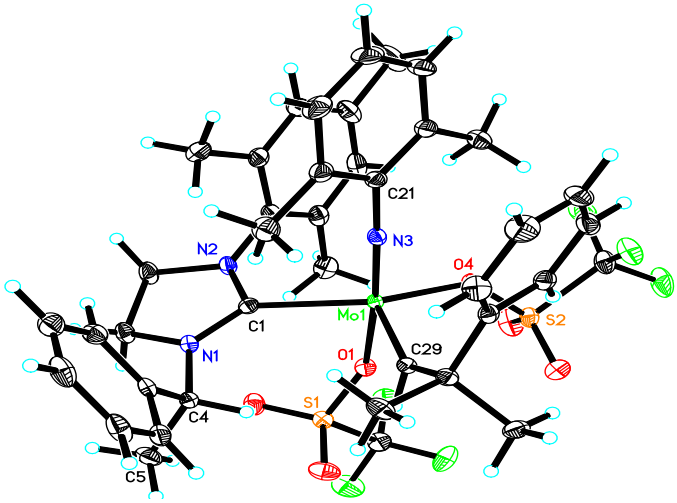


Table 18.1. Crystal data and structure refinement for **18**.

Empirical formula	$C_{41}H_{47}Cl_2F_6MoN_3O_6S_2$
Formula weight	1022.78
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	monoclinic, $P2_1$
Unit cell dimensions	a = 10.9444(5) Å, α = 90°
	b = 18.0372(9) Å, β = 111.600(2)°
	c = 11.9649(6) Å, γ = 90°
Volume	2196.08(18) $Å^3$
Z, Calculated density	2, 1.547 Mg/m^3
Absorption coefficient	0.590 mm^{-1}
F(000)	1048
Crystal size	0.64 x 0.53 x 0.26 mm
Theta range for data collection	1.83 to 28.3°.
Limiting indices	-14<=h<=14, -24<=k<=24, -15<=l<=15
Reflections collected / unique	56698 / 10934 [R(int) = 0.0215]
Completeness to theta = 28.36	99.8 %
Absorption correction	semi-empirical from equivalents
Max. and min. transmission	0.7457 and 0.6921
Refinement method	full-matrix least-squares on F^2
Data / restraints / parameters	10934 / 1 / 559
Goodness-of-fit on F^2	1.032
Final R indices [I>2σ(I)]	R1 = 0.0171, wR2 = 0.0422
R indices (all data)	R1 = 0.0191, wR2 = 0.0431
Absolute structure parameter	-0.033(11)
Extinction coefficient	0.0021(2)
Largest diff. peak and hole	0.260 and -0.275 $e \cdot Å^{-3}$

Table 18.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **18**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	4747(1)	258(1)	7858(1)	9(1)
S(1)	4137(1)	-183(1)	10437(1)	13(1)
F(1)	2849(1)	-1439(1)	9957(1)	29(1)
O(1)	3866(1)	-113(1)	9135(1)	14(1)
N(1)	6181(1)	1311(1)	10257(1)	13(1)
C(1)	5312(1)	1176(1)	9162(1)	12(1)
S(2)	2334(1)	-985(1)	6745(1)	16(1)
F(2)	1626(1)	-477(1)	9808(1)	24(1)
O(2)	5294(1)	-610(1)	11060(1)	22(1)
C(2)	5759(1)	1932(1)	10846(1)	17(1)
N(2)	4362(1)	1697(1)	8866(1)	14(1)
N(3)	5234(1)	675(1)	6791(1)	12(1)
O(3)	3950(1)	494(1)	10980(1)	20(1)
F(3)	2871(1)	-879(1)	11556(1)	30(1)
C(3)	4608(2)	2269(1)	9805(1)	19(1)
F(4)	887(1)	-569(1)	4561(1)	30(1)
O(4)	3061(1)	-289(1)	6730(1)	15(1)
C(4)	7319(1)	846(1)	10927(1)	14(1)
F(5)	2547(1)	-1250(1)	4676(1)	26(1)
O(5)	1250(1)	-871(1)	7112(1)	26(1)
C(5)	7446(2)	755(1)	12242(1)	20(1)
F(6)	852(1)	-1743(1)	4883(1)	33(1)
C(6)	8602(1)	1148(1)	10879(1)	14(1)
O(6)	3187(1)	-1605(1)	7222(1)	24(1)
C(7)	8754(1)	1867(1)	10555(1)	18(1)
C(8)	9974(2)	2116(1)	10580(1)	22(1)
C(9)	11032(2)	1640(1)	10912(1)	23(1)
C(10)	10891(2)	916(1)	11228(1)	22(1)
C(11)	9686(2)	672(1)	11225(1)	18(1)
C(12)	3408(1)	1802(1)	7666(1)	15(1)
C(13)	3754(2)	2261(1)	6870(1)	18(1)
C(14)	2842(2)	2373(1)	5725(1)	22(1)
C(15)	1604(2)	2040(1)	5334(2)	24(1)
C(16)	1279(2)	1607(1)	6140(1)	22(1)
C(17)	2150(2)	1487(1)	7325(1)	18(1)
C(18)	5068(2)	2647(1)	7270(2)	21(1)
C(19)	658(2)	2156(1)	4058(2)	36(1)
C(20)	1681(1)	1066(1)	8173(2)	21(1)
C(21)	5551(1)	1052(1)	5921(1)	14(1)
C(22)	6771(2)	1411(1)	6244(1)	17(1)
C(23)	7006(2)	1826(1)	5357(2)	24(1)
C(24)	6074(2)	1875(1)	4206(2)	28(1)
C(25)	4883(2)	1501(1)	3899(1)	25(1)
C(26)	4595(2)	1084(1)	4741(1)	18(1)

C(27)	7793(2)	1365(1)	7489(2)	22(1)
C(28)	3312(2)	680(1)	4428(1)	21(1)
C(29)	6064(1)	-477(1)	8368(1)	12(1)
C(30)	7101(1)	-863(1)	8012(1)	13(1)
C(31)	8458(1)	-640(1)	8922(1)	20(1)
C(32)	6932(2)	-1706(1)	8144(1)	19(1)
C(33)	6948(1)	-717(1)	6714(1)	13(1)
C(34)	7986(2)	-491(1)	6379(2)	20(1)
C(35)	7809(2)	-407(1)	5177(2)	28(1)
C(36)	6605(2)	-545(1)	4283(2)	25(1)
C(37)	5563(2)	-774(1)	4600(1)	21(1)
C(38)	5736(1)	-862(1)	5795(1)	15(1)
C(39)	2784(1)	-778(1)	10426(1)	18(1)
C(40)	1610(2)	-1140(1)	5120(2)	21(1)
C(1X)	9171(2)	8025(1)	1999(2)	21(1)
Cl(1X)	10575(1)	8470(1)	1926(1)	23(1)
Cl(2X)	7871(1)	8651(1)	1805(1)	26(1)

Table 18.3. Bond lengths [Å] and angles [°] for **18**.

Mo(1)-N(3)	1.7264(12)
Mo(1)-C(29)	1.8869(14)
Mo(1)-O(4)	2.0895(10)
Mo(1)-O(1)	2.1908(10)
Mo(1)-C(1)	2.2015(14)
S(1)-O(3)	1.4334(11)
S(1)-O(2)	1.4340(11)
S(1)-O(1)	1.4793(10)
S(1)-C(39)	1.8248(15)
F(1)-C(39)	1.3299(19)
N(1)-C(1)	1.3277(18)
N(1)-C(4)	1.4706(18)
N(1)-C(2)	1.4851(18)
C(1)-N(2)	1.3489(18)
S(2)-O(5)	1.4233(11)
S(2)-O(6)	1.4329(12)
S(2)-O(4)	1.4895(10)
S(2)-C(40)	1.8305(17)
F(2)-C(39)	1.3256(17)
C(2)-C(3)	1.533(2)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
N(2)-C(12)	1.4429(18)
N(2)-C(3)	1.4759(18)
N(3)-C(21)	1.3897(19)
F(3)-C(39)	1.3334(18)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
F(4)-C(40)	1.322(2)

C(4)-C(6)	1.5260(19)
C(4)-C(5)	1.537(2)
C(4)-H(4)	1.0000
F(5)-C(40)	1.3324(19)
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800
F(6)-C(40)	1.3338(18)
C(6)-C(7)	1.382(2)
C(6)-C(11)	1.398(2)
C(7)-C(8)	1.399(2)
C(7)-H(7)	0.9500
C(8)-C(9)	1.378(2)
C(8)-H(8)	0.9500
C(9)-C(10)	1.384(2)
C(9)-H(9)	0.9500
C(10)-C(11)	1.389(2)
C(10)-H(10)	0.9500
C(11)-H(11)	0.9500
C(12)-C(17)	1.404(2)
C(12)-C(13)	1.415(2)
C(13)-C(14)	1.381(2)
C(13)-C(18)	1.508(2)
C(14)-C(15)	1.396(2)
C(14)-H(14)	0.9500
C(15)-C(16)	1.385(3)
C(15)-C(19)	1.510(2)
C(16)-C(17)	1.404(2)
C(16)-H(16)	0.9500
C(17)-C(20)	1.501(2)
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-C(22)	1.405(2)
C(21)-C(26)	1.415(2)
C(22)-C(23)	1.398(2)
C(22)-C(27)	1.500(2)
C(23)-C(24)	1.382(2)
C(23)-H(23)	0.9500
C(24)-C(25)	1.391(3)
C(24)-H(24)	0.9500
C(25)-C(26)	1.384(2)
C(25)-H(25)	0.9500
C(26)-C(28)	1.501(2)

C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-C(30)	1.5196(19)
C(29)-H(29)	0.9500
C(30)-C(33)	1.522(2)
C(30)-C(31)	1.5361(19)
C(30)-C(32)	1.548(2)
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(34)	1.397(2)
C(33)-C(38)	1.401(2)
C(34)-C(35)	1.387(2)
C(34)-H(34)	0.9500
C(35)-C(36)	1.380(3)
C(35)-H(35)	0.9500
C(36)-C(37)	1.391(2)
C(36)-H(36)	0.9500
C(37)-C(38)	1.382(2)
C(37)-H(37)	0.9500
C(38)-H(38)	0.9500
C(1X)-Cl(2X)	1.7636(17)
C(1X)-Cl(1X)	1.7643(16)
C(1X)-H(1X1)	0.9900
C(1X)-H(1X2)	0.9900

N(3)-Mo(1)-C(29)	97.92(6)
N(3)-Mo(1)-O(4)	99.66(5)
C(29)-Mo(1)-O(4)	105.36(5)
N(3)-Mo(1)-O(1)	169.77(5)
C(29)-Mo(1)-O(1)	92.28(5)
O(4)-Mo(1)-O(1)	78.20(4)
N(3)-Mo(1)-C(1)	96.54(5)
C(29)-Mo(1)-C(1)	108.49(5)
O(4)-Mo(1)-C(1)	139.81(4)
O(1)-Mo(1)-C(1)	79.42(4)
O(3)-S(1)-O(2)	117.94(7)
O(3)-S(1)-O(1)	113.43(6)
O(2)-S(1)-O(1)	112.93(6)
O(3)-S(1)-C(39)	104.68(7)
O(2)-S(1)-C(39)	104.28(7)
O(1)-S(1)-C(39)	101.20(6)
S(1)-O(1)-Mo(1)	142.28(6)

C(1)-N(1)-C(4)	126.02(12)
C(1)-N(1)-C(2)	111.85(11)
C(4)-N(1)-C(2)	121.41(11)
N(1)-C(1)-N(2)	109.51(12)
N(1)-C(1)-Mo(1)	138.56(10)
N(2)-C(1)-Mo(1)	110.45(9)
O(5)-S(2)-O(6)	118.98(8)
O(5)-S(2)-O(4)	113.04(7)
O(6)-S(2)-O(4)	112.92(6)
O(5)-S(2)-C(40)	105.39(7)
O(6)-S(2)-C(40)	105.55(7)
O(4)-S(2)-C(40)	98.06(7)
N(1)-C(2)-C(3)	102.70(11)
N(1)-C(2)-H(2A)	111.2
C(3)-C(2)-H(2A)	111.2
N(1)-C(2)-H(2B)	111.2
C(3)-C(2)-H(2B)	111.2
H(2A)-C(2)-H(2B)	109.1
C(1)-N(2)-C(12)	123.98(12)
C(1)-N(2)-C(3)	112.36(12)
C(12)-N(2)-C(3)	121.84(12)
C(21)-N(3)-Mo(1)	175.50(11)
N(2)-C(3)-C(2)	101.92(11)
N(2)-C(3)-H(3A)	111.4
C(2)-C(3)-H(3A)	111.4
N(2)-C(3)-H(3B)	111.4
C(2)-C(3)-H(3B)	111.4
H(3A)-C(3)-H(3B)	109.2
S(2)-O(4)-Mo(1)	137.62(6)
N(1)-C(4)-C(6)	112.52(11)
N(1)-C(4)-C(5)	110.92(12)
C(6)-C(4)-C(5)	109.77(11)
N(1)-C(4)-H(4)	107.8
C(6)-C(4)-H(4)	107.8
C(5)-C(4)-H(4)	107.8
C(4)-C(5)-H(5A)	109.5
C(4)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(4)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(7)-C(6)-C(11)	118.84(13)
C(7)-C(6)-C(4)	123.57(13)
C(11)-C(6)-C(4)	117.55(13)
C(6)-C(7)-C(8)	120.57(14)
C(6)-C(7)-H(7)	119.7
C(8)-C(7)-H(7)	119.7
C(9)-C(8)-C(7)	120.00(15)
C(9)-C(8)-H(8)	120.0
C(7)-C(8)-H(8)	120.0

C(8)-C(9)-C(10)	120.06(14)
C(8)-C(9)-H(9)	120.0
C(10)-C(9)-H(9)	120.0
C(9)-C(10)-C(11)	119.96(15)
C(9)-C(10)-H(10)	120.0
C(11)-C(10)-H(10)	120.0
C(10)-C(11)-C(6)	120.55(15)
C(10)-C(11)-H(11)	119.7
C(6)-C(11)-H(11)	119.7
C(17)-C(12)-C(13)	121.20(14)
C(17)-C(12)-N(2)	120.61(14)
C(13)-C(12)-N(2)	118.12(13)
C(14)-C(13)-C(12)	118.55(14)
C(14)-C(13)-C(18)	120.28(15)
C(12)-C(13)-C(18)	121.12(13)
C(13)-C(14)-C(15)	121.90(16)
C(13)-C(14)-H(14)	119.1
C(15)-C(14)-H(14)	119.1
C(16)-C(15)-C(14)	118.36(15)
C(16)-C(15)-C(19)	121.68(17)
C(14)-C(15)-C(19)	119.96(17)
C(15)-C(16)-C(17)	122.50(15)
C(15)-C(16)-H(16)	118.7
C(17)-C(16)-H(16)	118.7
C(12)-C(17)-C(16)	117.37(15)
C(12)-C(17)-C(20)	123.43(14)
C(16)-C(17)-C(20)	119.14(14)
C(13)-C(18)-H(18A)	109.5
C(13)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(13)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(15)-C(19)-H(19A)	109.5
C(15)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(15)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(17)-C(20)-H(20A)	109.5
C(17)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(17)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
N(3)-C(21)-C(22)	119.59(13)
N(3)-C(21)-C(26)	118.06(13)
C(22)-C(21)-C(26)	122.29(14)
C(23)-C(22)-C(21)	117.42(14)
C(23)-C(22)-C(27)	120.33(14)

C(21)-C(22)-C(27)	122.24(14)
C(24)-C(23)-C(22)	121.03(15)
C(24)-C(23)-H(23)	119.5
C(22)-C(23)-H(23)	119.5
C(23)-C(24)-C(25)	120.57(15)
C(23)-C(24)-H(24)	119.7
C(25)-C(24)-H(24)	119.7
C(26)-C(25)-C(24)	120.93(15)
C(26)-C(25)-H(25)	119.5
C(24)-C(25)-H(25)	119.5
C(25)-C(26)-C(21)	117.73(15)
C(25)-C(26)-C(28)	121.66(14)
C(21)-C(26)-C(28)	120.61(14)
C(22)-C(27)-H(27A)	109.5
C(22)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(22)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(26)-C(28)-H(28A)	109.5
C(26)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(26)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(30)-C(29)-Mo(1)	142.33(10)
C(30)-C(29)-H(29)	108.8
Mo(1)-C(29)-H(29)	108.8
C(29)-C(30)-C(33)	113.19(11)
C(29)-C(30)-C(31)	107.96(12)
C(33)-C(30)-C(31)	113.12(12)
C(29)-C(30)-C(32)	106.97(11)
C(33)-C(30)-C(32)	107.52(12)
C(31)-C(30)-C(32)	107.77(12)
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(34)-C(33)-C(38)	117.68(14)
C(34)-C(33)-C(30)	123.16(13)
C(38)-C(33)-C(30)	119.01(13)
C(35)-C(34)-C(33)	120.74(15)

C(35)-C(34)-H(34)	119.6
C(33)-C(34)-H(34)	119.6
C(36)-C(35)-C(34)	120.90(16)
C(36)-C(35)-H(35)	119.5
C(34)-C(35)-H(35)	119.5
C(35)-C(36)-C(37)	119.13(15)
C(35)-C(36)-H(36)	120.4
C(37)-C(36)-H(36)	120.4
C(38)-C(37)-C(36)	120.21(15)
C(38)-C(37)-H(37)	119.9
C(36)-C(37)-H(37)	119.9
C(37)-C(38)-C(33)	121.32(14)
C(37)-C(38)-H(38)	119.3
C(33)-C(38)-H(38)	119.3
F(2)-C(39)-F(1)	108.64(12)
F(2)-C(39)-F(3)	108.50(12)
F(1)-C(39)-F(3)	108.11(13)
F(2)-C(39)-S(1)	111.73(10)
F(1)-C(39)-S(1)	111.18(10)
F(3)-C(39)-S(1)	108.57(10)
F(4)-C(40)-F(5)	108.67(14)
F(4)-C(40)-F(6)	108.57(13)
F(5)-C(40)-F(6)	107.63(13)
F(4)-C(40)-S(2)	111.30(11)
F(5)-C(40)-S(2)	110.53(10)
F(6)-C(40)-S(2)	110.03(12)
Cl(2X)-C(1X)-Cl(1X)	112.20(9)
Cl(2X)-C(1X)-H(1X1)	109.2
Cl(1X)-C(1X)-H(1X1)	109.2
Cl(2X)-C(1X)-H(1X2)	109.2
Cl(1X)-C(1X)-H(1X2)	109.2
H(1X1)-C(1X)-H(1X2)	107.9

Table 18.4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **18**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	9(1)	10(1)	9(1)	-1(1)	3(1)	0(1)
S(1)	11(1)	17(1)	14(1)	0(1)	6(1)	-2(1)
F(1)	33(1)	16(1)	41(1)	-3(1)	17(1)	-6(1)
O(1)	14(1)	16(1)	15(1)	-1(1)	7(1)	-2(1)
N(1)	13(1)	13(1)	12(1)	-2(1)	4(1)	-1(1)
C(1)	12(1)	12(1)	13(1)	1(1)	6(1)	-2(1)
S(2)	15(1)	15(1)	17(1)	-3(1)	6(1)	-4(1)
F(2)	12(1)	31(1)	30(1)	0(1)	8(1)	-2(1)
O(2)	14(1)	31(1)	20(1)	7(1)	5(1)	4(1)
C(2)	18(1)	19(1)	15(1)	-6(1)	5(1)	1(1)
N(2)	13(1)	14(1)	13(1)	-4(1)	3(1)	1(1)

N(3)	11(1)	12(1)	12(1)	-2(1)	3(1)	1(1)
O(3)	23(1)	21(1)	19(1)	-5(1)	11(1)	-5(1)
F(3)	28(1)	41(1)	25(1)	8(1)	16(1)	-9(1)
C(3)	19(1)	19(1)	18(1)	-8(1)	4(1)	4(1)
F(4)	24(1)	37(1)	22(1)	-3(1)	-1(1)	3(1)
O(4)	13(1)	16(1)	14(1)	-2(1)	2(1)	-3(1)
C(4)	14(1)	12(1)	12(1)	0(1)	2(1)	-2(1)
F(5)	23(1)	36(1)	21(1)	-9(1)	10(1)	-6(1)
O(5)	19(1)	34(1)	28(1)	-9(1)	13(1)	-8(1)
C(5)	20(1)	27(1)	12(1)	4(1)	3(1)	-4(1)
F(6)	33(1)	36(1)	29(1)	-15(1)	11(1)	-22(1)
C(6)	13(1)	16(1)	10(1)	-3(1)	2(1)	-2(1)
O(6)	30(1)	17(1)	24(1)	1(1)	8(1)	1(1)
C(7)	16(1)	20(1)	16(1)	0(1)	4(1)	-1(1)
C(8)	23(1)	24(1)	20(1)	0(1)	7(1)	-9(1)
C(9)	17(1)	35(1)	19(1)	-10(1)	9(1)	-8(1)
C(10)	15(1)	30(1)	18(1)	-11(1)	3(1)	3(1)
C(11)	20(1)	16(1)	15(1)	-4(1)	3(1)	0(1)
C(12)	16(1)	14(1)	14(1)	-2(1)	3(1)	5(1)
C(13)	21(1)	12(1)	18(1)	-3(1)	5(1)	5(1)
C(14)	29(1)	18(1)	17(1)	1(1)	7(1)	8(1)
C(15)	23(1)	27(1)	16(1)	-5(1)	2(1)	13(1)
C(16)	14(1)	23(1)	23(1)	-10(1)	0(1)	5(1)
C(17)	16(1)	16(1)	20(1)	-5(1)	5(1)	5(1)
C(18)	25(1)	15(1)	24(1)	1(1)	9(1)	-1(1)
C(19)	35(1)	45(1)	19(1)	-6(1)	-2(1)	16(1)
C(20)	13(1)	21(1)	29(1)	-2(1)	7(1)	2(1)
C(21)	20(1)	12(1)	13(1)	1(1)	8(1)	1(1)
C(22)	22(1)	14(1)	18(1)	-1(1)	10(1)	0(1)
C(23)	32(1)	18(1)	28(1)	1(1)	19(1)	-5(1)
C(24)	48(1)	21(1)	22(1)	6(1)	22(1)	-1(1)
C(25)	41(1)	22(1)	14(1)	4(1)	11(1)	4(1)
C(26)	25(1)	14(1)	15(1)	1(1)	8(1)	4(1)
C(27)	17(1)	25(1)	23(1)	-1(1)	7(1)	-6(1)
C(28)	23(1)	22(1)	15(1)	0(1)	2(1)	2(1)
C(29)	13(1)	13(1)	11(1)	0(1)	3(1)	0(1)
C(30)	12(1)	15(1)	12(1)	1(1)	4(1)	1(1)
C(31)	14(1)	27(1)	14(1)	0(1)	2(1)	2(1)
C(32)	24(1)	15(1)	19(1)	4(1)	10(1)	5(1)
C(33)	15(1)	12(1)	14(1)	-2(1)	7(1)	2(1)
C(34)	18(1)	23(1)	22(1)	-1(1)	10(1)	-2(1)
C(35)	36(1)	27(1)	30(1)	1(1)	24(1)	-2(1)
C(36)	42(1)	23(1)	15(1)	2(1)	14(1)	4(1)
C(37)	25(1)	20(1)	16(1)	-3(1)	5(1)	6(1)
C(38)	17(1)	14(1)	17(1)	-1(1)	8(1)	3(1)
C(39)	17(1)	20(1)	20(1)	1(1)	9(1)	-3(1)
C(40)	18(1)	23(1)	21(1)	-7(1)	6(1)	-7(1)
C(1X)	21(1)	17(1)	26(1)	2(1)	7(1)	-4(1)
Cl(1X)	18(1)	28(1)	22(1)	0(1)	7(1)	-4(1)

Cl(2X)	23(1)	27(1)	33(1)	1(1)	15(1)	0(1)

Table 18.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **18**.

	x	y	z	U(eq)
H(2A)	6476	2298	11188	21
H(2B)	5472	1750	11490	21
H(3A)	3830	2341	10029	23
H(3B)	4853	2748	9544	23
H(4)	7170	343	10548	16
H(5A)	7690	1232	12659	31
H(5B)	8124	386	12638	31
H(5C)	6603	591	12268	31
H(7)	8024	2195	10314	21
H(8)	10073	2614	10368	27
H(9)	11859	1808	10924	28
H(10)	11618	586	11447	26
H(11)	9598	178	11461	22
H(14)	3063	2684	5188	26
H(16)	435	1383	5880	27
H(18A)	5313	2735	6572	32
H(18B)	5734	2334	7851	32
H(18C)	5010	3121	7646	32
H(19A)	908	1835	3516	55
H(19B)	686	2675	3830	55
H(19C)	-235	2031	4001	55
H(20A)	2328	1112	8994	32
H(20B)	1573	542	7942	32
H(20C)	837	1268	8138	32
H(23)	7820	2079	5548	28
H(24)	6248	2166	3619	33
H(25)	4259	1533	3100	30
H(27A)	8382	947	7535	33
H(27B)	7363	1291	8068	33
H(27C)	8302	1826	7676	33
H(28A)	2706	844	3637	32
H(28B)	2931	789	5034	32
H(28C)	3462	146	4409	32
H(29)	6087	-677	9110	15
H(31A)	9142	-916	8752	29
H(31B)	8505	-756	9737	29
H(31C)	8591	-107	8857	29
H(32A)	6030	-1851	7655	28
H(32B)	7113	-1825	8989	28
H(32C)	7547	-1977	7871	28
H(34)	8822	-393	6982	24
H(35)	8526	-254	4967	33

H(36)	6490	-484	3461	30
H(37)	4729	-869	3992	25
H(38)	5018	-1024	5999	18
H(1X1)	8875	7639	1368	26
H(1X2)	9406	7777	2789	26

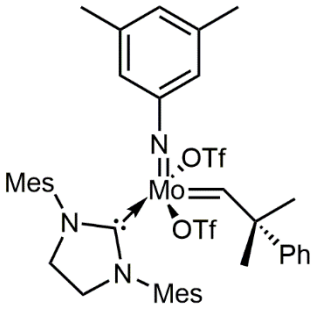
Table 18.6. Torsion angles [°] for **18**.

O(3)-S(1)-O(1)-Mo(1)	81.25(11)
O(2)-S(1)-O(1)-Mo(1)	-56.30(12)
C(39)-S(1)-O(1)-Mo(1)	-167.20(10)
N(3)-Mo(1)-O(1)-S(1)	-111.6(3)
C(29)-Mo(1)-O(1)-S(1)	64.27(11)
O(4)-Mo(1)-O(1)-S(1)	169.49(11)
C(1)-Mo(1)-O(1)-S(1)	-44.11(10)
C(4)-N(1)-C(1)-N(2)	176.38(12)
C(2)-N(1)-C(1)-N(2)	6.04(16)
C(4)-N(1)-C(1)-Mo(1)	12.3(2)
C(2)-N(1)-C(1)-Mo(1)	-158.01(12)
N(3)-Mo(1)-C(1)-N(1)	-113.40(15)
C(29)-Mo(1)-C(1)-N(1)	-12.76(16)
O(4)-Mo(1)-C(1)-N(1)	133.17(14)
O(1)-Mo(1)-C(1)-N(1)	76.10(15)
N(3)-Mo(1)-C(1)-N(2)	82.65(10)
C(29)-Mo(1)-C(1)-N(2)	-176.71(9)
O(4)-Mo(1)-C(1)-N(2)	-30.78(13)
O(1)-Mo(1)-C(1)-N(2)	-87.85(10)
C(1)-N(1)-C(2)-C(3)	-11.79(16)
C(4)-N(1)-C(2)-C(3)	177.36(12)
N(1)-C(1)-N(2)-C(12)	167.70(13)
Mo(1)-C(1)-N(2)-C(12)	-23.50(16)
N(1)-C(1)-N(2)-C(3)	2.89(17)
Mo(1)-C(1)-N(2)-C(3)	171.69(10)
C(29)-Mo(1)-N(3)-C(21)	-174.3(14)
O(4)-Mo(1)-N(3)-C(21)	78.6(14)
O(1)-Mo(1)-N(3)-C(21)	1.6(16)
C(1)-Mo(1)-N(3)-C(21)	-64.5(14)
C(1)-N(2)-C(3)-C(2)	-9.87(16)
C(12)-N(2)-C(3)-C(2)	-175.05(12)
N(1)-C(2)-C(3)-N(2)	12.09(15)
O(5)-S(2)-O(4)-Mo(1)	97.55(10)
O(6)-S(2)-O(4)-Mo(1)	-41.16(12)
C(40)-S(2)-O(4)-Mo(1)	-151.88(10)
N(3)-Mo(1)-O(4)-S(2)	148.01(10)
C(29)-Mo(1)-O(4)-S(2)	46.95(11)
O(1)-Mo(1)-O(4)-S(2)	-42.18(9)
C(1)-Mo(1)-O(4)-S(2)	-99.62(11)
C(1)-N(1)-C(4)-C(6)	100.60(15)
C(2)-N(1)-C(4)-C(6)	-89.92(15)

C(1)-N(1)-C(4)-C(5)	-136.00(14)
C(2)-N(1)-C(4)-C(5)	33.48(17)
N(1)-C(4)-C(6)-C(7)	17.37(19)
C(5)-C(4)-C(6)-C(7)	-106.68(16)
N(1)-C(4)-C(6)-C(11)	-164.94(12)
C(5)-C(4)-C(6)-C(11)	71.02(16)
C(11)-C(6)-C(7)-C(8)	-0.4(2)
C(4)-C(6)-C(7)-C(8)	177.29(14)
C(6)-C(7)-C(8)-C(9)	1.0(2)
C(7)-C(8)-C(9)-C(10)	-0.4(2)
C(8)-C(9)-C(10)-C(11)	-0.8(2)
C(9)-C(10)-C(11)-C(6)	1.4(2)
C(7)-C(6)-C(11)-C(10)	-0.8(2)
C(4)-C(6)-C(11)-C(10)	-178.65(13)
C(1)-N(2)-C(12)-C(17)	97.15(17)
C(3)-N(2)-C(12)-C(17)	-99.42(17)
C(1)-N(2)-C(12)-C(13)	-86.01(18)
C(3)-N(2)-C(12)-C(13)	77.42(18)
C(17)-C(12)-C(13)-C(14)	-2.4(2)
N(2)-C(12)-C(13)-C(14)	-179.23(13)
C(17)-C(12)-C(13)-C(18)	175.17(13)
N(2)-C(12)-C(13)-C(18)	-1.7(2)
C(12)-C(13)-C(14)-C(15)	-0.7(2)
C(18)-C(13)-C(14)-C(15)	-178.32(14)
C(13)-C(14)-C(15)-C(16)	2.1(2)
C(13)-C(14)-C(15)-C(19)	-177.68(15)
C(14)-C(15)-C(16)-C(17)	-0.5(2)
C(19)-C(15)-C(16)-C(17)	179.34(15)
C(13)-C(12)-C(17)-C(16)	3.9(2)
N(2)-C(12)-C(17)-C(16)	-179.33(13)
C(13)-C(12)-C(17)-C(20)	-173.15(13)
N(2)-C(12)-C(17)-C(20)	3.6(2)
C(15)-C(16)-C(17)-C(12)	-2.5(2)
C(15)-C(16)-C(17)-C(20)	174.72(14)
Mo(1)-N(3)-C(21)-C(22)	112.8(14)
Mo(1)-N(3)-C(21)-C(26)	-64.6(14)
N(3)-C(21)-C(22)-C(23)	-175.61(13)
C(26)-C(21)-C(22)-C(23)	1.7(2)
N(3)-C(21)-C(22)-C(27)	3.9(2)
C(26)-C(21)-C(22)-C(27)	-178.78(14)
C(21)-C(22)-C(23)-C(24)	-0.4(2)
C(27)-C(22)-C(23)-C(24)	-179.96(15)
C(22)-C(23)-C(24)-C(25)	-0.9(3)
C(23)-C(24)-C(25)-C(26)	1.1(3)
C(24)-C(25)-C(26)-C(21)	0.1(2)
C(24)-C(25)-C(26)-C(28)	179.62(15)
N(3)-C(21)-C(26)-C(25)	175.80(14)
C(22)-C(21)-C(26)-C(25)	-1.6(2)
N(3)-C(21)-C(26)-C(28)	-3.7(2)
C(22)-C(21)-C(26)-C(28)	178.95(14)

N(3)-Mo(1)-C(29)-C(30)	-15.64(17)
O(4)-Mo(1)-C(29)-C(30)	86.71(16)
O(1)-Mo(1)-C(29)-C(30)	165.10(16)
C(1)-Mo(1)-C(29)-C(30)	-115.30(16)
Mo(1)-C(29)-C(30)-C(33)	-13.2(2)
Mo(1)-C(29)-C(30)-C(31)	112.82(16)
Mo(1)-C(29)-C(30)-C(32)	-131.43(15)
C(29)-C(30)-C(33)-C(34)	130.63(14)
C(31)-C(30)-C(33)-C(34)	7.4(2)
C(32)-C(30)-C(33)-C(34)	-111.45(15)
C(29)-C(30)-C(33)-C(38)	-53.75(17)
C(31)-C(30)-C(33)-C(38)	-176.97(13)
C(32)-C(30)-C(33)-C(38)	64.17(16)
C(38)-C(33)-C(34)-C(35)	0.6(2)
C(30)-C(33)-C(34)-C(35)	176.26(15)
C(33)-C(34)-C(35)-C(36)	0.1(3)
C(34)-C(35)-C(36)-C(37)	-0.3(3)
C(35)-C(36)-C(37)-C(38)	-0.1(2)
C(36)-C(37)-C(38)-C(33)	0.7(2)
C(34)-C(33)-C(38)-C(37)	-1.0(2)
C(30)-C(33)-C(38)-C(37)	-176.85(13)
O(3)-S(1)-C(39)-F(2)	59.42(12)
O(2)-S(1)-C(39)-F(2)	-176.08(10)
O(1)-S(1)-C(39)-F(2)	-58.67(12)
O(3)-S(1)-C(39)-F(1)	-179.01(11)
O(2)-S(1)-C(39)-F(1)	-54.51(12)
O(1)-S(1)-C(39)-F(1)	62.90(12)
O(3)-S(1)-C(39)-F(3)	-60.20(12)
O(2)-S(1)-C(39)-F(3)	64.30(12)
O(1)-S(1)-C(39)-F(3)	-178.29(10)
O(5)-S(2)-C(40)-F(4)	58.82(13)
O(6)-S(2)-C(40)-F(4)	-174.44(11)
O(4)-S(2)-C(40)-F(4)	-57.85(12)
O(5)-S(2)-C(40)-F(5)	179.68(11)
O(6)-S(2)-C(40)-F(5)	-53.58(13)
O(4)-S(2)-C(40)-F(5)	63.01(12)
O(5)-S(2)-C(40)-F(6)	-61.58(13)
O(6)-S(2)-C(40)-F(6)	65.16(13)
O(4)-S(2)-C(40)-F(6)	-178.25(11)

Complex 19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OTf
Mes
Mo
N
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Ph
N
Mes

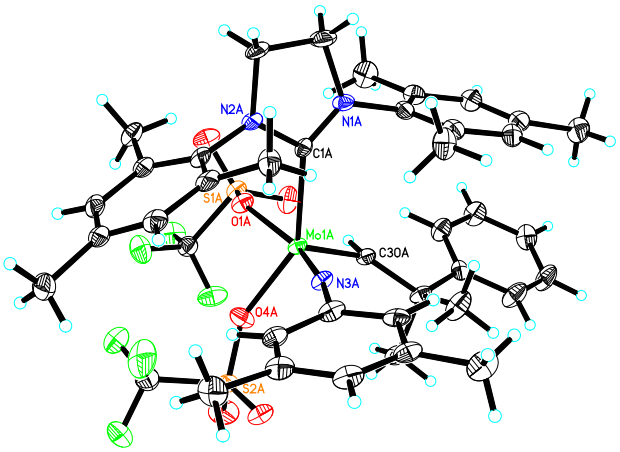

N2A
N1A
C1A
S1A
O1A
Mo1A
C30A
N3A
O4A
S2A

Table 19.1. Crystal data and structure refinement for **19**.

Empirical formula	$C_{41}H_{47}F_6MoN_3O_6S_2$
Formula weight	951.88
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, *P*c
Unit cell dimensions	a = 10.5710(6) Å α = 90°
	b = 20.9882(13) Å β = 96.356(3)°
	c = 19.0812(10) Å γ = 90°
Volume	4207.5(4) $Å^3$
Z, Calculated density	4, 1.503 Mg/m^3
Absorption coefficient	0.487 mm^{-1}
F(000)	1960
Crystal size	0.44 x 0.33 x 0.17 mm
Theta range for data collection	1.94 to 27.50 °.
Limiting indices	-13<=h<=13, -26<=k<=27, -24<=l<=24
Reflections collected / unique	37540 / 16193 [R(int) = 0.0482]
Completeness to theta = 27.50	98.1 %
Absorption correction	Numerical
Max. and min. transmission	0.9951 and 0.7340
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	16193 / 28 / 1089
Goodness-of-fit on F^2	1.032
Final R indices [I>2σ(I)]	R1 = 0.0468, wR2 = 0.1130
R indices (all data)	R1 = 0.0558, wR2 = 0.1179
Absolute structure parameter	0.04(2)
Largest diff. peak and hole	1.180 and -1.495 $e.Å^{-3}$

Table 19.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **19**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1A)	1776(1)	5290(1)	4098(1)	14(1)
C(1A)	2506(5)	4780(2)	3216(2)	15(1)
N(1A)	2180(4)	4231(2)	2891(2)	19(1)
C(2A)	2825(6)	4135(3)	2246(3)	35(1)
N(2A)	3283(4)	5104(2)	2829(2)	20(1)
N(3A)	3058(4)	5128(2)	4718(2)	15(1)
C(3A)	3534(6)	4756(2)	2187(3)	27(1)
C(4A)	1498(5)	3707(2)	3160(2)	19(1)
C(5A)	284(5)	3564(2)	2854(2)	21(1)
C(6A)	-326(5)	3039(2)	3112(3)	23(1)
C(7A)	251(5)	2673(2)	3659(3)	23(1)
C(8A)	1485(5)	2816(2)	3938(3)	23(1)
C(9A)	2140(5)	3333(2)	3692(3)	21(1)
C(10A)	-392(5)	3964(3)	2270(3)	31(1)
C(11A)	-460(5)	2131(2)	3960(3)	31(1)
C(12A)	3486(5)	3464(3)	3978(3)	31(1)
C(13A)	3939(5)	5678(2)	3059(2)	20(1)
C(14A)	3519(5)	6273(2)	2818(3)	22(1)
C(15A)	4155(5)	6811(2)	3088(3)	24(1)
C(16A)	5230(5)	6770(2)	3577(2)	21(1)
C(17A)	5709(5)	6173(2)	3757(3)	23(1)
C(18A)	5095(5)	5617(2)	3510(2)	22(1)
C(19A)	2425(5)	6348(3)	2228(3)	25(1)
C(20A)	5869(5)	7364(2)	3907(3)	29(1)
C(21A)	5664(5)	4979(2)	3702(3)	26(1)
C(22A)	4179(5)	5100(3)	5184(3)	19(1)
C(23A)	4947(5)	5643(2)	5264(2)	21(1)
C(24A)	6094(4)	5628(2)	5686(2)	22(1)
C(25A)	6430(5)	5073(2)	6074(3)	22(1)
C(26A)	5646(5)	4533(2)	6027(2)	22(1)
C(27A)	4523(5)	4545(2)	5560(2)	20(1)
C(28A)	6997(5)	6184(3)	5707(3)	28(1)
C(29A)	5977(5)	3959(3)	6475(3)	29(1)
C(30A)	527(5)	4742(2)	4387(2)	17(1)
C(31A)	139(4)	4391(2)	5016(2)	17(1)
C(32A)	1279(5)	4049(3)	5420(3)	31(1)
C(33A)	-321(6)	4907(3)	5509(3)	31(1)
C(34A)	-989(5)	3927(2)	4835(2)	18(1)
C(35A)	-1750(5)	3941(2)	4208(3)	25(1)
C(36A)	-2803(5)	3535(3)	4083(3)	28(1)
C(37A)	-3102(5)	3113(2)	4592(3)	27(1)
C(38A)	-2356(6)	3109(3)	5227(3)	33(1)
C(39A)	-1315(5)	3499(3)	5350(3)	32(1)
S(1A)	-654(1)	5803(1)	2847(1)	19(1)

O(1A)	651(3)	5710(2)	3216(2)	20(1)
O(2A)	-1565(3)	5375(2)	3090(2)	29(1)
O(3A)	-650(3)	5875(2)	2105(2)	26(1)
C(40A)	-1074(5)	6596(2)	3160(3)	24(1)
F(1A)	-1263(3)	6580(2)	3831(2)	32(1)
F(2A)	-2126(3)	6797(2)	2781(2)	32(1)
F(3A)	-138(3)	7005(1)	3086(2)	35(1)
S(2A)	1406(1)	6567(1)	5151(1)	21(1)
O(4A)	1226(4)	6164(2)	4512(2)	25(1)
O(5A)	2266(4)	6303(2)	5701(2)	31(1)
O(6A)	236(4)	6841(2)	5325(2)	38(1)
C(41A)	2258(5)	7232(2)	4809(3)	28(1)
F(4A)	2323(3)	7713(2)	5259(2)	42(1)
F(5A)	3453(3)	7058(2)	4721(2)	48(1)
F(6A)	1700(4)	7436(2)	4197(2)	41(1)
Mo(1B)	3359(1)	10093(1)	6741(1)	14(1)
N(1B)	1783(4)	9885(2)	7938(2)	18(1)
C(1B)	2624(4)	9552(2)	7611(2)	15(1)
N(2B)	2845(4)	8998(2)	7931(2)	19(1)
C(2B)	1413(6)	9555(2)	8568(3)	27(1)
N(3B)	2149(4)	9884(2)	6084(2)	17(1)
C(3B)	2008(5)	8897(2)	8500(3)	25(1)
C(4B)	1214(4)	10473(2)	7664(2)	18(1)
C(5B)	118(5)	10425(2)	7168(2)	22(1)
C(6B)	-364(5)	10980(3)	6855(3)	26(1)
C(7B)	160(5)	11564(3)	7021(3)	27(1)
C(8B)	1170(5)	11607(3)	7558(3)	27(1)
C(9B)	1690(5)	11059(2)	7902(3)	19(1)
C(10B)	-524(5)	9797(2)	6987(3)	26(1)
C(11B)	-336(6)	12157(3)	6627(3)	38(1)
C(12B)	2648(5)	11122(3)	8531(3)	26(1)
C(13B)	3560(5)	8469(2)	7711(2)	17(1)
C(14B)	2984(5)	8063(2)	7185(2)	19(1)
C(15B)	3669(5)	7540(2)	6992(2)	21(1)
C(16B)	4878(5)	7401(2)	7328(3)	24(1)
C(17B)	5382(5)	7799(2)	7880(3)	23(1)
C(18B)	4739(5)	8334(2)	8067(2)	21(1)
C(19B)	1653(5)	8186(3)	6842(3)	28(1)
C(20B)	5624(6)	6841(3)	7099(3)	34(1)
C(21B)	5346(5)	8765(3)	8655(3)	27(1)
C(22B)	1115(5)	9805(3)	5568(3)	21(1)
C(23B)	323(5)	10335(3)	5394(3)	22(1)
C(24B)	-755(5)	10259(3)	4919(3)	26(1)
C(25B)	-1012(5)	9667(3)	4614(3)	28(1)
C(26B)	-236(5)	9145(3)	4763(3)	27(1)
C(27B)	836(5)	9214(2)	5252(2)	21(1)
C(28B)	-1648(5)	10806(3)	4748(3)	39(2)
C(29B)	-541(5)	8512(3)	4403(3)	36(1)
C(30B)	4721(5)	9608(2)	6476(3)	18(1)
C(31B)	5208(5)	9265(2)	5857(2)	19(1)

C(32B)	4102(5)	8978(3)	5380(3)	27(1)
C(33B)	5838(5)	9801(2)	5448(3)	27(1)
C(34B)	6246(5)	8773(2)	6087(3)	19(1)
C(35B)	6701(5)	8381(2)	5568(3)	28(1)
C(36B)	7681(5)	7950(2)	5739(3)	30(1)
C(37B)	8224(5)	7888(2)	6424(3)	28(1)
C(38B)	7793(5)	8266(3)	6939(3)	31(1)
C(39B)	6821(5)	8712(2)	6775(3)	25(1)
S(1B)	5798(1)	10629(1)	7999(1)	19(1)
O(1B)	4504(3)	10530(2)	7627(2)	20(1)
O(2B)	5770(3)	10862(2)	8700(2)	28(1)
O(3B)	6662(4)	10121(2)	7895(2)	30(1)
C(40B)	6375(5)	11301(3)	7515(3)	27(1)
F(1B)	6532(3)	11128(2)	6860(2)	37(1)
F(2B)	5549(3)	11783(2)	7476(2)	36(1)
F(3B)	7487(3)	11505(2)	7837(2)	38(1)
S(2B)	3268(1)	11330(1)	5661(1)	29(1)
O(4B)	3690(3)	11020(2)	6343(2)	23(1)
O(5B)	3317(5)	10905(2)	5067(2)	53(1)
O(6B)	2138(4)	11686(2)	5657(3)	49(1)
C(41B)	4517(7)	11880(4)	5578(5)	66(3)
F(4B)	4283(4)	12193(2)	4955(3)	82(2)
F(5B)	5642(4)	11571(3)	5533(3)	78(1)
F(6B)	4705(6)	12282(2)	6082(3)	91(2)

Table 19.3. Bond lengths [Å] and angles [°] for **19**.

Mo(1A)-N(3A)	1.732(4)
Mo(1A)-C(30A)	1.879(5)
Mo(1A)-O(4A)	2.105(3)
Mo(1A)-O(1A)	2.140(3)
Mo(1A)-C(1A)	2.204(5)
C(1A)-N(1A)	1.336(6)
C(1A)-N(2A)	1.348(6)
N(1A)-C(4A)	1.441(6)
N(1A)-C(2A)	1.484(6)
C(2A)-C(3A)	1.514(7)
C(2A)-H(2A1)	0.9900
C(2A)-H(2A2)	0.9900
N(2A)-C(13A)	1.434(7)
N(2A)-C(3A)	1.476(6)
N(3A)-C(22A)	1.402(6)
C(3A)-H(3A1)	0.9900
C(3A)-H(3A2)	0.9900
C(4A)-C(5A)	1.383(7)
C(4A)-C(9A)	1.397(7)
C(5A)-C(6A)	1.394(7)
C(5A)-C(10A)	1.509(7)
C(6A)-C(7A)	1.383(7)

C(6A)-H(6A)	0.9500
C(7A)-C(8A)	1.385(7)
C(7A)-C(11A)	1.512(6)
C(8A)-C(9A)	1.397(7)
C(8A)-H(8A)	0.9500
C(9A)-C(12A)	1.492(7)
C(10A)-H(10A)	0.9800
C(10A)-H(10B)	0.9800
C(10A)-H(10C)	0.9800
C(11A)-H(11A)	0.9800
C(11A)-H(11B)	0.9800
C(11A)-H(11C)	0.9800
C(12A)-H(12A)	0.9800
C(12A)-H(12B)	0.9800
C(12A)-H(12C)	0.9800
C(13A)-C(14A)	1.387(7)
C(13A)-C(18A)	1.421(7)
C(14A)-C(15A)	1.383(7)
C(14A)-C(19A)	1.530(7)
C(15A)-C(16A)	1.391(7)
C(15A)-H(15A)	0.9500
C(16A)-C(17A)	1.381(7)
C(16A)-C(20A)	1.521(7)
C(17A)-C(18A)	1.392(7)
C(17A)-H(17A)	0.9500
C(18A)-C(21A)	1.497(7)
C(19A)-H(19A)	0.9800
C(19A)-H(19B)	0.9800
C(19A)-H(19C)	0.9800
C(20A)-H(20A)	0.9800
C(20A)-H(20B)	0.9800
C(20A)-H(20C)	0.9800
C(21A)-H(21A)	0.9800
C(21A)-H(21B)	0.9800
C(21A)-H(21C)	0.9800
C(22A)-C(27A)	1.394(7)
C(22A)-C(23A)	1.398(7)
C(23A)-C(24A)	1.379(7)
C(23A)-H(23A)	0.9500
C(24A)-C(25A)	1.405(7)
C(24A)-C(28A)	1.504(7)
C(25A)-C(26A)	1.401(7)
C(25A)-H(25A)	0.9500
C(26A)-C(27A)	1.403(7)
C(26A)-C(29A)	1.496(7)
C(27A)-H(27A)	0.9500
C(28A)-H(28A)	0.9800
C(28A)-H(28B)	0.9800
C(28A)-H(28C)	0.9800
C(29A)-H(29A)	0.9800

C(29A)-H(29B)	0.9800
C(29A)-H(29C)	0.9800
C(30A)-C(31A)	1.505(6)
C(30A)-H(30A)	0.981(10)
C(31A)-C(32A)	1.535(7)
C(31A)-C(34A)	1.548(7)
C(31A)-C(33A)	1.548(7)
C(32A)-H(32A)	0.9800
C(32A)-H(32B)	0.9800
C(32A)-H(32C)	0.9800
C(33A)-H(33A)	0.9800
C(33A)-H(33B)	0.9800
C(33A)-H(33C)	0.9800
C(34A)-C(35A)	1.367(7)
C(34A)-C(39A)	1.403(6)
C(35A)-C(36A)	1.400(7)
C(35A)-H(35A)	0.9500
C(36A)-C(37A)	1.378(7)
C(36A)-H(36A)	0.9500
C(37A)-C(38A)	1.369(8)
C(37A)-H(37A)	0.9500
C(38A)-C(39A)	1.371(8)
C(38A)-H(38A)	0.9500
C(39A)-H(39A)	0.9500
S(1A)-O(3A)	1.423(4)
S(1A)-O(2A)	1.432(4)
S(1A)-O(1A)	1.490(3)
S(1A)-C(40A)	1.838(5)
C(40A)-F(1A)	1.318(6)
C(40A)-F(2A)	1.327(6)
C(40A)-F(3A)	1.330(6)
S(2A)-O(5A)	1.423(4)
S(2A)-O(6A)	1.437(4)
S(2A)-O(4A)	1.476(3)
S(2A)-C(41A)	1.820(5)
C(41A)-F(6A)	1.320(6)
C(41A)-F(4A)	1.322(6)
C(41A)-F(5A)	1.342(6)
Mo(1B)-N(3B)	1.744(4)
Mo(1B)-C(30B)	1.879(5)
Mo(1B)-O(4B)	2.131(3)
Mo(1B)-O(1B)	2.170(3)
Mo(1B)-C(1B)	2.221(4)
N(1B)-C(1B)	1.337(6)
N(1B)-C(4B)	1.446(6)
N(1B)-C(2B)	1.477(6)
C(1B)-N(2B)	1.323(6)
N(2B)-C(13B)	1.431(6)
N(2B)-C(3B)	1.489(5)
C(2B)-C(3B)	1.529(7)

C(2B)-H(2B1)	0.9900
C(2B)-H(2B2)	0.9900
N(3B)-C(22B)	1.399(7)
C(3B)-H(3B1)	0.9900
C(3B)-H(3B2)	0.9900
C(4B)-C(9B)	1.385(7)
C(4B)-C(5B)	1.416(7)
C(5B)-C(6B)	1.380(7)
C(5B)-C(10B)	1.505(7)
C(6B)-C(7B)	1.369(8)
C(6B)-H(6B)	0.9500
C(7B)-C(8B)	1.398(8)
C(7B)-C(11B)	1.517(7)
C(8B)-C(9B)	1.406(7)
C(8B)-H(8B)	0.9500
C(9B)-C(12B)	1.489(7)
C(10B)-H(10D)	0.9800
C(10B)-H(10E)	0.9800
C(10B)-H(10F)	0.9800
C(11B)-H(11D)	0.9800
C(11B)-H(11E)	0.9800
C(11B)-H(11F)	0.9800
C(12B)-H(12D)	0.9800
C(12B)-H(12E)	0.9800
C(12B)-H(12F)	0.9800
C(13B)-C(18B)	1.381(7)
C(13B)-C(14B)	1.404(7)
C(14B)-C(15B)	1.387(7)
C(14B)-C(19B)	1.507(7)
C(15B)-C(16B)	1.395(7)
C(15B)-H(15B)	0.9500
C(16B)-C(17B)	1.403(7)
C(16B)-C(20B)	1.507(7)
C(17B)-C(18B)	1.379(7)
C(17B)-H(17B)	0.9500
C(18B)-C(21B)	1.527(7)
C(19B)-H(19D)	0.9800
C(19B)-H(19E)	0.9800
C(19B)-H(19F)	0.9800
C(20B)-H(20D)	0.9800
C(20B)-H(20E)	0.9800
C(20B)-H(20F)	0.9800
C(21B)-H(21D)	0.9800
C(21B)-H(21E)	0.9800
C(21B)-H(21F)	0.9800
C(22B)-C(27B)	1.395(7)
C(22B)-C(23B)	1.410(7)
C(23B)-C(24B)	1.384(8)
C(23B)-H(23B)	0.9500
C(24B)-C(25B)	1.386(8)

C(24B)-C(28B)	1.498(8)
C(25B)-C(26B)	1.379(8)
C(25B)-H(25B)	0.9500
C(26B)-C(27B)	1.395(7)
C(26B)-C(29B)	1.515(8)
C(27B)-H(27B)	0.9500
C(28B)-H(28D)	0.9800
C(28B)-H(28E)	0.9800
C(28B)-H(28F)	0.9800
C(29B)-H(29D)	0.9800
C(29B)-H(29E)	0.9800
C(29B)-H(29F)	0.9800
C(30B)-C(31B)	1.520(6)
C(30B)-H(30B)	0.986(10)
C(31B)-C(32B)	1.525(7)
C(31B)-C(34B)	1.536(7)
C(31B)-C(33B)	1.559(7)
C(32B)-H(32D)	0.9800
C(32B)-H(32E)	0.9800
C(32B)-H(32F)	0.9800
C(33B)-H(33D)	0.9800
C(33B)-H(33E)	0.9800
C(33B)-H(33F)	0.9800
C(34B)-C(39B)	1.391(7)
C(34B)-C(35B)	1.412(6)
C(35B)-C(36B)	1.386(8)
C(35B)-H(35B)	0.9500
C(36B)-C(37B)	1.374(8)
C(36B)-H(36B)	0.9500
C(37B)-C(38B)	1.379(8)
C(37B)-H(37B)	0.9500
C(38B)-C(39B)	1.399(8)
C(38B)-H(38B)	0.9500
C(39B)-H(39B)	0.9500
S(1B)-O(2B)	1.427(4)
S(1B)-O(3B)	1.432(4)
S(1B)-O(1B)	1.485(4)
S(1B)-C(40B)	1.827(5)
C(40B)-F(1B)	1.329(6)
C(40B)-F(2B)	1.333(6)
C(40B)-F(3B)	1.335(6)
S(2B)-O(6B)	1.408(4)
S(2B)-O(5B)	1.448(5)
S(2B)-O(4B)	1.479(4)
S(2B)-C(41B)	1.775(7)
C(41B)-F(6B)	1.277(10)
C(41B)-F(4B)	1.356(8)
C(41B)-F(5B)	1.366(10)

N(3A)-Mo(1A)-C(30A)	101.6(2)
N(3A)-Mo(1A)-O(4A)	98.16(16)
C(30A)-Mo(1A)-O(4A)	101.04(17)
N(3A)-Mo(1A)-O(1A)	160.57(15)
C(30A)-Mo(1A)-O(1A)	97.81(17)
O(4A)-Mo(1A)-O(1A)	77.56(13)
N(3A)-Mo(1A)-C(1A)	96.44(18)
C(30A)-Mo(1A)-C(1A)	104.09(18)
O(4A)-Mo(1A)-C(1A)	147.62(15)
O(1A)-Mo(1A)-C(1A)	79.08(15)
N(1A)-C(1A)-N(2A)	108.7(4)
N(1A)-C(1A)-Mo(1A)	132.8(3)
N(2A)-C(1A)-Mo(1A)	117.4(3)
C(1A)-N(1A)-C(4A)	127.3(4)
C(1A)-N(1A)-C(2A)	112.6(4)
C(4A)-N(1A)-C(2A)	119.1(4)
N(1A)-C(2A)-C(3A)	102.8(4)
N(1A)-C(2A)-H(2A1)	111.2
C(3A)-C(2A)-H(2A1)	111.2
N(1A)-C(2A)-H(2A2)	111.2
C(3A)-C(2A)-H(2A2)	111.2
H(2A1)-C(2A)-H(2A2)	109.1
C(1A)-N(2A)-C(13A)	124.0(4)
C(1A)-N(2A)-C(3A)	112.5(4)
C(13A)-N(2A)-C(3A)	123.0(4)
C(22A)-N(3A)-Mo(1A)	170.0(4)
N(2A)-C(3A)-C(2A)	103.2(4)
N(2A)-C(3A)-H(3A1)	111.1
C(2A)-C(3A)-H(3A1)	111.1
N(2A)-C(3A)-H(3A2)	111.1
C(2A)-C(3A)-H(3A2)	111.1
H(3A1)-C(3A)-H(3A2)	109.1
C(5A)-C(4A)-C(9A)	122.5(4)
C(5A)-C(4A)-N(1A)	119.5(4)
C(9A)-C(4A)-N(1A)	117.8(4)
C(4A)-C(5A)-C(6A)	117.8(5)
C(4A)-C(5A)-C(10A)	122.2(4)
C(6A)-C(5A)-C(10A)	120.0(5)
C(7A)-C(6A)-C(5A)	121.5(5)
C(7A)-C(6A)-H(6A)	119.2
C(5A)-C(6A)-H(6A)	119.2
C(6A)-C(7A)-C(8A)	119.2(5)
C(6A)-C(7A)-C(11A)	120.6(5)
C(8A)-C(7A)-C(11A)	120.2(5)
C(7A)-C(8A)-C(9A)	121.3(5)
C(7A)-C(8A)-H(8A)	119.4
C(9A)-C(8A)-H(8A)	119.4
C(4A)-C(9A)-C(8A)	117.5(5)
C(4A)-C(9A)-C(12A)	122.0(4)
C(8A)-C(9A)-C(12A)	120.5(5)

C(5A)-C(10A)-H(10A)	109.5
C(5A)-C(10A)-H(10B)	109.5
H(10A)-C(10A)-H(10B)	109.5
C(5A)-C(10A)-H(10C)	109.5
H(10A)-C(10A)-H(10C)	109.5
H(10B)-C(10A)-H(10C)	109.5
C(7A)-C(11A)-H(11A)	109.5
C(7A)-C(11A)-H(11B)	109.5
H(11A)-C(11A)-H(11B)	109.5
C(7A)-C(11A)-H(11C)	109.5
H(11A)-C(11A)-H(11C)	109.5
H(11B)-C(11A)-H(11C)	109.5
C(9A)-C(12A)-H(12A)	109.5
C(9A)-C(12A)-H(12B)	109.5
H(12A)-C(12A)-H(12B)	109.5
C(9A)-C(12A)-H(12C)	109.5
H(12A)-C(12A)-H(12C)	109.5
H(12B)-C(12A)-H(12C)	109.5
C(14A)-C(13A)-C(18A)	120.3(5)
C(14A)-C(13A)-N(2A)	122.0(5)
C(18A)-C(13A)-N(2A)	117.6(4)
C(15A)-C(14A)-C(13A)	119.1(5)
C(15A)-C(14A)-C(19A)	119.2(5)
C(13A)-C(14A)-C(19A)	121.6(4)
C(14A)-C(15A)-C(16A)	121.8(5)
C(14A)-C(15A)-H(15A)	119.1
C(16A)-C(15A)-H(15A)	119.1
C(17A)-C(16A)-C(15A)	118.2(5)
C(17A)-C(16A)-C(20A)	120.5(5)
C(15A)-C(16A)-C(20A)	121.3(5)
C(16A)-C(17A)-C(18A)	122.2(5)
C(16A)-C(17A)-H(17A)	118.9
C(18A)-C(17A)-H(17A)	118.9
C(17A)-C(18A)-C(13A)	117.9(5)
C(17A)-C(18A)-C(21A)	120.5(5)
C(13A)-C(18A)-C(21A)	121.7(5)
C(14A)-C(19A)-H(19A)	109.5
C(14A)-C(19A)-H(19B)	109.5
H(19A)-C(19A)-H(19B)	109.5
C(14A)-C(19A)-H(19C)	109.5
H(19A)-C(19A)-H(19C)	109.5
H(19B)-C(19A)-H(19C)	109.5
C(16A)-C(20A)-H(20A)	109.5
C(16A)-C(20A)-H(20B)	109.5
H(20A)-C(20A)-H(20B)	109.5
C(16A)-C(20A)-H(20C)	109.5
H(20A)-C(20A)-H(20C)	109.5
H(20B)-C(20A)-H(20C)	109.5
C(18A)-C(21A)-H(21A)	109.5
C(18A)-C(21A)-H(21B)	109.5

H(21A)-C(21A)-H(21B)	109.5
C(18A)-C(21A)-H(21C)	109.5
H(21A)-C(21A)-H(21C)	109.5
H(21B)-C(21A)-H(21C)	109.5
C(27A)-C(22A)-C(23A)	120.7(5)
C(27A)-C(22A)-N(3A)	121.1(5)
C(23A)-C(22A)-N(3A)	118.2(4)
C(24A)-C(23A)-C(22A)	120.5(5)
C(24A)-C(23A)-H(23A)	119.8
C(22A)-C(23A)-H(23A)	119.8
C(23A)-C(24A)-C(25A)	118.7(5)
C(23A)-C(24A)-C(28A)	120.8(5)
C(25A)-C(24A)-C(28A)	120.4(5)
C(26A)-C(25A)-C(24A)	121.6(5)
C(26A)-C(25A)-H(25A)	119.2
C(24A)-C(25A)-H(25A)	119.2
C(25A)-C(26A)-C(27A)	118.6(5)
C(25A)-C(26A)-C(29A)	121.0(5)
C(27A)-C(26A)-C(29A)	120.4(5)
C(22A)-C(27A)-C(26A)	119.7(5)
C(22A)-C(27A)-H(27A)	120.2
C(26A)-C(27A)-H(27A)	120.2
C(24A)-C(28A)-H(28A)	109.5
C(24A)-C(28A)-H(28B)	109.5
H(28A)-C(28A)-H(28B)	109.5
C(24A)-C(28A)-H(28C)	109.5
H(28A)-C(28A)-H(28C)	109.5
H(28B)-C(28A)-H(28C)	109.5
C(26A)-C(29A)-H(29A)	109.5
C(26A)-C(29A)-H(29B)	109.5
H(29A)-C(29A)-H(29B)	109.5
C(26A)-C(29A)-H(29C)	109.5
H(29A)-C(29A)-H(29C)	109.5
H(29B)-C(29A)-H(29C)	109.5
C(31A)-C(30A)-Mo(1A)	142.8(4)
C(31A)-C(30A)-H(30A)	115(3)
Mo(1A)-C(30A)-H(30A)	98(3)
C(30A)-C(31A)-C(32A)	111.2(4)
C(30A)-C(31A)-C(34A)	113.6(4)
C(32A)-C(31A)-C(34A)	111.2(4)
C(30A)-C(31A)-C(33A)	105.9(4)
C(32A)-C(31A)-C(33A)	107.7(4)
C(34A)-C(31A)-C(33A)	106.9(4)
C(31A)-C(32A)-H(32A)	109.5
C(31A)-C(32A)-H(32B)	109.5
H(32A)-C(32A)-H(32B)	109.5
C(31A)-C(32A)-H(32C)	109.5
H(32A)-C(32A)-H(32C)	109.5
H(32B)-C(32A)-H(32C)	109.5
C(31A)-C(33A)-H(33A)	109.5

C(31A)-C(33A)-H(33B)	109.5
H(33A)-C(33A)-H(33B)	109.5
C(31A)-C(33A)-H(33C)	109.5
H(33A)-C(33A)-H(33C)	109.5
H(33B)-C(33A)-H(33C)	109.5
C(35A)-C(34A)-C(39A)	117.5(5)
C(35A)-C(34A)-C(31A)	123.1(4)
C(39A)-C(34A)-C(31A)	119.2(4)
C(34A)-C(35A)-C(36A)	121.1(5)
C(34A)-C(35A)-H(35A)	119.5
C(36A)-C(35A)-H(35A)	119.5
C(37A)-C(36A)-C(35A)	120.7(5)
C(37A)-C(36A)-H(36A)	119.6
C(35A)-C(36A)-H(36A)	119.6
C(38A)-C(37A)-C(36A)	118.3(5)
C(38A)-C(37A)-H(37A)	120.9
C(36A)-C(37A)-H(37A)	120.9
C(37A)-C(38A)-C(39A)	121.4(5)
C(37A)-C(38A)-H(38A)	119.3
C(39A)-C(38A)-H(38A)	119.3
C(38A)-C(39A)-C(34A)	121.1(5)
C(38A)-C(39A)-H(39A)	119.5
C(34A)-C(39A)-H(39A)	119.5
O(3A)-S(1A)-O(2A)	117.7(2)
O(3A)-S(1A)-O(1A)	112.3(2)
O(2A)-S(1A)-O(1A)	112.7(2)
O(3A)-S(1A)-C(40A)	104.7(2)
O(2A)-S(1A)-C(40A)	105.5(2)
O(1A)-S(1A)-C(40A)	102.1(2)
S(1A)-O(1A)-Mo(1A)	146.1(2)
F(1A)-C(40A)-F(2A)	109.2(4)
F(1A)-C(40A)-F(3A)	108.3(4)
F(2A)-C(40A)-F(3A)	109.0(4)
F(1A)-C(40A)-S(1A)	111.2(3)
F(2A)-C(40A)-S(1A)	109.2(3)
F(3A)-C(40A)-S(1A)	109.9(3)
O(5A)-S(2A)-O(6A)	118.7(2)
O(5A)-S(2A)-O(4A)	113.6(2)
O(6A)-S(2A)-O(4A)	112.6(2)
O(5A)-S(2A)-C(41A)	105.2(2)
O(6A)-S(2A)-C(41A)	104.4(2)
O(4A)-S(2A)-C(41A)	99.6(2)
S(2A)-O(4A)-Mo(1A)	142.4(2)
F(6A)-C(41A)-F(4A)	108.2(4)
F(6A)-C(41A)-F(5A)	108.1(4)
F(4A)-C(41A)-F(5A)	107.9(5)
F(6A)-C(41A)-S(2A)	112.0(4)
F(4A)-C(41A)-S(2A)	110.2(3)
F(5A)-C(41A)-S(2A)	110.3(4)
N(3B)-Mo(1B)-C(30B)	101.1(2)

N(3B)-Mo(1B)-O(4B)	96.35(16)
C(30B)-Mo(1B)-O(4B)	103.74(17)
N(3B)-Mo(1B)-O(1B)	165.27(16)
C(30B)-Mo(1B)-O(1B)	93.48(17)
O(4B)-Mo(1B)-O(1B)	78.00(13)
N(3B)-Mo(1B)-C(1B)	96.83(17)
C(30B)-Mo(1B)-C(1B)	105.44(18)
O(4B)-Mo(1B)-C(1B)	144.86(15)
O(1B)-Mo(1B)-C(1B)	81.08(15)
C(1B)-N(1B)-C(4B)	123.2(4)
C(1B)-N(1B)-C(2B)	112.6(4)
C(4B)-N(1B)-C(2B)	123.9(4)
N(2B)-C(1B)-N(1B)	109.6(4)
N(2B)-C(1B)-Mo(1B)	137.4(3)
N(1B)-C(1B)-Mo(1B)	112.8(3)
C(1B)-N(2B)-C(13B)	128.2(4)
C(1B)-N(2B)-C(3B)	111.9(4)
C(13B)-N(2B)-C(3B)	118.7(4)
N(1B)-C(2B)-C(3B)	101.9(4)
N(1B)-C(2B)-H(2B1)	111.4
C(3B)-C(2B)-H(2B1)	111.4
N(1B)-C(2B)-H(2B2)	111.4
C(3B)-C(2B)-H(2B2)	111.4
H(2B1)-C(2B)-H(2B2)	109.3
C(22B)-N(3B)-Mo(1B)	171.8(4)
N(2B)-C(3B)-C(2B)	102.5(4)
N(2B)-C(3B)-H(3B1)	111.3
C(2B)-C(3B)-H(3B1)	111.3
N(2B)-C(3B)-H(3B2)	111.3
C(2B)-C(3B)-H(3B2)	111.3
H(3B1)-C(3B)-H(3B2)	109.2
C(9B)-C(4B)-C(5B)	121.5(5)
C(9B)-C(4B)-N(1B)	121.2(4)
C(5B)-C(4B)-N(1B)	117.2(4)
C(6B)-C(5B)-C(4B)	117.6(5)
C(6B)-C(5B)-C(10B)	120.3(5)
C(4B)-C(5B)-C(10B)	122.1(5)
C(7B)-C(6B)-C(5B)	122.4(5)
C(7B)-C(6B)-H(6B)	118.8
C(5B)-C(6B)-H(6B)	118.8
C(6B)-C(7B)-C(8B)	118.9(5)
C(6B)-C(7B)-C(11B)	120.7(5)
C(8B)-C(7B)-C(11B)	120.3(5)
C(7B)-C(8B)-C(9B)	121.1(5)
C(7B)-C(8B)-H(8B)	119.5
C(9B)-C(8B)-H(8B)	119.5
C(4B)-C(9B)-C(8B)	117.7(5)
C(4B)-C(9B)-C(12B)	122.2(4)
C(8B)-C(9B)-C(12B)	119.9(5)
C(5B)-C(10B)-H(10D)	109.5

C(5B)-C(10B)-H(10E)	109.5
H(10D)-C(10B)-H(10E)	109.5
C(5B)-C(10B)-H(10F)	109.5
H(10D)-C(10B)-H(10F)	109.5
H(10E)-C(10B)-H(10F)	109.5
C(7B)-C(11B)-H(11D)	109.5
C(7B)-C(11B)-H(11E)	109.5
H(11D)-C(11B)-H(11E)	109.5
C(7B)-C(11B)-H(11F)	109.5
H(11D)-C(11B)-H(11F)	109.5
H(11E)-C(11B)-H(11F)	109.5
C(9B)-C(12B)-H(12D)	109.5
C(9B)-C(12B)-H(12E)	109.5
H(12D)-C(12B)-H(12E)	109.5
C(9B)-C(12B)-H(12F)	109.5
H(12D)-C(12B)-H(12F)	109.5
H(12E)-C(12B)-H(12F)	109.5
C(18B)-C(13B)-C(14B)	121.5(4)
C(18B)-C(13B)-N(2B)	119.5(4)
C(14B)-C(13B)-N(2B)	118.6(4)
C(15B)-C(14B)-C(13B)	118.2(4)
C(15B)-C(14B)-C(19B)	120.7(5)
C(13B)-C(14B)-C(19B)	121.1(4)
C(14B)-C(15B)-C(16B)	121.5(5)
C(14B)-C(15B)-H(15B)	119.3
C(16B)-C(15B)-H(15B)	119.3
C(15B)-C(16B)-C(17B)	118.3(5)
C(15B)-C(16B)-C(20B)	120.8(5)
C(17B)-C(16B)-C(20B)	120.9(5)
C(18B)-C(17B)-C(16B)	121.4(5)
C(18B)-C(17B)-H(17B)	119.3
C(16B)-C(17B)-H(17B)	119.3
C(17B)-C(18B)-C(13B)	119.0(5)
C(17B)-C(18B)-C(21B)	119.6(5)
C(13B)-C(18B)-C(21B)	121.4(4)
C(14B)-C(19B)-H(19D)	109.5
C(14B)-C(19B)-H(19E)	109.5
H(19D)-C(19B)-H(19E)	109.5
C(14B)-C(19B)-H(19F)	109.5
H(19D)-C(19B)-H(19F)	109.5
H(19E)-C(19B)-H(19F)	109.5
C(16B)-C(20B)-H(20D)	109.5
C(16B)-C(20B)-H(20E)	109.5
H(20D)-C(20B)-H(20E)	109.5
C(16B)-C(20B)-H(20F)	109.5
H(20D)-C(20B)-H(20F)	109.5
H(20E)-C(20B)-H(20F)	109.5
C(18B)-C(21B)-H(21D)	109.5
C(18B)-C(21B)-H(21E)	109.5
H(21D)-C(21B)-H(21E)	109.5

C(18B)-C(21B)-H(21F)	109.5
H(21D)-C(21B)-H(21F)	109.5
H(21E)-C(21B)-H(21F)	109.5
C(27B)-C(22B)-N(3B)	121.4(5)
C(27B)-C(22B)-C(23B)	120.5(5)
N(3B)-C(22B)-C(23B)	118.0(5)
C(24B)-C(23B)-C(22B)	119.2(5)
C(24B)-C(23B)-H(23B)	120.4
C(22B)-C(23B)-H(23B)	120.4
C(23B)-C(24B)-C(25B)	119.1(5)
C(23B)-C(24B)-C(28B)	120.5(5)
C(25B)-C(24B)-C(28B)	120.4(5)
C(26B)-C(25B)-C(24B)	122.8(5)
C(26B)-C(25B)-H(25B)	118.6
C(24B)-C(25B)-H(25B)	118.6
C(25B)-C(26B)-C(27B)	118.4(5)
C(25B)-C(26B)-C(29B)	120.8(5)
C(27B)-C(26B)-C(29B)	120.8(5)
C(26B)-C(27B)-C(22B)	119.9(5)
C(26B)-C(27B)-H(27B)	120.0
C(22B)-C(27B)-H(27B)	120.0
C(24B)-C(28B)-H(28D)	109.5
C(24B)-C(28B)-H(28E)	109.5
H(28D)-C(28B)-H(28E)	109.5
C(24B)-C(28B)-H(28F)	109.5
H(28D)-C(28B)-H(28F)	109.5
H(28E)-C(28B)-H(28F)	109.5
C(26B)-C(29B)-H(29D)	109.5
C(26B)-C(29B)-H(29E)	109.5
H(29D)-C(29B)-H(29E)	109.5
C(26B)-C(29B)-H(29F)	109.5
H(29D)-C(29B)-H(29F)	109.5
H(29E)-C(29B)-H(29F)	109.5
C(31B)-C(30B)-Mo(1B)	143.3(4)
C(31B)-C(30B)-H(30B)	112(3)
Mo(1B)-C(30B)-H(30B)	101(3)
C(30B)-C(31B)-C(32B)	110.3(4)
C(30B)-C(31B)-C(34B)	112.9(4)
C(32B)-C(31B)-C(34B)	112.4(4)
C(30B)-C(31B)-C(33B)	104.3(4)
C(32B)-C(31B)-C(33B)	109.2(4)
C(34B)-C(31B)-C(33B)	107.3(4)
C(31B)-C(32B)-H(32D)	109.5
C(31B)-C(32B)-H(32E)	109.5
H(32D)-C(32B)-H(32E)	109.5
C(31B)-C(32B)-H(32F)	109.5
H(32D)-C(32B)-H(32F)	109.5
H(32E)-C(32B)-H(32F)	109.5
C(31B)-C(33B)-H(33D)	109.5
C(31B)-C(33B)-H(33E)	109.5

H(33D)-C(33B)-H(33E)	109.5
C(31B)-C(33B)-H(33F)	109.5
H(33D)-C(33B)-H(33F)	109.5
H(33E)-C(33B)-H(33F)	109.5
C(39B)-C(34B)-C(35B)	117.5(5)
C(39B)-C(34B)-C(31B)	123.8(4)
C(35B)-C(34B)-C(31B)	118.7(4)
C(36B)-C(35B)-C(34B)	121.2(5)
C(36B)-C(35B)-H(35B)	119.4
C(34B)-C(35B)-H(35B)	119.4
C(37B)-C(36B)-C(35B)	120.6(5)
C(37B)-C(36B)-H(36B)	119.7
C(35B)-C(36B)-H(36B)	119.7
C(36B)-C(37B)-C(38B)	119.1(5)
C(36B)-C(37B)-H(37B)	120.4
C(38B)-C(37B)-H(37B)	120.4
C(37B)-C(38B)-C(39B)	121.1(5)
C(37B)-C(38B)-H(38B)	119.4
C(39B)-C(38B)-H(38B)	119.4
C(34B)-C(39B)-C(38B)	120.5(5)
C(34B)-C(39B)-H(39B)	119.8
C(38B)-C(39B)-H(39B)	119.8
O(2B)-S(1B)-O(3B)	117.7(2)
O(2B)-S(1B)-O(1B)	112.5(2)
O(3B)-S(1B)-O(1B)	113.4(2)
O(2B)-S(1B)-C(40B)	104.6(2)
O(3B)-S(1B)-C(40B)	104.5(3)
O(1B)-S(1B)-C(40B)	102.0(2)
S(1B)-O(1B)-Mo(1B)	146.8(2)
F(1B)-C(40B)-F(2B)	107.6(4)
F(1B)-C(40B)-F(3B)	109.0(4)
F(2B)-C(40B)-F(3B)	108.7(4)
F(1B)-C(40B)-S(1B)	110.4(4)
F(2B)-C(40B)-S(1B)	111.1(3)
F(3B)-C(40B)-S(1B)	110.0(4)
O(6B)-S(2B)-O(5B)	115.2(3)
O(6B)-S(2B)-O(4B)	114.3(2)
O(5B)-S(2B)-O(4B)	112.7(2)
O(6B)-S(2B)-C(41B)	107.0(4)
O(5B)-S(2B)-C(41B)	103.8(4)
O(4B)-S(2B)-C(41B)	102.1(3)
S(2B)-O(4B)-Mo(1B)	132.0(2)
F(6B)-C(41B)-F(4B)	109.8(7)
F(6B)-C(41B)-F(5B)	107.3(7)
F(4B)-C(41B)-F(5B)	104.5(7)
F(6B)-C(41B)-S(2B)	114.6(6)
F(4B)-C(41B)-S(2B)	109.2(5)
F(5B)-C(41B)-S(2B)	111.0(6)

Table 19.4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **19**. The anisotropic displacement factor exponent takes the form: $-2\ \pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1A)	9(1)	19(1)	13(1)	0(1)	4(1)	-1(1)
C(1A)	12(2)	18(2)	16(2)	4(2)	4(2)	1(2)
N(1A)	17(2)	24(2)	16(2)	-4(2)	7(2)	-4(2)
C(2A)	47(4)	36(3)	26(3)	-12(2)	24(3)	-14(3)
N(2A)	20(2)	23(2)	20(2)	-3(2)	16(2)	-5(2)
N(3A)	9(2)	24(2)	12(2)	2(2)	-1(1)	-1(2)
C(3A)	34(3)	31(3)	19(2)	-4(2)	18(2)	-7(2)
C(4A)	19(3)	17(2)	22(2)	-3(2)	9(2)	-3(2)
C(5A)	17(3)	24(3)	23(2)	-4(2)	2(2)	-3(2)
C(6A)	16(3)	25(3)	27(3)	-1(2)	5(2)	-3(2)
C(7A)	20(3)	23(3)	27(3)	-1(2)	12(2)	-3(2)
C(8A)	20(3)	20(3)	29(3)	2(2)	9(2)	3(2)
C(9A)	17(2)	22(3)	26(2)	-3(2)	8(2)	1(2)
C(10A)	21(3)	38(3)	32(3)	3(2)	-6(2)	-4(2)
C(11A)	26(3)	31(3)	39(3)	5(2)	19(2)	-2(2)
C(12A)	22(3)	29(3)	41(3)	9(2)	2(2)	2(2)
C(13A)	17(3)	24(3)	21(2)	2(2)	14(2)	-2(2)
C(14A)	21(3)	26(3)	22(2)	-1(2)	14(2)	-5(2)
C(15A)	27(3)	19(2)	28(3)	3(2)	17(2)	2(2)
C(16A)	20(3)	25(3)	21(2)	-2(2)	11(2)	-6(2)
C(17A)	17(3)	29(3)	23(2)	0(2)	9(2)	-2(2)
C(18A)	18(2)	30(3)	21(2)	1(2)	14(2)	-2(2)
C(19A)	23(3)	32(3)	21(2)	7(2)	6(2)	-4(2)
C(20A)	31(3)	26(3)	32(3)	0(2)	10(2)	-7(2)
C(21A)	21(3)	22(3)	37(3)	4(2)	13(2)	3(2)
C(22A)	8(2)	33(3)	17(2)	1(2)	4(2)	4(2)
C(23A)	19(3)	28(3)	19(2)	0(2)	9(2)	1(2)
C(24A)	13(2)	32(3)	24(2)	-4(2)	9(2)	2(2)
C(25A)	8(2)	37(3)	20(2)	-2(2)	5(2)	3(2)
C(26A)	17(3)	32(3)	17(2)	-2(2)	9(2)	5(2)
C(27A)	14(2)	30(3)	17(2)	-6(2)	9(2)	-2(2)
C(28A)	16(3)	34(3)	34(3)	-2(2)	0(2)	-6(2)
C(29A)	18(3)	41(3)	28(3)	5(2)	4(2)	10(2)
C(30A)	17(3)	21(2)	13(2)	-1(2)	2(2)	-2(2)
C(31A)	10(2)	29(3)	13(2)	1(2)	4(2)	-2(2)
C(32A)	16(3)	47(3)	28(3)	14(2)	1(2)	-6(2)
C(33A)	36(3)	36(3)	24(3)	-4(2)	19(3)	-9(2)
C(34A)	15(2)	15(2)	25(2)	1(2)	9(2)	2(2)
C(35A)	18(3)	30(3)	25(3)	5(2)	2(2)	-4(2)
C(36A)	20(3)	35(3)	30(3)	4(2)	-1(2)	-5(2)
C(37A)	14(3)	28(3)	40(3)	5(2)	7(2)	-1(2)
C(38A)	31(3)	41(3)	28(3)	12(2)	9(2)	-14(3)
C(39A)	27(3)	47(3)	23(3)	9(2)	4(2)	-10(3)
S(1A)	13(1)	25(1)	18(1)	2(1)	2(1)	0(1)
O(1A)	12(2)	29(2)	18(2)	1(1)	4(1)	-2(1)

O(2A)	14(2)	33(2)	40(2)	7(2)	3(2)	-6(2)
O(3A)	18(2)	43(2)	16(2)	0(1)	-3(1)	4(2)
C(40A)	23(3)	26(3)	23(2)	1(2)	4(2)	-1(2)
F(1A)	22(2)	50(2)	25(2)	-5(1)	5(1)	8(1)
F(2A)	22(2)	39(2)	35(2)	-1(1)	0(1)	10(1)
F(3A)	30(2)	26(2)	48(2)	0(1)	6(2)	-4(1)
S(2A)	22(1)	23(1)	18(1)	-3(1)	8(1)	-2(1)
O(4A)	28(2)	21(2)	26(2)	-6(1)	-3(2)	5(2)
O(5A)	42(2)	34(2)	17(2)	1(1)	8(2)	-1(2)
O(6A)	27(2)	47(2)	44(2)	-13(2)	26(2)	-2(2)
C(41A)	28(3)	27(3)	30(3)	-2(2)	8(2)	0(2)
F(4A)	59(2)	29(2)	40(2)	-9(1)	8(2)	-15(2)
F(5A)	33(2)	48(2)	68(2)	10(2)	31(2)	-2(2)
F(6A)	59(2)	39(2)	27(2)	8(1)	5(2)	-3(2)
Mo(1B)	9(1)	20(1)	14(1)	0(1)	5(1)	-1(1)
N(1B)	16(2)	23(2)	19(2)	-3(2)	10(2)	1(2)
C(1B)	8(2)	24(2)	16(2)	3(2)	7(2)	-1(2)
N(2B)	16(2)	24(2)	17(2)	2(2)	8(2)	-1(2)
C(2B)	31(3)	32(3)	19(2)	6(2)	16(2)	2(2)
N(3B)	11(2)	29(2)	12(2)	5(2)	3(2)	-1(2)
C(3B)	25(3)	34(3)	21(2)	3(2)	20(2)	-2(2)
C(4B)	10(2)	31(3)	15(2)	3(2)	9(2)	4(2)
C(5B)	16(3)	31(3)	22(2)	0(2)	15(2)	3(2)
C(6B)	13(2)	39(3)	26(3)	-2(2)	6(2)	8(2)
C(7B)	27(3)	30(3)	24(3)	6(2)	10(2)	9(2)
C(8B)	23(3)	31(3)	31(3)	2(2)	15(2)	1(2)
C(9B)	11(2)	26(3)	23(2)	4(2)	10(2)	4(2)
C(10B)	16(3)	33(3)	31(3)	-4(2)	5(2)	-6(2)
C(11B)	33(3)	41(3)	40(3)	6(3)	6(3)	12(3)
C(12B)	21(3)	29(3)	29(3)	-5(2)	12(2)	4(2)
C(13B)	18(2)	17(2)	19(2)	3(2)	11(2)	-1(2)
C(14B)	16(2)	27(3)	15(2)	6(2)	3(2)	4(2)
C(15B)	19(3)	27(3)	16(2)	0(2)	2(2)	-4(2)
C(16B)	17(3)	23(3)	32(3)	3(2)	7(2)	1(2)
C(17B)	14(2)	28(3)	27(3)	2(2)	1(2)	0(2)
C(18B)	19(3)	20(3)	24(2)	5(2)	7(2)	-4(2)
C(19B)	19(3)	35(3)	28(3)	-1(2)	6(2)	2(2)
C(20B)	29(3)	34(3)	42(3)	-11(2)	10(3)	7(2)
C(21B)	20(3)	31(3)	30(3)	-6(2)	3(2)	-4(2)
C(22B)	14(2)	37(3)	14(2)	8(2)	7(2)	2(2)
C(23B)	12(2)	29(3)	26(3)	6(2)	9(2)	-3(2)
C(24B)	16(2)	40(3)	23(2)	15(2)	15(2)	5(2)
C(25B)	9(2)	56(4)	21(3)	7(2)	3(2)	-4(2)
C(26B)	14(3)	50(3)	19(2)	0(2)	7(2)	-8(2)
C(27B)	14(2)	30(3)	21(2)	-2(2)	8(2)	-3(2)
C(28B)	11(3)	52(4)	53(4)	26(3)	4(2)	-4(2)
C(29B)	17(3)	61(4)	31(3)	-11(3)	2(2)	-9(3)
C(30B)	13(2)	22(3)	20(2)	0(2)	3(2)	-4(2)
C(31B)	18(2)	24(3)	18(2)	-3(2)	12(2)	-2(2)
C(32B)	15(3)	42(3)	25(3)	-9(2)	4(2)	5(2)

C(33B)	27(3)	30(3)	27(3)	4(2)	19(2)	5(2)
C(34B)	14(2)	19(2)	25(2)	-1(2)	9(2)	-2(2)
C(35B)	26(3)	30(3)	29(3)	-4(2)	7(2)	4(2)
C(36B)	26(3)	25(3)	43(3)	-6(2)	16(3)	2(2)
C(37B)	15(3)	19(3)	51(3)	4(2)	9(2)	3(2)
C(38B)	28(3)	35(3)	29(3)	3(2)	-6(2)	4(2)
C(39B)	22(3)	27(3)	27(3)	-1(2)	5(2)	2(2)
S(1B)	14(1)	26(1)	19(1)	-3(1)	3(1)	-1(1)
O(1B)	16(2)	27(2)	18(2)	-2(1)	5(1)	-1(1)
O(2B)	20(2)	47(2)	16(2)	-5(2)	3(2)	-9(2)
O(3B)	17(2)	33(2)	38(2)	-5(2)	-5(2)	3(2)
C(40B)	21(3)	36(3)	23(3)	0(2)	1(2)	-9(2)
F(1B)	23(2)	70(2)	20(2)	-1(1)	11(1)	-11(2)
F(2B)	34(2)	31(2)	44(2)	5(1)	5(2)	-3(2)
F(3B)	26(2)	58(2)	31(2)	-2(2)	3(1)	-22(2)
S(2B)	21(1)	38(1)	29(1)	15(1)	5(1)	-1(1)
O(4B)	24(2)	23(2)	24(2)	2(1)	8(2)	-5(1)
O(5B)	46(3)	88(4)	26(2)	10(2)	7(2)	12(3)
O(6B)	41(3)	46(3)	61(3)	22(2)	9(2)	13(2)
C(41B)	38(4)	77(6)	79(6)	52(5)	-15(4)	-19(4)
F(4B)	57(3)	89(3)	98(3)	63(3)	-3(2)	-18(2)
F(5B)	41(2)	107(3)	88(3)	45(3)	14(2)	-8(2)
F(6B)	129(4)	52(3)	83(3)	18(2)	-24(3)	-46(3)

Table 19.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **19**.

	x	y	z	U(eq)
H(2A1)	2199	4064	1828	42
H(2A2)	3419	3769	2301	42
H(3A1)	4457	4681	2178	32
H(3A2)	3202	4992	1756	32
H(6A)	-1158	2931	2907	27
H(8A)	1893	2557	4304	27
H(10A)	-121	4409	2332	46
H(10B)	-1314	3935	2287	46
H(10C)	-180	3807	1814	46
H(11A)	-1169	2301	4192	46
H(11B)	119	1896	4304	46
H(11C)	-791	1843	3578	46
H(12A)	4039	3410	3603	46
H(12B)	3745	3165	4362	46
H(12C)	3558	3901	4157	46
H(15A)	3849	7219	2935	29
H(17A)	6484	6140	4059	27
H(19A)	2769	6456	1787	38
H(19B)	1855	6688	2351	38
H(19C)	1950	5947	2168	38

H(20A)	6147	7284	4407	44
H(20B)	5263	7719	3865	44
H(20C)	6608	7472	3663	44
H(21A)	5923	4773	3279	39
H(21B)	5033	4712	3902	39
H(21C)	6410	5033	4050	39
H(23A)	4677	6025	5026	25
H(25A)	7207	5064	6376	26
H(27A)	4000	4177	5500	24
H(28A)	7583	6126	5349	42
H(28B)	7482	6209	6175	42
H(28C)	6512	6578	5613	42
H(29A)	6880	3857	6467	43
H(29B)	5456	3597	6292	43
H(29C)	5812	4048	6961	43
H(30A)	-180(30)	4870(20)	4040(20)	20
H(32A)	1605	3726	5115	46
H(32B)	1009	3843	5840	46
H(32C)	1950	4359	5563	46
H(33A)	374	5207	5645	46
H(33B)	-584	4704	5933	46
H(33C)	-1045	5137	5262	46
H(35A)	-1562	4230	3851	30
H(36A)	-3316	3552	3642	34
H(37A)	-3806	2832	4506	32
H(38A)	-2565	2830	5589	39
H(39A)	-806	3479	5792	39
H(2B1)	476	9527	8557	32
H(2B2)	1768	9771	9007	32
H(3B1)	2507	8766	8946	30
H(3B2)	1349	8571	8362	30
H(6B)	-1086	10955	6512	31
H(8B)	1511	12013	7693	33
H(10D)	121	9473	6921	40
H(10E)	-1100	9842	6550	40
H(10F)	-1011	9667	7371	40
H(11D)	-234	12111	6125	56
H(11E)	144	12530	6818	56
H(11F)	-1240	12214	6683	56
H(12D)	2218	11239	8942	38
H(12E)	3265	11453	8445	38
H(12F)	3091	10715	8622	38
H(15B)	3306	7269	6624	25
H(17B)	6184	7698	8132	28
H(19D)	1420	7860	6484	41
H(19E)	1617	8608	6619	41
H(19F)	1057	8172	7200	41
H(20D)	6486	6979	7028	52
H(20E)	5200	6669	6657	52
H(20F)	5671	6511	7464	52

H(21D)	5664	9153	8449	40
H(21E)	6054	8541	8924	40
H(21F)	4708	8879	8969	40
H(23B)	527	10739	5600	26
H(25B)	-1754	9619	4289	34
H(27B)	1376	8860	5371	25
H(28D)	-1865	10833	4236	58
H(28E)	-1238	11203	4922	58
H(28F)	-2425	10739	4975	58
H(29D)	-1464	8474	4281	54
H(29E)	-241	8164	4722	54
H(29F)	-117	8486	3972	54
H(30B)	5430(30)	9760(20)	6810(20)	21
H(32D)	3684	8651	5640	41
H(32E)	4422	8785	4967	41
H(32F)	3487	9313	5227	41
H(33D)	5209	10135	5312	40
H(33E)	6145	9621	5025	40
H(33F)	6555	9985	5752	40
H(35B)	6328	8412	5093	34
H(36B)	7981	7696	5380	36
H(37B)	8886	7588	6542	34
H(38B)	8163	8223	7414	38
H(39B)	6552	8974	7136	30

Table 19.6. Torsion angles [°] for **19**.

N(3A)-Mo(1A)-C(1A)-N(1A)	107.2(5)
C(30A)-Mo(1A)-C(1A)-N(1A)	3.4(5)
O(4A)-Mo(1A)-C(1A)-N(1A)	-136.4(4)
O(1A)-Mo(1A)-C(1A)-N(1A)	-92.0(5)
N(3A)-Mo(1A)-C(1A)-N(2A)	-86.4(4)
C(30A)-Mo(1A)-C(1A)-N(2A)	169.9(4)
O(4A)-Mo(1A)-C(1A)-N(2A)	30.0(6)
O(1A)-Mo(1A)-C(1A)-N(2A)	74.5(4)
N(2A)-C(1A)-N(1A)-C(4A)	171.5(5)
Mo(1A)-C(1A)-N(1A)-C(4A)	-21.1(8)
N(2A)-C(1A)-N(1A)-C(2A)	3.7(6)
Mo(1A)-C(1A)-N(1A)-C(2A)	171.0(4)
C(1A)-N(1A)-C(2A)-C(3A)	-5.0(6)
C(4A)-N(1A)-C(2A)-C(3A)	-173.9(5)
N(1A)-C(1A)-N(2A)-C(13A)	-172.3(5)
Mo(1A)-C(1A)-N(2A)-C(13A)	18.1(7)
N(1A)-C(1A)-N(2A)-C(3A)	-0.7(6)
Mo(1A)-C(1A)-N(2A)-C(3A)	-170.2(4)
C(30A)-Mo(1A)-N(3A)-C(22A)	-160.9(19)
O(4A)-Mo(1A)-N(3A)-C(22A)	-57.7(19)
O(1A)-Mo(1A)-N(3A)-C(22A)	18(2)
C(1A)-Mo(1A)-N(3A)-C(22A)	93.3(19)

C(1A)-N(2A)-C(3A)-C(2A)	-2.4(6)
C(13A)-N(2A)-C(3A)-C(2A)	169.4(5)
N(1A)-C(2A)-C(3A)-N(2A)	4.1(6)
C(1A)-N(1A)-C(4A)-C(5A)	112.5(6)
C(2A)-N(1A)-C(4A)-C(5A)	-80.3(6)
C(1A)-N(1A)-C(4A)-C(9A)	-72.2(6)
C(2A)-N(1A)-C(4A)-C(9A)	95.0(6)
C(9A)-C(4A)-C(5A)-C(6A)	2.6(7)
N(1A)-C(4A)-C(5A)-C(6A)	177.6(4)
C(9A)-C(4A)-C(5A)-C(10A)	-178.7(5)
N(1A)-C(4A)-C(5A)-C(10A)	-3.7(7)
C(4A)-C(5A)-C(6A)-C(7A)	0.5(7)
C(10A)-C(5A)-C(6A)-C(7A)	-178.3(5)
C(5A)-C(6A)-C(7A)-C(8A)	-2.7(7)
C(5A)-C(6A)-C(7A)-C(11A)	176.2(5)
C(6A)-C(7A)-C(8A)-C(9A)	1.9(7)
C(11A)-C(7A)-C(8A)-C(9A)	-177.0(4)
C(5A)-C(4A)-C(9A)-C(8A)	-3.3(7)
N(1A)-C(4A)-C(9A)-C(8A)	-178.4(4)
C(5A)-C(4A)-C(9A)-C(12A)	175.1(5)
N(1A)-C(4A)-C(9A)-C(12A)	0.0(7)
C(7A)-C(8A)-C(9A)-C(4A)	1.0(7)
C(7A)-C(8A)-C(9A)-C(12A)	-177.5(5)
C(1A)-N(2A)-C(13A)-C(14A)	-102.2(6)
C(3A)-N(2A)-C(13A)-C(14A)	87.0(6)
C(1A)-N(2A)-C(13A)-C(18A)	82.0(6)
C(3A)-N(2A)-C(13A)-C(18A)	-88.8(6)
C(18A)-C(13A)-C(14A)-C(15A)	-7.7(6)
N(2A)-C(13A)-C(14A)-C(15A)	176.6(4)
C(18A)-C(13A)-C(14A)-C(19A)	168.3(4)
N(2A)-C(13A)-C(14A)-C(19A)	-7.3(6)
C(13A)-C(14A)-C(15A)-C(16A)	2.2(7)
C(19A)-C(14A)-C(15A)-C(16A)	-174.0(4)
C(14A)-C(15A)-C(16A)-C(17A)	4.3(6)
C(14A)-C(15A)-C(16A)-C(20A)	-175.9(4)
C(15A)-C(16A)-C(17A)-C(18A)	-5.4(7)
C(20A)-C(16A)-C(17A)-C(18A)	174.8(4)
C(16A)-C(17A)-C(18A)-C(13A)	0.0(6)
C(16A)-C(17A)-C(18A)-C(21A)	178.4(4)
C(14A)-C(13A)-C(18A)-C(17A)	6.6(6)
N(2A)-C(13A)-C(18A)-C(17A)	-177.5(4)
C(14A)-C(13A)-C(18A)-C(21A)	-171.7(4)
N(2A)-C(13A)-C(18A)-C(21A)	4.1(6)
Mo(1A)-N(3A)-C(22A)-C(27A)	-170.7(17)
Mo(1A)-N(3A)-C(22A)-C(23A)	9(2)
C(27A)-C(22A)-C(23A)-C(24A)	3.6(7)
N(3A)-C(22A)-C(23A)-C(24A)	-176.3(4)
C(22A)-C(23A)-C(24A)-C(25A)	-4.7(6)
C(22A)-C(23A)-C(24A)-C(28A)	172.7(4)
C(23A)-C(24A)-C(25A)-C(26A)	1.8(7)

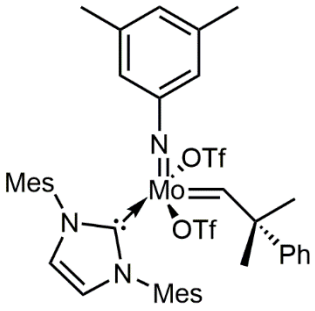
C(28A)-C(24A)-C(25A)-C(26A)	-175.7(4)
C(24A)-C(25A)-C(26A)-C(27A)	2.2(6)
C(24A)-C(25A)-C(26A)-C(29A)	-176.3(4)
C(23A)-C(22A)-C(27A)-C(26A)	0.5(7)
N(3A)-C(22A)-C(27A)-C(26A)	-179.5(4)
C(25A)-C(26A)-C(27A)-C(22A)	-3.4(6)
C(29A)-C(26A)-C(27A)-C(22A)	175.2(4)
N(3A)-Mo(1A)-C(30A)-C(31A)	24.2(6)
O(4A)-Mo(1A)-C(30A)-C(31A)	-76.7(6)
O(1A)-Mo(1A)-C(30A)-C(31A)	-155.4(6)
C(1A)-Mo(1A)-C(30A)-C(31A)	123.9(6)
Mo(1A)-C(30A)-C(31A)-C(32A)	-45.9(7)
Mo(1A)-C(30A)-C(31A)-C(34A)	-172.2(4)
Mo(1A)-C(30A)-C(31A)-C(33A)	70.8(7)
C(30A)-C(31A)-C(34A)-C(35A)	-14.5(6)
C(32A)-C(31A)-C(34A)-C(35A)	-140.8(5)
C(33A)-C(31A)-C(34A)-C(35A)	101.9(5)
C(30A)-C(31A)-C(34A)-C(39A)	170.1(4)
C(32A)-C(31A)-C(34A)-C(39A)	43.8(6)
C(33A)-C(31A)-C(34A)-C(39A)	-73.5(5)
C(39A)-C(34A)-C(35A)-C(36A)	-0.9(8)
C(31A)-C(34A)-C(35A)-C(36A)	-176.4(5)
C(34A)-C(35A)-C(36A)-C(37A)	0.3(8)
C(35A)-C(36A)-C(37A)-C(38A)	1.1(8)
C(36A)-C(37A)-C(38A)-C(39A)	-1.9(9)
C(37A)-C(38A)-C(39A)-C(34A)	1.3(9)
C(35A)-C(34A)-C(39A)-C(38A)	0.1(8)
C(31A)-C(34A)-C(39A)-C(38A)	175.8(5)
O(3A)-S(1A)-O(1A)-Mo(1A)	-150.4(3)
O(2A)-S(1A)-O(1A)-Mo(1A)	-14.7(4)
C(40A)-S(1A)-O(1A)-Mo(1A)	98.0(4)
N(3A)-Mo(1A)-O(1A)-S(1A)	-165.2(4)
C(30A)-Mo(1A)-O(1A)-S(1A)	13.6(4)
O(4A)-Mo(1A)-O(1A)-S(1A)	-86.0(4)
C(1A)-Mo(1A)-O(1A)-S(1A)	116.6(4)
O(3A)-S(1A)-C(40A)-F(1A)	172.4(3)
O(2A)-S(1A)-C(40A)-F(1A)	47.5(4)
O(1A)-S(1A)-C(40A)-F(1A)	-70.4(4)
O(3A)-S(1A)-C(40A)-F(2A)	51.8(4)
O(2A)-S(1A)-C(40A)-F(2A)	-73.1(4)
O(1A)-S(1A)-C(40A)-F(2A)	169.0(3)
O(3A)-S(1A)-C(40A)-F(3A)	-67.7(4)
O(2A)-S(1A)-C(40A)-F(3A)	167.4(3)
O(1A)-S(1A)-C(40A)-F(3A)	49.5(4)
O(5A)-S(2A)-O(4A)-Mo(1A)	1.5(5)
O(6A)-S(2A)-O(4A)-Mo(1A)	-137.1(4)
C(41A)-S(2A)-O(4A)-Mo(1A)	112.8(4)
N(3A)-Mo(1A)-O(4A)-S(2A)	-14.8(4)
C(30A)-Mo(1A)-O(4A)-S(2A)	88.8(4)
O(1A)-Mo(1A)-O(4A)-S(2A)	-175.6(4)

C(1A)-Mo(1A)-O(4A)-S(2A)	-130.8(4)
O(5A)-S(2A)-C(41A)-F(6A)	165.8(3)
O(6A)-S(2A)-C(41A)-F(6A)	-68.5(4)
O(4A)-S(2A)-C(41A)-F(6A)	48.0(4)
O(5A)-S(2A)-C(41A)-F(4A)	-73.6(4)
O(6A)-S(2A)-C(41A)-F(4A)	52.1(4)
O(4A)-S(2A)-C(41A)-F(4A)	168.6(4)
O(5A)-S(2A)-C(41A)-F(5A)	45.4(4)
O(6A)-S(2A)-C(41A)-F(5A)	171.1(4)
O(4A)-S(2A)-C(41A)-F(5A)	-72.4(4)
C(4B)-N(1B)-C(1B)-N(2B)	-171.5(4)
C(2B)-N(1B)-C(1B)-N(2B)	3.0(6)
C(4B)-N(1B)-C(1B)-Mo(1B)	12.3(6)
C(2B)-N(1B)-C(1B)-Mo(1B)	-173.1(3)
N(3B)-Mo(1B)-C(1B)-N(2B)	98.6(6)
C(30B)-Mo(1B)-C(1B)-N(2B)	-5.0(6)
O(4B)-Mo(1B)-C(1B)-N(2B)	-150.1(5)
O(1B)-Mo(1B)-C(1B)-N(2B)	-96.1(5)
N(3B)-Mo(1B)-C(1B)-N(1B)	-86.8(4)
C(30B)-Mo(1B)-C(1B)-N(1B)	169.7(4)
O(4B)-Mo(1B)-C(1B)-N(1B)	24.6(5)
O(1B)-Mo(1B)-C(1B)-N(1B)	78.5(4)
N(1B)-C(1B)-N(2B)-C(13B)	172.1(5)
Mo(1B)-C(1B)-N(2B)-C(13B)	-13.1(9)
N(1B)-C(1B)-N(2B)-C(3B)	5.5(6)
Mo(1B)-C(1B)-N(2B)-C(3B)	-179.8(4)
C(1B)-N(1B)-C(2B)-C(3B)	-9.6(6)
C(4B)-N(1B)-C(2B)-C(3B)	164.9(5)
C(30B)-Mo(1B)-N(3B)-C(22B)	-147(2)
O(4B)-Mo(1B)-N(3B)-C(22B)	-42(2)
O(1B)-Mo(1B)-N(3B)-C(22B)	25(3)
C(1B)-Mo(1B)-N(3B)-C(22B)	106(2)
C(1B)-N(2B)-C(3B)-C(2B)	-11.0(6)
C(13B)-N(2B)-C(3B)-C(2B)	-179.1(4)
N(1B)-C(2B)-C(3B)-N(2B)	11.4(5)
C(1B)-N(1B)-C(4B)-C(9B)	-97.7(6)
C(2B)-N(1B)-C(4B)-C(9B)	88.3(6)
C(1B)-N(1B)-C(4B)-C(5B)	85.2(6)
C(2B)-N(1B)-C(4B)-C(5B)	-88.8(6)
C(9B)-C(4B)-C(5B)-C(6B)	8.6(6)
N(1B)-C(4B)-C(5B)-C(6B)	-174.3(4)
C(9B)-C(4B)-C(5B)-C(10B)	-170.6(4)
N(1B)-C(4B)-C(5B)-C(10B)	6.5(6)
C(4B)-C(5B)-C(6B)-C(7B)	-1.6(7)
C(10B)-C(5B)-C(6B)-C(7B)	177.6(4)
C(5B)-C(6B)-C(7B)-C(8B)	-4.2(7)
C(5B)-C(6B)-C(7B)-C(11B)	175.4(5)
C(6B)-C(7B)-C(8B)-C(9B)	3.2(7)
C(11B)-C(7B)-C(8B)-C(9B)	-176.4(4)
C(5B)-C(4B)-C(9B)-C(8B)	-9.5(6)

N(1B)-C(4B)-C(9B)-C(8B)	173.5(4)
C(5B)-C(4B)-C(9B)-C(12B)	166.0(4)
N(1B)-C(4B)-C(9B)-C(12B)	-11.0(6)
C(7B)-C(8B)-C(9B)-C(4B)	3.5(7)
C(7B)-C(8B)-C(9B)-C(12B)	-172.1(4)
C(1B)-N(2B)-C(13B)-C(18B)	107.6(6)
C(3B)-N(2B)-C(13B)-C(18B)	-86.5(5)
C(1B)-N(2B)-C(13B)-C(14B)	-79.0(6)
C(3B)-N(2B)-C(13B)-C(14B)	86.9(5)
C(18B)-C(13B)-C(14B)-C(15B)	-4.5(6)
N(2B)-C(13B)-C(14B)-C(15B)	-177.8(4)
C(18B)-C(13B)-C(14B)-C(19B)	174.9(4)
N(2B)-C(13B)-C(14B)-C(19B)	1.6(6)
C(13B)-C(14B)-C(15B)-C(16B)	2.5(7)
C(19B)-C(14B)-C(15B)-C(16B)	-176.9(4)
C(14B)-C(15B)-C(16B)-C(17B)	1.3(7)
C(14B)-C(15B)-C(16B)-C(20B)	-178.3(5)
C(15B)-C(16B)-C(17B)-C(18B)	-3.5(7)
C(20B)-C(16B)-C(17B)-C(18B)	176.2(5)
C(16B)-C(17B)-C(18B)-C(13B)	1.6(7)
C(16B)-C(17B)-C(18B)-C(21B)	-177.9(4)
C(14B)-C(13B)-C(18B)-C(17B)	2.5(7)
N(2B)-C(13B)-C(18B)-C(17B)	175.7(4)
C(14B)-C(13B)-C(18B)-C(21B)	-178.0(4)
N(2B)-C(13B)-C(18B)-C(21B)	-4.8(6)
Mo(1B)-N(3B)-C(22B)-C(27B)	-174(2)
Mo(1B)-N(3B)-C(22B)-C(23B)	3(2)
C(27B)-C(22B)-C(23B)-C(24B)	1.6(6)
N(3B)-C(22B)-C(23B)-C(24B)	-175.7(4)
C(22B)-C(23B)-C(24B)-C(25B)	-1.4(6)
C(22B)-C(23B)-C(24B)-C(28B)	177.1(4)
C(23B)-C(24B)-C(25B)-C(26B)	-0.1(7)
C(28B)-C(24B)-C(25B)-C(26B)	-178.7(4)
C(24B)-C(25B)-C(26B)-C(27B)	1.4(7)
C(24B)-C(25B)-C(26B)-C(29B)	-178.5(5)
C(25B)-C(26B)-C(27B)-C(22B)	-1.3(7)
C(29B)-C(26B)-C(27B)-C(22B)	178.7(4)
N(3B)-C(22B)-C(27B)-C(26B)	177.0(4)
C(23B)-C(22B)-C(27B)-C(26B)	-0.2(7)
N(3B)-Mo(1B)-C(30B)-C(31B)	21.2(6)
O(4B)-Mo(1B)-C(30B)-C(31B)	-78.3(6)
O(1B)-Mo(1B)-C(30B)-C(31B)	-156.8(6)
C(1B)-Mo(1B)-C(30B)-C(31B)	121.5(6)
Mo(1B)-C(30B)-C(31B)-C(32B)	-34.2(7)
Mo(1B)-C(30B)-C(31B)-C(34B)	-160.9(4)
Mo(1B)-C(30B)-C(31B)-C(33B)	82.9(6)
C(30B)-C(31B)-C(34B)-C(39B)	-9.2(7)
C(32B)-C(31B)-C(34B)-C(39B)	-134.8(5)
C(33B)-C(31B)-C(34B)-C(39B)	105.1(5)
C(30B)-C(31B)-C(34B)-C(35B)	174.5(4)

C(32B)-C(31B)-C(34B)-C(35B)	48.9(6)
C(33B)-C(31B)-C(34B)-C(35B)	-71.2(6)
C(39B)-C(34B)-C(35B)-C(36B)	0.1(7)
C(31B)-C(34B)-C(35B)-C(36B)	176.7(5)
C(34B)-C(35B)-C(36B)-C(37B)	1.0(8)
C(35B)-C(36B)-C(37B)-C(38B)	-1.0(8)
C(36B)-C(37B)-C(38B)-C(39B)	-0.2(8)
C(35B)-C(34B)-C(39B)-C(38B)	-1.3(7)
C(31B)-C(34B)-C(39B)-C(38B)	-177.7(5)
C(37B)-C(38B)-C(39B)-C(34B)	1.4(8)
O(2B)-S(1B)-O(1B)-Mo(1B)	-164.1(3)
O(3B)-S(1B)-O(1B)-Mo(1B)	-27.4(5)
C(40B)-S(1B)-O(1B)-Mo(1B)	84.4(4)
N(3B)-Mo(1B)-O(1B)-S(1B)	-162.7(5)
C(30B)-Mo(1B)-O(1B)-S(1B)	9.3(4)
O(4B)-Mo(1B)-O(1B)-S(1B)	-94.0(4)
C(1B)-Mo(1B)-O(1B)-S(1B)	114.4(4)
O(2B)-S(1B)-C(40B)-F(1B)	175.5(4)
O(3B)-S(1B)-C(40B)-F(1B)	51.2(4)
O(1B)-S(1B)-C(40B)-F(1B)	-67.1(4)
O(2B)-S(1B)-C(40B)-F(2B)	-65.2(4)
O(3B)-S(1B)-C(40B)-F(2B)	170.5(3)
O(1B)-S(1B)-C(40B)-F(2B)	52.2(4)
O(2B)-S(1B)-C(40B)-F(3B)	55.3(4)
O(3B)-S(1B)-C(40B)-F(3B)	-69.0(4)
O(1B)-S(1B)-C(40B)-F(3B)	172.6(3)
O(6B)-S(2B)-O(4B)-Mo(1B)	93.3(3)
O(5B)-S(2B)-O(4B)-Mo(1B)	-40.8(4)
C(41B)-S(2B)-O(4B)-Mo(1B)	-151.6(4)
N(3B)-Mo(1B)-O(4B)-S(2B)	-12.5(3)
C(30B)-Mo(1B)-O(4B)-S(2B)	90.6(3)
O(1B)-Mo(1B)-O(4B)-S(2B)	-178.7(3)
C(1B)-Mo(1B)-O(4B)-S(2B)	-123.9(3)
O(6B)-S(2B)-C(41B)-F(6B)	62.1(6)
O(5B)-S(2B)-C(41B)-F(6B)	-175.6(6)
O(4B)-S(2B)-C(41B)-F(6B)	-58.3(6)
O(6B)-S(2B)-C(41B)-F(4B)	-61.6(7)
O(5B)-S(2B)-C(41B)-F(4B)	60.7(7)
O(4B)-S(2B)-C(41B)-F(4B)	178.1(6)
O(6B)-S(2B)-C(41B)-F(5B)	-176.2(5)
O(5B)-S(2B)-C(41B)-F(5B)	-53.9(6)
O(4B)-S(2B)-C(41B)-F(5B)	63.4(6)

Complex 20



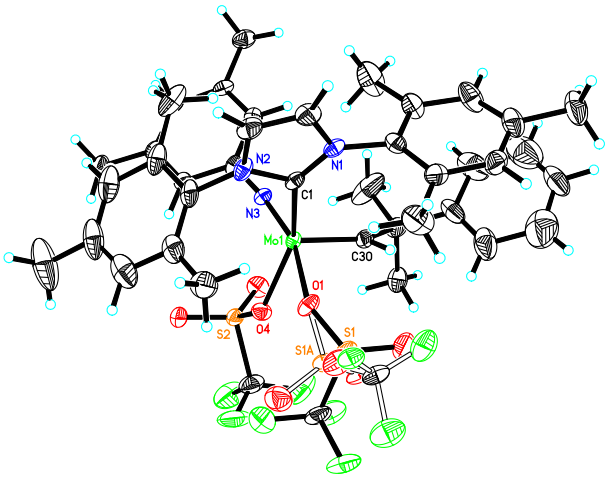


Table 20.1. Crystal data and structure refinement for **20**.

Empirical formula	$C_{41}H_{45}F_6MoN_3O_6S_2$
Formula weight	949.86
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, $P2_1/c$
Unit cell dimensions	a = 11.1860(5) Å, α = 90°
	b = 20.9570(10) Å, β = 106.252(2)°
	c = 19.9631(10) Å, γ = 90°
Volume	4492.8(4) $Å^3$
Z, Calculated density	4, 1.404 Mg/m^3
Absorption coefficient	0.456 mm^{-1}
F(000)	1952
Crystal size	0.34 x 0.29 x 0.23 mm
Theta range for data collection	1.44 to 28.29°
Limiting indices	-14<=h<=14, -26<=k<=27, -26<=l<=24
Reflections collected / unique	43001 / 11107 [R(int) = 0.0380]
Completeness to theta = 28.29	99.6 %
Absorption correction	Numerical
Max. and min. transmission	0.7457 and 0.6822
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11107 / 66 / 605
Goodness-of-fit on F2	1.043
Final R indices [I>2σ(I)]	R1 = 0.0785, wR2 = 0.1928
R indices (all data)	R1 = 0.0939, wR2 = 0.1992
Largest diff. peak and hole	1.868 and -0.947 $e.Å^{-3}$

****
REMARK: Disordered Solvent Electron-Density Squeezed by PLATON
****

Table 20.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **20**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	2801(1)	3673(1)	1837(1)	17(1)
N(1)	3328(4)	2111(2)	1963(2)	20(1)
C(1)	3639(4)	2729(3)	2101(3)	18(1)
N(2)	4807(4)	2705(2)	2555(3)	23(1)
C(2)	4281(5)	1710(3)	2317(3)	28(1)
N(3)	3720(4)	3876(2)	1310(2)	17(1)
C(3)	5198(5)	2082(3)	2688(3)	28(1)
C(4)	2190(5)	1853(3)	1508(3)	24(1)
C(5)	1289(6)	1623(3)	1812(3)	27(1)
C(6)	290(6)	1292(3)	1383(4)	35(1)
C(7)	162(6)	1190(3)	690(4)	36(1)
C(8)	1034(7)	1457(3)	408(3)	40(2)
C(9)	2070(6)	1790(3)	806(3)	32(1)
C(10)	1399(8)	1704(4)	2571(4)	48(2)
C(11)	-886(7)	791(4)	253(5)	52(2)
C(12)	3010(9)	2074(5)	497(4)	64(3)
C(13)	5522(5)	3267(3)	2824(3)	29(1)
C(14)	5320(6)	3574(3)	3397(3)	35(1)
C(15)	5969(7)	4142(3)	3604(4)	47(2)
C(16)	6810(7)	4381(4)	3271(4)	52(2)
C(17)	7060(6)	4024(4)	2743(4)	44(2)
C(18)	6420(5)	3460(3)	2498(3)	35(1)
C(19)	4534(6)	3292(4)	3837(4)	41(2)
C(20)	7466(11)	5005(4)	3493(6)	87(4)
C(21)	6701(6)	3086(4)	1928(4)	45(2)
C(22)	4566(4)	4074(3)	955(3)	19(1)
C(23)	4623(5)	3762(3)	340(3)	23(1)
C(24)	5499(5)	3949(3)	11(3)	22(1)
C(25)	6325(5)	4445(3)	297(3)	23(1)
C(26)	6284(5)	4755(3)	908(3)	22(1)
C(27)	5396(5)	4572(3)	1236(3)	21(1)
C(28)	5565(6)	3631(3)	-661(3)	32(1)
C(29)	7214(5)	5272(3)	1225(3)	30(1)
C(30)	1288(5)	3499(3)	1171(3)	23(1)
C(31)	531(5)	3633(4)	431(3)	36(2)
C(32)	-228(6)	4240(3)	482(3)	32(1)
C(33)	1361(7)	3801(6)	-42(4)	80(4)
C(34)	-379(7)	3103(4)	139(4)	52(2)
C(35)	-1182(7)	2910(4)	510(6)	60(2)
C(36)	-2077(10)	2427(5)	205(7)	85(3)
C(37)	-2042(8)	2196(4)	-460(5)	59(2)
C(38)	-1290(11)	2391(5)	-807(6)	84(3)

C(39)	-446(9)	2839(4)	-518(5)	67(3)
O(1)	2109(3)	3540(2)	2728(2)	25(1)
S(1)	1063(2)	3438(1)	3048(1)	24(1)
O(2)	1424(10)	3077(4)	3686(6)	33(2)
O(3)	-61(5)	3279(3)	2535(3)	39(1)
C(40)	815(8)	4241(5)	3336(4)	33(2)
F(1)	332(5)	4621(3)	2791(3)	44(1)
F(2)	1856(6)	4494(4)	3720(4)	54(2)
F(3)	-12(5)	4211(3)	3719(3)	47(1)
S(1A)	1189(5)	3884(3)	2939(3)	26(1)
O(2A)	175(15)	4165(9)	2431(9)	28(3)
O(3A)	1780(20)	4233(12)	3545(12)	40(5)
C(40A)	450(20)	3210(13)	3300(13)	31(5)
F(1A)	1290(20)	2862(10)	3726(13)	27(5)
F(2A)	-199(15)	2857(9)	2797(9)	45(4)
F(3A)	-288(16)	3468(9)	3645(9)	50(4)
S(2)	2833(1)	5250(1)	1870(1)	22(1)
O(4)	2552(4)	4629(2)	2147(2)	24(1)
O(5)	4015(4)	5502(2)	2255(2)	31(1)
O(6)	2518(4)	5276(2)	1124(2)	29(1)
C(41)	1698(6)	5758(3)	2109(4)	37(2)
F(4)	545(4)	5584(2)	1777(3)	54(1)
F(5)	1846(4)	6359(2)	1927(3)	61(1)
F(6)	1850(5)	5746(2)	2790(3)	58(1)

Table 20.3. Bond lengths [Å] and angles [°] for **20**.

Mo(1)-N(3)	1.717(4)
Mo(1)-C(30)	1.872(5)
Mo(1)-O(4)	2.139(4)
Mo(1)-O(1)	2.147(4)
Mo(1)-C(1)	2.188(5)
N(1)-C(1)	1.349(7)
N(1)-C(2)	1.386(7)
N(1)-C(4)	1.446(7)
C(1)-N(2)	1.366(6)
N(2)-C(3)	1.379(7)
N(2)-C(13)	1.440(7)
C(2)-C(3)	1.336(9)
C(2)-H(2)	0.9500
N(3)-C(22)	1.395(6)
C(3)-H(3)	0.9500
C(4)-C(9)	1.375(8)
C(4)-C(5)	1.400(8)
C(5)-C(6)	1.388(9)
C(5)-C(10)	1.495(9)
C(6)-C(7)	1.367(10)
C(6)-H(6)	0.9500
C(7)-C(8)	1.375(10)

C(7)-C(11)	1.503(9)
C(8)-C(9)	1.395(9)
C(8)-H(8)	0.9500
C(9)-C(12)	1.485(9)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.386(9)
C(13)-C(18)	1.401(9)
C(14)-C(15)	1.395(10)
C(14)-C(19)	1.526(10)
C(15)-C(16)	1.389(12)
C(15)-H(15)	0.9500
C(16)-C(17)	1.384(12)
C(16)-C(20)	1.503(11)
C(17)-C(18)	1.398(10)
C(17)-H(17)	0.9500
C(18)-C(21)	1.484(11)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(27)	1.404(7)
C(22)-C(23)	1.409(8)
C(23)-C(24)	1.380(7)
C(23)-H(23)	0.9500
C(24)-C(25)	1.402(8)
C(24)-C(28)	1.518(8)
C(25)-C(26)	1.395(8)
C(25)-H(25)	0.9500
C(26)-C(27)	1.387(7)
C(26)-C(29)	1.512(8)
C(27)-H(27)	0.9500
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800

C(30)-C(31)	1.509(8)
C(30)-H(30)	0.9500
C(31)-C(34)	1.509(10)
C(31)-C(33)	1.539(10)
C(31)-C(32)	1.549(9)
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-C(35)	1.376(13)
C(34)-C(39)	1.406(12)
C(35)-C(36)	1.433(13)
C(35)-H(35)	0.9500
C(36)-C(37)	1.425(15)
C(36)-H(36)	0.9500
C(37)-C(38)	1.296(16)
C(37)-H(37)	0.9500
C(38)-C(39)	1.342(14)
C(38)-H(38)	0.9500
C(39)-H(39)	0.9500
O(1)-S(1A)	1.415(7)
O(1)-S(1)	1.497(4)
S(1)-O(3)	1.421(6)
S(1)-O(2)	1.439(10)
S(1)-C(40)	1.823(9)
C(40)-F(2)	1.314(11)
C(40)-F(1)	1.334(10)
C(40)-F(3)	1.356(9)
S(1A)-O(3A)	1.41(2)
S(1A)-O(2A)	1.420(18)
S(1A)-C(40A)	1.88(3)
C(40A)-F(2A)	1.29(3)
C(40A)-F(1A)	1.30(4)
C(40A)-F(3A)	1.33(3)
S(2)-O(5)	1.431(4)
S(2)-O(6)	1.433(4)
S(2)-O(4)	1.482(4)
S(2)-C(41)	1.820(6)
C(41)-F(6)	1.322(8)
C(41)-F(4)	1.325(8)
C(41)-F(5)	1.334(8)

N(3)-Mo(1)-C(30)	101.0(2)
N(3)-Mo(1)-O(4)	95.31(17)
C(30)-Mo(1)-O(4)	102.85(19)
N(3)-Mo(1)-O(1)	162.87(18)
C(30)-Mo(1)-O(1)	95.7(2)
O(4)-Mo(1)-O(1)	77.03(15)

N(3)-Mo(1)-C(1)	94.78(19)
C(30)-Mo(1)-C(1)	103.7(2)
O(4)-Mo(1)-C(1)	149.14(17)
O(1)-Mo(1)-C(1)	84.97(16)
C(1)-N(1)-C(2)	111.1(5)
C(1)-N(1)-C(4)	128.2(4)
C(2)-N(1)-C(4)	120.6(5)
N(1)-C(1)-N(2)	104.2(4)
N(1)-C(1)-Mo(1)	138.5(4)
N(2)-C(1)-Mo(1)	117.3(4)
C(1)-N(2)-C(3)	110.8(5)
C(1)-N(2)-C(13)	123.1(4)
C(3)-N(2)-C(13)	126.0(5)
C(3)-C(2)-N(1)	106.8(5)
C(3)-C(2)-H(2)	126.6
N(1)-C(2)-H(2)	126.6
C(22)-N(3)-Mo(1)	173.0(4)
C(2)-C(3)-N(2)	107.0(5)
C(2)-C(3)-H(3)	126.5
N(2)-C(3)-H(3)	126.5
C(9)-C(4)-C(5)	122.1(5)
C(9)-C(4)-N(1)	119.6(5)
C(5)-C(4)-N(1)	118.1(5)
C(6)-C(5)-C(4)	117.2(6)
C(6)-C(5)-C(10)	120.4(6)
C(4)-C(5)-C(10)	122.3(6)
C(7)-C(6)-C(5)	122.8(6)
C(7)-C(6)-H(6)	118.6
C(5)-C(6)-H(6)	118.6
C(6)-C(7)-C(8)	117.7(6)
C(6)-C(7)-C(11)	121.2(7)
C(8)-C(7)-C(11)	121.1(7)
C(7)-C(8)-C(9)	122.8(6)
C(7)-C(8)-H(8)	118.6
C(9)-C(8)-H(8)	118.6
C(4)-C(9)-C(8)	117.3(6)
C(4)-C(9)-C(12)	120.4(6)
C(8)-C(9)-C(12)	122.4(6)
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(7)-C(11)-H(11A)	109.5
C(7)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(7)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5

C(9)-C(12)-H(12A)	109.5
C(9)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(9)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(18)	123.6(6)
C(14)-C(13)-N(2)	119.1(6)
C(18)-C(13)-N(2)	117.3(6)
C(13)-C(14)-C(15)	116.7(7)
C(13)-C(14)-C(19)	123.3(6)
C(15)-C(14)-C(19)	119.8(7)
C(16)-C(15)-C(14)	122.2(8)
C(16)-C(15)-H(15)	118.9
C(14)-C(15)-H(15)	118.9
C(17)-C(16)-C(15)	118.5(7)
C(17)-C(16)-C(20)	120.6(9)
C(15)-C(16)-C(20)	120.8(9)
C(16)-C(17)-C(18)	122.2(7)
C(16)-C(17)-H(17)	118.9
C(18)-C(17)-H(17)	118.9
C(17)-C(18)-C(13)	116.4(7)
C(17)-C(18)-C(21)	121.2(6)
C(13)-C(18)-C(21)	122.5(6)
C(14)-C(19)-H(19A)	109.5
C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-H(20A)	109.5
C(16)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(16)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(3)-C(22)-C(27)	119.0(5)
N(3)-C(22)-C(23)	120.5(5)
C(27)-C(22)-C(23)	120.5(5)
C(24)-C(23)-C(22)	119.6(5)
C(24)-C(23)-H(23)	120.2
C(22)-C(23)-H(23)	120.2
C(23)-C(24)-C(25)	119.4(5)
C(23)-C(24)-C(28)	120.9(5)

C(25)-C(24)-C(28)	119.7(5)
C(26)-C(25)-C(24)	121.5(5)
C(26)-C(25)-H(25)	119.2
C(24)-C(25)-H(25)	119.2
C(27)-C(26)-C(25)	119.2(5)
C(27)-C(26)-C(29)	120.0(5)
C(25)-C(26)-C(29)	120.8(5)
C(26)-C(27)-C(22)	119.8(5)
C(26)-C(27)-H(27)	120.1
C(22)-C(27)-H(27)	120.1
C(24)-C(28)-H(28A)	109.5
C(24)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(24)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(26)-C(29)-H(29A)	109.5
C(26)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(26)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(31)-C(30)-Mo(1)	143.9(5)
C(31)-C(30)-H(30)	108.1
Mo(1)-C(30)-H(30)	108.1
C(30)-C(31)-C(34)	112.0(6)
C(30)-C(31)-C(33)	111.9(5)
C(34)-C(31)-C(33)	112.8(7)
C(30)-C(31)-C(32)	104.9(5)
C(34)-C(31)-C(32)	107.9(5)
C(33)-C(31)-C(32)	106.7(7)
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(31)-C(33)-H(33A)	109.5
C(31)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(31)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(35)-C(34)-C(39)	120.9(8)
C(35)-C(34)-C(31)	118.7(7)
C(39)-C(34)-C(31)	120.3(9)
C(34)-C(35)-C(36)	117.6(10)
C(34)-C(35)-H(35)	121.2
C(36)-C(35)-H(35)	121.2
C(37)-C(36)-C(35)	115.9(11)

C(37)-C(36)-H(36)	122.0
C(35)-C(36)-H(36)	122.0
C(38)-C(37)-C(36)	125.6(9)
C(38)-C(37)-H(37)	117.2
C(36)-C(37)-H(37)	117.2
C(37)-C(38)-C(39)	118.3(11)
C(37)-C(38)-H(38)	120.8
C(39)-C(38)-H(38)	120.8
C(38)-C(39)-C(34)	121.6(12)
C(38)-C(39)-H(39)	119.2
C(34)-C(39)-H(39)	119.2
S(1A)-O(1)-S(1)	39.1(3)
S(1A)-O(1)-Mo(1)	129.9(3)
S(1)-O(1)-Mo(1)	151.4(3)
O(3)-S(1)-O(2)	119.1(5)
O(3)-S(1)-O(1)	111.4(3)
O(2)-S(1)-O(1)	113.2(5)
O(3)-S(1)-C(40)	105.1(4)
O(2)-S(1)-C(40)	103.6(5)
O(1)-S(1)-C(40)	102.1(3)
F(2)-C(40)-F(1)	108.9(8)
F(2)-C(40)-F(3)	108.8(7)
F(1)-C(40)-F(3)	107.6(7)
F(2)-C(40)-S(1)	111.6(6)
F(1)-C(40)-S(1)	110.9(6)
F(3)-C(40)-S(1)	108.9(6)
O(3A)-S(1A)-O(1)	108.2(11)
O(3A)-S(1A)-O(2A)	119.3(14)
O(1)-S(1A)-O(2A)	120.1(7)
O(3A)-S(1A)-C(40A)	102.3(13)
O(1)-S(1A)-C(40A)	99.6(8)
O(2A)-S(1A)-C(40A)	103.6(11)
F(2A)-C(40A)-F(1A)	109(2)
F(2A)-C(40A)-F(3A)	110(2)
F(1A)-C(40A)-F(3A)	109(2)
F(2A)-C(40A)-S(1A)	110.1(17)
F(1A)-C(40A)-S(1A)	110.6(18)
F(3A)-C(40A)-S(1A)	107.2(18)
O(5)-S(2)-O(6)	117.7(3)
O(5)-S(2)-O(4)	112.6(3)
O(6)-S(2)-O(4)	113.9(2)
O(5)-S(2)-C(41)	104.5(3)
O(6)-S(2)-C(41)	105.3(3)
O(4)-S(2)-C(41)	100.3(3)
S(2)-O(4)-Mo(1)	131.1(2)
F(6)-C(41)-F(4)	109.7(6)
F(6)-C(41)-F(5)	108.0(6)
F(4)-C(41)-F(5)	107.5(6)
F(6)-C(41)-S(2)	111.1(5)
F(4)-C(41)-S(2)	111.1(5)

F(5)-C(41)-S(2)	109.3(4)

Symmetry transformations used to generate equivalent atoms:

Table 20.4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **20**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11}+ ...+2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	13(1)	18(1)	18(1)	2(1)	3(1)	1(1)
N(1)	19(2)	23(2)	23(2)	5(2)	12(2)	2(2)
C(1)	15(2)	25(3)	16(2)	4(2)	7(2)	3(2)
N(2)	15(2)	23(2)	29(2)	8(2)	4(2)	3(2)
C(2)	30(3)	19(3)	35(3)	7(2)	8(2)	9(2)
N(3)	16(2)	20(2)	16(2)	4(2)	5(2)	3(2)
C(3)	25(3)	31(3)	27(3)	7(2)	5(2)	11(2)
C(4)	29(3)	19(2)	23(3)	-1(2)	5(2)	1(2)
C(5)	32(3)	21(3)	33(3)	2(2)	16(2)	-1(2)
C(6)	30(3)	23(3)	54(4)	2(3)	18(3)	-2(2)
C(7)	40(3)	21(3)	41(4)	4(3)	1(3)	-5(2)
C(8)	61(4)	34(4)	23(3)	-2(3)	7(3)	-15(3)
C(9)	43(3)	32(3)	24(3)	-3(2)	13(3)	-12(3)
C(10)	68(5)	41(4)	43(4)	-2(3)	30(4)	-12(4)
C(11)	49(4)	31(4)	69(5)	-2(4)	4(4)	-14(3)
C(12)	87(6)	80(6)	42(4)	-23(4)	46(4)	-52(5)
C(13)	20(3)	28(3)	30(3)	7(2)	-8(2)	1(2)
C(14)	30(3)	31(3)	33(3)	4(3)	-8(2)	6(2)
C(15)	55(4)	35(4)	35(4)	4(3)	-15(3)	6(3)
C(16)	44(4)	34(4)	56(5)	15(3)	-23(4)	-10(3)
C(17)	31(3)	45(4)	46(4)	23(3)	-7(3)	-9(3)
C(18)	20(3)	37(3)	38(3)	16(3)	-6(2)	0(2)
C(19)	37(3)	47(4)	32(3)	-2(3)	-1(3)	12(3)
C(20)	98(8)	39(5)	86(7)	17(5)	-38(6)	-27(5)
C(21)	23(3)	58(5)	55(4)	26(4)	13(3)	9(3)
C(22)	13(2)	24(3)	20(2)	7(2)	3(2)	1(2)
C(23)	22(2)	21(3)	25(3)	2(2)	5(2)	1(2)
C(24)	22(2)	22(3)	25(3)	5(2)	11(2)	7(2)
C(25)	16(2)	28(3)	29(3)	6(2)	9(2)	3(2)
C(26)	17(2)	24(3)	25(3)	6(2)	5(2)	3(2)
C(27)	19(2)	26(3)	18(2)	2(2)	3(2)	3(2)
C(28)	34(3)	31(3)	36(3)	3(3)	20(3)	2(3)
C(29)	20(3)	38(3)	32(3)	0(3)	7(2)	-6(2)
C(30)	17(2)	21(3)	31(3)	-2(2)	5(2)	3(2)
C(31)	19(3)	55(4)	27(3)	-11(3)	-3(2)	9(3)
C(32)	25(3)	36(3)	31(3)	8(3)	-1(2)	0(2)
C(33)	29(4)	184(12)	23(3)	0(5)	4(3)	20(5)
C(34)	31(3)	41(4)	61(5)	-29(4)	-22(3)	19(3)
C(35)	35(4)	37(4)	92(5)	-11(4)	-8(4)	3(3)
C(36)	58(5)	70(5)	116(7)	6(5)	6(5)	10(4)

C(37)	49(4)	33(4)	74(5)	-19(4)	-16(4)	8(3)
C(38)	84(6)	69(5)	79(6)	-16(5)	-7(5)	21(5)
C(39)	64(5)	60(5)	57(5)	-20(4)	-17(4)	24(4)
O(1)	20(2)	33(2)	25(2)	8(2)	13(2)	0(2)
S(1)	22(1)	34(1)	19(1)	4(1)	11(1)	-2(1)
O(2)	37(4)	37(5)	32(4)	11(4)	20(3)	-1(4)
O(3)	23(3)	60(4)	34(3)	-2(3)	8(2)	-7(3)
C(40)	29(4)	51(5)	25(4)	2(4)	18(3)	6(4)
F(1)	49(3)	45(3)	49(3)	19(3)	30(3)	12(2)
F(2)	45(4)	52(4)	65(5)	-24(4)	16(3)	-5(3)
F(3)	45(3)	61(4)	46(3)	0(3)	31(3)	16(3)
S(1A)	30(3)	34(3)	18(2)	5(2)	14(2)	4(2)
O(2A)	29(6)	38(7)	26(6)	9(5)	23(5)	2(5)
O(3A)	46(8)	45(8)	32(8)	-4(6)	15(6)	-3(7)
C(40A)	30(8)	38(8)	33(8)	2(6)	21(6)	4(6)
F(1A)	32(7)	35(8)	21(7)	4(6)	16(5)	1(6)
F(2A)	38(6)	52(7)	50(7)	10(6)	20(5)	-8(5)
F(3A)	51(7)	59(7)	45(7)	13(6)	23(6)	11(6)
S(2)	20(1)	20(1)	28(1)	-2(1)	10(1)	-2(1)
O(4)	28(2)	22(2)	24(2)	-2(2)	12(2)	-2(2)
O(5)	22(2)	32(2)	42(2)	-11(2)	11(2)	-7(2)
O(6)	36(2)	28(2)	24(2)	5(2)	10(2)	-1(2)
C(41)	35(3)	27(3)	56(4)	-2(3)	24(3)	7(3)
F(4)	25(2)	47(2)	94(4)	16(2)	23(2)	9(2)
F(5)	59(3)	23(2)	113(4)	7(2)	47(3)	6(2)
F(6)	67(3)	57(3)	67(3)	-14(2)	49(3)	7(2)

Table 20.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **20**.

	x	y	z	U(eq)
H(2)	4282	1257	2298	34
H(3)	5973	1944	2987	34
H(6)	-331	1130	1579	41
H(8)	926	1413	-79	48
H(10A)	620	1880	2626	72
H(10B)	2086	1997	2779	72
H(10C)	1563	1289	2805	72
H(11A)	-697	338	350	78
H(11B)	-986	876	-242	78
H(11C)	-1659	899	367	78
H(12A)	3144	2522	638	96
H(12B)	2711	2048	-13	96
H(12C)	3796	1839	661	96
H(15)	5831	4373	3985	57
H(17)	7686	4167	2540	53

H(19A)	5081	3093	4256	61
H(19B)	3968	2970	3564	61
H(19C)	4048	3631	3974	61
H(20A)	8253	4926	3851	131
H(20B)	6937	5282	3684	131
H(20C)	7635	5212	3089	131
H(21A)	7124	3360	1668	67
H(21B)	5923	2926	1612	67
H(21C)	7240	2725	2128	67
H(23)	4062	3424	153	28
H(25)	6926	4573	69	28
H(27)	5349	4783	1649	26
H(28A)	4927	3298	-791	48
H(28B)	6390	3440	-593	48
H(28C)	5421	3951	-1034	48
H(29A)	7107	5632	900	45
H(29B)	8060	5102	1315	45
H(29C)	7076	5416	1664	45
H(30)	820	3222	1377	28
H(32A)	-777	4345	19	48
H(32B)	343	4597	653	48
H(32C)	-731	4164	805	48
H(33A)	1838	3423	-102	119
H(33B)	1935	4144	173	119
H(33C)	838	3941	-498	119
H(35)	-1145	3090	952	72
H(36)	-2659	2271	433	102
H(37)	-2619	1871	-667	71
H(38)	-1335	2220	-1254	100
H(39)	120	2981	-763	81

Table 20.6. Torsion angles [°] for **20**.

C(2)-N(1)-C(1)-N(2)	-0.4(6)
C(4)-N(1)-C(1)-N(2)	-179.5(5)
C(2)-N(1)-C(1)-Mo(1)	-177.9(4)
C(4)-N(1)-C(1)-Mo(1)	3.0(9)
N(3)-Mo(1)-C(1)-N(1)	-109.0(5)
C(30)-Mo(1)-C(1)-N(1)	-6.5(6)
O(4)-Mo(1)-C(1)-N(1)	142.3(5)
O(1)-Mo(1)-C(1)-N(1)	88.2(5)
N(3)-Mo(1)-C(1)-N(2)	73.7(4)
C(30)-Mo(1)-C(1)-N(2)	176.3(4)
O(4)-Mo(1)-C(1)-N(2)	-35.0(6)
O(1)-Mo(1)-C(1)-N(2)	-89.1(4)
N(1)-C(1)-N(2)-C(3)	0.1(6)
Mo(1)-C(1)-N(2)-C(3)	178.2(4)
N(1)-C(1)-N(2)-C(13)	177.8(5)
Mo(1)-C(1)-N(2)-C(13)	-4.0(7)

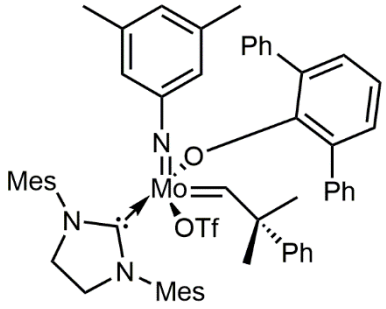
C(1)-N(1)-C(2)-C(3)	0.6(7)
C(4)-N(1)-C(2)-C(3)	179.8(5)
C(30)-Mo(1)-N(3)-C(22)	164(3)
O(4)-Mo(1)-N(3)-C(22)	60(3)
O(1)-Mo(1)-N(3)-C(22)	-3(4)
C(1)-Mo(1)-N(3)-C(22)	-91(3)
N(1)-C(2)-C(3)-N(2)	-0.5(7)
C(1)-N(2)-C(3)-C(2)	0.3(7)
C(13)-N(2)-C(3)-C(2)	-177.4(6)
C(1)-N(1)-C(4)-C(9)	85.1(7)
C(2)-N(1)-C(4)-C(9)	-93.9(7)
C(1)-N(1)-C(4)-C(5)	-100.5(6)
C(2)-N(1)-C(4)-C(5)	80.5(7)
C(9)-C(4)-C(5)-C(6)	3.6(9)
N(1)-C(4)-C(5)-C(6)	-170.6(5)
C(9)-C(4)-C(5)-C(10)	-178.5(6)
N(1)-C(4)-C(5)-C(10)	7.3(9)
C(4)-C(5)-C(6)-C(7)	-0.3(9)
C(10)-C(5)-C(6)-C(7)	-178.2(6)
C(5)-C(6)-C(7)-C(8)	-3.4(10)
C(5)-C(6)-C(7)-C(11)	175.8(6)
C(6)-C(7)-C(8)-C(9)	4.0(11)
C(11)-C(7)-C(8)-C(9)	-175.1(7)
C(5)-C(4)-C(9)-C(8)	-3.0(9)
N(1)-C(4)-C(9)-C(8)	171.1(6)
C(5)-C(4)-C(9)-C(12)	176.4(7)
N(1)-C(4)-C(9)-C(12)	-9.4(10)
C(7)-C(8)-C(9)-C(4)	-0.9(11)
C(7)-C(8)-C(9)-C(12)	179.7(8)
C(1)-N(2)-C(13)-C(14)	83.6(7)
C(3)-N(2)-C(13)-C(14)	-99.0(7)
C(1)-N(2)-C(13)-C(18)	-98.3(6)
C(3)-N(2)-C(13)-C(18)	79.0(7)
C(18)-C(13)-C(14)-C(15)	6.8(9)
N(2)-C(13)-C(14)-C(15)	-175.3(5)
C(18)-C(13)-C(14)-C(19)	-167.5(6)
N(2)-C(13)-C(14)-C(19)	10.5(8)
C(13)-C(14)-C(15)-C(16)	-2.1(9)
C(19)-C(14)-C(15)-C(16)	172.3(6)
C(14)-C(15)-C(16)-C(17)	-3.7(10)
C(14)-C(15)-C(16)-C(20)	178.2(7)
C(15)-C(16)-C(17)-C(18)	5.3(10)
C(20)-C(16)-C(17)-C(18)	-176.5(7)
C(16)-C(17)-C(18)-C(13)	-1.1(9)
C(16)-C(17)-C(18)-C(21)	179.7(6)
C(14)-C(13)-C(18)-C(17)	-5.3(8)
N(2)-C(13)-C(18)-C(17)	176.8(5)
C(14)-C(13)-C(18)-C(21)	174.0(6)
N(2)-C(13)-C(18)-C(21)	-4.0(8)
Mo(1)-N(3)-C(22)-C(27)	-22(3)

Mo(1)-N(3)-C(22)-C(23)	155(3)
N(3)-C(22)-C(23)-C(24)	-177.5(5)
C(27)-C(22)-C(23)-C(24)	-0.2(8)
C(22)-C(23)-C(24)-C(25)	0.4(8)
C(22)-C(23)-C(24)-C(28)	-178.6(5)
C(23)-C(24)-C(25)-C(26)	0.1(8)
C(28)-C(24)-C(25)-C(26)	179.1(5)
C(24)-C(25)-C(26)-C(27)	-0.7(8)
C(24)-C(25)-C(26)-C(29)	177.6(5)
C(25)-C(26)-C(27)-C(22)	0.9(8)
C(29)-C(26)-C(27)-C(22)	-177.5(5)
N(3)-C(22)-C(27)-C(26)	176.9(5)
C(23)-C(22)-C(27)-C(26)	-0.4(8)
N(3)-Mo(1)-C(30)-C(31)	-23.6(7)
O(4)-Mo(1)-C(30)-C(31)	74.5(7)
O(1)-Mo(1)-C(30)-C(31)	152.5(7)
C(1)-Mo(1)-C(30)-C(31)	-121.3(7)
Mo(1)-C(30)-C(31)-C(34)	154.2(6)
Mo(1)-C(30)-C(31)-C(33)	26.4(11)
Mo(1)-C(30)-C(31)-C(32)	-88.9(7)
C(30)-C(31)-C(34)-C(35)	53.1(8)
C(33)-C(31)-C(34)-C(35)	-179.6(7)
C(32)-C(31)-C(34)-C(35)	-61.9(8)
C(30)-C(31)-C(34)-C(39)	-130.4(7)
C(33)-C(31)-C(34)-C(39)	-3.1(9)
C(32)-C(31)-C(34)-C(39)	114.6(7)
C(39)-C(34)-C(35)-C(36)	0.6(11)
C(31)-C(34)-C(35)-C(36)	177.1(7)
C(34)-C(35)-C(36)-C(37)	-0.1(12)
C(35)-C(36)-C(37)-C(38)	-1.0(14)
C(36)-C(37)-C(38)-C(39)	1.5(16)
C(37)-C(38)-C(39)-C(34)	-1.0(14)
C(35)-C(34)-C(39)-C(38)	0.0(12)
C(31)-C(34)-C(39)-C(38)	-176.5(8)
N(3)-Mo(1)-O(1)-S(1A)	103.3(7)
C(30)-Mo(1)-O(1)-S(1A)	-63.4(5)
O(4)-Mo(1)-O(1)-S(1A)	38.5(5)
C(1)-Mo(1)-O(1)-S(1A)	-166.8(5)
N(3)-Mo(1)-O(1)-S(1)	158.0(6)
C(30)-Mo(1)-O(1)-S(1)	-8.8(6)
O(4)-Mo(1)-O(1)-S(1)	93.1(6)
C(1)-Mo(1)-O(1)-S(1)	-112.1(6)
S(1A)-O(1)-S(1)-O(3)	94.6(5)
Mo(1)-O(1)-S(1)-O(3)	12.1(7)
S(1A)-O(1)-S(1)-O(2)	-128.0(6)
Mo(1)-O(1)-S(1)-O(2)	149.5(6)
S(1A)-O(1)-S(1)-C(40)	-17.2(5)
Mo(1)-O(1)-S(1)-C(40)	-99.7(6)
O(3)-S(1)-C(40)-F(2)	-168.7(6)
O(2)-S(1)-C(40)-F(2)	65.5(7)

O(1)-S(1)-C(40)-F(2)	-52.3(6)
O(3)-S(1)-C(40)-F(1)	-47.0(6)
O(2)-S(1)-C(40)-F(1)	-172.8(6)
O(1)-S(1)-C(40)-F(1)	69.4(6)
O(3)-S(1)-C(40)-F(3)	71.2(6)
O(2)-S(1)-C(40)-F(3)	-54.6(7)
O(1)-S(1)-C(40)-F(3)	-172.4(5)
S(1)-O(1)-S(1A)-O(3A)	108.1(12)
Mo(1)-O(1)-S(1A)-O(3A)	-110.1(11)
S(1)-O(1)-S(1A)-O(2A)	-110.2(10)
Mo(1)-O(1)-S(1A)-O(2A)	31.6(11)
S(1)-O(1)-S(1A)-C(40A)	1.6(8)
Mo(1)-O(1)-S(1A)-C(40A)	143.5(9)
O(3A)-S(1A)-C(40A)-F(2A)	176.8(18)
O(1)-S(1A)-C(40A)-F(2A)	-72.1(17)
O(2A)-S(1A)-C(40A)-F(2A)	52.2(19)
O(3A)-S(1A)-C(40A)-F(1A)	-62(2)
O(1)-S(1A)-C(40A)-F(1A)	49(2)
O(2A)-S(1A)-C(40A)-F(1A)	173.3(19)
O(3A)-S(1A)-C(40A)-F(3A)	57(2)
O(1)-S(1A)-C(40A)-F(3A)	168.2(16)
O(2A)-S(1A)-C(40A)-F(3A)	-67.5(19)
O(5)-S(2)-O(4)-Mo(1)	-96.0(3)
O(6)-S(2)-O(4)-Mo(1)	41.3(4)
C(41)-S(2)-O(4)-Mo(1)	153.3(3)
N(3)-Mo(1)-O(4)-S(2)	12.3(3)
C(30)-Mo(1)-O(4)-S(2)	-90.3(4)
O(1)-Mo(1)-O(4)-S(2)	176.8(3)
C(1)-Mo(1)-O(4)-S(2)	120.9(4)
O(5)-S(2)-C(41)-F(6)	-58.7(5)
O(6)-S(2)-C(41)-F(6)	176.6(5)
O(4)-S(2)-C(41)-F(6)	58.1(5)
O(5)-S(2)-C(41)-F(4)	178.9(5)
O(6)-S(2)-C(41)-F(4)	54.2(5)
O(4)-S(2)-C(41)-F(4)	-64.3(5)
O(5)-S(2)-C(41)-F(5)	60.4(6)
O(6)-S(2)-C(41)-F(5)	-64.3(6)
O(4)-S(2)-C(41)-F(5)	177.2(5)

Symmetry transformations used to generate equivalent atoms:

Complex 21


Ph
N
O
Mes
Mo
Ph
N
OTf
Ph
N
Mes

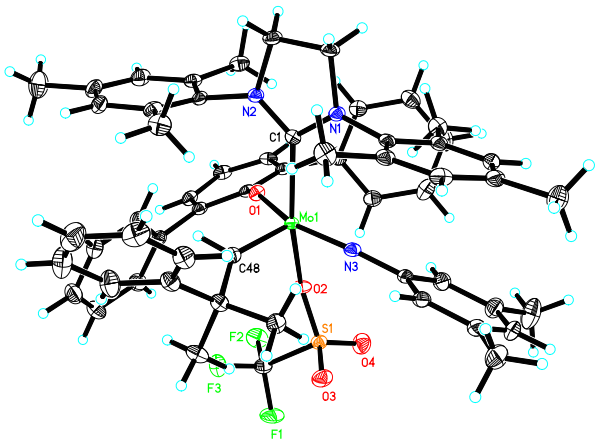

N2
C1
N1
O1
Mo1
C48
N3
O2
S1
F2
O4
F3
O3
F1

Table 21.1. Crystal data and structure refinement for **21**.

Empirical formula	$C_{59}H_{62}Cl_2F_3MoN_3O_4S$
Formula weight	1133.02
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, $P2_1/c$
Unit cell dimensions	a = 12.0834(5) Å α = 90°
	b = 18.1459(8) Å β = 97.644(2)°
	c = 26.6295(12) Å γ = 90°
Volume	5787.0(4) $Å^3$
Z, Calculated density	4, 1.300 Mg/m^3
Absorption coefficient	0.411 mm^{-1}
F(000)	2352
Crystal size	0.43 x 0.32 x 0.14 mm
Theta range for data collection	1.54 to 28.48 º.
Limiting indices	-16<=h<=16, -24<=k<=24, -35<=l<=33
Reflections collected / unique	63145 / 14428 [R(int) = 0.0373]
Completeness to theta = 28.48	98.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7457 and 0.6545
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	14428 / 0 / 668
Goodness-of-fit on F^2	1.048
Final R indices [I>2σ (I)]	R1 = 0.0390, wR2 = 0.0863
R indices (all data)	R1 = 0.0519, wR2 = 0.0912
Largest diff. peak and hole	1.149 and -1.141 $e.Å^{-3}$

****
REMARK: One disordered DCM squeezed by PLATON !
****

Table 21.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **21**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	2238(1)	162(1)	2586(1)	11(1)
S(1)	2282(1)	-1612(1)	2080(1)	15(1)
O(1)	1045(1)	-114(1)	2977(1)	14(1)
F(1)	2636(1)	-2979(1)	2351(1)	28(1)
N(1)	1974(1)	1899(1)	2419(1)	14(1)
C(1)	1940(2)	1343(1)	2749(1)	13(1)
F(2)	1274(1)	-2471(1)	2670(1)	26(1)
N(2)	1549(1)	1616(1)	3160(1)	15(1)
O(2)	1892(1)	-996(1)	2366(1)	18(1)
C(2)	1587(2)	2612(1)	2604(1)	18(1)
F(3)	2974(1)	-2205(1)	2965(1)	26(1)
N(3)	2723(1)	298(1)	2005(1)	14(1)
O(3)	3420(1)	-1558(1)	1987(1)	23(1)
C(3)	1282(2)	2412(1)	3122(1)	19(1)
C(4)	2421(2)	1930(1)	1948(1)	14(1)
O(4)	1472(1)	-1848(1)	1669(1)	26(1)
C(5)	1709(2)	1824(1)	1495(1)	15(1)
C(6)	2115(2)	1966(1)	1039(1)	19(1)
C(7)	3201(2)	2213(1)	1028(1)	21(1)
C(8)	3896(2)	2302(1)	1482(1)	20(1)
C(9)	3521(2)	2167(1)	1949(1)	16(1)
C(10)	529(2)	1559(1)	1502(1)	21(1)
C(11)	3608(2)	2382(2)	528(1)	33(1)
C(12)	4278(2)	2287(1)	2439(1)	23(1)
C(13)	1515(2)	1300(1)	3653(1)	14(1)
C(14)	2481(2)	1340(1)	4007(1)	17(1)
C(15)	2401(2)	1121(1)	4502(1)	21(1)
C(16)	1400(2)	885(1)	4651(1)	23(1)
C(17)	458(2)	869(1)	4291(1)	21(1)
C(18)	489(2)	1086(1)	3792(1)	16(1)
C(19)	3559(2)	1639(1)	3866(1)	24(1)
C(20)	1340(2)	642(2)	5189(1)	38(1)
C(21)	-569(2)	1131(1)	3426(1)	19(1)
C(22)	2904(2)	240(1)	1499(1)	15(1)
C(23)	3906(2)	481(1)	1350(1)	17(1)
C(24)	4097(2)	421(1)	848(1)	21(1)

C(25)	3265(2)	124(1)	496(1)	24(1)
C(26)	2257(2)	-127(1)	636(1)	24(1)
C(27)	2079(2)	-67(1)	1140(1)	20(1)
C(28)	5199(2)	668(2)	696(1)	30(1)
C(29)	1391(2)	-465(2)	244(1)	40(1)
C(30)	200(2)	-535(1)	3090(1)	13(1)
C(31)	348(2)	-1017(1)	3511(1)	14(1)
C(32)	-586(2)	-1361(1)	3666(1)	17(1)
C(33)	-1649(2)	-1237(1)	3418(1)	18(1)
C(34)	-1780(2)	-805(1)	2986(1)	16(1)
C(35)	-869(2)	-476(1)	2804(1)	14(1)
C(36)	1456(2)	-1179(1)	3807(1)	16(1)
C(37)	1762(2)	-1904(1)	3926(1)	22(1)
C(38)	2761(2)	-2064(1)	4229(1)	28(1)
C(39)	3468(2)	-1501(1)	4420(1)	27(1)
C(40)	3171(2)	-777(1)	4302(1)	22(1)
C(41)	2177(2)	-618(1)	3999(1)	18(1)
C(42)	-1085(2)	-102(1)	2300(1)	15(1)
C(43)	-1835(2)	481(1)	2221(1)	18(1)
C(44)	-2162(2)	759(1)	1739(1)	24(1)
C(45)	-1757(2)	450(1)	1324(1)	24(1)
C(46)	-1003(2)	-130(1)	1397(1)	25(1)
C(47)	-662(2)	-402(1)	1881(1)	20(1)
C(48)	3601(2)	57(1)	3026(1)	15(1)
C(49)	4843(2)	-79(1)	3025(1)	16(1)
C(50)	5204(2)	92(1)	2510(1)	19(1)
C(51)	5002(2)	-917(1)	3123(1)	22(1)
C(52)	5511(2)	368(1)	3452(1)	19(1)
C(53)	5656(2)	115(2)	3950(1)	28(1)
C(54)	6242(2)	527(2)	4338(1)	36(1)
C(55)	6697(2)	1203(2)	4238(1)	34(1)
C(56)	6570(2)	1458(1)	3745(1)	28(1)
C(57)	5987(2)	1046(1)	3357(1)	22(1)
C(58)	2290(2)	-2353(1)	2545(1)	18(1)
C(1X)	59(4)	7237(2)	5576(1)	71(1)
Cl(1)	604(1)	7520(1)	5019(1)	53(1)
Cl(2)	-1155(1)	6712(1)	5446(1)	70(1)

Table 21.3. Bond lengths [Å] and angles [°] for **21**.

Mo(1)-N(3)	1.7443(17)
Mo(1)-C(48)	1.8988(19)
Mo(1)-O(1)	1.9516(13)
Mo(1)-O(2)	2.2069(14)
Mo(1)-C(1)	2.225(2)
S(1)-O(3)	1.4318(16)
S(1)-O(4)	1.4335(16)
S(1)-O(2)	1.4651(15)
S(1)-C(58)	1.829(2)
O(1)-C(30)	1.341(2)
F(1)-C(58)	1.338(2)
N(1)-C(1)	1.343(3)
N(1)-C(4)	1.431(2)
N(1)-C(2)	1.483(3)
C(1)-N(2)	1.344(3)
F(2)-C(58)	1.331(2)
N(2)-C(13)	1.438(2)
N(2)-C(3)	1.480(3)
C(2)-C(3)	1.519(3)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
F(3)-C(58)	1.325(2)
N(3)-C(22)	1.397(2)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(9)	1.396(3)
C(4)-C(5)	1.399(3)
C(5)-C(6)	1.391(3)
C(5)-C(10)	1.508(3)
C(6)-C(7)	1.391(3)
C(6)-H(6)	0.9500
C(7)-C(8)	1.387(3)
C(7)-C(11)	1.512(3)
C(8)-C(9)	1.401(3)
C(8)-H(8)	0.9500
C(9)-C(12)	1.506(3)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800

C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(18)	1.395(3)
C(13)-C(14)	1.400(3)
C(14)-C(15)	1.394(3)
C(14)-C(19)	1.503(3)
C(15)-C(16)	1.389(3)
C(15)-H(15)	0.9500
C(16)-C(17)	1.386(3)
C(16)-C(20)	1.512(3)
C(17)-C(18)	1.392(3)
C(17)-H(17)	0.9500
C(18)-C(21)	1.503(3)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(23)	1.393(3)
C(22)-C(27)	1.402(3)
C(23)-C(24)	1.390(3)
C(23)-H(23)	0.9500
C(24)-C(25)	1.389(3)
C(24)-C(28)	1.509(3)
C(25)-C(26)	1.396(3)
C(25)-H(25)	0.9500
C(26)-C(27)	1.392(3)
C(26)-C(29)	1.506(3)
C(27)-H(27)	0.9500
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-C(35)	1.413(3)
C(30)-C(31)	1.414(3)
C(31)-C(32)	1.398(3)
C(31)-C(36)	1.490(3)

C(32)-C(33)	1.383(3)
C(32)-H(32)	0.9500
C(33)-C(34)	1.382(3)
C(33)-H(33)	0.9500
C(34)-C(35)	1.396(3)
C(34)-H(34)	0.9500
C(35)-C(42)	1.496(3)
C(36)-C(37)	1.392(3)
C(36)-C(41)	1.393(3)
C(37)-C(38)	1.389(3)
C(37)-H(37)	0.9500
C(38)-C(39)	1.385(4)
C(38)-H(38)	0.9500
C(39)-C(40)	1.386(3)
C(39)-H(39)	0.9500
C(40)-C(41)	1.387(3)
C(40)-H(40)	0.9500
C(41)-H(41)	0.9500
C(42)-C(43)	1.391(3)
C(42)-C(47)	1.398(3)
C(43)-C(44)	1.387(3)
C(43)-H(43)	0.9500
C(44)-C(45)	1.386(3)
C(44)-H(44)	0.9500
C(45)-C(46)	1.388(3)
C(45)-H(45)	0.9500
C(46)-C(47)	1.391(3)
C(46)-H(46)	0.9500
C(47)-H(47)	0.9500
C(48)-C(49)	1.521(3)
C(48)-H(48)	0.9500
C(49)-C(50)	1.526(3)
C(49)-C(52)	1.535(3)
C(49)-C(51)	1.551(3)
C(50)-H(50A)	0.9800
C(50)-H(50B)	0.9800
C(50)-H(50C)	0.9800
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800
C(52)-C(53)	1.393(3)
C(52)-C(57)	1.395(3)
C(53)-C(54)	1.389(3)
C(53)-H(53)	0.9500

C(54)-C(55)	1.384(4)
C(54)-H(54)	0.9500
C(55)-C(56)	1.382(4)
C(55)-H(55)	0.9500
C(56)-C(57)	1.390(3)
C(56)-H(56)	0.9500
C(57)-H(57)	0.9500
C(1X)-Cl(2)	1.745(5)
C(1X)-Cl(1)	1.778(4)
C(1X)-H(1X1)	0.9900
C(1X)-H(1X2)	0.9900

N(3)-Mo(1)-C(48)	101.25(8)
N(3)-Mo(1)-O(1)	150.26(7)
C(48)-Mo(1)-O(1)	106.69(7)
N(3)-Mo(1)-O(2)	88.42(7)
C(48)-Mo(1)-O(2)	100.77(7)
O(1)-Mo(1)-O(2)	76.68(6)
N(3)-Mo(1)-C(1)	96.85(7)
C(48)-Mo(1)-C(1)	97.24(8)
O(1)-Mo(1)-C(1)	89.63(6)
O(2)-Mo(1)-C(1)	159.88(6)
O(3)-S(1)-O(4)	117.53(10)
O(3)-S(1)-O(2)	114.85(9)
O(4)-S(1)-O(2)	113.00(9)
O(3)-S(1)-C(58)	104.33(9)
O(4)-S(1)-C(58)	103.88(10)
O(2)-S(1)-C(58)	100.51(9)
C(30)-O(1)-Mo(1)	154.76(13)
C(1)-N(1)-C(4)	130.72(17)
C(1)-N(1)-C(2)	113.52(16)
C(4)-N(1)-C(2)	115.42(15)
N(1)-C(1)-N(2)	107.58(17)
N(1)-C(1)-Mo(1)	125.14(14)
N(2)-C(1)-Mo(1)	126.70(14)
C(1)-N(2)-C(13)	130.73(17)
C(1)-N(2)-C(3)	113.60(16)
C(13)-N(2)-C(3)	114.84(16)
S(1)-O(2)-Mo(1)	143.33(9)
N(1)-C(2)-C(3)	102.59(16)
N(1)-C(2)-H(2A)	111.2
C(3)-C(2)-H(2A)	111.2
N(1)-C(2)-H(2B)	111.2
C(3)-C(2)-H(2B)	111.2

H(2A)-C(2)-H(2B)	109.2
C(22)-N(3)-Mo(1)	163.63(15)
N(2)-C(3)-C(2)	102.70(16)
N(2)-C(3)-H(3A)	111.2
C(2)-C(3)-H(3A)	111.2
N(2)-C(3)-H(3B)	111.2
C(2)-C(3)-H(3B)	111.2
H(3A)-C(3)-H(3B)	109.1
C(9)-C(4)-C(5)	121.34(18)
C(9)-C(4)-N(1)	118.68(18)
C(5)-C(4)-N(1)	119.37(18)
C(6)-C(5)-C(4)	118.61(19)
C(6)-C(5)-C(10)	120.97(18)
C(4)-C(5)-C(10)	120.42(18)
C(7)-C(6)-C(5)	121.4(2)
C(7)-C(6)-H(6)	119.3
C(5)-C(6)-H(6)	119.3
C(8)-C(7)-C(6)	118.86(19)
C(8)-C(7)-C(11)	121.0(2)
C(6)-C(7)-C(11)	120.2(2)
C(7)-C(8)-C(9)	121.56(19)
C(7)-C(8)-H(8)	119.2
C(9)-C(8)-H(8)	119.2
C(4)-C(9)-C(8)	118.19(19)
C(4)-C(9)-C(12)	121.00(18)
C(8)-C(9)-C(12)	120.81(19)
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(7)-C(11)-H(11A)	109.5
C(7)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(7)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(9)-C(12)-H(12A)	109.5
C(9)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(9)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5

C(18)-C(13)-C(14)	121.84(18)
C(18)-C(13)-N(2)	119.12(18)
C(14)-C(13)-N(2)	118.04(17)
C(15)-C(14)-C(13)	117.70(19)
C(15)-C(14)-C(19)	120.68(19)
C(13)-C(14)-C(19)	121.57(19)
C(16)-C(15)-C(14)	122.0(2)
C(16)-C(15)-H(15)	119.0
C(14)-C(15)-H(15)	119.0
C(17)-C(16)-C(15)	118.44(19)
C(17)-C(16)-C(20)	120.7(2)
C(15)-C(16)-C(20)	120.9(2)
C(16)-C(17)-C(18)	122.0(2)
C(16)-C(17)-H(17)	119.0
C(18)-C(17)-H(17)	119.0
C(17)-C(18)-C(13)	117.96(19)
C(17)-C(18)-C(21)	120.41(19)
C(13)-C(18)-C(21)	121.51(18)
C(14)-C(19)-H(19A)	109.5
C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-H(20A)	109.5
C(16)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(16)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(23)-C(22)-N(3)	120.36(18)
C(23)-C(22)-C(27)	119.68(19)
N(3)-C(22)-C(27)	119.95(18)
C(24)-C(23)-C(22)	120.8(2)
C(24)-C(23)-H(23)	119.6
C(22)-C(23)-H(23)	119.6
C(25)-C(24)-C(23)	118.7(2)
C(25)-C(24)-C(28)	121.2(2)

C(23)-C(24)-C(28)	120.1(2)
C(24)-C(25)-C(26)	121.7(2)
C(24)-C(25)-H(25)	119.1
C(26)-C(25)-H(25)	119.1
C(27)-C(26)-C(25)	118.9(2)
C(27)-C(26)-C(29)	121.2(2)
C(25)-C(26)-C(29)	119.9(2)
C(26)-C(27)-C(22)	120.2(2)
C(26)-C(27)-H(27)	119.9
C(22)-C(27)-H(27)	119.9
C(24)-C(28)-H(28A)	109.5
C(24)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(24)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(26)-C(29)-H(29A)	109.5
C(26)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(26)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
O(1)-C(30)-C(35)	120.21(17)
O(1)-C(30)-C(31)	120.78(17)
C(35)-C(30)-C(31)	118.93(17)
C(32)-C(31)-C(30)	119.22(18)
C(32)-C(31)-C(36)	117.35(18)
C(30)-C(31)-C(36)	123.42(17)
C(33)-C(32)-C(31)	121.41(19)
C(33)-C(32)-H(32)	119.3
C(31)-C(32)-H(32)	119.3
C(34)-C(33)-C(32)	119.09(18)
C(34)-C(33)-H(33)	120.5
C(32)-C(33)-H(33)	120.5
C(33)-C(34)-C(35)	121.49(18)
C(33)-C(34)-H(34)	119.3
C(35)-C(34)-H(34)	119.3
C(34)-C(35)-C(30)	119.18(18)
C(34)-C(35)-C(42)	116.97(17)
C(30)-C(35)-C(42)	123.80(17)
C(37)-C(36)-C(41)	118.26(19)
C(37)-C(36)-C(31)	120.04(19)
C(41)-C(36)-C(31)	121.57(18)
C(38)-C(37)-C(36)	120.9(2)

C(38)-C(37)-H(37)	119.5
C(36)-C(37)-H(37)	119.5
C(39)-C(38)-C(37)	120.3(2)
C(39)-C(38)-H(38)	119.8
C(37)-C(38)-H(38)	119.8
C(38)-C(39)-C(40)	119.2(2)
C(38)-C(39)-H(39)	120.4
C(40)-C(39)-H(39)	120.4
C(39)-C(40)-C(41)	120.5(2)
C(39)-C(40)-H(40)	119.7
C(41)-C(40)-H(40)	119.7
C(40)-C(41)-C(36)	120.8(2)
C(40)-C(41)-H(41)	119.6
C(36)-C(41)-H(41)	119.6
C(43)-C(42)-C(47)	118.38(19)
C(43)-C(42)-C(35)	120.87(18)
C(47)-C(42)-C(35)	120.11(18)
C(44)-C(43)-C(42)	121.1(2)
C(44)-C(43)-H(43)	119.4
C(42)-C(43)-H(43)	119.4
C(45)-C(44)-C(43)	120.2(2)
C(45)-C(44)-H(44)	119.9
C(43)-C(44)-H(44)	119.9
C(44)-C(45)-C(46)	119.4(2)
C(44)-C(45)-H(45)	120.3
C(46)-C(45)-H(45)	120.3
C(45)-C(46)-C(47)	120.4(2)
C(45)-C(46)-H(46)	119.8
C(47)-C(46)-H(46)	119.8
C(46)-C(47)-C(42)	120.5(2)
C(46)-C(47)-H(47)	119.8
C(42)-C(47)-H(47)	119.8
C(49)-C(48)-Mo(1)	142.21(15)
C(49)-C(48)-H(48)	108.9
Mo(1)-C(48)-H(48)	108.9
C(48)-C(49)-C(50)	111.64(16)
C(48)-C(49)-C(52)	109.59(17)
C(50)-C(49)-C(52)	111.95(17)
C(48)-C(49)-C(51)	105.04(16)
C(50)-C(49)-C(51)	107.80(18)
C(52)-C(49)-C(51)	110.60(17)
C(49)-C(50)-H(50A)	109.5
C(49)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5

C(49)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
C(49)-C(51)-H(51A)	109.5
C(49)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(49)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(53)-C(52)-C(57)	117.4(2)
C(53)-C(52)-C(49)	121.3(2)
C(57)-C(52)-C(49)	121.31(19)
C(54)-C(53)-C(52)	121.2(2)
C(54)-C(53)-H(53)	119.4
C(52)-C(53)-H(53)	119.4
C(55)-C(54)-C(53)	120.7(2)
C(55)-C(54)-H(54)	119.6
C(53)-C(54)-H(54)	119.6
C(56)-C(55)-C(54)	118.9(2)
C(56)-C(55)-H(55)	120.6
C(54)-C(55)-H(55)	120.6
C(55)-C(56)-C(57)	120.5(2)
C(55)-C(56)-H(56)	119.8
C(57)-C(56)-H(56)	119.8
C(56)-C(57)-C(52)	121.4(2)
C(56)-C(57)-H(57)	119.3
C(52)-C(57)-H(57)	119.3
F(3)-C(58)-F(2)	108.40(17)
F(3)-C(58)-F(1)	107.88(17)
F(2)-C(58)-F(1)	107.86(17)
F(3)-C(58)-S(1)	111.58(14)
F(2)-C(58)-S(1)	111.38(14)
F(1)-C(58)-S(1)	109.60(14)
Cl(2)-C(1X)-Cl(1)	112.74(18)
Cl(2)-C(1X)-H(1X1)	109.0
Cl(1)-C(1X)-H(1X1)	109.0
Cl(2)-C(1X)-H(1X2)	109.0
Cl(1)-C(1X)-H(1X2)	109.0
H(1X1)-C(1X)-H(1X2)	107.8

Table 21.4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **21**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^* U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	11(1)	9(1)	12(1)	1(1)	3(1)	0(1)
S(1)	18(1)	11(1)	17(1)	-1(1)	4(1)	0(1)
O(1)	15(1)	13(1)	15(1)	0(1)	5(1)	-3(1)
F(1)	35(1)	12(1)	40(1)	0(1)	12(1)	5(1)
N(1)	18(1)	11(1)	14(1)	0(1)	6(1)	1(1)
C(1)	11(1)	12(1)	15(1)	1(1)	2(1)	0(1)
F(2)	20(1)	25(1)	35(1)	6(1)	11(1)	-3(1)
N(2)	20(1)	11(1)	14(1)	1(1)	6(1)	2(1)
O(2)	20(1)	10(1)	26(1)	-3(1)	7(1)	0(1)
C(2)	25(1)	10(1)	20(1)	1(1)	8(1)	3(1)
F(3)	27(1)	31(1)	21(1)	5(1)	1(1)	-1(1)
N(3)	16(1)	10(1)	17(1)	1(1)	5(1)	1(1)
O(3)	23(1)	22(1)	25(1)	1(1)	12(1)	1(1)
C(3)	30(1)	10(1)	20(1)	0(1)	9(1)	3(1)
C(4)	19(1)	8(1)	17(1)	2(1)	5(1)	2(1)
O(4)	32(1)	23(1)	22(1)	-3(1)	-1(1)	-3(1)
C(5)	19(1)	10(1)	17(1)	1(1)	4(1)	1(1)
C(6)	26(1)	14(1)	16(1)	1(1)	4(1)	4(1)
C(7)	31(1)	14(1)	22(1)	5(1)	13(1)	5(1)
C(8)	20(1)	14(1)	28(1)	3(1)	12(1)	0(1)
C(9)	19(1)	10(1)	20(1)	2(1)	5(1)	0(1)
C(10)	21(1)	21(1)	23(1)	1(1)	2(1)	-1(1)
C(11)	40(1)	37(2)	26(1)	9(1)	19(1)	4(1)
C(12)	19(1)	23(1)	26(1)	3(1)	2(1)	-4(1)
C(13)	20(1)	10(1)	13(1)	-1(1)	6(1)	0(1)
C(14)	21(1)	12(1)	19(1)	-4(1)	4(1)	-3(1)
C(15)	29(1)	18(1)	15(1)	-3(1)	0(1)	1(1)
C(16)	37(1)	19(1)	14(1)	0(1)	9(1)	2(1)
C(17)	25(1)	18(1)	21(1)	1(1)	12(1)	0(1)
C(18)	19(1)	12(1)	19(1)	-2(1)	6(1)	1(1)
C(19)	20(1)	21(1)	29(1)	-1(1)	2(1)	-5(1)
C(20)	51(2)	46(2)	20(1)	9(1)	11(1)	2(1)
C(21)	16(1)	18(1)	25(1)	-3(1)	5(1)	0(1)
C(22)	20(1)	12(1)	15(1)	2(1)	5(1)	4(1)
C(23)	19(1)	15(1)	18(1)	1(1)	5(1)	3(1)
C(24)	23(1)	20(1)	20(1)	4(1)	9(1)	6(1)
C(25)	30(1)	28(1)	14(1)	1(1)	9(1)	6(1)
C(26)	31(1)	23(1)	19(1)	-2(1)	5(1)	0(1)
C(27)	22(1)	18(1)	20(1)	2(1)	5(1)	0(1)

C(28)	27(1)	40(2)	26(1)	5(1)	14(1)	2(1)
C(29)	44(2)	54(2)	20(1)	-6(1)	2(1)	-14(1)
C(30)	16(1)	10(1)	15(1)	-2(1)	6(1)	-1(1)
C(31)	18(1)	11(1)	15(1)	-2(1)	5(1)	0(1)
C(32)	22(1)	14(1)	16(1)	-1(1)	7(1)	-2(1)
C(33)	17(1)	14(1)	24(1)	-2(1)	10(1)	-4(1)
C(34)	14(1)	13(1)	23(1)	-3(1)	4(1)	1(1)
C(35)	17(1)	10(1)	16(1)	-2(1)	5(1)	0(1)
C(36)	18(1)	17(1)	13(1)	1(1)	5(1)	1(1)
C(37)	26(1)	17(1)	22(1)	2(1)	3(1)	0(1)
C(38)	34(1)	23(1)	27(1)	6(1)	1(1)	9(1)
C(39)	23(1)	36(1)	22(1)	5(1)	1(1)	8(1)
C(40)	23(1)	27(1)	16(1)	0(1)	2(1)	-3(1)
C(41)	21(1)	18(1)	16(1)	1(1)	4(1)	-1(1)
C(42)	14(1)	12(1)	20(1)	-1(1)	1(1)	-3(1)
C(43)	17(1)	17(1)	22(1)	-2(1)	2(1)	-2(1)
C(44)	20(1)	21(1)	28(1)	2(1)	-2(1)	1(1)
C(45)	22(1)	30(1)	20(1)	4(1)	-3(1)	-5(1)
C(46)	22(1)	34(1)	19(1)	-5(1)	5(1)	-5(1)
C(47)	17(1)	20(1)	22(1)	-1(1)	4(1)	0(1)
C(48)	15(1)	13(1)	16(1)	0(1)	3(1)	-1(1)
C(49)	14(1)	16(1)	19(1)	3(1)	3(1)	0(1)
C(50)	15(1)	25(1)	19(1)	3(1)	5(1)	0(1)
C(51)	18(1)	17(1)	31(1)	4(1)	3(1)	3(1)
C(52)	12(1)	22(1)	22(1)	2(1)	2(1)	0(1)
C(53)	27(1)	31(1)	24(1)	6(1)	0(1)	-5(1)
C(54)	34(1)	51(2)	21(1)	2(1)	-1(1)	-5(1)
C(55)	25(1)	44(2)	31(1)	-12(1)	-2(1)	-6(1)
C(56)	20(1)	29(1)	35(1)	-6(1)	6(1)	-5(1)
C(57)	16(1)	25(1)	24(1)	2(1)	4(1)	-2(1)
C(58)	19(1)	14(1)	21(1)	-1(1)	4(1)	0(1)
C(1X)	154(4)	32(2)	23(1)	-1(1)	2(2)	19(2)
Cl(1)	80(1)	40(1)	38(1)	3(1)	1(1)	6(1)
Cl(2)	76(1)	79(1)	59(1)	32(1)	22(1)	33(1)

Table 21.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **21**.

	x	y	z	U(eq)
H(2A)	931	2801	2378	21
H(2B)	2188	2987	2631	21
H(3A)	1733	2695	3393	23

H(3B)	480	2501	3140	23
H(6)	1641	1892	729	22
H(8)	4645	2459	1476	24
H(10A)	148	1525	1154	32
H(10B)	130	1907	1695	32
H(10C)	542	1072	1662	32
H(11A)	4370	2578	589	50
H(11B)	3115	2748	343	50
H(11C)	3603	1929	326	50
H(12A)	4106	2763	2585	34
H(12B)	5057	2285	2374	34
H(12C)	4164	1891	2677	34
H(15)	3051	1134	4746	25
H(17)	-229	704	4389	25
H(19A)	3483	2169	3802	35
H(19B)	3734	1390	3559	35
H(19C)	4161	1550	4144	35
H(20A)	577	707	5268	57
H(20B)	1854	939	5422	57
H(20C)	1550	121	5227	57
H(21A)	-900	1622	3446	29
H(21B)	-1098	758	3513	29
H(21C)	-401	1044	3081	29
H(23)	4465	687	1594	21
H(25)	3386	90	152	28
H(27)	1398	-235	1241	23
H(28A)	5426	1133	866	45
H(28B)	5118	739	328	45
H(28C)	5767	291	795	45
H(29A)	1670	-934	129	59
H(29B)	1237	-129	-45	59
H(29C)	703	-550	392	59
H(32)	-487	-1688	3947	20
H(33)	-2281	-1444	3543	21
H(34)	-2508	-732	2809	20
H(37)	1282	-2295	3799	26
H(38)	2959	-2562	4306	33
H(39)	4149	-1609	4628	33
H(40)	3652	-388	4431	27
H(41)	1985	-119	3920	22
H(43)	-2128	692	2502	22
H(44)	-2665	1164	1693	28
H(45)	-1993	633	993	29
H(46)	-718	-342	1114	30

H(47)	-138	-794	1927	23
H(48)	3456	108	3366	17
H(50A)	4806	-234	2253	29
H(50B)	6010	12	2526	29
H(50C)	5028	606	2420	29
H(51A)	4652	-1057	3421	33
H(51B)	5801	-1032	3184	33
H(51C)	4653	-1192	2827	33
H(53)	5348	-347	4027	33
H(54)	6332	343	4674	43
H(55)	7091	1486	4504	40
H(56)	6884	1919	3670	33
H(57)	5910	1229	3020	26
H(1X1)	632	6944	5790	85
H(1X2)	-104	7679	5771	85

Table 21.6. Torsion angles [^{0}] for **21**.

N(3)-Mo(1)-O(1)-C(30)	45.1(4)
C(48)-Mo(1)-O(1)-C(30)	-114.2(3)
O(2)-Mo(1)-O(1)-C(30)	-16.8(3)
C(1)-Mo(1)-O(1)-C(30)	148.3(3)
C(4)-N(1)-C(1)-N(2)	173.00(19)
C(2)-N(1)-C(1)-N(2)	0.1(2)
C(4)-N(1)-C(1)-Mo(1)	-15.3(3)
C(2)-N(1)-C(1)-Mo(1)	171.83(13)
N(3)-Mo(1)-C(1)-N(1)	9.91(17)
C(48)-Mo(1)-C(1)-N(1)	112.23(16)
O(1)-Mo(1)-C(1)-N(1)	-140.98(16)
O(2)-Mo(1)-C(1)-N(1)	-94.4(2)
N(3)-Mo(1)-C(1)-N(2)	-179.92(16)
C(48)-Mo(1)-C(1)-N(2)	-77.60(17)
O(1)-Mo(1)-C(1)-N(2)	29.19(16)
O(2)-Mo(1)-C(1)-N(2)	75.8(3)
N(1)-C(1)-N(2)-C(13)	-168.51(19)
Mo(1)-C(1)-N(2)-C(13)	19.9(3)
N(1)-C(1)-N(2)-C(3)	0.3(2)
Mo(1)-C(1)-N(2)-C(3)	-171.23(14)
O(3)-S(1)-O(2)-Mo(1)	20.35(19)
O(4)-S(1)-O(2)-Mo(1)	-118.24(15)
C(58)-S(1)-O(2)-Mo(1)	131.65(15)
N(3)-Mo(1)-O(2)-S(1)	33.01(16)
C(48)-Mo(1)-O(2)-S(1)	-68.14(17)

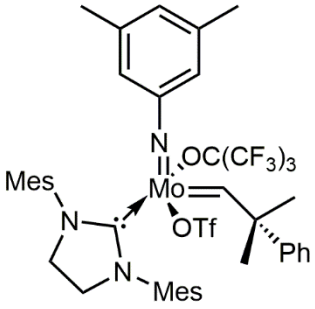
O(1)-Mo(1)-O(2)-S(1)	-172.95(17)
C(1)-Mo(1)-O(2)-S(1)	138.77(18)
C(1)-N(1)-C(2)-C(3)	-0.5(2)
C(4)-N(1)-C(2)-C(3)	-174.51(17)
C(48)-Mo(1)-N(3)-C(22)	126.8(5)
O(1)-Mo(1)-N(3)-C(22)	-33.0(6)
O(2)-Mo(1)-N(3)-C(22)	26.1(5)
C(1)-Mo(1)-N(3)-C(22)	-134.4(5)
C(1)-N(2)-C(3)-C(2)	-0.6(2)
C(13)-N(2)-C(3)-C(2)	170.10(16)
N(1)-C(2)-C(3)-N(2)	0.6(2)
C(1)-N(1)-C(4)-C(9)	-92.5(3)
C(2)-N(1)-C(4)-C(9)	80.3(2)
C(1)-N(1)-C(4)-C(5)	96.3(2)
C(2)-N(1)-C(4)-C(5)	-90.9(2)
C(9)-C(4)-C(5)-C(6)	-0.5(3)
N(1)-C(4)-C(5)-C(6)	170.37(18)
C(9)-C(4)-C(5)-C(10)	179.25(19)
N(1)-C(4)-C(5)-C(10)	-9.8(3)
C(4)-C(5)-C(6)-C(7)	-0.4(3)
C(10)-C(5)-C(6)-C(7)	179.8(2)
C(5)-C(6)-C(7)-C(8)	1.5(3)
C(5)-C(6)-C(7)-C(11)	-178.3(2)
C(6)-C(7)-C(8)-C(9)	-1.6(3)
C(11)-C(7)-C(8)-C(9)	178.2(2)
C(5)-C(4)-C(9)-C(8)	0.4(3)
N(1)-C(4)-C(9)-C(8)	-170.53(18)
C(5)-C(4)-C(9)-C(12)	179.43(19)
N(1)-C(4)-C(9)-C(12)	8.4(3)
C(7)-C(8)-C(9)-C(4)	0.6(3)
C(7)-C(8)-C(9)-C(12)	-178.4(2)
C(1)-N(2)-C(13)-C(18)	-109.1(2)
C(3)-N(2)-C(13)-C(18)	82.2(2)
C(1)-N(2)-C(13)-C(14)	82.1(3)
C(3)-N(2)-C(13)-C(14)	-86.6(2)
C(18)-C(13)-C(14)-C(15)	3.3(3)
N(2)-C(13)-C(14)-C(15)	171.75(18)
C(18)-C(13)-C(14)-C(19)	-174.2(2)
N(2)-C(13)-C(14)-C(19)	-5.7(3)
C(13)-C(14)-C(15)-C(16)	-1.4(3)
C(19)-C(14)-C(15)-C(16)	176.1(2)
C(14)-C(15)-C(16)-C(17)	0.0(3)
C(14)-C(15)-C(16)-C(20)	179.3(2)
C(15)-C(16)-C(17)-C(18)	-0.5(3)

C(20)-C(16)-C(17)-C(18)	-179.7(2)
C(16)-C(17)-C(18)-C(13)	2.3(3)
C(16)-C(17)-C(18)-C(21)	-174.0(2)
C(14)-C(13)-C(18)-C(17)	-3.7(3)
N(2)-C(13)-C(18)-C(17)	-172.05(18)
C(14)-C(13)-C(18)-C(21)	172.46(19)
N(2)-C(13)-C(18)-C(21)	4.1(3)
Mo(1)-N(3)-C(22)-C(23)	-154.8(4)
Mo(1)-N(3)-C(22)-C(27)	24.6(6)
N(3)-C(22)-C(23)-C(24)	179.57(19)
C(27)-C(22)-C(23)-C(24)	0.2(3)
C(22)-C(23)-C(24)-C(25)	0.6(3)
C(22)-C(23)-C(24)-C(28)	-178.5(2)
C(23)-C(24)-C(25)-C(26)	-1.1(3)
C(28)-C(24)-C(25)-C(26)	178.0(2)
C(24)-C(25)-C(26)-C(27)	0.8(4)
C(24)-C(25)-C(26)-C(29)	-178.4(2)
C(25)-C(26)-C(27)-C(22)	0.0(3)
C(29)-C(26)-C(27)-C(22)	179.2(2)
C(23)-C(22)-C(27)-C(26)	-0.5(3)
N(3)-C(22)-C(27)-C(26)	-179.88(19)
Mo(1)-O(1)-C(30)-C(35)	-78.3(3)
Mo(1)-O(1)-C(30)-C(31)	105.0(3)
O(1)-C(30)-C(31)-C(32)	170.17(18)
C(35)-C(30)-C(31)-C(32)	-6.6(3)
O(1)-C(30)-C(31)-C(36)	-9.5(3)
C(35)-C(30)-C(31)-C(36)	173.74(18)
C(30)-C(31)-C(32)-C(33)	-0.5(3)
C(36)-C(31)-C(32)-C(33)	179.15(18)
C(31)-C(32)-C(33)-C(34)	4.9(3)
C(32)-C(33)-C(34)-C(35)	-2.1(3)
C(33)-C(34)-C(35)-C(30)	-5.1(3)
C(33)-C(34)-C(35)-C(42)	172.39(19)
O(1)-C(30)-C(35)-C(34)	-167.47(18)
C(31)-C(30)-C(35)-C(34)	9.3(3)
O(1)-C(30)-C(35)-C(42)	15.3(3)
C(31)-C(30)-C(35)-C(42)	-167.94(18)
C(32)-C(31)-C(36)-C(37)	47.6(3)
C(30)-C(31)-C(36)-C(37)	-132.8(2)
C(32)-C(31)-C(36)-C(41)	-128.3(2)
C(30)-C(31)-C(36)-C(41)	51.4(3)
C(41)-C(36)-C(37)-C(38)	0.1(3)
C(31)-C(36)-C(37)-C(38)	-175.9(2)
C(36)-C(37)-C(38)-C(39)	0.3(4)

C(37)-C(38)-C(39)-C(40)	-0.3(4)
C(38)-C(39)-C(40)-C(41)	0.1(3)
C(39)-C(40)-C(41)-C(36)	0.3(3)
C(37)-C(36)-C(41)-C(40)	-0.4(3)
C(31)-C(36)-C(41)-C(40)	175.56(19)
C(34)-C(35)-C(42)-C(43)	60.0(3)
C(30)-C(35)-C(42)-C(43)	-122.7(2)
C(34)-C(35)-C(42)-C(47)	-110.6(2)
C(30)-C(35)-C(42)-C(47)	66.7(3)
C(47)-C(42)-C(43)-C(44)	0.2(3)
C(35)-C(42)-C(43)-C(44)	-170.56(19)
C(42)-C(43)-C(44)-C(45)	1.1(3)
C(43)-C(44)-C(45)-C(46)	-1.4(3)
C(44)-C(45)-C(46)-C(47)	0.5(3)
C(45)-C(46)-C(47)-C(42)	0.8(3)
C(43)-C(42)-C(47)-C(46)	-1.2(3)
C(35)-C(42)-C(47)-C(46)	169.67(19)
N(3)-Mo(1)-C(48)-C(49)	-15.0(2)
O(1)-Mo(1)-C(48)-C(49)	154.7(2)
O(2)-Mo(1)-C(48)-C(49)	75.5(2)
C(1)-Mo(1)-C(48)-C(49)	-113.5(2)
Mo(1)-C(48)-C(49)-C(50)	19.3(3)
Mo(1)-C(48)-C(49)-C(52)	143.9(2)
Mo(1)-C(48)-C(49)-C(51)	-97.3(2)
C(48)-C(49)-C(52)-C(53)	81.2(2)
C(50)-C(49)-C(52)-C(53)	-154.3(2)
C(51)-C(49)-C(52)-C(53)	-34.1(3)
C(48)-C(49)-C(52)-C(57)	-98.1(2)
C(50)-C(49)-C(52)-C(57)	26.3(3)
C(51)-C(49)-C(52)-C(57)	146.6(2)
C(57)-C(52)-C(53)-C(54)	0.6(4)
C(49)-C(52)-C(53)-C(54)	-178.7(2)
C(52)-C(53)-C(54)-C(55)	0.1(4)
C(53)-C(54)-C(55)-C(56)	-0.7(4)
C(54)-C(55)-C(56)-C(57)	0.5(4)
C(55)-C(56)-C(57)-C(52)	0.3(4)
C(53)-C(52)-C(57)-C(56)	-0.9(3)
C(49)-C(52)-C(57)-C(56)	178.5(2)
O(3)-S(1)-C(58)-F(3)	58.91(16)
O(4)-S(1)-C(58)-F(3)	-177.41(15)
O(2)-S(1)-C(58)-F(3)	-60.34(16)
O(3)-S(1)-C(58)-F(2)	-179.80(14)
O(4)-S(1)-C(58)-F(2)	-56.13(17)
O(2)-S(1)-C(58)-F(2)	60.95(16)

O(3)-S(1)-C(58)-F(1)	-60.52(16)
O(4)-S(1)-C(58)-F(1)	63.15(16)
O(2)-S(1)-C(58)-F(1)	-179.77(14)

Complex 22



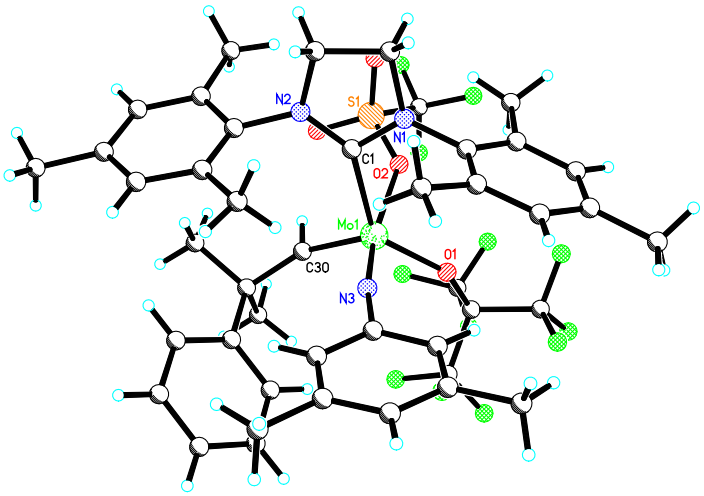


Table 22.1. Crystal data and structure refinement for **22**.

Empirical formula	$C_{44}H_{47}F_{12}MoN_3O_4S$
Formula weight	1037.85
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, *P*-1
Unit cell dimensions	a = 10.8567(6) Å, α = 103.491(3)°
	b = 11.0251(5) Å, β = 92.687(4)°
	c = 21.1863(12) Å, γ= 110.454(3)°
Volume	2287.4(2) A^3
Z, Calculated density	2, 1.507 Mg/m^3
Absorption coefficient	0.426 mm^{-1}
F(000)	1060
Crystal size	0.34 x 0.25 x 0.10 mm
Theta range for data collection	2.00 to 26.38 deg.
Limiting indices	-12<=h<=13, -13<=k<=13, -26<=l<=26
Reflections collected / unique	35917 / 9224 [R(int) = 0.0377]
Completeness to theta = 26.38	98.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7454 and 0.6558
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9224 / 6 / 594
Goodness-of-fit on F^2	1.054
Final R indices [I>2σ(I)]	R1 = 0.0650, wR2 = 0.1733
R indices (all data)	R1 = 0.0765, wR2 = 0.1771
Largest diff. peak and hole	2.455 and -1.245 $e.Å^{-3}$

Table 22.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **22** .U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Mo(1)	1767(1)	8639(1)	2631(1)	10(1)
S(1)	3491(1)	11321(1)	3989(1)	17(1)
O(1)	2175(4)	9779(4)	2001(2)	18(1)
F(1)	5364(4)	13256(4)	3661(2)	41(1)
N(1)	4112(4)	8046(4)	3116(2)	12(1)
C(1)	2891(5)	7919(5)	3271(2)	11(1)
O(2)	3152(3)	10621(4)	3287(2)	15(1)
N(2)	2753(4)	7529(4)	3824(2)	13(1)
F(2)	3489(4)	13521(4)	3707(2)	40(1)
C(2)	4930(5)	7799(6)	3618(3)	17(1)
O(3)	2357(4)	11309(4)	4313(2)	24(1)
N(3)	1014(4)	7099(4)	2071(2)	13(1)
F(3)	4727(4)	13822(4)	4597(2)	41(1)
C(3)	3915(5)	7241(5)	4050(3)	15(1)
F(4)	3104(4)	12696(4)	2329(2)	35(1)
O(4)	4512(4)	11043(5)	4318(2)	27(1)
C(4)	4528(5)	8125(5)	2482(3)	14(1)
F(5)	1216(4)	11635(3)	2592(2)	30(1)
C(5)	5318(5)	9335(5)	2375(3)	17(1)
F(6)	1297(4)	12483(4)	1769(2)	36(1)
C(6)	5701(5)	9315(6)	1750(3)	20(1)
F(7)	277(4)	8447(4)	983(2)	34(1)
C(7)	5355(6)	8145(6)	1253(3)	23(1)
F(8)	-502(3)	9801(4)	1573(2)	29(1)
C(8)	4616(6)	6946(6)	1384(3)	20(1)
F(9)	312(4)	10210(4)	704(2)	38(1)
C(9)	4196(5)	6899(5)	1993(3)	15(1)
F(10)	2916(5)	11833(5)	905(2)	46(1)
C(10)	5833(5)	10658(5)	2895(3)	19(1)
F(11)	4147(4)	11219(4)	1492(2)	37(1)
C(11)	5772(8)	8156(8)	582(3)	41(2)
F(12)	2737(5)	9740(5)	687(2)	45(1)
C(12)	3471(6)	5572(6)	2126(3)	21(1)
C(13)	1562(5)	7052(5)	4117(3)	14(1)
C(14)	1481(5)	7777(5)	4741(3)	16(1)
C(15)	357(6)	7235(6)	5028(3)	19(1)

C(16)	-655(5)	6016(6)	4728(3)	21(1)
C(17)	-499(5)	5292(5)	4119(3)	18(1)
C(18)	604(5)	5787(5)	3812(3)	16(1)
C(19)	2547(6)	9102(6)	5112(3)	23(1)
C(20)	-1891(6)	5486(7)	5032(3)	28(1)
C(21)	770(6)	4918(5)	3180(3)	20(1)
C(22)	609(5)	5906(5)	1565(2)	13(1)
C(23)	-424(5)	4759(5)	1607(3)	17(1)
C(24)	-736(6)	3559(6)	1118(3)	19(1)
C(25)	10(6)	3555(5)	598(3)	21(1)
C(26)	1016(6)	4697(6)	544(3)	19(1)
C(27)	1312(5)	5891(5)	1029(3)	16(1)
C(28)	-1843(7)	2308(6)	1159(3)	32(1)
C(29)	1810(6)	4645(6)	-21(3)	26(1)
C(30)	354(5)	8776(5)	3081(3)	15(1)
C(31)	-1103(5)	8274(5)	3161(3)	14(1)
C(32)	-1172(5)	8237(6)	3880(3)	19(1)
C(33)	-1615(6)	9377(6)	3063(3)	20(1)
C(34)	-1962(5)	6936(5)	2672(3)	16(1)
C(35)	-2171(5)	6859(5)	2011(3)	18(1)
C(36)	-3027(5)	5693(6)	1563(3)	22(1)
C(37)	-3684(5)	4566(6)	1770(3)	24(1)
C(38)	-3464(6)	4612(6)	2423(3)	26(1)
C(39)	-2606(5)	5782(6)	2874(3)	21(1)
C(40)	1855(6)	10509(6)	1638(3)	20(1)
C(41)	1865(6)	11853(6)	2086(3)	25(1)
C(42)	469(6)	9743(6)	1218(3)	26(1)
C(43)	2929(7)	10841(7)	1176(3)	31(1)
C(44)	4315(6)	13071(6)	3984(3)	27(1)

Table 22.3. Bond lengths [Å] and angles [^{0}] for **22**.

Mo(1)-N(3)	1.720(4)
Mo(1)-C(30)	1.876(5)
Mo(1)-O(1)	2.002(4)
Mo(1)-C(1)	2.232(5)
Mo(1)-O(2)	2.249(4)
S(1)-O(3)	1.435(4)
S(1)-O(4)	1.440(4)
S(1)-O(2)	1.470(4)
S(1)-C(44)	1.824(6)
O(1)-C(40)	1.349(6)
F(1)-C(44)	1.336(7)

N(1)-C(1)	1.348(6)
N(1)-C(4)	1.450(7)
N(1)-C(2)	1.486(6)
C(1)-N(2)	1.335(7)
N(2)-C(13)	1.445(6)
N(2)-C(3)	1.489(6)
F(2)-C(44)	1.338(8)
C(2)-C(3)	1.523(7)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
N(3)-C(22)	1.402(6)
F(3)-C(44)	1.325(7)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
F(4)-C(41)	1.333(7)
C(4)-C(5)	1.388(7)
C(4)-C(9)	1.414(7)
F(5)-C(41)	1.333(7)
C(5)-C(6)	1.404(8)
C(5)-C(10)	1.509(7)
F(6)-C(41)	1.338(7)
C(6)-C(7)	1.379(8)
C(6)-H(6)	0.9500
F(7)-C(42)	1.335(7)
C(7)-C(8)	1.386(8)
C(7)-C(11)	1.514(8)
F(8)-C(42)	1.334(7)
C(8)-C(9)	1.394(8)
C(8)-H(8)	0.9500
F(9)-C(42)	1.336(7)
C(9)-C(12)	1.498(8)
F(10)-C(43)	1.352(7)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
F(11)-C(43)	1.330(8)
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
F(12)-C(43)	1.344(8)
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(18)	1.395(7)

C(13)-C(14)	1.401(7)
C(14)-C(15)	1.395(8)
C(14)-C(19)	1.512(8)
C(15)-C(16)	1.386(8)
C(15)-H(15)	0.9500
C(16)-C(17)	1.401(8)
C(16)-C(20)	1.505(8)
C(17)-C(18)	1.392(8)
C(17)-H(17)	0.9500
C(18)-C(21)	1.512(7)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(23)	1.390(7)
C(22)-C(27)	1.399(7)
C(23)-C(24)	1.398(7)
C(23)-H(23)	0.9500
C(24)-C(25)	1.397(8)
C(24)-C(28)	1.504(8)
C(25)-C(26)	1.382(8)
C(25)-H(25)	0.9500
C(26)-C(27)	1.390(7)
C(26)-C(29)	1.509(8)
C(27)-H(27)	0.9500
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-C(31)	1.515(7)
C(30)-H(30)	0.9500
C(31)-C(34)	1.534(7)
C(31)-C(32)	1.538(7)
C(31)-C(33)	1.552(7)
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800

C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-C(35)	1.387(8)
C(34)-C(39)	1.396(8)
C(35)-C(36)	1.389(8)
C(35)-H(35)	0.9500
C(36)-C(37)	1.382(8)
C(36)-H(36)	0.9500
C(37)-C(38)	1.379(9)
C(37)-H(37)	0.9500
C(38)-C(39)	1.395(8)
C(38)-H(38)	0.9500
C(39)-H(39)	0.9500
C(40)-C(42)	1.550(8)
C(40)-C(41)	1.557(8)
C(40)-C(43)	1.559(9)

N(3)-Mo(1)-C(30)	101.3(2)
N(3)-Mo(1)-O(1)	98.33(18)
C(30)-Mo(1)-O(1)	112.84(19)
N(3)-Mo(1)-C(1)	94.87(18)
C(30)-Mo(1)-C(1)	104.1(2)
O(1)-Mo(1)-C(1)	137.21(17)
N(3)-Mo(1)-O(2)	167.76(16)
C(30)-Mo(1)-O(2)	90.83(18)
O(1)-Mo(1)-O(2)	78.48(14)
C(1)-Mo(1)-O(2)	80.14(15)
O(3)-S(1)-O(4)	117.5(3)
O(3)-S(1)-O(2)	113.7(2)
O(4)-S(1)-O(2)	113.4(2)
O(3)-S(1)-C(44)	104.1(3)
O(4)-S(1)-C(44)	103.3(3)
O(2)-S(1)-C(44)	102.6(3)
C(40)-O(1)-Mo(1)	152.0(4)
C(1)-N(1)-C(4)	125.4(4)
C(1)-N(1)-C(2)	112.4(4)
C(4)-N(1)-C(2)	120.9(4)
N(2)-C(1)-N(1)	108.9(4)
N(2)-C(1)-Mo(1)	137.1(4)
N(1)-C(1)-Mo(1)	113.4(3)
S(1)-O(2)-Mo(1)	138.7(2)
C(1)-N(2)-C(13)	128.7(4)
C(1)-N(2)-C(3)	112.2(4)

C(13)-N(2)-C(3)	117.1(4)
N(1)-C(2)-C(3)	102.1(4)
N(1)-C(2)-H(2A)	111.3
C(3)-C(2)-H(2A)	111.3
N(1)-C(2)-H(2B)	111.3
C(3)-C(2)-H(2B)	111.3
H(2A)-C(2)-H(2B)	109.2
C(22)-N(3)-Mo(1)	169.8(4)
N(2)-C(3)-C(2)	102.7(4)
N(2)-C(3)-H(3A)	111.2
C(2)-C(3)-H(3A)	111.2
N(2)-C(3)-H(3B)	111.2
C(2)-C(3)-H(3B)	111.2
H(3A)-C(3)-H(3B)	109.1
C(5)-C(4)-C(9)	121.2(5)
C(5)-C(4)-N(1)	121.5(5)
C(9)-C(4)-N(1)	117.1(5)
C(4)-C(5)-C(6)	117.8(5)
C(4)-C(5)-C(10)	124.1(5)
C(6)-C(5)-C(10)	118.1(5)
C(7)-C(6)-C(5)	122.6(5)
C(7)-C(6)-H(6)	118.7
C(5)-C(6)-H(6)	118.7
C(6)-C(7)-C(8)	118.2(5)
C(6)-C(7)-C(11)	121.5(6)
C(8)-C(7)-C(11)	120.3(6)
C(7)-C(8)-C(9)	122.0(5)
C(7)-C(8)-H(8)	119.0
C(9)-C(8)-H(8)	119.0
C(8)-C(9)-C(4)	118.1(5)
C(8)-C(9)-C(12)	120.1(5)
C(4)-C(9)-C(12)	121.8(5)
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(7)-C(11)-H(11A)	109.5
C(7)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(7)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5

C(9)-C(12)-H(12A)	109.5
C(9)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(9)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(18)-C(13)-C(14)	121.4(5)
C(18)-C(13)-N(2)	118.8(5)
C(14)-C(13)-N(2)	119.2(5)
C(15)-C(14)-C(13)	117.6(5)
C(15)-C(14)-C(19)	119.2(5)
C(13)-C(14)-C(19)	123.3(5)
C(16)-C(15)-C(14)	123.0(5)
C(16)-C(15)-H(15)	118.5
C(14)-C(15)-H(15)	118.5
C(15)-C(16)-C(17)	117.5(5)
C(15)-C(16)-C(20)	121.9(5)
C(17)-C(16)-C(20)	120.6(6)
C(18)-C(17)-C(16)	121.8(5)
C(18)-C(17)-H(17)	119.1
C(16)-C(17)-H(17)	119.1
C(17)-C(18)-C(13)	118.6(5)
C(17)-C(18)-C(21)	119.5(5)
C(13)-C(18)-C(21)	121.8(5)
C(14)-C(19)-H(19A)	109.5
C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-H(20A)	109.5
C(16)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(16)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(23)-C(22)-C(27)	121.0(5)
C(23)-C(22)-N(3)	121.1(5)

C(27)-C(22)-N(3)	117.8(5)
C(22)-C(23)-C(24)	119.7(5)
C(22)-C(23)-H(23)	120.2
C(24)-C(23)-H(23)	120.2
C(25)-C(24)-C(23)	118.3(5)
C(25)-C(24)-C(28)	121.4(5)
C(23)-C(24)-C(28)	120.3(5)
C(26)-C(25)-C(24)	122.4(5)
C(26)-C(25)-H(25)	118.8
C(24)-C(25)-H(25)	118.8
C(25)-C(26)-C(27)	118.9(5)
C(25)-C(26)-C(29)	120.7(5)
C(27)-C(26)-C(29)	120.3(5)
C(26)-C(27)-C(22)	119.6(5)
C(26)-C(27)-H(27)	120.2
C(22)-C(27)-H(27)	120.2
C(24)-C(28)-H(28A)	109.5
C(24)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(24)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(26)-C(29)-H(29A)	109.5
C(26)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(26)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(31)-C(30)-Mo(1)	151.2(4)
C(31)-C(30)-H(30)	104.4
Mo(1)-C(30)-H(30)	104.4
C(30)-C(31)-C(34)	114.9(4)
C(30)-C(31)-C(32)	106.8(4)
C(34)-C(31)-C(32)	113.0(4)
C(30)-C(31)-C(33)	106.1(4)
C(34)-C(31)-C(33)	108.8(4)
C(32)-C(31)-C(33)	106.9(4)
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(31)-C(33)-H(33A)	109.5

C(31)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(31)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(35)-C(34)-C(39)	117.8(5)
C(35)-C(34)-C(31)	120.1(5)
C(39)-C(34)-C(31)	122.0(5)
C(34)-C(35)-C(36)	121.6(5)
C(34)-C(35)-H(35)	119.2
C(36)-C(35)-H(35)	119.2
C(37)-C(36)-C(35)	120.2(5)
C(37)-C(36)-H(36)	119.9
C(35)-C(36)-H(36)	119.9
C(38)-C(37)-C(36)	119.1(5)
C(38)-C(37)-H(37)	120.4
C(36)-C(37)-H(37)	120.4
C(37)-C(38)-C(39)	120.8(6)
C(37)-C(38)-H(38)	119.6
C(39)-C(38)-H(38)	119.6
C(38)-C(39)-C(34)	120.5(5)
C(38)-C(39)-H(39)	119.8
C(34)-C(39)-H(39)	119.8
O(1)-C(40)-C(42)	112.3(5)
O(1)-C(40)-C(41)	110.6(5)
C(42)-C(40)-C(41)	108.5(5)
O(1)-C(40)-C(43)	107.6(5)
C(42)-C(40)-C(43)	109.2(5)
C(41)-C(40)-C(43)	108.6(5)
F(5)-C(41)-F(4)	107.4(5)
F(5)-C(41)-F(6)	107.5(5)
F(4)-C(41)-F(6)	107.5(5)
F(5)-C(41)-C(40)	110.7(5)
F(4)-C(41)-C(40)	110.8(5)
F(6)-C(41)-C(40)	112.9(5)
F(8)-C(42)-F(7)	107.2(5)
F(8)-C(42)-F(9)	107.5(5)
F(7)-C(42)-F(9)	107.1(5)
F(8)-C(42)-C(40)	111.4(5)
F(7)-C(42)-C(40)	110.1(5)
F(9)-C(42)-C(40)	113.3(5)
F(11)-C(43)-F(12)	107.0(6)
F(11)-C(43)-F(10)	107.1(5)
F(12)-C(43)-F(10)	108.0(5)

F(11)-C(43)-C(40)	111.6(5)
F(12)-C(43)-C(40)	109.7(5)
F(10)-C(43)-C(40)	113.2(5)
F(3)-C(44)-F(1)	108.3(5)
F(3)-C(44)-F(2)	107.8(5)
F(1)-C(44)-F(2)	107.7(5)
F(3)-C(44)-S(1)	109.0(5)
F(1)-C(44)-S(1)	112.3(4)
F(2)-C(44)-S(1)	111.6(4)

Symmetry transformations used to generate equivalent atoms:

Table 22.4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **22**. The anisotropic displacement factor exponent takes the form: $-2\ \pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	7(1)	7(1)	16(1)	3(1)	2(1)	3(1)
S(1)	12(1)	16(1)	20(1)	1(1)	2(1)	4(1)
O(1)	19(2)	13(2)	24(2)	8(2)	2(2)	5(2)
F(1)	36(2)	20(2)	56(3)	-1(2)	27(2)	-1(2)
N(1)	7(2)	13(2)	19(2)	5(2)	2(2)	6(2)
C(1)	9(2)	7(2)	16(2)	0(2)	0(2)	3(2)
O(2)	9(2)	10(2)	25(2)	4(1)	2(1)	2(1)
N(2)	6(2)	17(2)	19(2)	7(2)	2(2)	6(2)
F(2)	50(3)	21(2)	53(3)	9(2)	13(2)	17(2)
C(2)	11(2)	21(3)	22(3)	8(2)	0(2)	7(2)
O(3)	18(2)	25(2)	28(2)	2(2)	8(2)	8(2)
N(3)	10(2)	11(2)	19(2)	8(2)	2(2)	5(2)
F(3)	29(2)	28(2)	44(2)	-17(2)	8(2)	-1(2)
C(3)	8(2)	18(3)	24(3)	10(2)	2(2)	7(2)
F(4)	31(2)	17(2)	50(2)	7(2)	-8(2)	1(2)
O(4)	18(2)	37(3)	25(2)	7(2)	-2(2)	10(2)
C(4)	8(2)	18(3)	22(3)	7(2)	4(2)	10(2)
F(5)	36(2)	21(2)	35(2)	4(2)	7(2)	15(2)
C(5)	10(2)	14(3)	27(3)	7(2)	3(2)	5(2)
F(6)	37(2)	17(2)	57(3)	17(2)	-3(2)	11(2)
C(6)	13(3)	20(3)	33(3)	14(2)	10(2)	7(2)
F(7)	39(2)	21(2)	31(2)	-2(2)	-7(2)	6(2)
C(7)	18(3)	29(3)	25(3)	11(2)	9(2)	11(2)
F(8)	19(2)	26(2)	41(2)	15(2)	2(2)	5(2)
C(8)	21(3)	24(3)	21(3)	4(2)	4(2)	16(2)
F(9)	36(2)	48(2)	30(2)	22(2)	-6(2)	10(2)
C(9)	8(2)	16(3)	23(3)	5(2)	2(2)	6(2)
F(10)	50(3)	56(3)	53(3)	43(2)	15(2)	25(2)
C(10)	16(3)	6(2)	34(3)	7(2)	8(2)	2(2)
F(11)	22(2)	44(2)	55(3)	30(2)	12(2)	12(2)
C(11)	48(5)	50(5)	26(4)	12(3)	18(3)	15(4)

F(12)	53(3)	53(3)	34(2)	13(2)	21(2)	23(2)
C(12)	19(3)	18(3)	25(3)	3(2)	4(2)	9(2)
C(13)	11(2)	17(3)	19(3)	12(2)	5(2)	6(2)
C(14)	12(3)	20(3)	19(3)	9(2)	2(2)	8(2)
C(15)	21(3)	27(3)	17(3)	10(2)	6(2)	15(2)
C(16)	15(3)	33(3)	25(3)	17(2)	7(2)	16(2)
C(17)	11(2)	15(3)	27(3)	10(2)	0(2)	4(2)
C(18)	14(3)	16(3)	20(3)	8(2)	1(2)	7(2)
C(19)	26(3)	24(3)	19(3)	2(2)	4(2)	11(3)
C(20)	20(3)	36(4)	35(3)	21(3)	12(3)	12(3)
C(21)	24(3)	14(3)	22(3)	5(2)	5(2)	8(2)
C(22)	9(2)	13(2)	18(3)	3(2)	-1(2)	6(2)
C(23)	16(3)	18(3)	18(3)	5(2)	1(2)	8(2)
C(24)	18(3)	16(3)	25(3)	3(2)	-3(2)	9(2)
C(25)	24(3)	12(3)	24(3)	-2(2)	-4(2)	9(2)
C(26)	21(3)	23(3)	17(3)	2(2)	0(2)	14(2)
C(27)	11(2)	18(3)	19(3)	5(2)	0(2)	5(2)
C(28)	31(4)	17(3)	41(4)	2(3)	2(3)	5(3)
C(29)	24(3)	31(3)	20(3)	0(2)	3(2)	12(3)
C(30)	16(3)	9(2)	19(3)	3(2)	0(2)	3(2)
C(31)	9(2)	12(2)	23(3)	4(2)	3(2)	5(2)
C(32)	13(3)	20(3)	26(3)	7(2)	6(2)	7(2)
C(33)	19(3)	20(3)	26(3)	7(2)	4(2)	11(2)
C(34)	12(2)	16(2)	19(2)	4(1)	3(1)	6(1)
C(35)	8(2)	18(3)	29(3)	10(2)	6(2)	4(2)
C(36)	12(3)	27(3)	25(3)	3(2)	1(2)	8(2)
C(37)	10(3)	15(3)	38(3)	1(2)	-1(2)	-1(2)
C(38)	13(3)	19(3)	44(4)	11(3)	8(2)	-1(2)
C(39)	14(3)	24(3)	30(3)	12(2)	6(2)	8(2)
C(40)	24(3)	17(3)	21(3)	10(2)	2(2)	9(2)
C(41)	23(3)	14(3)	36(3)	8(2)	-1(2)	4(2)
C(42)	32(3)	25(3)	21(3)	9(2)	0(2)	10(3)
C(43)	36(4)	28(3)	35(4)	19(3)	8(3)	9(3)
C(44)	19(3)	19(3)	33(3)	-2(2)	12(2)	1(2)

Table 22.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **22**.

	x	y	z	U(eq)
H(2A)	5651	8641	3869	20
H(2B)	5321	7139	3415	20
H(3A)	3688	6264	3982	18

H(3B)	4245	7703	4520	18
H(6)	6219	10139	1666	24
H(8)	4388	6132	1049	24
H(10A)	5362	11226	2806	28
H(10B)	6785	11110	2892	28
H(10C)	5685	10497	3326	28
H(11A)	5446	8745	400	62
H(11B)	5396	7242	291	62
H(11C)	6743	8486	620	62
H(12A)	3238	4857	1716	31
H(12B)	2659	5585	2306	31
H(12C)	4041	5408	2442	31
H(15)	282	7722	5449	23
H(17)	-1165	4439	3911	21
H(19A)	2180	9811	5178	35
H(19B)	3291	9321	4860	35
H(19C)	2861	9032	5539	35
H(20A)	-1700	5881	5507	41
H(20B)	-2186	4507	4937	41
H(20C)	-2592	5726	4849	41
H(21A)	-3	4073	3046	30
H(21B)	1575	4726	3248	30
H(21C)	846	5392	2838	30
H(23)	-914	4792	1966	20
H(25)	-182	2737	270	25
H(27)	1987	6691	996	19
H(28A)	-2606	2111	833	48
H(28B)	-2104	2444	1599	48
H(28C)	-1540	1553	1072	48
H(29A)	2289	4045	-2	39
H(29B)	2447	5549	9	39
H(29C)	1209	4308	-436	39
H(30)	753	9551	3440	18
H(32A)	-858	7548	3961	28
H(32B)	-2092	8023	3967	28
H(32C)	-611	9115	4169	28
H(33A)	-1084	10234	3379	30
H(33B)	-2548	9124	3133	30
H(33C)	-1538	9470	2616	30
H(35)	-1718	7623	1860	21
H(36)	-3161	5671	1114	26
H(37)	-4279	3770	1467	28
H(38)	-3903	3837	2568	31
H(39)	-2459	5795	3322	26

Table 22.6. Torsion angles [°] for **22**.

N(3)-Mo(1)-O(1)-C(40)	88.9(8)
C(30)-Mo(1)-O(1)-C(40)	-17.1(8)
C(1)-Mo(1)-O(1)-C(40)	-164.5(7)
O(2)-Mo(1)-O(1)-C(40)	-103.1(8)
C(4)-N(1)-C(1)-N(2)	163.9(4)
C(2)-N(1)-C(1)-N(2)	-3.4(6)
C(4)-N(1)-C(1)-Mo(1)	-23.2(6)
C(2)-N(1)-C(1)-Mo(1)	169.6(3)
N(3)-Mo(1)-C(1)-N(2)	-98.2(5)
C(30)-Mo(1)-C(1)-N(2)	4.7(6)
O(1)-Mo(1)-C(1)-N(2)	153.9(5)
O(2)-Mo(1)-C(1)-N(2)	93.0(5)
N(3)-Mo(1)-C(1)-N(1)	91.6(4)
C(30)-Mo(1)-C(1)-N(1)	-165.5(4)
O(1)-Mo(1)-C(1)-N(1)	-16.2(5)
O(2)-Mo(1)-C(1)-N(1)	-77.1(3)
O(3)-S(1)-O(2)-Mo(1)	-49.5(4)
O(4)-S(1)-O(2)-Mo(1)	88.1(4)
C(44)-S(1)-O(2)-Mo(1)	-161.2(3)
N(3)-Mo(1)-O(2)-S(1)	-124.8(7)
C(30)-Mo(1)-O(2)-S(1)	46.1(4)
O(1)-Mo(1)-O(2)-S(1)	159.2(3)
C(1)-Mo(1)-O(2)-S(1)	-58.1(3)
N(1)-C(1)-N(2)-C(13)	-168.6(5)
Mo(1)-C(1)-N(2)-C(13)	20.9(8)
N(1)-C(1)-N(2)-C(3)	-5.4(6)
Mo(1)-C(1)-N(2)-C(3)	-175.8(4)
C(1)-N(1)-C(2)-C(3)	10.1(5)
C(4)-N(1)-C(2)-C(3)	-157.8(4)
C(30)-Mo(1)-N(3)-C(22)	171(2)
O(1)-Mo(1)-N(3)-C(22)	56(2)
C(1)-Mo(1)-N(3)-C(22)	-84(2)
O(2)-Mo(1)-N(3)-C(22)	-18(3)
C(1)-N(2)-C(3)-C(2)	11.3(6)
C(13)-N(2)-C(3)-C(2)	176.7(4)
N(1)-C(2)-C(3)-N(2)	-11.9(5)
C(1)-N(1)-C(4)-C(5)	103.8(6)
C(2)-N(1)-C(4)-C(5)	-89.9(6)
C(1)-N(1)-C(4)-C(9)	-81.9(6)
C(2)-N(1)-C(4)-C(9)	84.4(6)
C(9)-C(4)-C(5)-C(6)	4.4(7)
N(1)-C(4)-C(5)-C(6)	178.5(4)

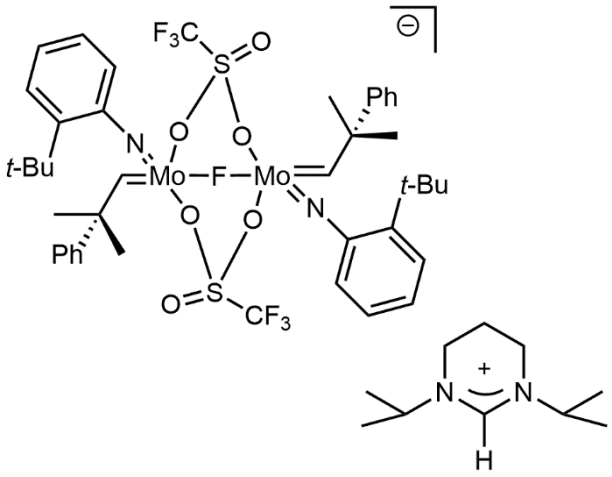
C(9)-C(4)-C(5)-C(10)	-173.2(5)
N(1)-C(4)-C(5)-C(10)	0.9(8)
C(4)-C(5)-C(6)-C(7)	-2.0(8)
C(10)-C(5)-C(6)-C(7)	175.8(5)
C(5)-C(6)-C(7)-C(8)	-0.9(8)
C(5)-C(6)-C(7)-C(11)	179.4(6)
C(6)-C(7)-C(8)-C(9)	1.4(8)
C(11)-C(7)-C(8)-C(9)	-179.0(6)
C(7)-C(8)-C(9)-C(4)	1.0(8)
C(7)-C(8)-C(9)-C(12)	-176.2(5)
C(5)-C(4)-C(9)-C(8)	-4.0(7)
N(1)-C(4)-C(9)-C(8)	-178.4(4)
C(5)-C(4)-C(9)-C(12)	173.2(5)
N(1)-C(4)-C(9)-C(12)	-1.2(7)
C(1)-N(2)-C(13)-C(18)	70.7(7)
C(3)-N(2)-C(13)-C(18)	-91.9(6)
C(1)-N(2)-C(13)-C(14)	-118.3(6)
C(3)-N(2)-C(13)-C(14)	79.1(6)
C(18)-C(13)-C(14)-C(15)	-4.7(8)
N(2)-C(13)-C(14)-C(15)	-175.4(4)
C(18)-C(13)-C(14)-C(19)	175.2(5)
N(2)-C(13)-C(14)-C(19)	4.4(8)
C(13)-C(14)-C(15)-C(16)	1.0(8)
C(19)-C(14)-C(15)-C(16)	-178.9(5)
C(14)-C(15)-C(16)-C(17)	2.4(8)
C(14)-C(15)-C(16)-C(20)	-176.8(5)
C(15)-C(16)-C(17)-C(18)	-2.2(8)
C(20)-C(16)-C(17)-C(18)	176.9(5)
C(16)-C(17)-C(18)-C(13)	-1.3(8)
C(16)-C(17)-C(18)-C(21)	175.5(5)
C(14)-C(13)-C(18)-C(17)	4.8(8)
N(2)-C(13)-C(18)-C(17)	175.7(4)
C(14)-C(13)-C(18)-C(21)	-171.9(5)
N(2)-C(13)-C(18)-C(21)	-1.1(7)
Mo(1)-N(3)-C(22)-C(23)	160.5(18)
Mo(1)-N(3)-C(22)-C(27)	-17(2)
C(27)-C(22)-C(23)-C(24)	2.3(8)
N(3)-C(22)-C(23)-C(24)	-175.1(5)
C(22)-C(23)-C(24)-C(25)	-0.1(8)
C(22)-C(23)-C(24)-C(28)	179.5(5)
C(23)-C(24)-C(25)-C(26)	-1.6(8)
C(28)-C(24)-C(25)-C(26)	178.8(5)
C(24)-C(25)-C(26)-C(27)	1.0(8)
C(24)-C(25)-C(26)-C(29)	179.2(5)

C(25)-C(26)-C(27)-C(22)	1.3(8)
C(29)-C(26)-C(27)-C(22)	-176.9(5)
C(23)-C(22)-C(27)-C(26)	-3.0(8)
N(3)-C(22)-C(27)-C(26)	174.6(5)
N(3)-Mo(1)-C(30)-C(31)	-8.5(8)
O(1)-Mo(1)-C(30)-C(31)	95.6(8)
C(1)-Mo(1)-C(30)-C(31)	-106.5(8)
O(2)-Mo(1)-C(30)-C(31)	173.5(8)
Mo(1)-C(30)-C(31)-C(34)	5.5(10)
Mo(1)-C(30)-C(31)-C(32)	131.6(7)
Mo(1)-C(30)-C(31)-C(33)	-114.7(8)
C(30)-C(31)-C(34)-C(35)	-67.0(6)
C(32)-C(31)-C(34)-C(35)	170.1(5)
C(33)-C(31)-C(34)-C(35)	51.6(6)
C(30)-C(31)-C(34)-C(39)	116.1(6)
C(32)-C(31)-C(34)-C(39)	-6.8(7)
C(33)-C(31)-C(34)-C(39)	-125.3(5)
C(39)-C(34)-C(35)-C(36)	2.2(8)
C(31)-C(34)-C(35)-C(36)	-174.8(5)
C(34)-C(35)-C(36)-C(37)	-0.8(8)
C(35)-C(36)-C(37)-C(38)	-0.8(8)
C(36)-C(37)-C(38)-C(39)	0.9(9)
C(37)-C(38)-C(39)-C(34)	0.6(9)
C(35)-C(34)-C(39)-C(38)	-2.1(8)
C(31)-C(34)-C(39)-C(38)	174.8(5)
Mo(1)-O(1)-C(40)-C(42)	-50.0(9)
Mo(1)-O(1)-C(40)-C(41)	71.4(9)
Mo(1)-O(1)-C(40)-C(43)	-170.2(6)
O(1)-C(40)-C(41)-F(5)	-46.7(6)
C(42)-C(40)-C(41)-F(5)	77.0(6)
C(43)-C(40)-C(41)-F(5)	-164.5(5)
O(1)-C(40)-C(41)-F(4)	72.3(6)
C(42)-C(40)-C(41)-F(4)	-164.0(5)
C(43)-C(40)-C(41)-F(4)	-45.5(6)
O(1)-C(40)-C(41)-F(6)	-167.1(5)
C(42)-C(40)-C(41)-F(6)	-43.5(6)
C(43)-C(40)-C(41)-F(6)	75.1(6)
O(1)-C(40)-C(42)-F(8)	80.3(6)
C(41)-C(40)-C(42)-F(8)	-42.4(6)
C(43)-C(40)-C(42)-F(8)	-160.5(5)
O(1)-C(40)-C(42)-F(7)	-38.5(7)
C(41)-C(40)-C(42)-F(7)	-161.2(5)
C(43)-C(40)-C(42)-F(7)	80.7(6)
O(1)-C(40)-C(42)-F(9)	-158.4(5)

C(41)-C(40)-C(42)-F(9)	79.0(6)
C(43)-C(40)-C(42)-F(9)	-39.2(7)
O(1)-C(40)-C(43)-F(11)	-43.7(7)
C(42)-C(40)-C(43)-F(11)	-165.8(5)
C(41)-C(40)-C(43)-F(11)	76.1(6)
O(1)-C(40)-C(43)-F(12)	74.7(6)
C(42)-C(40)-C(43)-F(12)	-47.4(6)
C(41)-C(40)-C(43)-F(12)	-165.6(5)
O(1)-C(40)-C(43)-F(10)	-164.6(5)
C(42)-C(40)-C(43)-F(10)	73.3(7)
C(41)-C(40)-C(43)-F(10)	-44.8(7)
O(3)-S(1)-C(44)-F(3)	63.8(5)
O(4)-S(1)-C(44)-F(3)	-59.4(5)
O(2)-S(1)-C(44)-F(3)	-177.5(4)
O(3)-S(1)-C(44)-F(1)	-176.2(5)
O(4)-S(1)-C(44)-F(1)	60.6(5)
O(2)-S(1)-C(44)-F(1)	-57.5(5)
O(3)-S(1)-C(44)-F(2)	-55.1(5)
O(4)-S(1)-C(44)-F(2)	-178.4(4)
O(2)-S(1)-C(44)-F(2)	63.6(4)

Symmetry transformations used to generate equivalent atoms:

Complex 24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S
O
O
O
Ph
N
t-Bu
Mo
F
Mo
N
t-Bu
O
O
O
Ph
O
S
CF3
+
N
N
H

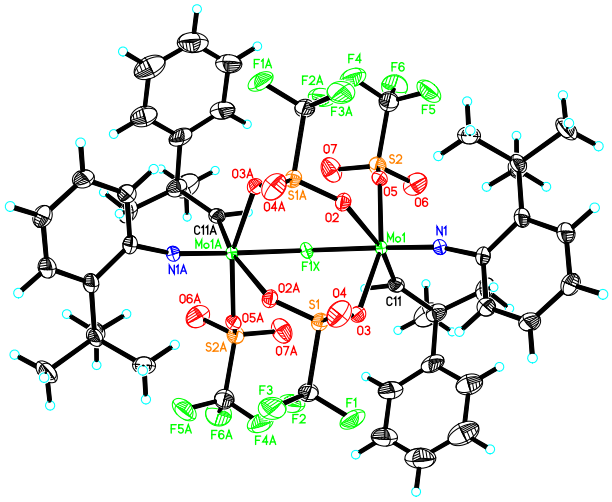

F1A
F2A
F4
F6
F3A
F5
07
S2
03A
S1A
O5
O4A
O2
06
C11A
Mo1A
Mo1
N1
N1A
F1X
O2A
06A
O4
S1
C11
O5A
O3
S2A
07A
F3
F1
F5A
F6A
F2
F4A

Table 24.1. Crystal data and structure refinement for **24**.

Empirical formula	$C_{54}H_{71}F_{13}Mo_2N_4O_{12}S_4$
Formula weight	1535.27
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, *C*2/c
Unit cell dimensions	a = 26.6357(18) Å, α = 90°
	b = 13.7056(8) Å, β = 122.487(5)°
	c = 24.6539(15) Å, γ = 90°
Volume	7591.7(8) $Å^3$
Z, Calculated density	4, 1.343 Mg/m^3
Absorption coefficient	0.523 mm^{-1}
F(000)	3136
Crystal size	0.53 x 0.37 x 0.07 mm
Theta range for data collection	1.74 to 28.33 deg.
Reflections collected / unique	79157 / 9420 [R(int) = 0.0404]
Completeness to theta =	28.33 99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7457 and 0.6839
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9420 / 31 / 424
Goodness-of-fit on F^2	1.033
Final R indices [I>2σ(I)]	R1 = 0.0376, wR2 = 0.0918
R indices (all data)	R1 = 0.0530, wR2 = 0.0974
Largest diff. peak and hole	1.377 and -0.659 $e.Å^{-3}$

****
REMARK: Disordered Solvent density (Et2O) squeezed by PLATON
****

Table 24.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **24**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	864(1)	9947(1)	2799(1)	14(1)
S(1)	321(1)	11506(1)	3379(1)	20(1)
F(1X)	0	9526(1)	2500	16(1)
F(1)	912(1)	11673(1)	4624(1)	44(1)
N(1)	1516(1)	10554(1)	3042(1)	19(1)
C(1)	1986(1)	11221(2)	3319(1)	23(1)
S(2)	645(1)	8281(1)	1755(1)	25(1)
O(2)	292(1)	11254(1)	2096(1)	20(1)
F(2)	207(1)	10616(1)	4245(1)	46(1)
C(2)	2312(1)	11472(2)	3035(1)	27(1)
O(3)	742(1)	10738(1)	3475(1)	21(1)
F(3)	1(1)	12152(2)	4134(1)	57(1)
C(3)	2770(1)	12147(2)	3377(1)	34(1)
F(4)	105(1)	8823(2)	550(1)	49(1)
O(4)	497(1)	12469(1)	3339(1)	35(1)
C(4)	2901(1)	12553(2)	3953(1)	36(1)
O(5)	682(1)	9328(1)	1942(1)	20(1)
F(5)	1052(1)	8978(2)	1076(1)	53(1)
C(5)	2574(1)	12297(2)	4217(1)	33(1)
C(6)	2119(1)	11632(2)	3904(1)	26(1)
O(6)	1176(1)	7746(2)	2160(1)	43(1)
F(6)	656(1)	7556(1)	791(1)	53(1)
O(7)	91(1)	7839(1)	1579(1)	41(1)
C(7)	2170(1)	11032(2)	2395(1)	32(1)
C(8)	1532(1)	11313(2)	1860(1)	36(1)
C(9)	2591(2)	11450(3)	2202(2)	49(1)
C(10)	2244(1)	9927(2)	2447(1)	35(1)
C(11)	1172(1)	8840(2)	3344(1)	21(1)
C(12)	1754(1)	8427(2)	3897(1)	30(1)
C(13)	2273(1)	8639(2)	3818(1)	40(1)
C(14)	1703(2)	7317(2)	3927(2)	47(1)
C(15)	1816(1)	8914(2)	4494(1)	33(1)
C(16)	1386(2)	8741(3)	4645(2)	55(1)
C(17)	1416(2)	9183(3)	5166(2)	64(1)
C(18)	1863(2)	9811(3)	5532(2)	56(1)
C(19)	2290(2)	10006(2)	5405(2)	51(1)
C(20)	2267(2)	9543(2)	4873(1)	41(1)
C(21)	363(1)	11473(2)	4142(1)	32(1)
C(22)	609(1)	8428(2)	998(1)	36(1)
C(1X)	0	14290(3)	2500	39(1)
N(1X)	-388(1)	14703(2)	2596(2)	53(1)
C(2X)	-795(2)	14097(3)	2690(2)	52(1)

C(3XA)	-526(4)	15770(6)	2362(5)	68(2)
C(3XB)	-314(4)	15751(5)	2818(4)	60(2)
C(4X)	0	16238(4)	2500	69(2)
C(5X)	-767(2)	14389(4)	3285(2)	85(1)
C(6X)	-1404(2)	14096(4)	2109(2)	87(1)

Table 24.3. Bond lengths [Å] and angles [°] for **24**.

Mo(1)-N(1)	1.7186(19)
Mo(1)-C(11)	1.896(2)
Mo(1)-O(5)	2.0800(15)
Mo(1)-F(1X)	2.0844(5)
Mo(1)-O(3)	2.1535(15)
Mo(1)-O(2)	2.3868(16)
S(1)-O(4)	1.4211(18)
S(1)-O(2)#1	1.4481(16)
S(1)-O(3)	1.4622(16)
S(1)-C(21)	1.825(3)
F(1X)-Mo(1)#1	2.0843(5)
F(1)-C(21)	1.325(3)
N(1)-C(1)	1.398(3)
C(1)-C(6)	1.405(3)
C(1)-C(2)	1.417(3)
S(2)-O(6)	1.421(2)
S(2)-O(7)	1.430(2)
S(2)-O(5)	1.4941(17)
S(2)-C(22)	1.830(3)
O(2)-S(1)#1	1.4481(16)
F(2)-C(21)	1.315(3)
C(2)-C(3)	1.397(3)
C(2)-C(7)	1.534(4)
F(3)-C(21)	1.332(3)
C(3)-C(4)	1.384(4)
C(3)-H(3)	0.9500
F(4)-C(22)	1.312(3)
C(4)-C(5)	1.385(4)
C(4)-H(4)	0.9500
F(5)-C(22)	1.326(3)
C(5)-C(6)	1.376(4)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
F(6)-C(22)	1.331(3)
C(7)-C(10)	1.523(4)
C(7)-C(8)	1.540(4)
C(7)-C(9)	1.544(3)
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800

C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-C(12)	1.521(3)
C(11)-H(11)	1.02(2)
C(12)-C(13)	1.525(4)
C(12)-C(14)	1.534(4)
C(12)-C(15)	1.540(4)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-C(20)	1.362(4)
C(15)-C(16)	1.400(4)
C(16)-C(17)	1.384(5)
C(16)-H(16)	0.9500
C(17)-C(18)	1.349(6)
C(17)-H(17)	0.9500
C(18)-C(19)	1.358(5)
C(18)-H(18)	0.9500
C(19)-C(20)	1.427(5)
C(19)-H(19)	0.9500
C(20)-H(20)	0.9500
C(1X)-N(1X)	1.308(3)
C(1X)-N(1X)#1	1.308(3)
C(1X)-H(1X)	0.90(5)
N(1X)-C(2X)	1.478(4)
N(1X)-C(3XB)	1.513(8)
N(1X)-C(3XA)	1.543(8)
C(2X)-C(6X)	1.478(5)
C(2X)-C(5X)	1.484(5)
C(2X)-H(2X)	1.0000
C(3XA)-C(4X)	1.407(9)
C(3XA)-H(3X1)	0.9900
C(3XA)-H(3X2)	0.9900
C(3XB)-C(4X)	1.569(8)
C(3XB)-H(3X3)	0.9900
C(3XB)-H(3X4)	0.9900
C(4X)-C(3XA)#1	1.407(9)
C(4X)-C(3XB)#1	1.569(8)
C(4X)-H(4X1)	0.9766
C(4X)-H(4X3)	0.9770
C(5X)-H(5X1)	0.9800
C(5X)-H(5X2)	0.9800
C(5X)-H(5X3)	0.9800
C(6X)-H(6X1)	0.9800

C(6X)-H(6X2)	0.9800
C(6X)-H(6X3)	0.9800
N(1)-Mo(1)-C(11)	99.70(10)
N(1)-Mo(1)-O(5)	100.96(8)
C(11)-Mo(1)-O(5)	99.75(8)
N(1)-Mo(1)-F(1X)	167.08(8)
C(11)-Mo(1)-F(1X)	90.27(8)
O(5)-Mo(1)-F(1X)	85.27(5)
N(1)-Mo(1)-O(3)	91.83(8)
C(11)-Mo(1)-O(3)	92.42(8)
O(5)-Mo(1)-O(3)	160.51(6)
F(1X)-Mo(1)-O(3)	79.47(5)
N(1)-Mo(1)-O(2)	91.24(7)
C(11)-Mo(1)-O(2)	168.37(8)
O(5)-Mo(1)-O(2)	81.88(6)
F(1X)-Mo(1)-O(2)	78.35(5)
O(3)-Mo(1)-O(2)	83.21(6)
O(4)-S(1)-O(2)#1	115.84(11)
O(4)-S(1)-O(3)	115.25(11)
O(2)#1-S(1)-O(3)	113.10(9)
O(4)-S(1)-C(21)	104.74(13)
O(2)#1-S(1)-C(21)	104.33(11)
O(3)-S(1)-C(21)	101.33(11)
Mo(1)#1-F(1X)-Mo(1)	147.86(9)
C(1)-N(1)-Mo(1)	163.77(17)
N(1)-C(1)-C(6)	115.4(2)
N(1)-C(1)-C(2)	122.9(2)
C(6)-C(1)-C(2)	121.8(2)
O(6)-S(2)-O(7)	118.10(14)
O(6)-S(2)-O(5)	113.73(11)
O(7)-S(2)-O(5)	112.86(11)
O(6)-S(2)-C(22)	105.08(13)
O(7)-S(2)-C(22)	104.87(13)
O(5)-S(2)-C(22)	99.57(12)
S(1)#1-O(2)-Mo(1)	140.21(9)
C(3)-C(2)-C(1)	115.5(2)
C(3)-C(2)-C(7)	122.2(2)
C(1)-C(2)-C(7)	122.3(2)
S(1)-O(3)-Mo(1)	131.12(10)
C(4)-C(3)-C(2)	122.9(2)
C(4)-C(3)-H(3)	118.6
C(2)-C(3)-H(3)	118.6
C(3)-C(4)-C(5)	120.3(2)
C(3)-C(4)-H(4)	119.8
C(5)-C(4)-H(4)	119.8
S(2)-O(5)-Mo(1)	130.18(10)
C(6)-C(5)-C(4)	119.4(2)
C(6)-C(5)-H(5)	120.3
C(4)-C(5)-H(5)	120.3

C(5)-C(6)-C(1)	120.1(2)
C(5)-C(6)-H(6)	119.9
C(1)-C(6)-H(6)	119.9
C(10)-C(7)-C(2)	110.9(2)
C(10)-C(7)-C(8)	110.8(2)
C(2)-C(7)-C(8)	109.3(2)
C(10)-C(7)-C(9)	108.1(2)
C(2)-C(7)-C(9)	110.7(2)
C(8)-C(7)-C(9)	107.0(2)
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(7)-C(10)-H(10A)	109.5
C(7)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(7)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(12)-C(11)-Mo(1)	141.07(19)
C(12)-C(11)-H(11)	111.8(17)
Mo(1)-C(11)-H(11)	106.8(17)
C(11)-C(12)-C(13)	111.9(2)
C(11)-C(12)-C(14)	109.8(2)
C(13)-C(12)-C(14)	107.7(2)
C(11)-C(12)-C(15)	103.32(19)
C(13)-C(12)-C(15)	113.6(2)
C(14)-C(12)-C(15)	110.6(2)
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(20)-C(15)-C(16)	118.0(3)
C(20)-C(15)-C(12)	122.2(3)

C(16)-C(15)-C(12)	119.8(3)
C(17)-C(16)-C(15)	121.7(4)
C(17)-C(16)-H(16)	119.1
C(15)-C(16)-H(16)	119.1
C(18)-C(17)-C(16)	119.3(4)
C(18)-C(17)-H(17)	120.4
C(16)-C(17)-H(17)	120.4
C(17)-C(18)-C(19)	121.3(3)
C(17)-C(18)-H(18)	119.3
C(19)-C(18)-H(18)	119.3
C(18)-C(19)-C(20)	119.7(3)
C(18)-C(19)-H(19)	120.1
C(20)-C(19)-H(19)	120.1
C(15)-C(20)-C(19)	119.9(3)
C(15)-C(20)-H(20)	120.0
C(19)-C(20)-H(20)	120.0
F(2)-C(21)-F(1)	109.0(2)
F(2)-C(21)-F(3)	109.0(2)
F(1)-C(21)-F(3)	108.1(2)
F(2)-C(21)-S(1)	111.72(18)
F(1)-C(21)-S(1)	110.25(19)
F(3)-C(21)-S(1)	108.8(2)
F(4)-C(22)-F(5)	108.5(3)
F(4)-C(22)-F(6)	108.3(2)
F(5)-C(22)-F(6)	107.8(2)
F(4)-C(22)-S(2)	111.90(18)
F(5)-C(22)-S(2)	111.10(19)
F(6)-C(22)-S(2)	109.2(2)
N(1X)-C(1X)-N(1X)#1	128.7(4)
N(1X)-C(1X)-H(1X)	115.64(19)
N(1X)#1-C(1X)-H(1X)	115.6(2)
C(1X)-N(1X)-C(2X)	120.2(3)
C(1X)-N(1X)-C(3XB)	120.9(4)
C(2X)-N(1X)-C(3XB)	116.3(4)
C(1X)-N(1X)-C(3XA)	113.3(4)
C(2X)-N(1X)-C(3XA)	123.0(4)
C(3XB)-N(1X)-C(3XA)	36.2(4)
C(6X)-C(2X)-N(1X)	111.4(3)
C(6X)-C(2X)-C(5X)	113.8(4)
N(1X)-C(2X)-C(5X)	110.5(3)
C(6X)-C(2X)-H(2X)	106.9
N(1X)-C(2X)-H(2X)	106.9
C(5X)-C(2X)-H(2X)	106.9
C(4X)-C(3XA)-N(1X)	109.6(6)
C(4X)-C(3XA)-H(3X1)	109.7
N(1X)-C(3XA)-H(3X1)	109.7
C(4X)-C(3XA)-H(3X2)	109.7
N(1X)-C(3XA)-H(3X2)	109.7
H(3X1)-C(3XA)-H(3X2)	108.2
N(1X)-C(3XB)-C(4X)	103.0(5)

N(1X)-C(3XB)-H(3X3)	111.2
C(4X)-C(3XB)-H(3X3)	111.2
N(1X)-C(3XB)-H(3X4)	111.2
C(4X)-C(3XB)-H(3X4)	111.2
H(3X3)-C(3XB)-H(3X4)	109.1
C(3XA)-C(4X)-C(3XA)#1	125.8(7)
C(3XA)-C(4X)-C(3XB)	36.7(4)
C(3XA)#1-C(4X)-C(3XB)	114.5(5)
C(3XA)-C(4X)-C(3XB)#1	114.5(5)
C(3XA)#1-C(4X)-C(3XB)#1	36.7(4)
C(3XB)-C(4X)-C(3XB)#1	129.7(6)
C(3XA)-C(4X)-H(4X1)	106.3
C(3XA)#1-C(4X)-H(4X1)	106.3
C(3XB)-C(4X)-H(4X1)	78.1
C(3XB)#1-C(4X)-H(4X1)	136.8
C(3XA)-C(4X)-H(4X3)	137.1
C(3XA)#1-C(4X)-H(4X3)	80.3
C(3XB)-C(4X)-H(4X3)	104.6
C(3XB)#1-C(4X)-H(4X3)	105.9
H(4X1)-C(4X)-H(4X3)	31.3
C(2X)-C(5X)-H(5X1)	109.5
C(2X)-C(5X)-H(5X2)	109.5
H(5X1)-C(5X)-H(5X2)	109.5
C(2X)-C(5X)-H(5X3)	109.5
H(5X1)-C(5X)-H(5X3)	109.5
H(5X2)-C(5X)-H(5X3)	109.5
C(2X)-C(6X)-H(6X1)	109.5
C(2X)-C(6X)-H(6X2)	109.5
H(6X1)-C(6X)-H(6X2)	109.5
C(2X)-C(6X)-H(6X3)	109.5
H(6X1)-C(6X)-H(6X3)	109.5
H(6X2)-C(6X)-H(6X3)	109.5

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,-z+1/2

Table 24.4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **24**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11}+ ...+2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	11(1)	17(1)	14(1)	0(1)	7(1)	0(1)
S(1)	19(1)	19(1)	20(1)	-5(1)	9(1)	-1(1)
F(1X)	14(1)	17(1)	20(1)	0	11(1)	0
F(1)	36(1)	60(1)	21(1)	-17(1)	5(1)	-3(1)
N(1)	14(1)	26(1)	17(1)	-1(1)	9(1)	0(1)
C(1)	16(1)	28(1)	22(1)	-3(1)	9(1)	-5(1)
S(2)	25(1)	24(1)	27(1)	-5(1)	15(1)	1(1)
O(2)	16(1)	22(1)	20(1)	4(1)	8(1)	-1(1)
F(2)	54(1)	60(1)	30(1)	-4(1)	28(1)	-12(1)
C(2)	20(1)	37(1)	26(1)	-7(1)	14(1)	-10(1)
O(3)	17(1)	27(1)	18(1)	-3(1)	9(1)	3(1)
F(3)	50(1)	80(1)	37(1)	-19(1)	22(1)	24(1)
C(3)	27(1)	47(2)	29(1)	-8(1)	17(1)	-16(1)
F(4)	48(1)	67(1)	24(1)	-5(1)	14(1)	10(1)
O(4)	36(1)	21(1)	38(1)	-5(1)	12(1)	-8(1)
C(4)	29(1)	45(2)	29(1)	-13(1)	13(1)	-20(1)
O(5)	19(1)	25(1)	18(1)	-2(1)	12(1)	1(1)
F(5)	57(1)	75(1)	51(1)	-23(1)	44(1)	-23(1)
C(5)	34(2)	43(2)	23(1)	-12(1)	15(1)	-14(1)
C(6)	25(1)	32(1)	24(1)	-4(1)	14(1)	-5(1)
O(6)	42(1)	40(1)	37(1)	-3(1)	16(1)	18(1)
F(6)	59(1)	56(1)	48(1)	-26(1)	32(1)	2(1)
O(7)	42(1)	34(1)	55(1)	-14(1)	32(1)	-14(1)
C(7)	26(1)	50(2)	27(1)	-13(1)	19(1)	-20(1)
C(8)	38(2)	47(2)	23(1)	-3(1)	17(1)	-13(1)
C(9)	48(2)	76(2)	42(2)	-27(2)	36(2)	-38(2)
C(10)	27(1)	53(2)	32(2)	-14(1)	20(1)	-10(1)
C(11)	22(1)	25(1)	18(1)	-1(1)	12(1)	4(1)
C(12)	30(1)	29(1)	24(1)	4(1)	10(1)	11(1)
C(13)	23(1)	51(2)	36(2)	4(1)	9(1)	19(1)
C(14)	52(2)	30(2)	41(2)	11(1)	12(2)	19(1)
C(15)	34(2)	35(1)	19(1)	9(1)	6(1)	17(1)
C(16)	46(2)	91(3)	24(2)	4(2)	17(2)	8(2)
C(17)	52(2)	115(4)	28(2)	7(2)	23(2)	17(2)
C(18)	66(3)	68(2)	33(2)	9(2)	26(2)	26(2)
C(19)	62(2)	37(2)	34(2)	4(1)	12(2)	8(2)
C(20)	49(2)	37(2)	29(2)	8(1)	15(1)	7(1)
C(21)	26(1)	44(2)	24(1)	-13(1)	13(1)	3(1)
C(22)	32(2)	47(2)	30(2)	-14(1)	17(1)	0(1)
C(1X)	50(3)	21(2)	48(3)	0	28(2)	0
N(1X)	51(2)	30(1)	84(2)	-6(1)	40(2)	0(1)
C(2X)	45(2)	57(2)	62(2)	4(2)	33(2)	1(2)
C(3XA)	68(4)	51(3)	71(4)	-6(3)	29(3)	21(3)

C(3XB)	76(4)	45(3)	60(3)	-5(3)	38(3)	5(3)
C(4X)	94(3)	44(2)	80(3)	0	53(3)	0
C(5X)	80(3)	102(3)	72(3)	-6(2)	40(2)	6(2)
C(6X)	71(3)	112(3)	77(3)	-2(2)	40(2)	-7(2)

Table 24.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **24**.

	x	y	z	U(eq)
H(3)	3002	12335	3206	41
H(4)	3217	13011	4167	43
H(5)	2663	12578	4612	40
H(6)	1893	11449	4083	32
H(8A)	1250	11056	1964	54
H(8B)	1441	11038	1450	54
H(8C)	1497	12026	1825	54
H(9A)	2542	12159	2154	74
H(9B)	2494	11160	1793	74
H(9C)	3004	11295	2536	74
H(10A)	2649	9763	2798	53
H(10B)	2174	9666	2042	53
H(10C)	1956	9642	2533	53
H(11)	816(11)	8430(20)	3257(14)	40(8)
H(13A)	2197	8340	3420	60
H(13B)	2640	8368	4185	60
H(13C)	2317	9346	3800	60
H(14A)	1382	7160	3995	71
H(14B)	2079	7054	4282	71
H(14C)	1615	7027	3521	71
H(16)	1066	8309	4383	66
H(17)	1124	9045	5265	77
H(18)	1880	10124	5885	67
H(19)	2603	10447	5669	61
H(20)	2566	9674	4784	50
H(1X)	0	13630(40)	2500	46
H(2X)	-645	13411	2755	63
H(3X1)	-823	15786	1893	81
H(3X2)	-697	16116	2580	81
H(3X3)	-63	15797	3293	72
H(3X4)	-704	16060	2665	72
H(4X1)	113	16677	2860	83
H(4X3)	294	16679	2829	83
H(5X1)	-352	14370	3649	127
H(5X2)	-1006	13938	3364	127
H(5X3)	-923	15053	3235	127
H(6X1)	-1673	13760	2204	130
H(6X2)	-1404	13758	1759	130

H(6X3)	-1538	14770	1980	130

Table 24.6. Torsion angles [°] for **24**.

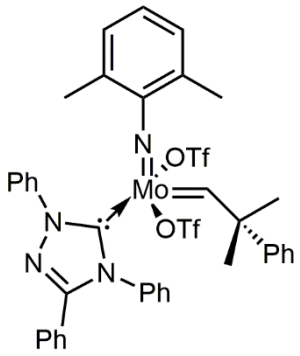
N(1)-Mo(1)-F(1X)-Mo(1)#1	5.8(3)
C(11)-Mo(1)-F(1X)-Mo(1)#1	146.52(7)
O(5)-Mo(1)-F(1X)-Mo(1)#1	-113.71(4)
O(3)-Mo(1)-F(1X)-Mo(1)#1	54.11(4)
O(2)-Mo(1)-F(1X)-Mo(1)#1	-31.05(4)
C(11)-Mo(1)-N(1)-C(1)	-107.4(6)
O(5)-Mo(1)-N(1)-C(1)	150.6(6)
F(1X)-Mo(1)-N(1)-C(1)	32.6(8)
O(3)-Mo(1)-N(1)-C(1)	-14.7(6)
O(2)-Mo(1)-N(1)-C(1)	68.6(6)
Mo(1)-N(1)-C(1)-C(6)	33.1(7)
Mo(1)-N(1)-C(1)-C(2)	-146.9(5)
N(1)-Mo(1)-O(2)-S(1)#1	176.10(16)
C(11)-Mo(1)-O(2)-S(1)#1	-23.7(5)
O(5)-Mo(1)-O(2)-S(1)#1	75.20(16)
F(1X)-Mo(1)-O(2)-S(1)#1	-11.61(15)
O(3)-Mo(1)-O(2)-S(1)#1	-92.21(16)
N(1)-C(1)-C(2)-C(3)	-179.7(2)
C(6)-C(1)-C(2)-C(3)	0.2(4)
N(1)-C(1)-C(2)-C(7)	0.3(4)
C(6)-C(1)-C(2)-C(7)	-179.8(3)
O(4)-S(1)-O(3)-Mo(1)	-85.03(16)
O(2)#1-S(1)-O(3)-Mo(1)	51.45(16)
C(21)-S(1)-O(3)-Mo(1)	162.54(14)
N(1)-Mo(1)-O(3)-S(1)	107.96(14)
C(11)-Mo(1)-O(3)-S(1)	-152.25(15)
O(5)-Mo(1)-O(3)-S(1)	-23.4(3)
F(1X)-Mo(1)-O(3)-S(1)	-62.43(13)
O(2)-Mo(1)-O(3)-S(1)	16.93(13)
C(1)-C(2)-C(3)-C(4)	-0.3(4)
C(7)-C(2)-C(3)-C(4)	179.7(3)
C(2)-C(3)-C(4)-C(5)	0.1(5)
O(6)-S(2)-O(5)-Mo(1)	-58.71(17)
O(7)-S(2)-O(5)-Mo(1)	79.34(16)
C(22)-S(2)-O(5)-Mo(1)	-169.95(13)
N(1)-Mo(1)-O(5)-S(2)	116.70(13)
C(11)-Mo(1)-O(5)-S(2)	14.73(14)
F(1X)-Mo(1)-O(5)-S(2)	-74.73(12)
O(3)-Mo(1)-O(5)-S(2)	-113.16(19)
O(2)-Mo(1)-O(5)-S(2)	-153.61(13)
C(3)-C(4)-C(5)-C(6)	0.2(5)
C(4)-C(5)-C(6)-C(1)	-0.3(4)
N(1)-C(1)-C(6)-C(5)	180.0(2)
C(2)-C(1)-C(6)-C(5)	0.0(4)
C(3)-C(2)-C(7)-C(10)	119.2(3)

C(1)-C(2)-C(7)-C(10)	-60.8(3)
C(3)-C(2)-C(7)-C(8)	-118.4(3)
C(1)-C(2)-C(7)-C(8)	61.6(3)
C(3)-C(2)-C(7)-C(9)	-0.7(4)
C(1)-C(2)-C(7)-C(9)	179.3(3)
N(1)-Mo(1)-C(11)-C(12)	5.5(3)
O(5)-Mo(1)-C(11)-C(12)	108.5(3)
F(1X)-Mo(1)-C(11)-C(12)	-166.3(3)
O(3)-Mo(1)-C(11)-C(12)	-86.8(3)
O(2)-Mo(1)-C(11)-C(12)	-154.4(3)
Mo(1)-C(11)-C(12)-C(13)	-38.7(4)
Mo(1)-C(11)-C(12)-C(14)	-158.2(2)
Mo(1)-C(11)-C(12)-C(15)	83.9(3)
C(11)-C(12)-C(15)-C(20)	-115.6(3)
C(13)-C(12)-C(15)-C(20)	5.8(4)
C(14)-C(12)-C(15)-C(20)	127.0(3)
C(11)-C(12)-C(15)-C(16)	61.9(3)
C(13)-C(12)-C(15)-C(16)	-176.7(3)
C(14)-C(12)-C(15)-C(16)	-55.5(3)
C(20)-C(15)-C(16)-C(17)	-0.6(5)
C(12)-C(15)-C(16)-C(17)	-178.2(3)
C(15)-C(16)-C(17)-C(18)	1.3(6)
C(16)-C(17)-C(18)-C(19)	-1.1(6)
C(17)-C(18)-C(19)-C(20)	0.3(5)
C(16)-C(15)-C(20)-C(19)	-0.1(4)
C(12)-C(15)-C(20)-C(19)	177.4(2)
C(18)-C(19)-C(20)-C(15)	0.3(5)
O(4)-S(1)-C(21)-F(2)	179.53(18)
O(2)#1-S(1)-C(21)-F(2)	57.4(2)
O(3)-S(1)-C(21)-F(2)	-60.3(2)
O(4)-S(1)-C(21)-F(1)	-59.2(2)
O(2)#1-S(1)-C(21)-F(1)	178.67(18)
O(3)-S(1)-C(21)-F(1)	61.0(2)
O(4)-S(1)-C(21)-F(3)	59.2(2)
O(2)#1-S(1)-C(21)-F(3)	-63.0(2)
O(3)-S(1)-C(21)-F(3)	179.38(18)
O(6)-S(2)-C(22)-F(4)	173.3(2)
O(7)-S(2)-C(22)-F(4)	48.1(2)
O(5)-S(2)-C(22)-F(4)	-68.8(2)
O(6)-S(2)-C(22)-F(5)	-65.3(2)
O(7)-S(2)-C(22)-F(5)	169.5(2)
O(5)-S(2)-C(22)-F(5)	52.6(2)
O(6)-S(2)-C(22)-F(6)	53.5(2)
O(7)-S(2)-C(22)-F(6)	-71.7(2)
O(5)-S(2)-C(22)-F(6)	171.37(18)
N(1X)#1-C(1X)-N(1X)-C(2X)	179.4(4)
N(1X)#1-C(1X)-N(1X)-C(3XB)	-19.8(4)
N(1X)#1-C(1X)-N(1X)-C(3XA)	20.2(4)
C(1X)-N(1X)-C(2X)-C(6X)	-104.7(4)
C(3XB)-N(1X)-C(2X)-C(6X)	93.6(5)

C(3XA)-N(1X)-C(2X)-C(6X)	52.4(6)
C(1X)-N(1X)-C(2X)-C(5X)	127.7(3)
C(3XB)-N(1X)-C(2X)-C(5X)	-34.0(6)
C(3XA)-N(1X)-C(2X)-C(5X)	-75.1(6)
C(1X)-N(1X)-C(3XA)-C(4X)	-38.8(7)
C(2X)-N(1X)-C(3XA)-C(4X)	162.6(4)
C(3XB)-N(1X)-C(3XA)-C(4X)	72.2(8)
C(1X)-N(1X)-C(3XB)-C(4X)	32.2(7)
C(2X)-N(1X)-C(3XB)-C(4X)	-166.3(4)
C(3XA)-N(1X)-C(3XB)-C(4X)	-55.6(7)
N(1X)-C(3XA)-C(4X)-C(3XA)#1	18.5(3)
N(1X)-C(3XA)-C(4X)-C(3XB)	-65.1(7)
N(1X)-C(3XA)-C(4X)-C(3XB)#1	59.2(6)
N(1X)-C(3XB)-C(4X)-C(3XA)	63.4(7)
N(1X)-C(3XB)-C(4X)-C(3XA)#1	-54.2(6)
N(1X)-C(3XB)-C(4X)-C(3XB)#1	-14.3(3)

Symmetry transformations used to generate equivalent atoms: #1 -x,y,-z+1/2

Complex 25



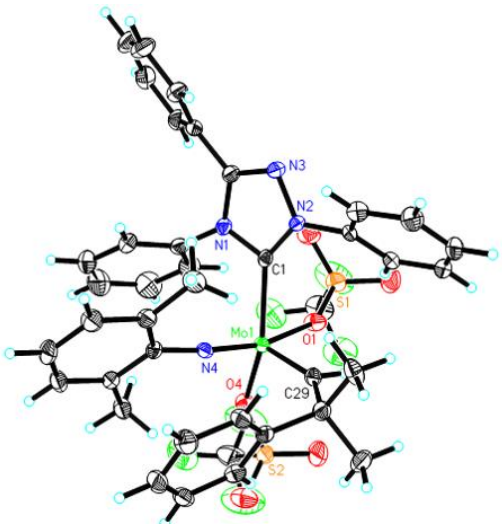


Table 25.1. Crystal data and structure refinement for **25**.

Empirical formula	$C_{42}H_{41}F_6MoN_4O_6$
Formula weight	979.85
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, *C*2/c
Unit cell dimensions	a = 28.1045(14) Å, α = 90°
	b = 14.1361(7) Å, β= 111.926(2)°
	c = 24.4793(11) Å, γ = 90°
Volume	9021.9(8) $Å^3$
Z, Calculated density	8, 1.443 Mg/m^3
Absorption coefficient	0.459 mm^{-1}
F(000)	4008
Crystal size	0.23 x 0.21 x 0.12 mm
Theta range for data collection	1.56 to 28.34°
Limiting indices	-34<=h<=37, -18<=k<=18, -32<=l<=23
Reflections collected / unique	47260 / 11226 [R(int) = 0.0646]
Completeness to theta =	28.34 99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7454 and 0.7061
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11226 / 6 / 56
Goodness-of-fit on F^2	1.048
Final R indices [I>2σ(I)]	R1 = 0.0414, wR2 = 0.0780
R indices (all data)	R1 = 0.0897, wR2 = 0.0865
Largest diff. peak and hole	0.738 and -0.543 $e.Å^{-3}$

Table 25.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **25**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)	
Mo(1)	1571(1)	7301(1)	925(1)	16(1)	
S(1)	1894(1)	9701(1)	1178(1)	28(1)	
N(1)	1680(1)	7604(1)	2212(1)	18(1)	
F(1)	923(1)	10120(1)	688(1)	57(1)	
O(1)	1753(1)	8776(1)	882(1)	28(1)	
C(1)	1969(1)	7493(2)	1874(1)	16(1)	
C(2)	2000(1)	7624(2)	2798(1)	20(1)	
S(2)	881(1)	7775(1)	-497(1)	25(1)	
N(2)	2449(1)	7468(1)	2273(1)	17(1)	
N(3)	2476(1)	7539(1)	2848(1)	21(1)	
O(2)	1846(1)	9733(1)	1738(1)	31(1)	
F(2)	1356(1)	10457(1)	158(1)	70(1)	
C(3)	1126(1)	7629(2)	1980(1)	22(1)	
O(3)	2349(1)	10081(1)	1139(1)	45(1)	
F(3)	1430(1)	11317(1)	911(1)	76(1)	
O(4)	973(1)	7689(1)	135(1)	23(1)	
N(4)	1328(1)	6260(1)	1074(1)	17(1)	
F(4)	-77(1)	7987(2)	-616(1)	71(1)	
C(4)	878(1)	8355(2)	1602(1)	33(1)	
O(5)	743(1)	6904(1)	-806(1)	38(1)	
F(5)	340(1)	9283(1)	-491(1)	78(1)	
C(5)	345(1)	8362(2)	1373(1)	44(1)	
F(6)	117(1)	8567(2)	-1321(1)	83(1)	
C(6)	73(1)	7674(3)	1530(2)	47(1)	
O(6)	1239(1)	8367(2)	-612(1)	54(1)	
C(7)	327(1)	6965(2)	1912(1)	36(1)	
C(8)	858(1)	6935(2)	2139(1)	26(1)	
C(9)	2924(1)	7359(2)	2186(1)	19(1)	
C(10)	3032(1)	7919(2)	1783(1)	23(1)	
C(11)	3498(1)	7807(2)	1721(1)	30(1)	
C(12)	3849(1)	7158(2)	2061(1)	35(1)	
C(13)	3741(1)	6610(2)	2468(1)	32(1)	
C(14)	3270(1)	6706(2)	2531(1)	27(1)	
C(15)	1832(1)	7727(2)	3300(1)	21(1)	
C(16)	1488(1)	8431(2)	3301(1)	27(1)	
C(17)	1348(1)	8526(2)	3783(1)	31(1)	
C(18)	1544(1)	7920(2)	4256(1)	35(1)	
C(19)	1884(1)	7220(2)	4254(1)	34(1)	
C(20)	2030(1)	7121(2)	3774(1)	25(1)	
C(21)	1111(1)	5478(2)	1239(1)	18(1)	
C(22)	588(1)	5318(2)	919(1)	20(1)	
C(23)	363(1)	4540(2)	1072(1)	27(1)	

C(24)	648(1)	3949(2)	1526(1)	31(1)
C(25)	1159(1)	4130(2)	1840(1)	29(1)
C(26)	1405(1)	4903(2)	1710(1)	21(1)
C(27)	294(1)	5990(2)	433(1)	26(1)
C(28)	1959(1)	5103(2)	2075(1)	26(1)
C(29)	2084(1)	6778(2)	699(1)	20(1)
C(30)	2294(1)	5866(2)	548(1)	21(1)
C(31)	2376(1)	6034(2)	-35(1)	32(1)
C(32)	2823(1)	5682(2)	1031(1)	30(1)
C(33)	1924(1)	5040(2)	469(1)	20(1)
C(34)	2051(1)	4247(2)	830(1)	23(1)
C(35)	1705(1)	3503(2)	747(1)	31(1)
C(36)	1235(1)	3536(2)	292(1)	31(1)
C(37)	1108(1)	4307(2)	-82(1)	26(1)
C(38)	1448(1)	5052(2)	8(1)	23(1)
C(39)	1370(2)	10438(2)	701(2)	46(1)
C(40)	281(2)	8444(2)	-740(1)	48(1)
O(1X)	0	5075(2)	2500	71(1)
C(1X)	399(1)	4569(3)	2900(2)	54(1)
C(2X)	809(2)	5161(3)	3298(2)	91(2)

Table 25.3. Bond lengths [Å] and angles [°] for **25**.

Mo(1)-N(4)	1.7183(19)
Mo(1)-C(29)	1.878(3)
Mo(1)-O(4)	2.1085(17)
Mo(1)-O(1)	2.1584(16)
Mo(1)-C(1)	2.186(2)
S(1)-O(3)	1.422(2)
S(1)-O(2)	1.4267(18)
S(1)-O(1)	1.4756(17)
S(1)-C(39)	1.827(4)
N(1)-C(1)	1.366(3)
N(1)-C(2)	1.380(3)
N(1)-C(3)	1.443(3)
F(1)-C(39)	1.324(4)
C(1)-N(2)	1.339(3)
C(2)-N(3)	1.302(3)
C(2)-C(15)	1.478(3)
S(2)-O(6)	1.415(2)
S(2)-O(5)	1.420(2)
S(2)-O(4)	1.4757(17)
S(2)-C(40)	1.830(4)
N(2)-N(3)	1.385(3)
N(2)-C(9)	1.437(3)
F(2)-C(39)	1.314(4)
C(3)-C(8)	1.378(4)
C(3)-C(4)	1.385(4)
F(3)-C(39)	1.333(3)

N(4)-C(21)	1.393(3)
F(4)-C(40)	1.321(4)
C(4)-C(5)	1.388(4)
C(4)-H(4)	0.9500
F(5)-C(40)	1.314(4)
C(5)-C(6)	1.380(5)
C(5)-H(5)	0.9500
F(6)-C(40)	1.333(3)
C(6)-C(7)	1.374(4)
C(6)-H(6)	0.9500
C(7)-C(8)	1.386(4)
C(7)-H(7)	0.9500
C(8)-H(8)	0.9500
C(9)-C(14)	1.378(4)
C(9)-C(10)	1.384(3)
C(10)-C(11)	1.383(4)
C(10)-H(10)	0.9500
C(11)-C(12)	1.376(4)
C(11)-H(11)	0.9500
C(12)-C(13)	1.383(4)
C(12)-H(12)	0.9500
C(13)-C(14)	1.394(4)
C(13)-H(13)	0.9500
C(14)-H(14)	0.9500
C(15)-C(20)	1.382(4)
C(15)-C(16)	1.390(4)
C(16)-C(17)	1.383(3)
C(16)-H(16)	0.9500
C(17)-C(18)	1.378(4)
C(17)-H(17)	0.9500
C(18)-C(19)	1.378(4)
C(18)-H(18)	0.9500
C(19)-C(20)	1.387(3)
C(19)-H(19)	0.9500
C(20)-H(20)	0.9500
C(21)-C(26)	1.401(3)
C(21)-C(22)	1.402(3)
C(22)-C(23)	1.388(3)
C(22)-C(27)	1.505(3)
C(23)-C(24)	1.383(4)
C(23)-H(23)	0.9500
C(24)-C(25)	1.377(4)
C(24)-H(24)	0.9500
C(25)-C(26)	1.391(3)
C(25)-H(25)	0.9500
C(26)-C(28)	1.503(4)
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-H(28A)	0.9800

C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-C(30)	1.520(3)
C(29)-H(29)	0.89(2)
C(30)-C(33)	1.528(3)
C(30)-C(32)	1.536(4)
C(30)-C(31)	1.546(3)
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(34)	1.389(3)
C(33)-C(38)	1.391(4)
C(34)-C(35)	1.395(4)
C(34)-H(34)	0.9500
C(35)-C(36)	1.374(4)
C(35)-H(35)	0.9500
C(36)-C(37)	1.382(4)
C(36)-H(36)	0.9500
C(37)-C(38)	1.384(4)
C(37)-H(37)	0.9500
C(38)-H(38)	0.9500
O(1X)-C(1X)#1	1.380(4)
O(1X)-C(1X)	1.380(4)
C(1X)-C(2X)	1.463(5)
C(1X)-H(1X1)	0.9900
C(1X)-H(1X2)	0.9900
C(2X)-H(2X1)	0.9800
C(2X)-H(2X2)	0.9800
C(2X)-H(2X3)	0.9800

N(4)-Mo(1)-C(29)	97.76(10)
N(4)-Mo(1)-O(4)	99.96(8)
C(29)-Mo(1)-O(4)	105.60(9)
N(4)-Mo(1)-O(1)	163.32(8)
C(29)-Mo(1)-O(1)	98.29(9)
O(4)-Mo(1)-O(1)	80.01(7)
N(4)-Mo(1)-C(1)	88.06(8)
C(29)-Mo(1)-C(1)	102.63(10)
O(4)-Mo(1)-C(1)	149.21(8)
O(1)-Mo(1)-C(1)	84.04(7)
O(3)-S(1)-O(2)	117.62(13)
O(3)-S(1)-O(1)	112.62(12)
O(2)-S(1)-O(1)	113.24(10)
O(3)-S(1)-C(39)	105.77(15)
O(2)-S(1)-C(39)	104.69(14)
O(1)-S(1)-C(39)	100.73(13)
C(1)-N(1)-C(2)	109.0(2)

C(1)-N(1)-C(3)	124.2(2)
C(2)-N(1)-C(3)	126.69(19)
S(1)-O(1)-Mo(1)	148.98(11)
N(2)-C(1)-N(1)	103.1(2)
N(2)-C(1)-Mo(1)	138.37(17)
N(1)-C(1)-Mo(1)	118.26(18)
N(3)-C(2)-N(1)	110.2(2)
N(3)-C(2)-C(15)	124.4(2)
N(1)-C(2)-C(15)	125.4(2)
O(6)-S(2)-O(5)	118.69(13)
O(6)-S(2)-O(4)	113.42(12)
O(5)-S(2)-O(4)	113.15(11)
O(6)-S(2)-C(40)	105.54(16)
O(5)-S(2)-C(40)	103.92(14)
O(4)-S(2)-C(40)	99.24(13)
C(1)-N(2)-N(3)	113.4(2)
C(1)-N(2)-C(9)	129.33(19)
N(3)-N(2)-C(9)	117.26(19)
C(2)-N(3)-N(2)	104.2(2)
C(8)-C(3)-C(4)	121.6(3)
C(8)-C(3)-N(1)	119.6(2)
C(4)-C(3)-N(1)	118.8(2)
S(2)-O(4)-Mo(1)	138.64(11)
C(21)-N(4)-Mo(1)	173.24(17)
C(3)-C(4)-C(5)	118.3(3)
C(3)-C(4)-H(4)	120.9
C(5)-C(4)-H(4)	120.9
C(6)-C(5)-C(4)	120.7(3)
C(6)-C(5)-H(5)	119.7
C(4)-C(5)-H(5)	119.7
C(7)-C(6)-C(5)	120.1(3)
C(7)-C(6)-H(6)	119.9
C(5)-C(6)-H(6)	119.9
C(6)-C(7)-C(8)	120.3(3)
C(6)-C(7)-H(7)	119.9
C(8)-C(7)-H(7)	119.9
C(3)-C(8)-C(7)	119.1(3)
C(3)-C(8)-H(8)	120.5
C(7)-C(8)-H(8)	120.5
C(14)-C(9)-C(10)	121.8(2)
C(14)-C(9)-N(2)	117.6(2)
C(10)-C(9)-N(2)	120.5(2)
C(11)-C(10)-C(9)	118.8(3)
C(11)-C(10)-H(10)	120.6
C(9)-C(10)-H(10)	120.6
C(12)-C(11)-C(10)	120.2(3)
C(12)-C(11)-H(11)	119.9
C(10)-C(11)-H(11)	119.9
C(11)-C(12)-C(13)	120.6(3)
C(11)-C(12)-H(12)	119.7

C(13)-C(12)-H(12)	119.7
C(12)-C(13)-C(14)	119.9(3)
C(12)-C(13)-H(13)	120.1
C(14)-C(13)-H(13)	120.1
C(9)-C(14)-C(13)	118.7(3)
C(9)-C(14)-H(14)	120.7
C(13)-C(14)-H(14)	120.7
C(20)-C(15)-C(16)	120.2(2)
C(20)-C(15)-C(2)	119.0(2)
C(16)-C(15)-C(2)	120.8(2)
C(17)-C(16)-C(15)	119.5(3)
C(17)-C(16)-H(16)	120.3
C(15)-C(16)-H(16)	120.3
C(18)-C(17)-C(16)	120.3(3)
C(18)-C(17)-H(17)	119.8
C(16)-C(17)-H(17)	119.8
C(19)-C(18)-C(17)	120.2(3)
C(19)-C(18)-H(18)	119.9
C(17)-C(18)-H(18)	119.9
C(18)-C(19)-C(20)	120.0(3)
C(18)-C(19)-H(19)	120.0
C(20)-C(19)-H(19)	120.0
C(15)-C(20)-C(19)	119.8(3)
C(15)-C(20)-H(20)	120.1
C(19)-C(20)-H(20)	120.1
N(4)-C(21)-C(26)	120.8(2)
N(4)-C(21)-C(22)	116.6(2)
C(26)-C(21)-C(22)	122.6(2)
C(23)-C(22)-C(21)	117.7(2)
C(23)-C(22)-C(27)	122.8(2)
C(21)-C(22)-C(27)	119.4(2)
C(24)-C(23)-C(22)	120.7(3)
C(24)-C(23)-H(23)	119.7
C(22)-C(23)-H(23)	119.7
C(25)-C(24)-C(23)	120.5(2)
C(25)-C(24)-H(24)	119.8
C(23)-C(24)-H(24)	119.8
C(24)-C(25)-C(26)	121.5(3)
C(24)-C(25)-H(25)	119.3
C(26)-C(25)-H(25)	119.3
C(25)-C(26)-C(21)	117.0(2)
C(25)-C(26)-C(28)	120.2(2)
C(21)-C(26)-C(28)	122.8(2)
C(22)-C(27)-H(27A)	109.5
C(22)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(22)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(26)-C(28)-H(28A)	109.5

C(26)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(26)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(30)-C(29)-Mo(1)	144.7(2)
C(30)-C(29)-H(29)	111.3(15)
Mo(1)-C(29)-H(29)	103.8(15)
C(29)-C(30)-C(33)	111.8(2)
C(29)-C(30)-C(32)	108.0(2)
C(33)-C(30)-C(32)	112.6(2)
C(29)-C(30)-C(31)	107.4(2)
C(33)-C(30)-C(31)	109.2(2)
C(32)-C(30)-C(31)	107.6(2)
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(34)-C(33)-C(38)	117.8(2)
C(34)-C(33)-C(30)	122.4(2)
C(38)-C(33)-C(30)	119.8(2)
C(33)-C(34)-C(35)	121.2(3)
C(33)-C(34)-H(34)	119.4
C(35)-C(34)-H(34)	119.4
C(36)-C(35)-C(34)	119.9(3)
C(36)-C(35)-H(35)	120.1
C(34)-C(35)-H(35)	120.1
C(35)-C(36)-C(37)	119.7(3)
C(35)-C(36)-H(36)	120.1
C(37)-C(36)-H(36)	120.1
C(36)-C(37)-C(38)	120.2(3)
C(36)-C(37)-H(37)	119.9
C(38)-C(37)-H(37)	119.9
C(37)-C(38)-C(33)	121.1(2)
C(37)-C(38)-H(38)	119.4
C(33)-C(38)-H(38)	119.4
F(2)-C(39)-F(1)	108.4(3)
F(2)-C(39)-F(3)	108.9(3)
F(1)-C(39)-F(3)	107.9(3)
F(2)-C(39)-S(1)	111.8(3)
F(1)-C(39)-S(1)	110.7(2)
F(3)-C(39)-S(1)	109.2(2)

F(5)-C(40)-F(4)	108.2(3)
F(5)-C(40)-F(6)	108.0(3)
F(4)-C(40)-F(6)	108.7(3)
F(5)-C(40)-S(2)	112.0(2)
F(4)-C(40)-S(2)	111.2(2)
F(6)-C(40)-S(2)	108.8(3)
C(1X)#1-O(1X)-C(1X)	117.6(4)
O(1X)-C(1X)-C(2X)	113.9(3)
O(1X)-C(1X)-H(1X1)	108.8
C(2X)-C(1X)-H(1X1)	108.8
O(1X)-C(1X)-H(1X2)	108.8
C(2X)-C(1X)-H(1X2)	108.8
H(1X1)-C(1X)-H(1X2)	107.7
C(1X)-C(2X)-H(2X1)	109.5
C(1X)-C(2X)-H(2X2)	109.5
H(2X1)-C(2X)-H(2X2)	109.5
C(1X)-C(2X)-H(2X3)	109.5
H(2X1)-C(2X)-H(2X3)	109.5
H(2X2)-C(2X)-H(2X3)	109.5

Symmetry transformations used to generate equivalent atoms: #1 -x,y,-z+1/2

Table 25.4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **25**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11}+...+2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	19(1)	14(1)	15(1)	1(1)	6(1)	-3(1)
S(1)	39(1)	16(1)	29(1)	-2(1)	13(1)	-7(1)
N(1)	21(1)	17(1)	18(1)	1(1)	9(1)	-2(1)
F(1)	48(1)	46(1)	60(1)	14(1)	2(1)	10(1)
O(1)	47(1)	14(1)	23(1)	0(1)	13(1)	-8(1)
C(1)	20(1)	13(1)	20(1)	0(1)	11(1)	-2(1)
C(2)	23(2)	19(1)	19(1)	-2(1)	10(1)	-3(1)
S(2)	26(1)	28(1)	20(1)	3(1)	6(1)	-5(1)
N(2)	20(1)	19(1)	14(1)	-1(1)	7(1)	-3(1)
N(3)	25(1)	24(1)	16(1)	-1(1)	9(1)	-3(1)
O(2)	40(1)	25(1)	29(1)	-8(1)	13(1)	-2(1)
F(2)	103(2)	53(1)	41(1)	25(1)	12(1)	-10(1)
C(3)	20(1)	29(1)	18(1)	-4(1)	8(1)	1(1)
O(3)	53(2)	35(1)	57(1)	-12(1)	33(1)	-21(1)
F(3)	100(2)	15(1)	86(2)	3(1)	4(1)	5(1)
O(4)	21(1)	24(1)	21(1)	5(1)	4(1)	1(1)
N(4)	16(1)	17(1)	14(1)	-1(1)	4(1)	-2(1)
F(4)	31(1)	90(2)	80(2)	-12(1)	8(1)	6(1)
C(4)	28(2)	34(2)	35(2)	4(1)	12(1)	5(1)
O(5)	47(1)	31(1)	29(1)	-7(1)	9(1)	-2(1)
F(5)	87(2)	39(1)	76(2)	-6(1)	-6(1)	30(1)

C(5)	32(2)	51(2)	45(2)	9(2)	8(2)	14(2)
F(6)	96(2)	82(2)	36(1)	17(1)	-16(1)	30(1)
C(6)	19(2)	68(2)	52(2)	-6(2)	12(2)	1(2)
O(6)	57(2)	74(2)	37(1)	3(1)	22(1)	-33(1)
C(7)	25(2)	51(2)	38(2)	-5(2)	16(2)	-8(2)
C(8)	27(2)	32(2)	24(1)	-1(1)	14(1)	-3(1)
C(9)	15(1)	25(1)	18(1)	-6(1)	7(1)	-8(1)
C(10)	21(2)	29(2)	20(1)	-6(1)	8(1)	-9(1)
C(11)	27(2)	43(2)	23(1)	-6(1)	13(1)	-14(1)
C(12)	18(2)	56(2)	34(2)	-13(2)	14(1)	-7(2)
C(13)	21(2)	43(2)	32(2)	-1(1)	8(1)	4(1)
C(14)	27(2)	29(2)	24(1)	-2(1)	10(1)	-2(1)
C(15)	22(1)	23(1)	19(1)	-6(1)	9(1)	-7(1)
C(16)	30(2)	25(1)	29(2)	-2(1)	14(1)	-4(1)
C(17)	33(2)	26(2)	41(2)	-10(1)	22(2)	-4(1)
C(18)	48(2)	36(2)	32(2)	-8(1)	29(2)	-9(2)
C(19)	50(2)	33(2)	23(1)	0(1)	19(1)	-3(2)
C(20)	30(2)	24(2)	23(1)	-1(1)	13(1)	0(1)
C(21)	21(2)	17(1)	17(1)	1(1)	9(1)	-3(1)
C(22)	20(2)	22(1)	18(1)	0(1)	8(1)	-3(1)
C(23)	21(2)	31(2)	26(1)	1(1)	6(1)	-9(1)
C(24)	37(2)	28(2)	30(2)	7(1)	15(1)	-10(1)
C(25)	35(2)	25(1)	23(1)	8(1)	7(1)	-6(1)
C(26)	23(2)	20(1)	19(1)	2(1)	6(1)	-1(1)
C(27)	21(2)	28(2)	27(2)	5(1)	6(1)	-4(1)
C(28)	27(2)	23(1)	25(1)	5(1)	4(1)	1(1)
C(29)	25(2)	18(1)	19(1)	1(1)	9(1)	-7(1)
C(30)	24(2)	19(1)	23(1)	-1(1)	11(1)	-3(1)
C(31)	43(2)	28(2)	33(2)	-5(1)	26(2)	-7(2)
C(32)	18(2)	26(2)	43(2)	-3(1)	8(1)	-2(1)
C(33)	23(2)	19(1)	20(1)	-5(1)	12(1)	-3(1)
C(34)	24(2)	21(1)	23(1)	-2(1)	7(1)	-3(1)
C(35)	41(2)	21(1)	32(2)	0(1)	14(2)	-6(1)
C(36)	36(2)	22(1)	38(2)	-11(1)	19(2)	-11(1)
C(37)	20(2)	31(2)	26(2)	-10(1)	7(1)	-4(1)
C(38)	28(2)	22(1)	21(1)	-1(1)	11(1)	2(1)
C(39)	65(3)	18(2)	46(2)	7(1)	12(2)	-2(2)
C(40)	52(2)	39(2)	34(2)	1(2)	-5(2)	5(2)
O(1X)	129(4)	28(2)	27(2)	0	-3(2)	0
C(1X)	54(3)	55(2)	65(3)	7(2)	37(2)	11(2)
C(2X)	129(4)	67(3)	40(2)	8(2)	-10(2)	-8(3)

Table 25.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **25**.

	x	y	z	U(eq)
H(4)	1066	8837	1501	39
H(5)	167	8846	1106	53
H(6)	-292	7689	1374	56
H(7)	138	6495	2021	44
H(8)	1035	6443	2400	32
H(10)	2790	8371	1553	28
H(11)	3577	8181	1443	36
H(12)	4168	7085	2015	42
H(13)	3987	6169	2705	39
H(14)	3190	6328	2806	32
H(16)	1350	8845	2974	32
H(17)	1115	9010	3789	37
H(18)	1445	7986	4585	42
H(19)	2019	6804	4581	40
H(20)	2265	6639	3772	30
H(23)	10	4412	861	32
H(24)	490	3415	1623	37
H(25)	1349	3718	2152	34
H(27A)	-58	5761	238	39
H(27B)	460	6026	145	39
H(27C)	290	6619	599	39
H(28A)	2115	5442	1835	40
H(28B)	2140	4505	2212	40
H(28C)	1981	5492	2415	40
H(29)	2248(9)	7279(17)	639(10)	12(6)
H(31A)	2053	6241	-340	47
H(31B)	2490	5445	-159	47
H(31C)	2638	6524	24	47
H(32A)	3045	6230	1063	45
H(32B)	2976	5120	929	45
H(32C)	2784	5579	1407	45
H(34)	2378	4211	1139	28
H(35)	1794	2974	1005	37
H(36)	998	3030	235	37
H(37)	787	4325	-402	31
H(38)	1355	5582	-249	28
H(1X1)	545	4145	2681	65
H(1X2)	261	4166	3137	65
H(2X1)	967	5525	3070	136
H(2X2)	1068	4759	3582	136
H(2X3)	666	5596	3508	136

Table 25.6. Torsion angles [°] for **25**.

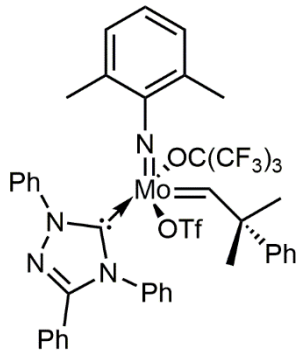
O(3)-S(1)-O(1)-Mo(1)	125.1(2)
O(2)-S(1)-O(1)-Mo(1)	-11.4(3)
C(39)-S(1)-O(1)-Mo(1)	-122.6(3)
N(4)-Mo(1)-O(1)-S(1)	41.4(5)
C(29)-Mo(1)-O(1)-S(1)	-122.7(3)
O(4)-Mo(1)-O(1)-S(1)	132.8(3)
C(1)-Mo(1)-O(1)-S(1)	-20.7(3)
C(2)-N(1)-C(1)-N(2)	-1.1(2)
C(3)-N(1)-C(1)-N(2)	-177.2(2)
C(2)-N(1)-C(1)-Mo(1)	174.41(15)
C(3)-N(1)-C(1)-Mo(1)	-1.7(3)
N(4)-Mo(1)-C(1)-N(2)	109.5(2)
C(29)-Mo(1)-C(1)-N(2)	11.9(3)
O(4)-Mo(1)-C(1)-N(2)	-144.2(2)
O(1)-Mo(1)-C(1)-N(2)	-85.3(2)
N(4)-Mo(1)-C(1)-N(1)	-63.92(17)
C(29)-Mo(1)-C(1)-N(1)	-161.45(17)
O(4)-Mo(1)-C(1)-N(1)	42.4(2)
O(1)-Mo(1)-C(1)-N(1)	101.36(17)
C(1)-N(1)-C(2)-N(3)	0.6(3)
C(3)-N(1)-C(2)-N(3)	176.6(2)
C(1)-N(1)-C(2)-C(15)	-179.5(2)
C(3)-N(1)-C(2)-C(15)	-3.5(4)
N(1)-C(1)-N(2)-N(3)	1.3(2)
Mo(1)-C(1)-N(2)-N(3)	-172.74(17)
N(1)-C(1)-N(2)-C(9)	179.7(2)
Mo(1)-C(1)-N(2)-C(9)	5.6(4)
N(1)-C(2)-N(3)-N(2)	0.2(3)
C(15)-C(2)-N(3)-N(2)	-179.7(2)
C(1)-N(2)-N(3)-C(2)	-1.0(3)
C(9)-N(2)-N(3)-C(2)	-179.6(2)
C(1)-N(1)-C(3)-C(8)	116.6(3)
C(2)-N(1)-C(3)-C(8)	-58.8(3)
C(1)-N(1)-C(3)-C(4)	-63.5(3)
C(2)-N(1)-C(3)-C(4)	121.1(3)
O(6)-S(2)-O(4)-Mo(1)	-55.2(2)
O(5)-S(2)-O(4)-Mo(1)	83.75(19)
C(40)-S(2)-O(4)-Mo(1)	-166.70(18)
N(4)-Mo(1)-O(4)-S(2)	-111.22(17)
C(29)-Mo(1)-O(4)-S(2)	-10.18(19)
O(1)-Mo(1)-O(4)-S(2)	85.72(17)
C(1)-Mo(1)-O(4)-S(2)	145.63(16)
C(29)-Mo(1)-N(4)-C(21)	155.5(16)
O(4)-Mo(1)-N(4)-C(21)	-97.1(16)
O(1)-Mo(1)-N(4)-C(21)	-8.7(18)
C(1)-Mo(1)-N(4)-C(21)	53.0(16)
C(8)-C(3)-C(4)-C(5)	-1.3(4)
N(1)-C(3)-C(4)-C(5)	178.9(2)

C(3)-C(4)-C(5)-C(6)	1.4(5)
C(4)-C(5)-C(6)-C(7)	-0.6(5)
C(5)-C(6)-C(7)-C(8)	-0.4(5)
C(4)-C(3)-C(8)-C(7)	0.3(4)
N(1)-C(3)-C(8)-C(7)	-179.9(2)
C(6)-C(7)-C(8)-C(3)	0.6(4)
C(1)-N(2)-C(9)-C(14)	-132.1(3)
N(3)-N(2)-C(9)-C(14)	46.2(3)
C(1)-N(2)-C(9)-C(10)	50.2(3)
N(3)-N(2)-C(9)-C(10)	-131.5(2)
C(14)-C(9)-C(10)-C(11)	0.9(4)
N(2)-C(9)-C(10)-C(11)	178.5(2)
C(9)-C(10)-C(11)-C(12)	-0.8(4)
C(10)-C(11)-C(12)-C(13)	-0.1(4)
C(11)-C(12)-C(13)-C(14)	0.8(4)
C(10)-C(9)-C(14)-C(13)	-0.1(4)
N(2)-C(9)-C(14)-C(13)	-177.8(2)
C(12)-C(13)-C(14)-C(9)	-0.7(4)
N(3)-C(2)-C(15)-C(20)	-47.5(4)
N(1)-C(2)-C(15)-C(20)	132.6(3)
N(3)-C(2)-C(15)-C(16)	131.3(3)
N(1)-C(2)-C(15)-C(16)	-48.6(4)
C(20)-C(15)-C(16)-C(17)	0.4(4)
C(2)-C(15)-C(16)-C(17)	-178.4(2)
C(15)-C(16)-C(17)-C(18)	-0.6(4)
C(16)-C(17)-C(18)-C(19)	0.4(4)
C(17)-C(18)-C(19)-C(20)	-0.1(4)
C(16)-C(15)-C(20)-C(19)	-0.1(4)
C(2)-C(15)-C(20)-C(19)	178.7(2)
C(18)-C(19)-C(20)-C(15)	-0.1(4)
Mo(1)-N(4)-C(21)-C(26)	-92.8(16)
Mo(1)-N(4)-C(21)-C(22)	85.9(16)
N(4)-C(21)-C(22)-C(23)	179.6(2)
C(26)-C(21)-C(22)-C(23)	-1.7(4)
N(4)-C(21)-C(22)-C(27)	-0.9(3)
C(26)-C(21)-C(22)-C(27)	177.7(2)
C(21)-C(22)-C(23)-C(24)	0.2(4)
C(27)-C(22)-C(23)-C(24)	-179.2(3)
C(22)-C(23)-C(24)-C(25)	0.8(4)
C(23)-C(24)-C(25)-C(26)	-0.2(4)
C(24)-C(25)-C(26)-C(21)	-1.2(4)
C(24)-C(25)-C(26)-C(28)	177.7(2)
N(4)-C(21)-C(26)-C(25)	-179.2(2)
C(22)-C(21)-C(26)-C(25)	2.2(4)
N(4)-C(21)-C(26)-C(28)	1.9(4)
C(22)-C(21)-C(26)-C(28)	-176.7(2)
N(4)-Mo(1)-C(29)-C(30)	9.9(3)
O(4)-Mo(1)-C(29)-C(30)	-92.7(3)
O(1)-Mo(1)-C(29)-C(30)	-174.6(3)
C(1)-Mo(1)-C(29)-C(30)	99.7(3)

Mo(1)-C(29)-C(30)-C(33)	11.3(4)
Mo(1)-C(29)-C(30)-C(32)	-113.2(3)
Mo(1)-C(29)-C(30)-C(31)	131.1(3)
C(29)-C(30)-C(33)-C(34)	-117.3(3)
C(32)-C(30)-C(33)-C(34)	4.5(3)
C(31)-C(30)-C(33)-C(34)	123.9(3)
C(29)-C(30)-C(33)-C(38)	64.9(3)
C(32)-C(30)-C(33)-C(38)	-173.3(2)
C(31)-C(30)-C(33)-C(38)	-53.8(3)
C(38)-C(33)-C(34)-C(35)	-2.3(4)
C(30)-C(33)-C(34)-C(35)	180.0(2)
C(33)-C(34)-C(35)-C(36)	1.8(4)
C(34)-C(35)-C(36)-C(37)	0.0(4)
C(35)-C(36)-C(37)-C(38)	-1.3(4)
C(36)-C(37)-C(38)-C(33)	0.8(4)
C(34)-C(33)-C(38)-C(37)	1.0(4)
C(30)-C(33)-C(38)-C(37)	178.8(2)
O(3)-S(1)-C(39)-F(2)	56.8(3)
O(2)-S(1)-C(39)-F(2)	-178.3(2)
O(1)-S(1)-C(39)-F(2)	-60.6(2)
O(3)-S(1)-C(39)-F(1)	177.6(2)
O(2)-S(1)-C(39)-F(1)	-57.5(2)
O(1)-S(1)-C(39)-F(1)	60.2(2)
O(3)-S(1)-C(39)-F(3)	-63.7(3)
O(2)-S(1)-C(39)-F(3)	61.2(3)
O(1)-S(1)-C(39)-F(3)	178.9(2)
O(6)-S(2)-C(40)-F(5)	-54.4(3)
O(5)-S(2)-C(40)-F(5)	180.0(2)
O(4)-S(2)-C(40)-F(5)	63.2(3)
O(6)-S(2)-C(40)-F(4)	-175.5(2)
O(5)-S(2)-C(40)-F(4)	58.8(3)
O(4)-S(2)-C(40)-F(4)	-57.9(2)
O(6)-S(2)-C(40)-F(6)	64.9(3)
O(5)-S(2)-C(40)-F(6)	-60.8(3)
O(4)-S(2)-C(40)-F(6)	-177.6(2)
C(1X)#1-O(1X)-C(1X)-C(2X)	178.8(4)

Symmetry transformations used to generate equivalent atoms: #1 -x,y,-z+1/2

Complex 26



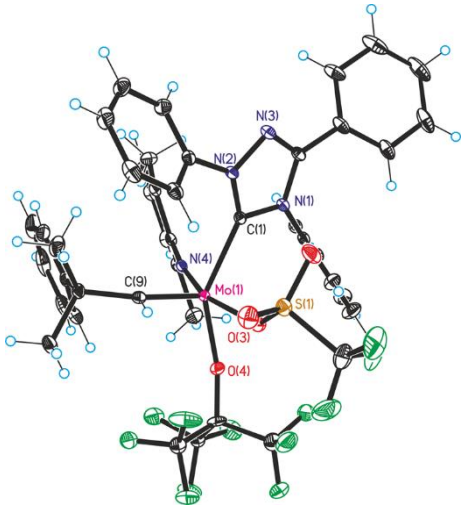


Table 26.1. Crystal data and structure refinement for **26**

Empirical formula	$C_{43}H_{36}F_{12}MoN_4O_4SxEt_2O$
Formula weight	1102.88
Temperature	183(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$ (no. 14)
Unit cell dimensions	a = 14.5345(7) Å , α = 90°
	b = 15.8850(7) Å, β = 97.229(2)°
	c = 21.3143(10) Å, γ = 90°
Volume	4881.9(4) $Å^3$
Z	4
Density (calculated)	1.501 Mg/m^3
Absorption coefficient	0.406 mm^{-1}
F(000)	2248
Crystal size	0.180 x 0.110 x 0.090 mm^3
Theta range for data collection	2.055 to 25.250°.
Index ranges	-17<=h<=17, -19<=k<=19, -25<=l<=25
Reflections collected	120951
Independent reflections	8818 [R(int) = 0.0642]
Completeness to theta =	25.242° 99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.901 and 0.858
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8818 / 0 / 689
Goodness-of-fit on F^2	1.055
Final R indices [I>2sigma(I)]	R1 = 0.0457, wR2 = 0.1144
R indices (all data)	R1 = 0.0576, wR2 = 0.1202
Extinction coefficient	n/a
Largest diff. peak and hole	1.420 and -0.613 $e.Å^{-3}$

Table 26.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **26**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	7470(1)	5244(1)	3071(1)	21(1)
N(1)	6259(2)	4720(2)	1850(1)	24(1)
N(2)	5253(2)	5240(2)	2374(1)	24(1)
N(3)	4763(2)	4933(2)	1825(1)	30(1)
N(4)	7378(2)	4177(2)	3217(1)	24(1)
C(1)	6173(2)	5115(2)	2409(1)	23(1)
C(2)	5395(2)	4611(2)	1512(2)	27(1)
C(3)	7256(2)	3304(2)	3244(1)	25(1)
C(4)	6371(2)	2959(2)	3262(1)	29(1)
C(5)	6293(3)	2088(2)	3299(2)	36(1)
C(6)	7053(3)	1581(2)	3307(2)	41(1)
C(7)	7918(3)	1925(2)	3279(2)	40(1)
C(8)	8047(2)	2791(2)	3247(2)	32(1)
C(9)	7066(2)	5652(2)	3821(2)	26(1)
C(10)	6883(2)	5402(2)	4481(2)	29(1)
C(11)	5871(3)	5632(3)	4554(2)	50(1)
C(12)	7503(3)	5941(2)	4964(2)	44(1)
C(13)	9654(2)	5816(2)	3344(2)	41(1)
C(17)	7659(4)	7704(3)	1816(2)	65(1)
C(18)	9051(9)	8612(7)	5008(4)	165(4)
C(19)	10024(8)	8630(7)	5377(4)	191(6)
C(20)	8281(5)	9114(8)	3997(5)	157(4)
C(21)	8408(7)	9399(6)	3406(5)	139(4)
C(41)	5511(2)	3496(2)	3236(2)	37(1)
C(81)	8981(3)	3168(2)	3223(2)	44(1)
C(101)	7131(2)	4411(2)	1680(1)	26(1)
C(102)	7780(3)	4979(2)	1510(2)	40(1)
C(103)	8603(3)	4670(3)	1335(2)	54(1)
C(104)	8765(3)	3815(3)	1326(2)	50(1)
C(105)	8113(3)	3258(2)	1499(2)	40(1)
C(106)	7291(2)	3555(2)	1681(2)	31(1)
C(201)	4700(2)	5586(2)	2824(2)	29(1)
C(202)	4896(2)	6365(2)	3094(2)	35(1)
C(203)	4288(3)	6687(3)	3495(2)	48(1)
C(204)	3512(3)	6242(3)	3608(2)	54(1)
C(205)	3333(3)	5466(3)	3335(2)	50(1)
C(206)	3924(2)	5129(3)	2942(2)	39(1)
C(301)	5173(3)	4199(2)	891(2)	37(1)
C(302)	5747(3)	4272(2)	416(2)	43(1)
C(303)	5475(4)	3912(3)	-174(2)	60(1)
C(304)	4649(4)	3492(3)	-286(2)	74(2)
C(305)	4084(4)	3420(3)	178(3)	74(2)
C(306)	4342(3)	3770(3)	778(2)	54(1)

C(401)	7092(2)	4474(2)	4620(1)	30(1)
C(402)	6411(3)	3898(3)	4734(2)	48(1)
C(403)	6647(5)	3061(3)	4868(2)	72(2)
C(404)	7533(6)	2790(3)	4894(2)	76(2)
C(405)	8221(4)	3348(3)	4787(2)	61(1)
C(406)	7999(3)	4183(2)	4652(2)	40(1)
S(1)	6901(1)	7133(1)	2284(1)	37(1)
O(1)	7514(2)	6475(1)	2584(1)	32(1)
O(2)	6191(2)	6827(2)	1818(1)	51(1)
O(3)	6624(2)	7746(2)	2723(1)	57(1)
O(4)	8859(2)	5393(2)	3156(1)	32(1)
O(5)	9122(3)	8969(3)	4391(2)	107(1)
F(1)	7157(3)	8294(2)	1490(2)	97(1)
F(2)	8356(2)	8071(2)	2165(2)	99(1)
F(3)	8006(3)	7196(2)	1416(2)	104(1)
F(4)	10266(2)	7010(2)	3933(1)	64(1)
F(7)	10895(2)	6411(2)	2853(1)	88(1)
F(10)	11174(2)	5540(2)	3905(1)	69(1)
C(14)	9563(5)	6477(5)	3871(4)	41(2)
F(5)	8800(7)	6923(6)	3698(6)	80(4)
F(6)	9505(4)	6138(3)	4416(2)	60(2)
C(15)	9999(6)	6241(7)	2769(4)	51(2)
F(8)	9582(4)	6941(5)	2638(4)	95(3)
F(9)	9874(7)	5717(9)	2265(4)	108(5)
C(16)	10396(5)	5153(6)	3631(4)	37(2)
F(11)	10051(4)	4673(4)	4075(3)	58(2)
F(12)	10637(5)	4664(5)	3189(3)	72(2)
C(14A)	9508(7)	6669(7)	3635(6)	35(2)
F(5A)	9233(7)	7265(5)	3158(7)	105(5)
F(6A)	8857(13)	6664(13)	3985(11)	142(11)
C(15A)	10178(8)	5930(9)	2731(6)	45(3)
F(8A)	9534(12)	6278(12)	2273(6)	109(6)
F(9A)	10501(9)	5233(10)	2559(8)	142(7)
C(16A)	10291(10)	5290(9)	3831(9)	61(4)
F(11A)	9976(6)	5331(8)	4353(4)	90(5)
F(12A)	10381(9)	4519(7)	3589(11)	138(9)

Table 26.3. Bond lengths [Å] and angles [°] for **26**.

Mo(1)-N(4)	1.731(3)
Mo(1)-C(9)	1.885(3)
Mo(1)-O(4)	2.018(2)
Mo(1)-C(1)	2.218(3)
Mo(1)-O(1)	2.219(2)
N(1)-C(1)	1.367(4)
N(1)-C(2)	1.377(4)
N(1)-C(101)	1.446(4)
N(2)-C(1)	1.344(4)
N(2)-N(3)	1.379(4)
N(2)-C(201)	1.436(4)

N(3)-C(2)	1.307(4)
N(4)-C(3)	1.401(4)
C(2)-C(301)	1.476(5)
C(3)-C(4)	1.403(5)
C(3)-C(8)	1.408(5)
C(4)-C(5)	1.392(5)
C(4)-C(41)	1.508(5)
C(5)-C(6)	1.365(5)
C(5)-H(5)	0.9500
C(6)-C(7)	1.380(6)
C(6)-H(6)	0.9500
C(7)-C(8)	1.391(5)
C(7)-H(7)	0.9500
C(8)-C(81)	1.489(5)
C(9)-C(10)	1.518(4)
C(9)-H(9)	0.94(3)
C(10)-C(401)	1.527(5)
C(10)-C(12)	1.540(5)
C(10)-C(11)	1.541(5)
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-O(4)	1.353(4)
C(13)-C(14A)	1.516(10)
C(13)-C(15)	1.538(9)
C(13)-C(16A)	1.548(15)
C(13)-C(14)	1.555(8)
C(13)-C(16)	1.576(9)
C(13)-C(15A)	1.603(13)
C(17)-F(2)	1.315(6)
C(17)-F(3)	1.320(6)
C(17)-F(1)	1.328(5)
C(17)-S(1)	1.820(5)
C(18)-O(5)	1.448(10)
C(18)-C(19)	1.530(14)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-C(21)	1.374(12)
C(20)-O(5)	1.411(8)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800

C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(81)-H(81A)	0.9800
C(81)-H(81B)	0.9800
C(81)-H(81C)	0.9800
C(101)-C(106)	1.380(5)
C(101)-C(102)	1.387(5)
C(102)-C(103)	1.387(6)
C(102)-H(102)	0.9500
C(103)-C(104)	1.379(6)
C(103)-H(103)	0.9500
C(104)-C(105)	1.379(6)
C(104)-H(104)	0.9500
C(105)-C(106)	1.384(5)
C(105)-H(105)	0.9500
C(106)-H(106)	0.9500
C(201)-C(202)	1.379(5)
C(201)-C(206)	1.390(5)
C(202)-C(203)	1.401(5)
C(202)-H(202)	0.9500
C(203)-C(204)	1.378(6)
C(203)-H(203)	0.9500
C(204)-C(205)	1.374(7)
C(204)-H(204)	0.9500
C(205)-C(206)	1.381(5)
C(205)-H(205)	0.9500
C(206)-H(206)	0.9500
C(301)-C(306)	1.382(6)
C(301)-C(302)	1.395(6)
C(302)-C(303)	1.393(5)
C(302)-H(302)	0.9500
C(303)-C(304)	1.368(8)
C(303)-H(303)	0.9500
C(304)-C(305)	1.369(8)
C(304)-H(304)	0.9500
C(305)-C(306)	1.401(6)
C(305)-H(305)	0.9500
C(306)-H(306)	0.9500
C(401)-C(406)	1.391(5)
C(401)-C(402)	1.391(5)
C(402)-C(403)	1.393(7)
C(402)-H(402)	0.9500
C(403)-C(404)	1.353(8)
C(403)-H(403)	0.9500
C(404)-C(405)	1.376(8)
C(404)-H(404)	0.9500
C(405)-C(406)	1.387(6)
C(405)-H(405)	0.9500
C(406)-H(406)	0.9500

S(1)-O(2)	1.424(3)
S(1)-O(3)	1.442(3)
S(1)-O(1)	1.467(2)
F(4)-C(14A)	1.317(10)
F(4)-C(14)	1.321(8)
F(7)-C(15A)	1.292(12)
F(7)-C(15)	1.320(9)
F(10)-C(16A)	1.334(15)
F(10)-C(16)	1.354(8)
C(14)-F(6)	1.292(11)
C(14)-F(5)	1.329(12)
C(15)-F(8)	1.280(14)
C(15)-F(9)	1.353(14)
C(16)-F(12)	1.303(13)
C(16)-F(11)	1.360(10)
C(14A)-F(6A)	1.28(2)
C(14A)-F(5A)	1.410(17)
C(15A)-F(9A)	1.274(19)
C(15A)-F(8A)	1.38(2)
C(16A)-F(11A)	1.26(2)
C(16A)-F(12A)	1.34(2)

N(4)-Mo(1)-C(9)	98.39(13)
N(4)-Mo(1)-O(4)	101.37(10)
C(9)-Mo(1)-O(4)	107.35(11)
N(4)-Mo(1)-C(1)	86.87(11)
C(9)-Mo(1)-C(1)	103.91(12)
O(4)-Mo(1)-C(1)	145.98(10)
N(4)-Mo(1)-O(1)	162.55(10)
C(9)-Mo(1)-O(1)	97.13(12)
O(4)-Mo(1)-O(1)	81.46(9)
C(1)-Mo(1)-O(1)	81.70(10)
C(1)-N(1)-C(2)	109.7(3)
C(1)-N(1)-C(101)	123.5(3)
C(2)-N(1)-C(101)	126.6(3)
C(1)-N(2)-N(3)	113.5(2)
C(1)-N(2)-C(201)	130.9(3)
N(3)-N(2)-C(201)	115.4(2)
C(2)-N(3)-N(2)	104.5(3)
C(3)-N(4)-Mo(1)	171.9(2)
N(2)-C(1)-N(1)	102.6(2)
N(2)-C(1)-Mo(1)	141.4(2)
N(1)-C(1)-Mo(1)	115.7(2)
N(3)-C(2)-N(1)	109.7(3)
N(3)-C(2)-C(301)	122.9(3)
N(1)-C(2)-C(301)	127.4(3)
N(4)-C(3)-C(4)	120.6(3)
N(4)-C(3)-C(8)	117.7(3)
C(4)-C(3)-C(8)	121.7(3)
C(5)-C(4)-C(3)	118.0(3)

C(5)-C(4)-C(41)	119.5(3)
C(3)-C(4)-C(41)	122.5(3)
C(6)-C(5)-C(4)	121.1(3)
C(6)-C(5)-H(5)	119.5
C(4)-C(5)-H(5)	119.5
C(5)-C(6)-C(7)	120.4(3)
C(5)-C(6)-H(6)	119.8
C(7)-C(6)-H(6)	119.8
C(6)-C(7)-C(8)	121.5(3)
C(6)-C(7)-H(7)	119.2
C(8)-C(7)-H(7)	119.2
C(7)-C(8)-C(3)	117.2(3)
C(7)-C(8)-C(81)	121.8(3)
C(3)-C(8)-C(81)	121.0(3)
C(10)-C(9)-Mo(1)	143.7(2)
C(10)-C(9)-H(9)	111.1(19)
Mo(1)-C(9)-H(9)	104.6(19)
C(9)-C(10)-C(401)	112.2(3)
C(9)-C(10)-C(12)	108.6(3)
C(401)-C(10)-C(12)	108.7(3)
C(9)-C(10)-C(11)	108.2(3)
C(401)-C(10)-C(11)	112.3(3)
C(12)-C(10)-C(11)	106.7(3)
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
O(4)-C(13)-C(14A)	114.1(5)
O(4)-C(13)-C(15)	109.6(4)
O(4)-C(13)-C(16A)	110.3(6)
C(14A)-C(13)-C(16A)	108.1(8)
O(4)-C(13)-C(14)	113.7(4)
C(15)-C(13)-C(14)	110.2(6)
O(4)-C(13)-C(16)	107.5(4)
C(15)-C(13)-C(16)	109.0(5)
C(14)-C(13)-C(16)	106.7(5)
O(4)-C(13)-C(15A)	106.9(5)
C(14A)-C(13)-C(15A)	109.8(7)
C(16A)-C(13)-C(15A)	107.5(8)
F(2)-C(17)-F(3)	107.9(5)
F(2)-C(17)-F(1)	108.5(4)
F(3)-C(17)-F(1)	108.9(4)

F(2)-C(17)-S(1)	112.8(4)
F(3)-C(17)-S(1)	110.8(3)
F(1)-C(17)-S(1)	107.9(4)
O(5)-C(18)-C(19)	107.1(8)
O(5)-C(18)-H(18A)	110.3
C(19)-C(18)-H(18A)	110.3
O(5)-C(18)-H(18B)	110.3
C(19)-C(18)-H(18B)	110.3
H(18A)-C(18)-H(18B)	108.6
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(21)-C(20)-O(5)	113.1(8)
C(21)-C(20)-H(20A)	109.0
O(5)-C(20)-H(20A)	109.0
C(21)-C(20)-H(20B)	109.0
O(5)-C(20)-H(20B)	109.0
H(20A)-C(20)-H(20B)	107.8
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(4)-C(41)-H(41A)	109.5
C(4)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(4)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(8)-C(81)-H(81A)	109.5
C(8)-C(81)-H(81B)	109.5
H(81A)-C(81)-H(81B)	109.5
C(8)-C(81)-H(81C)	109.5
H(81A)-C(81)-H(81C)	109.5
H(81B)-C(81)-H(81C)	109.5
C(106)-C(101)-C(102)	121.4(3)
C(106)-C(101)-N(1)	119.2(3)
C(102)-C(101)-N(1)	119.4(3)
C(101)-C(102)-C(103)	118.6(4)
C(101)-C(102)-H(102)	120.7
C(103)-C(102)-H(102)	120.7
C(104)-C(103)-C(102)	120.4(4)
C(104)-C(103)-H(103)	119.8
C(102)-C(103)-H(103)	119.8
C(103)-C(104)-C(105)	120.3(4)
C(103)-C(104)-H(104)	119.9

C(105)-C(104)-H(104)	119.9
C(104)-C(105)-C(106)	120.1(4)
C(104)-C(105)-H(105)	119.9
C(106)-C(105)-H(105)	119.9
C(101)-C(106)-C(105)	119.1(3)
C(101)-C(106)-H(106)	120.4
C(105)-C(106)-H(106)	120.4
C(202)-C(201)-C(206)	121.5(3)
C(202)-C(201)-N(2)	121.2(3)
C(206)-C(201)-N(2)	117.2(3)
C(201)-C(202)-C(203)	118.0(4)
C(201)-C(202)-H(202)	121.0
C(203)-C(202)-H(202)	121.0
C(204)-C(203)-C(202)	120.8(4)
C(204)-C(203)-H(203)	119.6
C(202)-C(203)-H(203)	119.6
C(205)-C(204)-C(203)	120.1(4)
C(205)-C(204)-H(204)	119.9
C(203)-C(204)-H(204)	119.9
C(204)-C(205)-C(206)	120.4(4)
C(204)-C(205)-H(205)	119.8
C(206)-C(205)-H(205)	119.8
C(205)-C(206)-C(201)	119.2(4)
C(205)-C(206)-H(206)	120.4
C(201)-C(206)-H(206)	120.4
C(306)-C(301)-C(302)	120.3(3)
C(306)-C(301)-C(2)	117.5(4)
C(302)-C(301)-C(2)	122.1(3)
C(303)-C(302)-C(301)	119.6(4)
C(303)-C(302)-H(302)	120.2
C(301)-C(302)-H(302)	120.2
C(304)-C(303)-C(302)	120.0(5)
C(304)-C(303)-H(303)	120.0
C(302)-C(303)-H(303)	120.0
C(303)-C(304)-C(305)	120.6(4)
C(303)-C(304)-H(304)	119.7
C(305)-C(304)-H(304)	119.7
C(304)-C(305)-C(306)	120.7(5)
C(304)-C(305)-H(305)	119.7
C(306)-C(305)-H(305)	119.7
C(301)-C(306)-C(305)	118.9(5)
C(301)-C(306)-H(306)	120.6
C(305)-C(306)-H(306)	120.6
C(406)-C(401)-C(402)	117.6(4)
C(406)-C(401)-C(10)	119.7(3)
C(402)-C(401)-C(10)	122.7(3)
C(401)-C(402)-C(403)	120.1(5)
C(401)-C(402)-H(402)	120.0
C(403)-C(402)-H(402)	120.0
C(404)-C(403)-C(402)	121.3(5)

C(404)-C(403)-H(403)	119.3
C(402)-C(403)-H(403)	119.3
C(403)-C(404)-C(405)	119.7(4)
C(403)-C(404)-H(404)	120.1
C(405)-C(404)-H(404)	120.1
C(404)-C(405)-C(406)	119.7(5)
C(404)-C(405)-H(405)	120.1
C(406)-C(405)-H(405)	120.1
C(405)-C(406)-C(401)	121.5(4)
C(405)-C(406)-H(406)	119.3
C(401)-C(406)-H(406)	119.3
O(2)-S(1)-O(3)	116.50(19)
O(2)-S(1)-O(1)	114.08(16)
O(3)-S(1)-O(1)	113.72(17)
O(2)-S(1)-C(17)	102.9(2)
O(3)-S(1)-C(17)	104.8(2)
O(1)-S(1)-C(17)	102.53(19)
S(1)-O(1)-Mo(1)	141.26(14)
C(13)-O(4)-Mo(1)	153.1(2)
C(20)-O(5)-C(18)	116.7(8)
F(6)-C(14)-F(4)	108.3(6)
F(6)-C(14)-F(5)	109.0(9)
F(4)-C(14)-F(5)	107.1(7)
F(6)-C(14)-C(13)	113.0(6)
F(4)-C(14)-C(13)	111.8(6)
F(5)-C(14)-C(13)	107.6(8)
F(8)-C(15)-F(7)	106.5(8)
F(8)-C(15)-F(9)	110.4(10)
F(7)-C(15)-F(9)	105.4(8)
F(8)-C(15)-C(13)	111.2(8)
F(7)-C(15)-C(13)	113.4(7)
F(9)-C(15)-C(13)	109.8(8)
F(12)-C(16)-F(10)	107.3(7)
F(12)-C(16)-F(11)	109.0(9)
F(10)-C(16)-F(11)	108.4(6)
F(12)-C(16)-C(13)	110.6(7)
F(10)-C(16)-C(13)	111.0(6)
F(11)-C(16)-C(13)	110.5(6)
F(6A)-C(14A)-F(4)	110.9(12)
F(6A)-C(14A)-F(5A)	105.1(15)
F(4)-C(14A)-F(5A)	102.5(8)
F(6A)-C(14A)-C(13)	112.6(12)
F(4)-C(14A)-C(13)	114.5(8)
F(5A)-C(14A)-C(13)	110.3(9)
F(9A)-C(15A)-F(7)	104.8(11)
F(9A)-C(15A)-F(8A)	112.7(15)
F(7)-C(15A)-F(8A)	111.2(11)
F(9A)-C(15A)-C(13)	111.5(11)
F(7)-C(15A)-C(13)	111.0(9)
F(8A)-C(15A)-C(13)	105.8(11)

F(11A)-C(16A)-F(10)	109.4(13)
F(11A)-C(16A)-F(12A)	116.9(17)
F(10)-C(16A)-F(12A)	100.3(13)
F(11A)-C(16A)-C(13)	108.2(12)
F(10)-C(16A)-C(13)	113.8(11)
F(12A)-C(16A)-C(13)	108.3(13)

Symmetry transformations used to generate equivalent atoms:

Table 26.4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **26**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	19(1)	25(1)	20(1)	0(1)	1(1)	-1(1)
N(1)	24(1)	26(1)	22(1)	-3(1)	0(1)	4(1)
N(2)	23(1)	28(1)	22(1)	-3(1)	-1(1)	2(1)
N(3)	27(1)	32(2)	28(1)	-5(1)	-4(1)	4(1)
N(4)	22(1)	33(2)	18(1)	-1(1)	0(1)	2(1)
C(1)	26(2)	22(2)	22(2)	0(1)	1(1)	1(1)
C(2)	29(2)	24(2)	26(2)	-2(1)	-4(1)	5(1)
C(3)	34(2)	22(2)	18(1)	-1(1)	-1(1)	1(1)
C(4)	34(2)	30(2)	20(2)	-1(1)	-3(1)	-1(1)
C(5)	45(2)	30(2)	30(2)	-3(2)	-2(2)	-8(2)
C(6)	57(2)	27(2)	37(2)	-3(2)	1(2)	0(2)
C(7)	52(2)	30(2)	36(2)	-1(2)	6(2)	14(2)
C(8)	37(2)	34(2)	26(2)	-1(1)	3(1)	4(2)
C(9)	22(2)	26(2)	29(2)	0(1)	0(1)	1(1)
C(10)	29(2)	35(2)	25(2)	-4(1)	7(1)	5(1)
C(11)	39(2)	71(3)	41(2)	9(2)	17(2)	18(2)
C(12)	60(3)	41(2)	29(2)	-7(2)	1(2)	-3(2)
C(13)	16(2)	46(2)	61(2)	-4(2)	4(2)	-11(2)
C(17)	86(4)	48(3)	63(3)	22(2)	20(3)	4(3)
C(18)	225(13)	179(10)	102(7)	-3(7)	62(8)	-20(9)
C(19)	273(13)	203(10)	80(5)	-18(6)	-48(7)	174(10)
C(20)	73(5)	270(14)	121(7)	-14(8)	-15(5)	42(6)
C(21)	145(8)	111(6)	145(8)	-21(6)	-51(6)	31(6)
C(41)	30(2)	35(2)	46(2)	4(2)	1(2)	-3(2)
C(81)	36(2)	43(2)	55(2)	-1(2)	10(2)	10(2)
C(101)	27(2)	29(2)	21(2)	-4(1)	2(1)	3(1)
C(102)	44(2)	32(2)	46(2)	-7(2)	19(2)	-4(2)
C(103)	47(2)	55(3)	66(3)	-13(2)	30(2)	-13(2)
C(104)	35(2)	62(3)	54(2)	-18(2)	16(2)	7(2)
C(105)	39(2)	38(2)	43(2)	-10(2)	5(2)	13(2)
C(106)	32(2)	32(2)	29(2)	-2(1)	2(1)	3(1)
C(201)	25(2)	36(2)	24(2)	0(1)	1(1)	9(1)
C(202)	34(2)	39(2)	30(2)	-4(2)	-2(1)	11(2)
C(203)	54(3)	51(2)	38(2)	-13(2)	-3(2)	26(2)
C(204)	42(2)	81(3)	40(2)	-2(2)	12(2)	27(2)

C(205)	35(2)	72(3)	46(2)	5(2)	16(2)	12(2)
C(206)	32(2)	45(2)	41(2)	1(2)	6(2)	6(2)
C(301)	42(2)	33(2)	32(2)	-8(2)	-10(2)	16(2)
C(302)	55(2)	43(2)	28(2)	-7(2)	-6(2)	22(2)
C(303)	85(3)	60(3)	31(2)	-12(2)	-9(2)	42(3)
C(304)	92(4)	73(3)	48(3)	-33(3)	-29(3)	36(3)
C(305)	68(3)	68(3)	75(4)	-33(3)	-33(3)	11(3)
C(306)	46(2)	57(3)	53(3)	-23(2)	-17(2)	5(2)
C(401)	37(2)	35(2)	18(2)	-2(1)	3(1)	-1(2)
C(402)	61(3)	52(2)	34(2)	-8(2)	16(2)	-21(2)
C(403)	138(5)	41(3)	42(3)	-6(2)	28(3)	-35(3)
C(404)	164(6)	35(2)	29(2)	2(2)	10(3)	13(3)
C(405)	94(4)	50(3)	33(2)	-1(2)	-14(2)	28(3)
C(406)	47(2)	41(2)	29(2)	-2(2)	-6(2)	8(2)
S(1)	44(1)	30(1)	35(1)	5(1)	2(1)	2(1)
O(1)	31(1)	31(1)	34(1)	9(1)	-1(1)	-3(1)
O(2)	53(2)	53(2)	42(2)	6(1)	-15(1)	1(1)
O(3)	66(2)	50(2)	57(2)	-5(1)	13(2)	4(2)
O(4)	24(1)	39(1)	34(1)	3(1)	4(1)	-2(1)
O(5)	88(3)	112(4)	119(4)	-4(3)	10(3)	20(3)
F(1)	127(3)	66(2)	99(2)	58(2)	22(2)	20(2)
F(2)	91(2)	73(2)	132(3)	26(2)	9(2)	-38(2)
F(3)	160(4)	79(2)	89(2)	21(2)	82(2)	16(2)
F(4)	52(2)	57(2)	80(2)	-10(1)	0(1)	-25(1)
F(7)	62(2)	143(3)	63(2)	-5(2)	22(1)	-55(2)
F(10)	30(1)	89(2)	83(2)	-18(2)	-15(1)	-1(1)
F(5)	39(4)	44(3)	150(10)	-34(5)	-12(6)	3(3)
F(6)	56(3)	78(4)	49(3)	-18(2)	16(2)	-20(3)
F(8)	78(4)	118(6)	86(5)	47(5)	0(3)	-39(4)
F(9)	81(8)	208(13)	40(4)	-34(7)	27(4)	-79(8)
F(11)	48(3)	55(4)	67(4)	21(3)	-11(2)	0(2)
F(12)	44(3)	97(6)	75(5)	-30(4)	10(3)	20(3)
F(5A)	86(7)	65(5)	152(12)	-6(6)	-38(8)	-14(5)
F(6A)	97(15)	160(20)	190(20)	-142(17)	85(15)	-70(14)
F(8A)	104(11)	184(17)	43(6)	0(10)	23(6)	-68(10)
F(9A)	70(7)	206(15)	164(14)	-114(12)	64(9)	-35(8)
F(11A)	70(5)	125(11)	70(6)	49(7)	-6(4)	-22(6)
F(12A)	81(11)	51(6)	250(20)	11(13)	-99(13)	3(7)

Table 26.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **26**.

	x	y	z	U(eq)
H(5)	5702	1842	3319	43
H(6)	6985	987	3332	49
H(7)	8439	1562	3281	47
H(9)	7050(20)	6240(20)	3772(15)	20(8)
H(11A)	5739	5475	4978	74

H(11B)	5781	6239	4493	74
H(11C)	5451	5328	4237	74
H(12A)	7393	5786	5393	66
H(12B)	8156	5841	4915	66
H(12C)	7357	6537	4891	66
H(18A)	8818	8027	4965	198
H(18B)	8618	8947	5230	198
H(19A)	10004	8392	5799	287
H(19B)	10446	8296	5152	287
H(19C)	10246	9212	5416	287
H(20A)	7921	8584	3954	188
H(20B)	7913	9534	4202	188
H(21A)	7803	9488	3155	209
H(21B)	8752	9931	3444	209
H(21C)	8760	8980	3196	209
H(41A)	5232	3558	2795	56
H(41B)	5677	4052	3414	56
H(41C)	5066	3227	3481	56
H(81A)	9442	2718	3222	66
H(81B)	9142	3529	3593	66
H(81C)	8973	3504	2837	66
H(102)	7663	5567	1512	48
H(103)	9058	5050	1221	65
H(104)	9327	3609	1201	60
H(105)	8228	2670	1493	48
H(106)	6843	3174	1805	38
H(202)	5427	6673	3010	42
H(203)	4412	7220	3690	58
H(204)	3101	6471	3876	65
H(205)	2799	5160	3416	60
H(206)	3801	4592	2754	47
H(302)	6319	4566	494	52
H(303)	5863	3959	-499	72
H(304)	4466	3249	-690	89
H(305)	3510	3129	94	89
H(306)	3953	3713	1102	65
H(402)	5785	4076	4719	58
H(403)	6175	2673	4943	87
H(404)	7680	2217	4985	92
H(405)	8844	3161	4806	73
H(406)	8478	4565	4580	48

Table 26.6. Torsion angles [°] for **26**.

C(1)-N(2)-N(3)-C(2)	0.0(4)
C(201)-N(2)-N(3)-C(2)	-176.3(3)
N(3)-N(2)-C(1)-N(1)	0.7(3)
C(201)-N(2)-C(1)-N(1)	176.3(3)
N(3)-N(2)-C(1)-Mo(1)	-172.6(3)

C(201)-N(2)-C(1)-Mo(1)	2.9(6)
C(2)-N(1)-C(1)-N(2)	-1.2(3)
C(101)-N(1)-C(1)-N(2)	-176.4(3)
C(2)-N(1)-C(1)-Mo(1)	174.2(2)
C(101)-N(1)-C(1)-Mo(1)	-1.0(4)
N(2)-N(3)-C(2)-N(1)	-0.8(3)
N(2)-N(3)-C(2)-C(301)	179.4(3)
C(1)-N(1)-C(2)-N(3)	1.3(4)
C(101)-N(1)-C(2)-N(3)	176.4(3)
C(1)-N(1)-C(2)-C(301)	-178.8(3)
C(101)-N(1)-C(2)-C(301)	-3.8(5)
N(4)-C(3)-C(4)-C(5)	-179.0(3)
C(8)-C(3)-C(4)-C(5)	1.5(5)
N(4)-C(3)-C(4)-C(41)	1.8(5)
C(8)-C(3)-C(4)-C(41)	-177.8(3)
C(3)-C(4)-C(5)-C(6)	-1.0(5)
C(41)-C(4)-C(5)-C(6)	178.3(3)
C(4)-C(5)-C(6)-C(7)	0.0(5)
C(5)-C(6)-C(7)-C(8)	0.5(6)
C(6)-C(7)-C(8)-C(3)	0.0(5)
C(6)-C(7)-C(8)-C(81)	179.4(3)
N(4)-C(3)-C(8)-C(7)	179.5(3)
C(4)-C(3)-C(8)-C(7)	-1.0(5)
N(4)-C(3)-C(8)-C(81)	0.0(5)
C(4)-C(3)-C(8)-C(81)	179.6(3)
N(4)-Mo(1)-C(9)-C(10)	15.1(4)
O(4)-Mo(1)-C(9)-C(10)	-89.7(4)
C(1)-Mo(1)-C(9)-C(10)	103.9(4)
O(1)-Mo(1)-C(9)-C(10)	-172.9(4)
Mo(1)-C(9)-C(10)-C(401)	0.0(5)
Mo(1)-C(9)-C(10)-C(12)	120.2(4)
Mo(1)-C(9)-C(10)-C(11)	-124.4(4)
C(1)-N(1)-C(101)-C(106)	107.3(4)
C(2)-N(1)-C(101)-C(106)	-67.1(4)
C(1)-N(1)-C(101)-C(102)	-73.9(4)
C(2)-N(1)-C(101)-C(102)	111.6(4)
C(106)-C(101)-C(102)-C(103)	0.2(6)
N(1)-C(101)-C(102)-C(103)	-178.6(3)
C(101)-C(102)-C(103)-C(104)	0.7(7)
C(102)-C(103)-C(104)-C(105)	-0.8(7)
C(103)-C(104)-C(105)-C(106)	0.1(6)
C(102)-C(101)-C(106)-C(105)	-0.8(5)
N(1)-C(101)-C(106)-C(105)	177.9(3)
C(104)-C(105)-C(106)-C(101)	0.7(5)
C(1)-N(2)-C(201)-C(202)	53.7(5)
N(3)-N(2)-C(201)-C(202)	-130.9(3)
C(1)-N(2)-C(201)-C(206)	-130.7(4)
N(3)-N(2)-C(201)-C(206)	44.8(4)
C(206)-C(201)-C(202)-C(203)	0.1(5)
N(2)-C(201)-C(202)-C(203)	175.6(3)

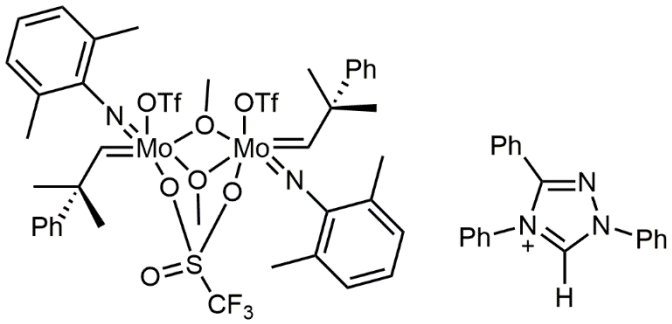
C(201)-C(202)-C(203)-C(204)	-0.8(5)
C(202)-C(203)-C(204)-C(205)	0.9(6)
C(203)-C(204)-C(205)-C(206)	-0.3(6)
C(204)-C(205)-C(206)-C(201)	-0.3(6)
C(202)-C(201)-C(206)-C(205)	0.4(5)
N(2)-C(201)-C(206)-C(205)	-175.2(3)
N(3)-C(2)-C(301)-C(306)	-33.0(5)
N(1)-C(2)-C(301)-C(306)	147.2(4)
N(3)-C(2)-C(301)-C(302)	143.6(4)
N(1)-C(2)-C(301)-C(302)	-36.3(5)
C(306)-C(301)-C(302)-C(303)	0.2(5)
C(2)-C(301)-C(302)-C(303)	-176.2(3)
C(301)-C(302)-C(303)-C(304)	0.2(6)
C(302)-C(303)-C(304)-C(305)	-0.1(7)
C(303)-C(304)-C(305)-C(306)	-0.3(8)
C(302)-C(301)-C(306)-C(305)	-0.7(6)
C(2)-C(301)-C(306)-C(305)	175.9(4)
C(304)-C(305)-C(306)-C(301)	0.8(7)
C(9)-C(10)-C(401)-C(406)	65.8(4)
C(12)-C(10)-C(401)-C(406)	-54.3(4)
C(11)-C(10)-C(401)-C(406)	-172.2(3)
C(9)-C(10)-C(401)-C(402)	-116.0(3)
C(12)-C(10)-C(401)-C(402)	124.0(3)
C(11)-C(10)-C(401)-C(402)	6.1(5)
C(406)-C(401)-C(402)-C(403)	-0.6(5)
C(10)-C(401)-C(402)-C(403)	-178.9(3)
C(401)-C(402)-C(403)-C(404)	0.3(6)
C(402)-C(403)-C(404)-C(405)	0.1(7)
C(403)-C(404)-C(405)-C(406)	-0.2(6)
C(404)-C(405)-C(406)-C(401)	-0.2(6)
C(402)-C(401)-C(406)-C(405)	0.6(5)
C(10)-C(401)-C(406)-C(405)	178.9(3)
F(2)-C(17)-S(1)-O(2)	177.5(4)
F(3)-C(17)-S(1)-O(2)	-61.4(4)
F(1)-C(17)-S(1)-O(2)	57.7(4)
F(2)-C(17)-S(1)-O(3)	55.2(4)
F(3)-C(17)-S(1)-O(3)	176.3(4)
F(1)-C(17)-S(1)-O(3)	-64.6(4)
F(2)-C(17)-S(1)-O(1)	-63.8(4)
F(3)-C(17)-S(1)-O(1)	57.3(4)
F(1)-C(17)-S(1)-O(1)	176.4(3)
O(2)-S(1)-O(1)-Mo(1)	-51.8(3)
O(3)-S(1)-O(1)-Mo(1)	85.1(3)
C(17)-S(1)-O(1)-Mo(1)	-162.3(3)
C(14A)-C(13)-O(4)-Mo(1)	-4.3(9)
C(15)-C(13)-O(4)-Mo(1)	-104.2(7)
C(16A)-C(13)-O(4)-Mo(1)	117.5(9)
C(14)-C(13)-O(4)-Mo(1)	19.7(8)
C(16)-C(13)-O(4)-Mo(1)	137.5(5)
C(15A)-C(13)-O(4)-Mo(1)	-125.9(7)

C(21)-C(20)-O(5)-C(18)	-175.8(9)
C(19)-C(18)-O(5)-C(20)	-172.2(8)
O(4)-C(13)-C(14)-F(6)	72.9(7)
C(15)-C(13)-C(14)-F(6)	-163.6(6)
C(16)-C(13)-C(14)-F(6)	-45.4(7)
O(4)-C(13)-C(14)-F(4)	-164.7(5)
C(15)-C(13)-C(14)-F(4)	-41.2(8)
C(16)-C(13)-C(14)-F(4)	77.0(7)
O(4)-C(13)-C(14)-F(5)	-47.4(9)
C(15)-C(13)-C(14)-F(5)	76.1(9)
C(16)-C(13)-C(14)-F(5)	-165.7(8)
O(4)-C(13)-C(15)-F(8)	82.3(8)
C(14)-C(13)-C(15)-F(8)	-43.5(8)
C(16)-C(13)-C(15)-F(8)	-160.3(7)
O(4)-C(13)-C(15)-F(7)	-157.7(6)
C(14)-C(13)-C(15)-F(7)	76.4(9)
C(16)-C(13)-C(15)-F(7)	-40.3(9)
O(4)-C(13)-C(15)-F(9)	-40.1(11)
C(14)-C(13)-C(15)-F(9)	-166.0(9)
C(16)-C(13)-C(15)-F(9)	77.3(10)
O(4)-C(13)-C(16)-F(12)	69.1(7)
C(15)-C(13)-C(16)-F(12)	-49.5(8)
C(14)-C(13)-C(16)-F(12)	-168.6(7)
O(4)-C(13)-C(16)-F(10)	-171.9(5)
C(15)-C(13)-C(16)-F(10)	69.4(7)
C(14)-C(13)-C(16)-F(10)	-49.6(7)
O(4)-C(13)-C(16)-F(11)	-51.7(8)
C(15)-C(13)-C(16)-F(11)	-170.4(7)
C(14)-C(13)-C(16)-F(11)	70.6(8)
O(4)-C(13)-C(14A)-F(6A)	38.9(17)
C(16A)-C(13)-C(14A)-F(6A)	-84.2(17)
C(15A)-C(13)-C(14A)-F(6A)	158.8(15)
O(4)-C(13)-C(14A)-F(4)	166.9(7)
C(16A)-C(13)-C(14A)-F(4)	43.8(11)
C(15A)-C(13)-C(14A)-F(4)	-73.2(10)
O(4)-C(13)-C(14A)-F(5A)	-78.2(9)
C(16A)-C(13)-C(14A)-F(5A)	158.7(10)
C(15A)-C(13)-C(14A)-F(5A)	41.7(10)
O(4)-C(13)-C(15A)-F(9A)	-70.8(11)
C(14A)-C(13)-C(15A)-F(9A)	165.0(11)
C(16A)-C(13)-C(15A)-F(9A)	47.6(13)
O(4)-C(13)-C(15A)-F(7)	172.8(8)
C(14A)-C(13)-C(15A)-F(7)	48.6(11)
C(16A)-C(13)-C(15A)-F(7)	-68.8(11)
O(4)-C(13)-C(15A)-F(8A)	52.0(13)
C(14A)-C(13)-C(15A)-F(8A)	-72.2(13)
C(16A)-C(13)-C(15A)-F(8A)	170.5(12)
O(4)-C(13)-C(16A)-F(11A)	-76.1(12)
C(14A)-C(13)-C(16A)-F(11A)	49.2(12)
C(15A)-C(13)-C(16A)-F(11A)	167.6(10)

O(4)-C(13)-C(16A)-F(10)	162.1(10)
C(14A)-C(13)-C(16A)-F(10)	-72.6(13)
C(15A)-C(13)-C(16A)-F(10)	45.8(14)
O(4)-C(13)-C(16A)-F(12A)	51.4(16)
C(14A)-C(13)-C(16A)-F(12A)	176.7(14)
C(15A)-C(13)-C(16A)-F(12A)	-64.8(16)

Symmetry transformations used to generate equivalent atoms:

Complex 27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OTf
N
Mo
Mo
O
O
O
O
N
Ph
O
S
CF3
Ph
N
N
Ph
Ph
N
+
H

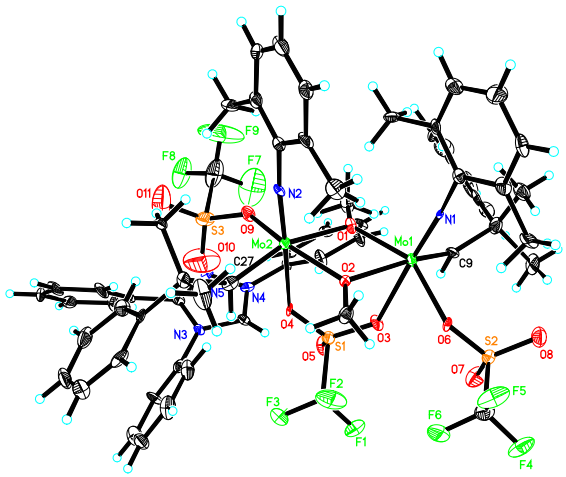

F9
F8
F7
O11
S3
O9
N2
O1
Mo2
Mo1
N1
O10
C27
C9
O2
N5
N4
N3
O4
O3
O6
S2
O8
O5
S1
O7
F5
F2
F3
F6
F1
F4

Table 27.1. Crystal data and structure refinement for **27**.

Empirical formula	$C_{68}H_{72}F_9Mo_2N_5O_{11}S_3$
Formula weight	1594.37
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, *P*na2_1
Unit cell dimensions	a = 20.454(3)Å, α = 90°
	b = 21.169(2) Å, β = 90°
	c = 16.515(2) Å, γ = 90°
Volume	7151.3(15) $Å^3$
Z, Calculated density	4, 1.481 Mg/m^3
Absorption coefficient	0.523 mm^{-1}
F(000)	3264
Crystal size	0.21 x 0.06 x 0.04 mm
Theta range for data collection	1.56 to 25.08°
Limiting indices	-21<=h<=24, -25<=k<=17, -19<=l<=19
Reflections collected / unique	31575 / 12298 [R(int) = 0.1039]
Completeness to theta = 25.08	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7137 and 0.6523
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12298 / 127 / 897
Goodness-of-fit on F^2	0.963
Final R indices [I>2σ(I)]	R1 = 0.0584, wR2 = 0.0767
R indices (all data)	R1 = 0.1229, wR2 = 0.0880
Absolute structure parameter	-0.06(3)
Largest diff. peak and hole	0.944 and -0.606 e.$Å^{-3}$

Table 27.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **27**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	9638(1)	2950(1)	6915(1)	11(1)
Mo(2)	9917(1)	2165(1)	8713(1)	11(1)
S(1)	9591(1)	3810(1)	8732(1)	13(1)
S(2)	8414(1)	3831(1)	6262(1)	15(1)
S(3)	11154(1)	2463(1)	10043(1)	23(1)
O(1)	10356(3)	2711(2)	7699(3)	13(1)
F(1)	8555(2)	4520(2)	8795(3)	41(1)
N(1)	9659(3)	2351(2)	6215(3)	6(1)
C(1)	9665(4)	1824(3)	5713(4)	12(2)
O(2)	9187(3)	2417(2)	7957(3)	12(1)
F(2)	8354(2)	3533(2)	8852(3)	43(1)
N(2)	10070(3)	1394(2)	8434(3)	11(2)
C(2)	9163(4)	1737(3)	5121(5)	18(2)
O(3)	9511(3)	3749(2)	7862(3)	16(1)
F(3)	8748(2)	4012(2)	9886(3)	37(1)
N(3)	10961(3)	4291(2)	11100(4)	13(2)
C(3)	9176(4)	1204(3)	4653(5)	24(2)
F(4)	7207(2)	4226(2)	6223(3)	37(1)
O(4)	9769(2)	3220(2)	9136(3)	9(1)
N(4)	11635(3)	4507(3)	10145(4)	17(2)
C(4)	9676(5)	757(3)	4750(5)	29(2)
O(5)	9961(3)	4347(2)	8983(2)	18(1)
F(5)	7308(2)	3215(2)	6327(3)	35(1)
N(5)	12018(3)	4358(3)	10804(4)	16(2)
C(5)	10161(4)	847(3)	5308(4)	20(2)
O(6)	8671(2)	3258(2)	6689(3)	10(1)
F(6)	7501(3)	3799(2)	7361(3)	41(2)
C(6)	10169(4)	1376(3)	5797(4)	13(2)
O(7)	8634(3)	4412(2)	6600(3)	28(2)
C(7)	8641(4)	2231(3)	5030(4)	19(2)
F(7)	12051(3)	3057(3)	9294(4)	88(2)
C(8)	10724(4)	1489(3)	6413(4)	17(2)
F(8)	12378(3)	2643(2)	10379(3)	45(2)
O(8)	8409(3)	3769(2)	5398(3)	25(2)
O(9)	10838(3)	2341(2)	9258(3)	16(1)
F(9)	12217(3)	2067(3)	9377(4)	98(2)
C(9)	10093(4)	3582(3)	6300(4)	14(2)
C(10)	10413(4)	3709(3)	5481(4)	20(2)
O(10)	10995(4)	3027(3)	10416(4)	75(2)
C(11)	10051(4)	4289(3)	5116(5)	26(2)
O(11)	11145(4)	1902(3)	10558(4)	65(2)
C(12)	10321(4)	3160(3)	4879(4)	23(2)
C(13)	11140(4)	3841(3)	5644(4)	18(2)
C(14)	11425(5)	4439(4)	5564(5)	25(2)

C(15)	12086(5)	4522(4)	5712(5)	39(3)
C(16)	12486(5)	4032(4)	5921(5)	35(2)
C(17)	12206(5)	3441(4)	5995(5)	33(3)
C(18)	11557(4)	3344(4)	5845(4)	21(2)
C(19)	10218(4)	794(3)	8140(4)	14(2)
C(20)	9764(4)	474(3)	7654(4)	19(2)
C(21)	9932(5)	-120(3)	7357(4)	21(2)
C(22)	10532(5)	-376(4)	7516(5)	34(3)
C(23)	10986(4)	-56(3)	7963(5)	23(2)
C(24)	10846(4)	539(3)	8286(4)	16(2)
C(25)	9117(4)	776(4)	7453(5)	25(2)
C(26)	11332(4)	894(3)	8795(5)	22(2)
C(27)	9420(4)	2000(3)	9676(4)	13(2)
C(28)	9217(4)	1452(3)	10227(5)	14(2)
C(29)	9761(4)	945(3)	10262(4)	18(2)
C(30)	8595(5)	1156(3)	9873(5)	32(3)
C(31)	9116(4)	1699(3)	11092(4)	11(2)
C(32)	9630(4)	1977(3)	11499(5)	20(2)
C(33)	9569(5)	2200(4)	12286(5)	27(2)
C(34)	8970(5)	2154(4)	12673(5)	27(2)
C(35)	8465(5)	1894(4)	12292(5)	32(3)
C(36)	8522(4)	1658(3)	11507(5)	20(2)
C(37)	8765(4)	3969(4)	9093(5)	19(2)
C(38)	7558(5)	3758(4)	6571(6)	28(2)
C(39)	12000(5)	2517(5)	9759(6)	42(3)
C(40)	11011(4)	2961(4)	7707(4)	24(2)
C(41)	8515(4)	2268(3)	8042(5)	18(2)
C(42)	11013(4)	4468(3)	10308(5)	14(2)
C(43)	11596(4)	4226(3)	11378(5)	13(2)
C(44)	10365(4)	4221(3)	11541(4)	15(2)
C(45)	10265(4)	4578(3)	12219(4)	18(2)
C(46)	9671(4)	4514(3)	12646(5)	26(2)
C(47)	9198(4)	4106(4)	12365(5)	22(2)
C(48)	9309(5)	3752(4)	11672(5)	26(2)
C(49)	9885(4)	3812(3)	11254(5)	24(2)
C(50)	11927(4)	4649(3)	9374(5)	14(2)
C(51)	11619(4)	4449(3)	8679(5)	22(2)
C(52)	11903(5)	4585(4)	7926(5)	29(2)
C(53)	12477(4)	4928(3)	7902(5)	25(2)
C(54)	12770(4)	5128(3)	8600(5)	20(2)
C(55)	12495(5)	4997(3)	9354(5)	22(2)
C(56)	11759(4)	4023(3)	12195(4)	11(2)
C(57)	11527(4)	3448(3)	12474(5)	22(2)
C(58)	11674(4)	3243(3)	13243(5)	25(2)
C(59)	12055(4)	3633(3)	13737(6)	26(2)
C(60)	12288(4)	4206(3)	13472(5)	22(2)
C(61)	12139(4)	4391(3)	12693(5)	26(2)
C(1X)	2916(5)	6619(3)	7687(5)	27(2)
C(2X)	3584(5)	6547(3)	7755(5)	24(2)
C(3X)	3887(5)	6560(4)	8499(5)	32(3)

C(4X)	3529(5)	6656(3)	9191(5)	31(3)
C(5X)	2877(5)	6736(3)	9115(5)	29(3)
C(6X)	2551(4)	6722(3)	8392(5)	22(2)
C(7X)	2577(4)	6590(3)	6856(6)	37(2)

Table 27.3. Bond lengths [Å] and angles [°] for **27**.

Mo(1)-N(1)	1.716(5)
Mo(1)-C(9)	1.920(7)
Mo(1)-O(1)	2.024(5)
Mo(1)-O(6)	2.114(5)
Mo(1)-O(2)	2.256(5)
Mo(1)-O(3)	2.317(4)
Mo(2)-N(2)	1.725(5)
Mo(2)-C(27)	1.920(7)
Mo(2)-O(2)	2.018(5)
Mo(2)-O(9)	2.122(5)
Mo(2)-O(1)	2.223(4)
Mo(2)-O(4)	2.361(4)
S(1)-O(5)	1.428(5)
S(1)-O(3)	1.453(5)
S(1)-O(4)	1.460(4)
S(1)-C(37)	1.822(8)
S(2)-O(7)	1.423(5)
S(2)-O(8)	1.433(5)
S(2)-O(6)	1.498(4)
S(2)-C(38)	1.830(9)
S(3)-O(10)	1.383(6)
S(3)-O(11)	1.462(6)
S(3)-O(9)	1.471(5)
S(3)-C(39)	1.796(10)
O(1)-C(40)	1.441(9)
F(1)-C(37)	1.336(8)
N(1)-C(1)	1.391(8)
C(1)-C(6)	1.409(10)
C(1)-C(2)	1.429(11)
O(2)-C(41)	1.416(8)
F(2)-C(37)	1.310(8)
N(2)-C(19)	1.393(8)
C(2)-C(3)	1.367(10)
C(2)-C(7)	1.503(10)
F(3)-C(37)	1.313(8)
N(3)-C(42)	1.364(9)
N(3)-C(43)	1.384(10)
N(3)-C(44)	1.429(10)
C(3)-C(4)	1.403(10)
C(3)-H(3)	0.9500
F(4)-C(38)	1.350(9)
N(4)-C(42)	1.303(10)

N(4)-N(5)	1.378(8)
N(4)-C(50)	1.439(9)
C(4)-C(5)	1.367(11)
C(4)-H(4)	0.9500
F(5)-C(38)	1.322(9)
N(5)-C(43)	1.312(9)
C(5)-C(6)	1.383(9)
C(5)-H(5)	0.9500
F(6)-C(38)	1.313(8)
C(6)-C(8)	1.541(10)
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
F(7)-C(39)	1.381(10)
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
F(8)-C(39)	1.310(10)
F(9)-C(39)	1.226(11)
C(9)-C(10)	1.527(10)
C(9)-H(9)	0.9500
C(10)-C(13)	1.537(11)
C(10)-C(12)	1.541(9)
C(10)-C(11)	1.554(10)
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(18)	1.396(10)
C(13)-C(14)	1.400(10)
C(14)-C(15)	1.386(12)
C(14)-H(14)	0.9500
C(15)-C(16)	1.365(12)
C(15)-H(15)	0.9500
C(16)-C(17)	1.381(11)
C(16)-H(16)	0.9500
C(17)-C(18)	1.364(11)
C(17)-H(17)	0.9500
C(18)-H(18)	0.9500
C(19)-C(20)	1.401(10)
C(19)-C(24)	1.413(10)
C(20)-C(21)	1.393(9)
C(20)-C(25)	1.507(10)
C(21)-C(22)	1.366(12)
C(21)-H(21)	0.9500
C(22)-C(23)	1.366(11)
C(22)-H(22)	0.9500
C(23)-C(24)	1.398(9)

C(23)-H(23)	0.9500
C(24)-C(26)	1.503(10)
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-C(28)	1.532(9)
C(27)-H(27)	0.9500
C(28)-C(31)	1.534(10)
C(28)-C(30)	1.534(11)
C(28)-C(29)	1.548(10)
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-C(32)	1.379(10)
C(31)-C(36)	1.399(11)
C(32)-C(33)	1.389(9)
C(32)-H(32)	0.9500
C(33)-C(34)	1.385(11)
C(33)-H(33)	0.9500
C(34)-C(35)	1.330(12)
C(34)-H(34)	0.9500
C(35)-C(36)	1.393(10)
C(35)-H(35)	0.9500
C(36)-H(36)	0.9500
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-H(42)	0.84(7)
C(43)-C(56)	1.455(10)
C(44)-C(45)	1.366(9)
C(44)-C(49)	1.392(10)
C(45)-C(46)	1.412(11)
C(45)-H(45)	0.9500
C(46)-C(47)	1.379(11)
C(46)-H(46)	0.9500
C(47)-C(48)	1.387(10)
C(47)-H(47)	0.9500
C(48)-C(49)	1.371(11)
C(48)-H(48)	0.9500
C(49)-H(49)	0.9500
C(50)-C(51)	1.376(11)

C(50)-C(55)	1.375(11)
C(51)-C(52)	1.402(11)
C(51)-H(51)	0.9500
C(52)-C(53)	1.382(11)
C(52)-H(52)	0.9500
C(53)-C(54)	1.368(11)
C(53)-H(53)	0.9500
C(54)-C(55)	1.394(10)
C(54)-H(54)	0.9500
C(55)-H(55)	0.9500
C(56)-C(61)	1.375(10)
C(56)-C(57)	1.385(10)
C(57)-C(58)	1.374(10)
C(57)-H(57)	0.9500
C(58)-C(59)	1.399(11)
C(58)-H(58)	0.9500
C(59)-C(60)	1.376(9)
C(59)-H(59)	0.9500
C(60)-C(61)	1.379(10)
C(60)-H(60)	0.9500
C(61)-H(61)	0.9500
C(1X)-C(2X)	1.380(11)
C(1X)-C(6X)	1.400(11)
C(1X)-C(7X)	1.538(12)
C(2X)-C(3X)	1.377(11)
C(2X)-H(2X)	0.9500
C(3X)-C(4X)	1.372(11)
C(3X)-H(3X)	0.9500
C(4X)-C(5X)	1.351(12)
C(4X)-H(4X)	0.9500
C(5X)-C(6X)	1.366(11)
C(5X)-H(5X)	0.9500
C(6X)-H(6X)	0.9500
C(7X)-H(7X1)	0.9800
C(7X)-H(7X2)	0.9800
C(7X)-H(7X3)	0.9800

N(1)-Mo(1)-C(9)	98.4(3)
N(1)-Mo(1)-O(1)	103.1(2)
C(9)-Mo(1)-O(1)	99.2(3)
N(1)-Mo(1)-O(6)	97.6(2)
C(9)-Mo(1)-O(6)	98.4(3)
O(1)-Mo(1)-O(6)	150.36(18)
N(1)-Mo(1)-O(2)	98.9(2)
C(9)-Mo(1)-O(2)	161.9(2)
O(1)-Mo(1)-O(2)	71.52(17)
O(6)-Mo(1)-O(2)	84.64(18)
N(1)-Mo(1)-O(3)	175.0(2)
C(9)-Mo(1)-O(3)	84.5(2)
O(1)-Mo(1)-O(3)	80.34(17)

O(6)-Mo(1)-O(3)	77.86(17)
O(2)-Mo(1)-O(3)	78.71(16)
N(2)-Mo(2)-C(27)	98.3(3)
N(2)-Mo(2)-O(2)	102.7(2)
C(27)-Mo(2)-O(2)	99.7(3)
N(2)-Mo(2)-O(9)	96.7(2)
C(27)-Mo(2)-O(9)	98.6(3)
O(2)-Mo(2)-O(9)	150.90(18)
N(2)-Mo(2)-O(1)	102.6(2)
C(27)-Mo(2)-O(1)	158.8(2)
O(2)-Mo(2)-O(1)	72.33(18)
O(9)-Mo(2)-O(1)	82.52(19)
N(2)-Mo(2)-O(4)	176.5(2)
C(27)-Mo(2)-O(4)	81.9(2)
O(2)-Mo(2)-O(4)	80.68(17)
O(9)-Mo(2)-O(4)	79.74(17)
O(1)-Mo(2)-O(4)	77.44(15)
O(5)-S(1)-O(3)	114.7(3)
O(5)-S(1)-O(4)	114.5(3)
O(3)-S(1)-O(4)	113.8(3)
O(5)-S(1)-C(37)	104.5(3)
O(3)-S(1)-C(37)	103.6(3)
O(4)-S(1)-C(37)	103.9(3)
O(7)-S(2)-O(8)	118.1(3)
O(7)-S(2)-O(6)	113.8(3)
O(8)-S(2)-O(6)	113.4(3)
O(7)-S(2)-C(38)	105.4(4)
O(8)-S(2)-C(38)	105.2(4)
O(6)-S(2)-C(38)	97.9(3)
O(10)-S(3)-O(11)	116.1(4)
O(10)-S(3)-O(9)	116.2(4)
O(11)-S(3)-O(9)	111.3(3)
O(10)-S(3)-C(39)	106.8(5)
O(11)-S(3)-C(39)	102.5(4)
O(9)-S(3)-C(39)	101.8(4)
C(40)-O(1)-Mo(1)	126.1(4)
C(40)-O(1)-Mo(2)	124.1(4)
Mo(1)-O(1)-Mo(2)	108.6(2)
C(1)-N(1)-Mo(1)	174.2(5)
N(1)-C(1)-C(6)	119.1(7)
N(1)-C(1)-C(2)	120.4(7)
C(6)-C(1)-C(2)	120.4(7)
C(41)-O(2)-Mo(2)	126.7(4)
C(41)-O(2)-Mo(1)	125.7(4)
Mo(2)-O(2)-Mo(1)	107.5(2)
C(19)-N(2)-Mo(2)	174.5(5)
C(3)-C(2)-C(1)	118.6(7)
C(3)-C(2)-C(7)	122.1(7)
C(1)-C(2)-C(7)	119.2(6)
S(1)-O(3)-Mo(1)	136.1(3)

C(42)-N(3)-C(43)	105.8(7)
C(42)-N(3)-C(44)	125.7(7)
C(43)-N(3)-C(44)	128.4(6)
C(2)-C(3)-C(4)	120.5(8)
C(2)-C(3)-H(3)	119.8
C(4)-C(3)-H(3)	119.8
S(1)-O(4)-Mo(2)	134.8(3)
C(42)-N(4)-N(5)	112.1(7)
C(42)-N(4)-C(50)	127.0(7)
N(5)-N(4)-C(50)	120.8(7)
C(5)-C(4)-C(3)	120.8(7)
C(5)-C(4)-H(4)	119.6
C(3)-C(4)-H(4)	119.6
C(43)-N(5)-N(4)	104.3(7)
C(4)-C(5)-C(6)	121.0(8)
C(4)-C(5)-H(5)	119.5
C(6)-C(5)-H(5)	119.5
S(2)-O(6)-Mo(1)	131.4(3)
C(5)-C(6)-C(1)	118.7(7)
C(5)-C(6)-C(8)	121.3(7)
C(1)-C(6)-C(8)	120.0(6)
C(2)-C(7)-H(7A)	109.5
C(2)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(2)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(6)-C(8)-H(8A)	109.5
C(6)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(6)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
S(3)-O(9)-Mo(2)	142.7(3)
C(10)-C(9)-Mo(1)	143.1(5)
C(10)-C(9)-H(9)	108.5
Mo(1)-C(9)-H(9)	108.5
C(9)-C(10)-C(13)	106.9(6)
C(9)-C(10)-C(12)	112.7(6)
C(13)-C(10)-C(12)	111.6(7)
C(9)-C(10)-C(11)	106.3(6)
C(13)-C(10)-C(11)	112.6(6)
C(12)-C(10)-C(11)	106.8(6)
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5

C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(18)-C(13)-C(14)	116.7(8)
C(18)-C(13)-C(10)	119.8(7)
C(14)-C(13)-C(10)	123.4(7)
C(15)-C(14)-C(13)	120.4(8)
C(15)-C(14)-H(14)	119.8
C(13)-C(14)-H(14)	119.8
C(16)-C(15)-C(14)	122.1(8)
C(16)-C(15)-H(15)	119.0
C(14)-C(15)-H(15)	119.0
C(15)-C(16)-C(17)	117.6(9)
C(15)-C(16)-H(16)	121.2
C(17)-C(16)-H(16)	121.2
C(18)-C(17)-C(16)	121.6(8)
C(18)-C(17)-H(17)	119.2
C(16)-C(17)-H(17)	119.2
C(17)-C(18)-C(13)	121.6(8)
C(17)-C(18)-H(18)	119.2
C(13)-C(18)-H(18)	119.2
N(2)-C(19)-C(20)	119.7(7)
N(2)-C(19)-C(24)	119.0(7)
C(20)-C(19)-C(24)	121.1(7)
C(21)-C(20)-C(19)	118.2(8)
C(21)-C(20)-C(25)	121.5(7)
C(19)-C(20)-C(25)	120.3(6)
C(22)-C(21)-C(20)	120.9(8)
C(22)-C(21)-H(21)	119.6
C(20)-C(21)-H(21)	119.6
C(21)-C(22)-C(23)	121.1(7)
C(21)-C(22)-H(22)	119.5
C(23)-C(22)-H(22)	119.5
C(22)-C(23)-C(24)	121.0(8)
C(22)-C(23)-H(23)	119.5
C(24)-C(23)-H(23)	119.5
C(23)-C(24)-C(19)	117.7(7)
C(23)-C(24)-C(26)	121.9(7)
C(19)-C(24)-C(26)	120.4(6)
C(20)-C(25)-H(25A)	109.5
C(20)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(20)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(24)-C(26)-H(26A)	109.5
C(24)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5

C(24)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(28)-C(27)-Mo(2)	140.7(5)
C(28)-C(27)-H(27)	109.7
Mo(2)-C(27)-H(27)	109.7
C(27)-C(28)-C(31)	109.4(5)
C(27)-C(28)-C(30)	107.9(6)
C(31)-C(28)-C(30)	112.5(7)
C(27)-C(28)-C(29)	110.7(6)
C(31)-C(28)-C(29)	107.4(6)
C(30)-C(28)-C(29)	109.0(6)
C(28)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(28)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(28)-C(30)-H(30A)	109.5
C(28)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(28)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(32)-C(31)-C(36)	116.7(7)
C(32)-C(31)-C(28)	119.7(7)
C(36)-C(31)-C(28)	123.5(7)
C(31)-C(32)-C(33)	122.2(9)
C(31)-C(32)-H(32)	118.9
C(33)-C(32)-H(32)	118.9
C(34)-C(33)-C(32)	119.1(9)
C(34)-C(33)-H(33)	120.4
C(32)-C(33)-H(33)	120.4
C(35)-C(34)-C(33)	119.9(8)
C(35)-C(34)-H(34)	120.1
C(33)-C(34)-H(34)	120.1
C(34)-C(35)-C(36)	121.6(10)
C(34)-C(35)-H(35)	119.2
C(36)-C(35)-H(35)	119.2
C(35)-C(36)-C(31)	120.4(8)
C(35)-C(36)-H(36)	119.8
C(31)-C(36)-H(36)	119.8
F(2)-C(37)-F(3)	109.5(7)
F(2)-C(37)-F(1)	107.2(7)
F(3)-C(37)-F(1)	107.3(6)
F(2)-C(37)-S(1)	111.4(5)
F(3)-C(37)-S(1)	111.4(6)
F(1)-C(37)-S(1)	109.8(5)
F(6)-C(38)-F(5)	109.1(8)
F(6)-C(38)-F(4)	109.1(7)

F(5)-C(38)-F(4)	107.6(7)
F(6)-C(38)-S(2)	110.9(7)
F(5)-C(38)-S(2)	111.0(6)
F(4)-C(38)-S(2)	109.2(6)
F(9)-C(39)-F(8)	110.3(9)
F(9)-C(39)-F(7)	109.2(9)
F(8)-C(39)-F(7)	102.8(8)
F(9)-C(39)-S(3)	115.7(7)
F(8)-C(39)-S(3)	112.2(7)
F(7)-C(39)-S(3)	105.7(7)
O(1)-C(40)-H(40A)	109.5
O(1)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
O(1)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
O(2)-C(41)-H(41A)	109.5
O(2)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
O(2)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
N(4)-C(42)-N(3)	107.0(7)
N(4)-C(42)-H(42)	128(5)
N(3)-C(42)-H(42)	125(5)
N(5)-C(43)-N(3)	110.8(7)
N(5)-C(43)-C(56)	125.6(8)
N(3)-C(43)-C(56)	123.5(7)
C(45)-C(44)-C(49)	121.2(8)
C(45)-C(44)-N(3)	119.2(7)
C(49)-C(44)-N(3)	119.6(7)
C(44)-C(45)-C(46)	119.0(8)
C(44)-C(45)-H(45)	120.5
C(46)-C(45)-H(45)	120.5
C(47)-C(46)-C(45)	119.7(8)
C(47)-C(46)-H(46)	120.1
C(45)-C(46)-H(46)	120.1
C(46)-C(47)-C(48)	120.1(8)
C(46)-C(47)-H(47)	119.9
C(48)-C(47)-H(47)	119.9
C(49)-C(48)-C(47)	120.4(8)
C(49)-C(48)-H(48)	119.8
C(47)-C(48)-H(48)	119.8
C(48)-C(49)-C(44)	119.5(8)
C(48)-C(49)-H(49)	120.3
C(44)-C(49)-H(49)	120.3
C(51)-C(50)-C(55)	122.2(8)
C(51)-C(50)-N(4)	118.9(8)
C(55)-C(50)-N(4)	118.9(7)
C(50)-C(51)-C(52)	119.1(8)

C(50)-C(51)-H(51)	120.5
C(52)-C(51)-H(51)	120.5
C(53)-C(52)-C(51)	119.1(9)
C(53)-C(52)-H(52)	120.5
C(51)-C(52)-H(52)	120.5
C(54)-C(53)-C(52)	120.7(9)
C(54)-C(53)-H(53)	119.6
C(52)-C(53)-H(53)	119.6
C(53)-C(54)-C(55)	121.0(8)
C(53)-C(54)-H(54)	119.5
C(55)-C(54)-H(54)	119.5
C(50)-C(55)-C(54)	117.9(8)
C(50)-C(55)-H(55)	121.0
C(54)-C(55)-H(55)	121.0
C(61)-C(56)-C(57)	119.6(7)
C(61)-C(56)-C(43)	121.1(7)
C(57)-C(56)-C(43)	119.4(7)
C(58)-C(57)-C(56)	120.6(8)
C(58)-C(57)-H(57)	119.7
C(56)-C(57)-H(57)	119.7
C(57)-C(58)-C(59)	118.4(7)
C(57)-C(58)-H(58)	120.8
C(59)-C(58)-H(58)	120.8
C(60)-C(59)-C(58)	121.8(8)
C(60)-C(59)-H(59)	119.1
C(58)-C(59)-H(59)	119.1
C(59)-C(60)-C(61)	118.1(8)
C(59)-C(60)-H(60)	120.9
C(61)-C(60)-H(60)	120.9
C(56)-C(61)-C(60)	121.4(7)
C(56)-C(61)-H(61)	119.3
C(60)-C(61)-H(61)	119.3
C(2X)-C(1X)-C(6X)	118.5(9)
C(2X)-C(1X)-C(7X)	120.9(8)
C(6X)-C(1X)-C(7X)	120.6(9)
C(3X)-C(2X)-C(1X)	121.0(9)
C(3X)-C(2X)-H(2X)	119.5
C(1X)-C(2X)-H(2X)	119.5
C(4X)-C(3X)-C(2X)	120.5(10)
C(4X)-C(3X)-H(3X)	119.8
C(2X)-C(3X)-H(3X)	119.8
C(5X)-C(4X)-C(3X)	117.8(9)
C(5X)-C(4X)-H(4X)	121.1
C(3X)-C(4X)-H(4X)	121.1
C(4X)-C(5X)-C(6X)	124.1(9)
C(4X)-C(5X)-H(5X)	118.0
C(6X)-C(5X)-H(5X)	118.0
C(5X)-C(6X)-C(1X)	118.1(9)
C(5X)-C(6X)-H(6X)	120.9
C(1X)-C(6X)-H(6X)	120.9

C(1X)-C(7X)-H(7X1)	109.5
C(1X)-C(7X)-H(7X2)	109.5
H(7X1)-C(7X)-H(7X2)	109.5
C(1X)-C(7X)-H(7X3)	109.5
H(7X1)-C(7X)-H(7X3)	109.5
H(7X2)-C(7X)-H(7X3)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 27.4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **27**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	13(1)	11(1)	8(1)	0(1)	0(1)	1(1)
Mo(2)	14(1)	10(1)	10(1)	0(1)	0(1)	1(1)
S(1)	17(1)	11(1)	12(1)	-2(1)	-1(1)	1(1)
S(2)	16(1)	15(1)	14(1)	3(1)	-1(1)	2(1)
S(3)	13(1)	30(1)	25(1)	-9(1)	-6(1)	4(1)
O(1)	17(4)	13(2)	8(3)	1(2)	0(2)	-5(2)
F(1)	42(4)	43(3)	39(3)	10(3)	1(3)	27(2)
N(1)	6(3)	8(2)	4(2)	-1(2)	-4(2)	2(2)
C(1)	14(3)	11(2)	11(3)	3(2)	2(2)	-3(2)
O(2)	10(4)	15(3)	9(3)	2(2)	0(2)	4(2)
F(2)	15(3)	55(3)	58(4)	-19(3)	10(3)	-8(2)
N(2)	11(4)	14(3)	7(4)	1(2)	5(3)	0(3)
C(2)	28(6)	11(4)	16(5)	-6(4)	-3(4)	-4(4)
O(3)	28(4)	12(2)	8(3)	-6(2)	-1(3)	0(2)
F(3)	41(4)	51(3)	20(3)	1(2)	10(3)	18(3)
N(3)	21(5)	10(3)	7(4)	-4(3)	1(3)	4(3)
C(3)	30(5)	31(4)	11(4)	-3(3)	-5(3)	-5(4)
F(4)	15(3)	36(3)	60(4)	18(3)	0(3)	5(2)
O(4)	11(3)	8(2)	6(2)	5(2)	-2(2)	1(2)
N(4)	17(5)	15(3)	18(4)	0(3)	3(4)	8(3)
C(4)	38(7)	20(4)	30(6)	-6(4)	-6(5)	5(5)
O(5)	26(4)	16(2)	11(3)	-1(2)	-5(3)	-7(3)
F(5)	14(3)	16(2)	76(4)	0(3)	-6(3)	-8(2)
N(5)	17(5)	17(3)	15(4)	2(3)	0(4)	9(3)
C(5)	29(6)	12(4)	18(5)	-3(4)	4(4)	-1(4)
O(6)	10(3)	13(2)	8(3)	2(2)	-5(2)	0(2)
F(6)	35(4)	54(3)	33(4)	8(3)	16(3)	16(3)
C(6)	15(5)	18(4)	7(4)	4(3)	2(4)	0(4)
O(7)	34(4)	11(3)	39(4)	-1(2)	-9(3)	-1(3)
C(7)	9(4)	31(4)	16(4)	-4(3)	7(3)	-4(3)
F(7)	72(5)	105(4)	86(4)	32(4)	-17(3)	-24(4)
C(8)	15(6)	17(4)	20(5)	-1(4)	5(4)	7(4)
F(8)	34(4)	53(3)	49(4)	18(3)	-26(3)	-22(3)
O(8)	28(3)	29(2)	17(3)	6(2)	-1(2)	0(2)
O(9)	16(4)	22(3)	11(3)	-3(2)	-1(3)	-2(2)
F(9)	49(4)	118(4)	127(5)	-95(4)	-7(3)	21(4)
C(9)	16(5)	14(4)	11(5)	1(3)	6(4)	4(4)

C(10)	21(6)	22(4)	17(5)	8(4)	1(4)	2(4)
O(10)	63(5)	73(4)	89(5)	-56(4)	-25(4)	12(4)
C(11)	29(6)	31(4)	19(5)	19(4)	5(5)	-3(5)
O(11)	60(5)	88(4)	45(4)	34(3)	-10(3)	-15(4)
C(12)	35(6)	18(4)	17(5)	2(3)	8(4)	-1(4)
C(13)	26(6)	23(4)	4(5)	1(4)	5(4)	-2(4)
C(14)	27(7)	32(5)	18(5)	-1(4)	4(4)	3(5)
C(15)	63(9)	39(6)	16(6)	-1(4)	6(5)	-28(6)
C(16)	31(4)	44(3)	31(3)	-6(3)	4(3)	-2(3)
C(17)	29(7)	55(6)	14(6)	4(4)	-5(4)	27(5)
C(18)	32(7)	27(5)	5(5)	1(4)	2(4)	6(4)
C(19)	15(3)	16(3)	10(3)	1(2)	2(2)	1(2)
C(20)	30(7)	17(4)	9(5)	-6(3)	3(4)	2(4)
C(21)	36(7)	15(4)	12(5)	2(3)	2(4)	0(4)
C(22)	72(9)	14(4)	14(5)	1(4)	11(5)	8(5)
C(23)	32(7)	22(4)	13(5)	8(4)	6(4)	11(4)
C(24)	25(4)	12(3)	12(4)	4(3)	4(3)	-2(3)
C(25)	22(6)	30(5)	23(5)	-3(4)	1(4)	-4(4)
C(26)	26(6)	18(4)	21(5)	-8(4)	2(5)	8(4)
C(27)	8(4)	11(3)	20(4)	0(3)	-3(3)	-3(3)
C(28)	12(5)	14(4)	15(5)	5(3)	3(4)	-5(4)
C(29)	31(5)	10(3)	13(4)	5(3)	12(3)	9(3)
C(30)	48(8)	27(5)	22(6)	1(4)	-1(5)	-25(5)
C(31)	12(5)	9(4)	11(5)	7(3)	-1(4)	0(4)
C(32)	21(6)	20(4)	20(5)	4(4)	2(4)	1(4)
C(33)	42(7)	22(4)	18(5)	0(4)	-13(5)	5(5)
C(34)	48(8)	23(5)	11(5)	1(4)	6(5)	3(5)
C(35)	39(8)	35(5)	22(6)	6(4)	8(5)	10(5)
C(36)	10(6)	25(4)	26(6)	4(4)	-11(4)	3(4)
C(37)	13(6)	28(5)	16(5)	2(4)	7(4)	0(4)
C(38)	25(7)	31(5)	29(6)	5(5)	5(4)	7(5)
C(39)	28(7)	55(6)	42(7)	16(6)	-21(5)	-14(6)
C(40)	20(4)	35(4)	16(4)	5(4)	-2(3)	-4(4)
C(41)	14(4)	20(3)	19(4)	7(3)	-1(3)	-2(3)
C(42)	16(4)	15(3)	10(4)	-3(3)	3(3)	2(3)
C(43)	15(5)	11(4)	12(5)	-6(3)	1(4)	-1(4)
C(44)	20(6)	10(4)	15(4)	0(3)	-3(4)	3(4)
C(45)	12(6)	27(4)	15(5)	-6(4)	8(4)	-2(4)
C(46)	34(7)	21(4)	22(5)	2(4)	4(5)	-7(4)
C(47)	18(6)	34(5)	14(5)	-2(4)	2(4)	1(4)
C(48)	31(7)	23(4)	24(6)	7(4)	-5(4)	-16(4)
C(49)	36(7)	20(4)	15(5)	2(4)	-4(5)	-3(5)
C(50)	18(6)	15(4)	8(5)	4(4)	7(4)	4(4)
C(51)	28(6)	28(4)	10(5)	2(4)	2(5)	-6(4)
C(52)	31(7)	46(6)	9(6)	5(4)	5(5)	0(5)
C(53)	30(7)	26(5)	18(6)	-4(4)	10(5)	11(4)
C(54)	15(5)	19(4)	24(6)	9(4)	13(4)	4(3)
C(55)	36(7)	15(4)	16(6)	-6(4)	2(4)	11(4)
C(56)	16(4)	11(3)	7(4)	-1(3)	3(3)	3(3)
C(57)	30(7)	27(5)	9(5)	-7(4)	5(4)	1(4)

C(58)	35(7)	17(4)	24(6)	3(4)	23(5)	1(4)
C(59)	29(6)	37(4)	12(5)	12(5)	4(5)	17(4)
C(60)	26(6)	22(4)	17(6)	-5(4)	0(4)	9(4)
C(61)	38(7)	21(4)	18(6)	9(4)	10(5)	-2(4)
C(1X)	34(7)	21(4)	27(6)	6(4)	-2(5)	-7(5)
C(2X)	29(7)	18(4)	26(6)	2(4)	6(5)	1(4)
C(3X)	29(7)	34(5)	31(7)	8(4)	-5(5)	-2(4)
C(4X)	43(8)	22(5)	28(6)	7(4)	-9(5)	-2(5)
C(5X)	49(8)	15(4)	22(6)	7(4)	10(5)	-10(5)
C(6X)	17(6)	22(4)	27(6)	12(4)	1(5)	-9(4)
C(7X)	46(7)	35(5)	31(6)	6(5)	-14(6)	-4(4)

Table 27.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **27**.

	x	y	z	U(eq)
H(3)	8845	1137	4259	29
H(4)	9677	387	4425	35
H(5)	10498	540	5360	24
H(7A)	8829	2610	4782	28
H(7B)	8464	2338	5564	28
H(7C)	8290	2068	4685	28
H(8A)	10945	1088	6528	26
H(8B)	10540	1660	6915	26
H(8C)	11039	1790	6187	26
H(9)	10136	3949	6626	17
H(11A)	10041	4632	5515	40
H(11B)	9603	4169	4974	40
H(11C)	10282	4432	4629	40
H(12A)	10536	3264	4366	35
H(12B)	9853	3092	4785	35
H(12C)	10515	2775	5105	35
H(14)	11163	4789	5407	30
H(15)	12267	4934	5666	47
H(16)	12940	4095	6012	42
H(17)	12471	3094	6153	39
H(18)	11386	2927	5878	26
H(21)	9626	-350	7041	25
H(22)	10634	-784	7312	40
H(23)	11402	-241	8055	27
H(25A)	8856	820	7947	37
H(25B)	8881	511	7064	37
H(25C)	9192	1194	7215	37
H(26A)	11125	1023	9304	33
H(26B)	11480	1270	8500	33
H(26C)	11707	621	8911	33
H(27)	9242	2384	9876	16
H(29A)	9790	730	9738	27

H(29B)	9657	636	10685	27
H(29C)	10181	1147	10385	27
H(30A)	8249	1475	9850	48
H(30B)	8454	805	10218	48
H(30C)	8686	999	9327	48
H(32)	10039	2017	11232	24
H(33)	9934	2381	12556	33
H(34)	8920	2307	13210	33
H(35)	8055	1868	12561	39
H(36)	8154	1469	11252	24
H(40A)	11314	2644	7492	35
H(40B)	11135	3067	8264	35
H(40C)	11030	3342	7371	35
H(41A)	8412	1896	7712	26
H(41B)	8250	2627	7863	26
H(41C)	8420	2176	8612	26
H(42)	10700(40)	4530(30)	9990(40)	16
H(45)	10591	4866	12399	22
H(46)	9598	4752	13126	31
H(47)	8795	4067	12646	27
H(48)	8984	3466	11486	31
H(49)	9955	3577	10772	28
H(51)	11219	4222	8710	27
H(52)	11703	4443	7440	34
H(53)	12670	5025	7394	29
H(54)	13168	5359	8571	23
H(55)	12693	5145	9839	27
H(57)	11263	3193	12131	26
H(58)	11520	2847	13434	30
H(59)	12157	3497	14271	31
H(60)	12545	4467	13816	26
H(61)	12303	4782	12496	31
H(2X)	3839	6487	7280	29
H(3X)	4346	6503	8534	38
H(4X)	3733	6666	9708	37
H(5X)	2629	6808	9593	35
H(6X)	2091	6780	8370	26
H(7X1)	2902	6497	6437	56
H(7X2)	2371	6998	6740	56
H(7X3)	2244	6258	6861	56

Table 27.6. Torsion angles [°] for **27**.

N(1)-Mo(1)-O(1)-C(40)	98.8(5)
C(9)-Mo(1)-O(1)-C(40)	-2.2(6)
O(6)-Mo(1)-O(1)-C(40)	-128.0(5)
O(2)-Mo(1)-O(1)-C(40)	-166.1(5)
O(3)-Mo(1)-O(1)-C(40)	-84.9(5)
N(1)-Mo(1)-O(1)-Mo(2)	-93.8(3)

C(9)-Mo(1)-O(1)-Mo(2)	165.3(3)
O(6)-Mo(1)-O(1)-Mo(2)	39.5(4)
O(2)-Mo(1)-O(1)-Mo(2)	1.35(17)
O(3)-Mo(1)-O(1)-Mo(2)	82.6(2)
N(2)-Mo(2)-O(1)-C(40)	-94.2(5)
C(27)-Mo(2)-O(1)-C(40)	95.6(9)
O(2)-Mo(2)-O(1)-C(40)	166.3(5)
O(9)-Mo(2)-O(1)-C(40)	1.1(5)
O(4)-Mo(2)-O(1)-C(40)	82.2(5)
N(2)-Mo(2)-O(1)-Mo(1)	98.0(3)
C(27)-Mo(2)-O(1)-Mo(1)	-72.2(7)
O(2)-Mo(2)-O(1)-Mo(1)	-1.50(19)
O(9)-Mo(2)-O(1)-Mo(1)	-166.7(2)
O(4)-Mo(2)-O(1)-Mo(1)	-85.6(2)
C(9)-Mo(1)-N(1)-C(1)	161(6)
O(1)-Mo(1)-N(1)-C(1)	59(6)
O(6)-Mo(1)-N(1)-C(1)	-100(6)
O(2)-Mo(1)-N(1)-C(1)	-14(6)
O(3)-Mo(1)-N(1)-C(1)	-75(7)
Mo(1)-N(1)-C(1)-C(6)	-67(6)
Mo(1)-N(1)-C(1)-C(2)	113(5)
N(2)-Mo(2)-O(2)-C(41)	79.7(5)
C(27)-Mo(2)-O(2)-C(41)	-21.2(6)
O(9)-Mo(2)-O(2)-C(41)	-149.5(5)
O(1)-Mo(2)-O(2)-C(41)	179.0(5)
O(4)-Mo(2)-O(2)-C(41)	-101.3(5)
N(2)-Mo(2)-O(2)-Mo(1)	-98.0(2)
C(27)-Mo(2)-O(2)-Mo(1)	161.1(2)
O(9)-Mo(2)-O(2)-Mo(1)	32.8(5)
O(1)-Mo(2)-O(2)-Mo(1)	1.34(17)
O(4)-Mo(2)-O(2)-Mo(1)	81.03(19)
N(1)-Mo(1)-O(2)-C(41)	-78.2(5)
C(9)-Mo(1)-O(2)-C(41)	119.4(9)
O(1)-Mo(1)-O(2)-C(41)	-179.2(5)
O(6)-Mo(1)-O(2)-C(41)	18.7(5)
O(3)-Mo(1)-O(2)-C(41)	97.3(5)
N(1)-Mo(1)-O(2)-Mo(2)	99.5(3)
C(9)-Mo(1)-O(2)-Mo(2)	-62.9(9)
O(1)-Mo(1)-O(2)-Mo(2)	-1.48(19)
O(6)-Mo(1)-O(2)-Mo(2)	-163.6(2)
O(3)-Mo(1)-O(2)-Mo(2)	-85.0(2)
C(27)-Mo(2)-N(2)-C(19)	171(6)
O(2)-Mo(2)-N(2)-C(19)	69(6)
O(9)-Mo(2)-N(2)-C(19)	-89(6)
O(1)-Mo(2)-N(2)-C(19)	-6(6)
O(4)-Mo(2)-N(2)-C(19)	-96(7)
N(1)-C(1)-C(2)-C(3)	-178.3(7)
C(6)-C(1)-C(2)-C(3)	1.3(12)
N(1)-C(1)-C(2)-C(7)	1.9(11)
C(6)-C(1)-C(2)-C(7)	-178.4(7)

O(5)-S(1)-O(3)-Mo(1)	131.3(4)
O(4)-S(1)-O(3)-Mo(1)	-3.3(6)
C(37)-S(1)-O(3)-Mo(1)	-115.5(5)
N(1)-Mo(1)-O(3)-S(1)	101(2)
C(9)-Mo(1)-O(3)-S(1)	-133.6(5)
O(1)-Mo(1)-O(3)-S(1)	-33.2(4)
O(6)-Mo(1)-O(3)-S(1)	126.6(5)
O(2)-Mo(1)-O(3)-S(1)	39.7(4)
C(1)-C(2)-C(3)-C(4)	-0.4(12)
C(7)-C(2)-C(3)-C(4)	179.3(7)
O(5)-S(1)-O(4)-Mo(2)	-138.0(4)
O(3)-S(1)-O(4)-Mo(2)	-3.3(5)
C(37)-S(1)-O(4)-Mo(2)	108.7(4)
N(2)-Mo(2)-O(4)-S(1)	131(3)
C(27)-Mo(2)-O(4)-S(1)	-135.5(5)
O(2)-Mo(2)-O(4)-S(1)	-34.2(4)
O(9)-Mo(2)-O(4)-S(1)	124.2(4)
O(1)-Mo(2)-O(4)-S(1)	39.6(4)
C(2)-C(3)-C(4)-C(5)	-0.6(13)
C(42)-N(4)-N(5)-C(43)	0.0(8)
C(50)-N(4)-N(5)-C(43)	-176.7(6)
C(3)-C(4)-C(5)-C(6)	0.8(13)
O(7)-S(2)-O(6)-Mo(1)	-57.8(5)
O(8)-S(2)-O(6)-Mo(1)	81.0(4)
C(38)-S(2)-O(6)-Mo(1)	-168.6(4)
N(1)-Mo(1)-O(6)-S(2)	-105.8(4)
C(9)-Mo(1)-O(6)-S(2)	-6.1(4)
O(1)-Mo(1)-O(6)-S(2)	119.9(4)
O(2)-Mo(1)-O(6)-S(2)	155.9(4)
O(3)-Mo(1)-O(6)-S(2)	76.3(4)
C(4)-C(5)-C(6)-C(1)	0.1(11)
C(4)-C(5)-C(6)-C(8)	-178.5(7)
N(1)-C(1)-C(6)-C(5)	178.5(6)
C(2)-C(1)-C(6)-C(5)	-1.2(11)
N(1)-C(1)-C(6)-C(8)	-2.9(10)
C(2)-C(1)-C(6)-C(8)	177.5(7)
O(10)-S(3)-O(9)-Mo(2)	-66.2(6)
O(11)-S(3)-O(9)-Mo(2)	69.7(6)
C(39)-S(3)-O(9)-Mo(2)	178.3(5)
N(2)-Mo(2)-O(9)-S(3)	-112.3(5)
C(27)-Mo(2)-O(9)-S(3)	-12.8(5)
O(2)-Mo(2)-O(9)-S(3)	115.7(5)
O(1)-Mo(2)-O(9)-S(3)	145.8(5)
O(4)-Mo(2)-O(9)-S(3)	67.3(5)
N(1)-Mo(1)-C(9)-C(10)	2.2(10)
O(1)-Mo(1)-C(9)-C(10)	107.0(10)
O(6)-Mo(1)-C(9)-C(10)	-96.9(10)
O(2)-Mo(1)-C(9)-C(10)	164.6(7)
O(3)-Mo(1)-C(9)-C(10)	-173.7(10)
Mo(1)-C(9)-C(10)-C(13)	-118.2(9)

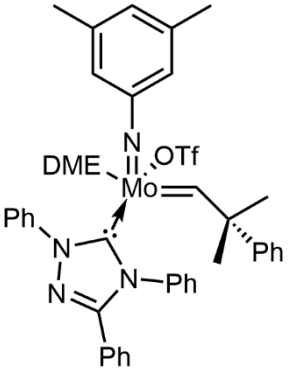
Mo(1)-C(9)-C(10)-C(12)	4.7(13)
Mo(1)-C(9)-C(10)-C(11)	121.3(9)
C(9)-C(10)-C(13)-C(18)	74.2(8)
C(12)-C(10)-C(13)-C(18)	-49.4(9)
C(11)-C(10)-C(13)-C(18)	-169.5(7)
C(9)-C(10)-C(13)-C(14)	-109.2(8)
C(12)-C(10)-C(13)-C(14)	127.2(8)
C(11)-C(10)-C(13)-C(14)	7.1(10)
C(18)-C(13)-C(14)-C(15)	-2.5(12)
C(10)-C(13)-C(14)-C(15)	-179.2(7)
C(13)-C(14)-C(15)-C(16)	1.5(13)
C(14)-C(15)-C(16)-C(17)	-1.0(14)
C(15)-C(16)-C(17)-C(18)	1.6(13)
C(16)-C(17)-C(18)-C(13)	-2.9(13)
C(14)-C(13)-C(18)-C(17)	3.2(11)
C(10)-C(13)-C(18)-C(17)	-180.0(7)
Mo(2)-N(2)-C(19)-C(20)	-86(6)
Mo(2)-N(2)-C(19)-C(24)	89(6)
N(2)-C(19)-C(20)-C(21)	178.8(6)
C(24)-C(19)-C(20)-C(21)	3.8(11)
N(2)-C(19)-C(20)-C(25)	-0.2(11)
C(24)-C(19)-C(20)-C(25)	-175.3(7)
C(19)-C(20)-C(21)-C(22)	-1.9(11)
C(25)-C(20)-C(21)-C(22)	177.1(7)
C(20)-C(21)-C(22)-C(23)	-0.7(12)
C(21)-C(22)-C(23)-C(24)	1.4(13)
C(22)-C(23)-C(24)-C(19)	0.5(11)
C(22)-C(23)-C(24)-C(26)	178.6(7)
N(2)-C(19)-C(24)-C(23)	-178.2(6)
C(20)-C(19)-C(24)-C(23)	-3.1(11)
N(2)-C(19)-C(24)-C(26)	3.6(11)
C(20)-C(19)-C(24)-C(26)	178.8(7)
N(2)-Mo(2)-C(27)-C(28)	7.7(9)
O(2)-Mo(2)-C(27)-C(28)	112.3(8)
O(9)-Mo(2)-C(27)-C(28)	-90.5(8)
O(1)-Mo(2)-C(27)-C(28)	178.0(6)
O(4)-Mo(2)-C(27)-C(28)	-168.7(9)
Mo(2)-C(27)-C(28)-C(31)	151.2(7)
Mo(2)-C(27)-C(28)-C(30)	-86.1(10)
Mo(2)-C(27)-C(28)-C(29)	33.1(11)
C(27)-C(28)-C(31)-C(32)	-60.4(9)
C(30)-C(28)-C(31)-C(32)	179.7(6)
C(29)-C(28)-C(31)-C(32)	59.7(8)
C(27)-C(28)-C(31)-C(36)	119.8(7)
C(30)-C(28)-C(31)-C(36)	-0.2(9)
C(29)-C(28)-C(31)-C(36)	-120.1(8)
C(36)-C(31)-C(32)-C(33)	0.8(10)
C(28)-C(31)-C(32)-C(33)	-179.0(6)
C(31)-C(32)-C(33)-C(34)	-1.2(11)
C(32)-C(33)-C(34)-C(35)	0.5(12)

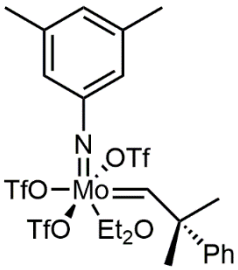
C(33)-C(34)-C(35)-C(36)	0.6(12)
C(34)-C(35)-C(36)-C(31)	-1.0(12)
C(32)-C(31)-C(36)-C(35)	0.3(10)
C(28)-C(31)-C(36)-C(35)	-179.9(6)
O(5)-S(1)-C(37)-F(2)	175.2(5)
O(3)-S(1)-C(37)-F(2)	54.8(6)
O(4)-S(1)-C(37)-F(2)	-64.4(6)
O(5)-S(1)-C(37)-F(3)	-62.1(6)
O(3)-S(1)-C(37)-F(3)	177.4(5)
O(4)-S(1)-C(37)-F(3)	58.2(6)
O(5)-S(1)-C(37)-F(1)	56.6(6)
O(3)-S(1)-C(37)-F(1)	-63.8(6)
O(4)-S(1)-C(37)-F(1)	177.0(5)
O(7)-S(2)-C(38)-F(6)	-55.3(7)
O(8)-S(2)-C(38)-F(6)	179.2(6)
O(6)-S(2)-C(38)-F(6)	62.2(7)
O(7)-S(2)-C(38)-F(5)	-176.6(6)
O(8)-S(2)-C(38)-F(5)	57.8(7)
O(6)-S(2)-C(38)-F(5)	-59.2(6)
O(7)-S(2)-C(38)-F(4)	64.9(7)
O(8)-S(2)-C(38)-F(4)	-60.6(6)
O(6)-S(2)-C(38)-F(4)	-177.6(6)
O(10)-S(3)-C(39)-F(9)	-176.1(8)
O(11)-S(3)-C(39)-F(9)	61.4(9)
O(9)-S(3)-C(39)-F(9)	-53.9(8)
O(10)-S(3)-C(39)-F(8)	56.2(8)
O(11)-S(3)-C(39)-F(8)	-66.3(7)
O(9)-S(3)-C(39)-F(8)	178.4(6)
O(10)-S(3)-C(39)-F(7)	-55.1(8)
O(11)-S(3)-C(39)-F(7)	-177.6(6)
O(9)-S(3)-C(39)-F(7)	67.2(7)
N(5)-N(4)-C(42)-N(3)	0.3(8)
C(50)-N(4)-C(42)-N(3)	176.8(6)
C(43)-N(3)-C(42)-N(4)	-0.4(8)
C(44)-N(3)-C(42)-N(4)	176.9(6)
N(4)-N(5)-C(43)-N(3)	-0.3(8)
N(4)-N(5)-C(43)-C(56)	178.2(6)
C(42)-N(3)-C(43)-N(5)	0.5(8)
C(44)-N(3)-C(43)-N(5)	-176.8(6)
C(42)-N(3)-C(43)-C(56)	-178.1(6)
C(44)-N(3)-C(43)-C(56)	4.7(10)
C(42)-N(3)-C(44)-C(45)	-120.5(8)
C(43)-N(3)-C(44)-C(45)	56.3(9)
C(42)-N(3)-C(44)-C(49)	56.6(9)
C(43)-N(3)-C(44)-C(49)	-126.7(8)
C(49)-C(44)-C(45)-C(46)	2.1(11)
N(3)-C(44)-C(45)-C(46)	179.1(7)
C(44)-C(45)-C(46)-C(47)	-1.5(11)
C(45)-C(46)-C(47)-C(48)	1.0(11)
C(46)-C(47)-C(48)-C(49)	-1.1(12)

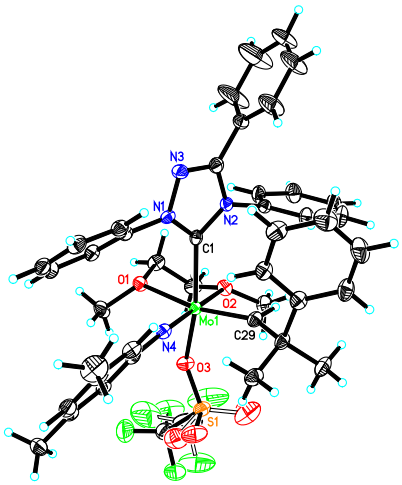
C(47)-C(48)-C(49)-C(44)	1.6(12)
C(45)-C(44)-C(49)-C(48)	-2.1(11)
N(3)-C(44)-C(49)-C(48)	-179.1(7)
C(42)-N(4)-C(50)-C(51)	-33.1(11)
N(5)-N(4)-C(50)-C(51)	143.1(7)
C(42)-N(4)-C(50)-C(55)	144.9(8)
N(5)-N(4)-C(50)-C(55)	-38.9(10)
C(55)-C(50)-C(51)-C(52)	2.2(11)
N(4)-C(50)-C(51)-C(52)	-179.8(7)
C(50)-C(51)-C(52)-C(53)	-1.4(11)
C(51)-C(52)-C(53)-C(54)	0.6(12)
C(52)-C(53)-C(54)-C(55)	-0.7(11)
C(51)-C(50)-C(55)-C(54)	-2.3(11)
N(4)-C(50)-C(55)-C(54)	179.8(6)
C(53)-C(54)-C(55)-C(50)	1.5(10)
N(5)-C(43)-C(56)-C(61)	58.7(11)
N(3)-C(43)-C(56)-C(61)	-122.9(8)
N(5)-C(43)-C(56)-C(57)	-121.2(9)
N(3)-C(43)-C(56)-C(57)	57.1(10)
C(61)-C(56)-C(57)-C(58)	-0.1(12)
C(43)-C(56)-C(57)-C(58)	179.9(7)
C(56)-C(57)-C(58)-C(59)	0.8(12)
C(57)-C(58)-C(59)-C(60)	-0.6(12)
C(58)-C(59)-C(60)-C(61)	-0.4(12)
C(57)-C(56)-C(61)-C(60)	-0.9(12)
C(43)-C(56)-C(61)-C(60)	179.1(8)
C(59)-C(60)-C(61)-C(56)	1.2(12)
C(6X)-C(1X)-C(2X)-C(3X)	1.5(12)
C(7X)-C(1X)-C(2X)-C(3X)	-178.8(7)
C(1X)-C(2X)-C(3X)-C(4X)	-1.0(12)
C(2X)-C(3X)-C(4X)-C(5X)	-0.1(12)
C(3X)-C(4X)-C(5X)-C(6X)	0.7(12)
C(4X)-C(5X)-C(6X)-C(1X)	-0.2(12)
C(2X)-C(1X)-C(6X)-C(5X)	-0.9(12)
C(7X)-C(1X)-C(6X)-C(5X)	179.3(6)

Symmetry transformations used to generate equivalent atoms:

Complex 28


N
OTf
DME
Mo
Ph
N
N
N
Ph
Ph
Ph


N
OTf
TfO
Mo
TfO
Et2O
Ph


N3
N1
N2
C1
O1
O2
Mo1
C29
N4
O3
S1

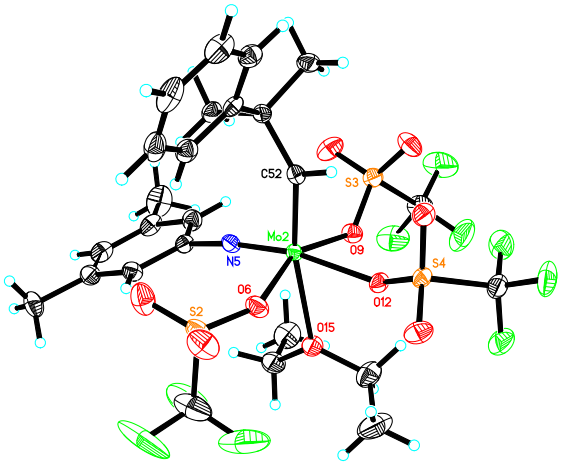

C52
S3
Mo2
O9
N5
S4
O6
O12
S2
O15

Table 28.1. Crystal data and structure refinement for **28**.

Empirical formula	$C_{72}H_{87}F_{12}Mo_2N_5O_{16}S_4$
Formula weight	1826.59
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, *P*-1
Unit cell dimensions	a = 15.7115(9) Å, α = 98.805(3)°
	b = 17.0859(10) Å, β = 110.138(2)°
	c = 19.5275(11) Å, γ = 107.808(3)°
Volume	4485.8(4) $Å^3$
Z, Calculated density	2, 1.352 Mg/m^3
Absorption coefficient	0.457 mm^{-1}
F(000)	1876
Crystal size	0.77 x 0.33 x 0.20 mm
Theta range for data collection	1.98 to 28.31°
Limiting indices	-20<=h<=20, -22<=k<=22, -25<=l<=26
Reflections collected / unique	82675 / 22188 [R(int) = 0.0383]
Completeness to theta = 28.31	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7457 and 0.6623
Refinement method	Full-matrix least-squares on F°
Data / restraints / parameters	22188 / 123 / 1066
Goodness-of-fit on F^2	1.023
Final R indices [I>2σ(I)]	R1 = 0.0444, wR2 = 0.1101
R indices (all data)	R1 = 0.0730, wR2 = 0.1215
Largest diff. peak and hole	1.387 and -0.623 e.$Å^{-3}$

****
REMARK: Disordered solvent electron density (Et_2O) squeezed by PLATON !
****

Table 28.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **28**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	2202(1)	3333(1)	2231(1)	15(1)
N(1)	1327(2)	4603(2)	1430(1)	17(1)
O(1)	3436(1)	3942(1)	1860(1)	20(1)
C(1)	1847(2)	4474(2)	2083(2)	17(1)
O(2)	3626(1)	4143(1)	3313(1)	22(1)
N(2)	2012(2)	5185(2)	2623(1)	18(1)
C(2)	1577(2)	5688(2)	2268(2)	21(1)
N(3)	1146(2)	5346(2)	1536(1)	22(1)
C(3)	952(2)	4102(2)	652(2)	18(1)
N(4)	1308(2)	2632(2)	1372(1)	18(1)
C(4)	-18(2)	3906(2)	176(2)	22(1)
C(5)	-378(2)	3432(2)	-576(2)	26(1)
C(6)	222(2)	3155(2)	-844(2)	27(1)
C(7)	1199(2)	3373(2)	-368(2)	25(1)
C(8)	1577(2)	3867(2)	386(2)	21(1)
C(9)	2514(2)	5404(2)	3444(2)	19(1)
C(10)	3511(2)	5913(2)	3800(2)	26(1)
C(11)	3975(2)	6180(2)	4587(2)	31(1)
C(12)	3438(2)	5929(2)	5006(2)	32(1)
C(13)	2444(2)	5414(2)	4643(2)	31(1)
C(14)	1967(2)	5159(2)	3855(2)	25(1)
C(15)	1639(2)	6526(2)	2666(2)	24(1)
C(16)	2500(4)	7235(3)	2927(3)	76(2)
C(17)	2581(4)	8033(3)	3304(4)	87(2)
C(18)	1773(3)	8111(3)	3386(2)	47(1)
C(19)	931(3)	7410(3)	3143(3)	54(1)
C(20)	855(3)	6612(2)	2775(2)	44(1)
C(21)	729(2)	1995(2)	675(2)	20(1)
C(22)	1145(2)	1486(2)	398(2)	22(1)
C(23)	591(2)	857(2)	-298(2)	26(1)
C(24)	-380(3)	757(2)	-703(2)	32(1)
C(25)	-806(2)	1258(2)	-436(2)	30(1)
C(26)	-242(2)	1888(2)	271(2)	24(1)
C(27)	1032(3)	301(2)	-612(2)	38(1)
C(28)	-1863(3)	1139(3)	-889(2)	45(1)
C(29)	1479(2)	3109(2)	2845(2)	20(1)
C(30)	498(2)	2557(2)	2820(2)	21(1)
C(31)	-76(2)	1751(2)	2138(2)	28(1)
C(32)	719(2)	2271(2)	3554(2)	31(1)
C(33)	-95(2)	3132(2)	2781(2)	24(1)
C(34)	-433(2)	3332(2)	3325(2)	32(1)
C(35)	-947(3)	3868(3)	3270(2)	39(1)

C(36)	-1137(2)	4216(2)	2666(2)	38(1)
C(37)	-817(2)	4014(2)	2110(2)	30(1)
C(38)	-299(2)	3484(2)	2167(2)	24(1)
S(1)	2802(1)	1682(1)	2602(1)	27(1)
O(3)	3010(1)	2514(1)	2420(1)	22(1)
O(4)	1868(4)	1031(4)	2086(4)	44(1)
O(5)	3039(5)	1784(5)	3384(3)	50(2)
C(39)	3690(5)	1356(4)	2386(4)	37(1)
F(1)	4598(4)	1937(3)	2800(4)	65(2)
F(2)	3677(3)	627(3)	2542(2)	47(1)
F(3)	3481(4)	1228(3)	1648(3)	68(1)
O(4A)	2210(6)	974(5)	1948(4)	47(2)
O(5A)	2576(8)	1669(8)	3239(5)	62(3)
C(39A)	4018(6)	1650(5)	2889(5)	55(3)
F(1A)	4682(5)	2276(4)	3511(5)	89(2)
F(2A)	3998(5)	904(4)	3038(5)	75(2)
F(3A)	4323(8)	1738(7)	2327(6)	85(3)
C(40)	3646(2)	3427(2)	1330(2)	28(1)
C(41)	4308(2)	4603(2)	2473(2)	24(1)
C(42)	4512(2)	4320(2)	3175(2)	25(1)
C(43)	3803(2)	3985(2)	4052(2)	29(1)
Mo(2)	6434(1)	7304(1)	2257(1)	15(1)
S(2)	6507(1)	6924(1)	3952(1)	26(1)
S(3)	6412(1)	7565(1)	630(1)	21(1)
S(4)	3890(1)	6218(1)	1459(1)	18(1)
F(4)	7221(2)	8591(1)	4446(1)	70(1)
N(5)	7694(2)	7793(2)	2741(1)	20(1)
F(5)	5716(3)	7965(2)	4280(2)	82(1)
O(6)	6101(2)	6982(1)	3170(1)	25(1)
F(6)	6886(3)	7937(2)	5231(1)	91(1)
F(7)	6679(2)	9155(1)	623(1)	46(1)
O(7)	5816(2)	6271(2)	4090(1)	35(1)
F(8)	6175(2)	8266(2)	-473(1)	57(1)
O(8)	7494(2)	6964(2)	4219(1)	38(1)
O(9)	6307(2)	7834(1)	1351(1)	22(1)
F(9)	5176(2)	8270(2)	60(1)	54(1)
F(10)	3553(1)	6700(1)	217(1)	38(1)
O(10)	5676(2)	6757(1)	128(1)	33(1)
F(11)	2254(1)	5955(1)	326(1)	42(1)
O(11)	7413(2)	7742(2)	753(1)	35(1)
O(12)	4850(1)	6939(1)	1756(1)	20(1)
F(12)	3078(1)	7278(1)	997(1)	39(1)
O(13)	3875(1)	5426(1)	1078(1)	23(1)
O(14)	3444(2)	6191(1)	1989(1)	29(1)
O(15)	6268(2)	8635(1)	2684(1)	24(1)
C(44)	8691(2)	8303(2)	3150(2)	19(1)
C(45)	9136(2)	8416(2)	3935(2)	22(1)
C(46)	10111(2)	8974(2)	4355(2)	25(1)
C(47)	10619(2)	9410(2)	3978(2)	26(1)
C(48)	10191(2)	9296(2)	3195(2)	26(1)

C(49)	9220(2)	8730(2)	2778(2)	25(1)
C(50)	10601(2)	9100(2)	5197(2)	35(1)
C(51)	10767(3)	9755(2)	2796(2)	44(1)
C(52)	6339(2)	6213(2)	1756(1)	17(1)
C(53)	6955(2)	5710(2)	1650(2)	18(1)
C(54)	8061(2)	6267(2)	2015(2)	22(1)
C(55)	6629(2)	5344(2)	790(2)	24(1)
C(56)	6749(2)	5002(2)	2043(2)	19(1)
C(57)	7021(2)	5237(2)	2830(2)	24(1)
C(58)	6861(2)	4622(2)	3206(2)	30(1)
C(59)	6430(2)	3761(2)	2815(2)	34(1)
C(60)	6147(2)	3515(2)	2036(2)	32(1)
C(61)	6298(2)	4131(2)	1650(2)	24(1)
C(62)	6598(4)	7909(3)	4509(2)	50(1)
C(63)	6086(3)	8362(2)	189(2)	33(1)
C(64)	3150(2)	6559(2)	706(2)	26(1)
C(65)	4775(3)	8689(3)	2757(3)	56(1)
C(66)	5408(2)	8820(2)	2324(2)	34(1)
C(67)	7148(2)	9399(2)	3132(2)	30(1)
C(68)	7583(3)	9856(2)	2652(2)	38(1)
O(1X)	1158(2)	7152(2)	5298(2)	44(1)
C(1X)	2167(4)	7378(4)	5556(3)	85(2)
C(2X)	2714(4)	8112(3)	6262(3)	78(2)
C(3X)	560(4)	6423(4)	4675(3)	74(2)
C(4X)	-471(3)	6264(3)	4417(3)	68(1)

Table 28.3. Bond lengths [Å] and angles [°] for **28**.

Mo(1)-N(4)	1.719(2)
Mo(1)-C(29)	1.919(3)
Mo(1)-O(3)	2.1515(19)
Mo(1)-C(1)	2.219(3)
Mo(1)-O(1)	2.3092(18)
Mo(1)-O(2)	2.3107(19)
N(1)-C(1)	1.350(3)
N(1)-N(3)	1.383(3)
N(1)-C(3)	1.437(3)
O(1)-C(40)	1.445(3)
O(1)-C(41)	1.448(3)
C(1)-N(2)	1.370(3)
O(2)-C(42)	1.459(3)
O(2)-C(43)	1.458(3)
N(2)-C(2)	1.380(4)
N(2)-C(9)	1.450(3)
C(2)-N(3)	1.296(4)
C(2)-C(15)	1.478(4)
C(3)-C(4)	1.384(4)
C(3)-C(8)	1.387(4)
N(4)-C(21)	1.397(3)

C(4)-C(5)	1.385(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.387(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.386(4)
C(6)-H(6)	0.9500
C(7)-C(8)	1.394(4)
C(7)-H(7)	0.9500
C(8)-H(8)	0.9500
C(9)-C(14)	1.384(4)
C(9)-C(10)	1.388(4)
C(10)-C(11)	1.383(4)
C(10)-H(10)	0.9500
C(11)-C(12)	1.389(4)
C(11)-H(11)	0.9500
C(12)-C(13)	1.386(5)
C(12)-H(12)	0.9500
C(13)-C(14)	1.386(4)
C(13)-H(13)	0.9500
C(14)-H(14)	0.9500
C(15)-C(20)	1.365(4)
C(15)-C(16)	1.375(5)
C(16)-C(17)	1.392(6)
C(16)-H(16)	0.9500
C(17)-C(18)	1.375(6)
C(17)-H(17)	0.9500
C(18)-C(19)	1.355(6)
C(18)-H(18)	0.9500
C(19)-C(20)	1.390(5)
C(19)-H(19)	0.9500
C(20)-H(20)	0.9500
C(21)-C(22)	1.386(4)
C(21)-C(26)	1.394(4)
C(22)-C(23)	1.388(4)
C(22)-H(22)	0.9500
C(23)-C(24)	1.396(5)
C(23)-C(27)	1.508(5)
C(24)-C(25)	1.381(5)
C(24)-H(24)	0.9500
C(25)-C(26)	1.402(4)
C(25)-C(28)	1.519(5)
C(26)-H(26)	0.9500
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-C(30)	1.521(4)
C(29)-H(29)	0.9500

C(30)-C(31)	1.528(4)
C(30)-C(33)	1.541(4)
C(30)-C(32)	1.544(4)
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(34)	1.383(4)
C(33)-C(38)	1.406(4)
C(34)-C(35)	1.387(5)
C(34)-H(34)	0.9500
C(35)-C(36)	1.384(5)
C(35)-H(35)	0.9500
C(36)-C(37)	1.383(5)
C(36)-H(36)	0.9500
C(37)-C(38)	1.384(4)
C(37)-H(37)	0.9500
C(38)-H(38)	0.9500
S(1)-O(5A)	1.407(8)
S(1)-O(4A)	1.408(7)
S(1)-O(5)	1.410(5)
S(1)-O(4)	1.431(5)
S(1)-O(3)	1.485(2)
S(1)-C(39)	1.802(6)
S(1)-C(39A)	1.818(8)
C(39)-F(2)	1.323(7)
C(39)-F(3)	1.328(8)
C(39)-F(1)	1.330(8)
C(39A)-F(1A)	1.326(8)
C(39A)-F(2A)	1.343(8)
C(39A)-F(3A)	1.350(9)
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(41)-C(42)	1.487(4)
C(41)-H(41A)	0.9900
C(41)-H(41B)	0.9900
C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
Mo(2)-N(5)	1.723(2)
Mo(2)-C(52)	1.904(3)
Mo(2)-O(9)	2.0855(19)
Mo(2)-O(6)	2.1267(19)
Mo(2)-O(12)	2.1742(19)
Mo(2)-O(15)	2.422(2)

S(2)-O(8)	1.431(2)
S(2)-O(7)	1.431(2)
S(2)-O(6)	1.470(2)
S(2)-C(62)	1.794(4)
S(3)-O(10)	1.426(2)
S(3)-O(11)	1.433(2)
S(3)-O(9)	1.492(2)
S(3)-C(63)	1.829(3)
S(4)-O(13)	1.430(2)
S(4)-O(14)	1.434(2)
S(4)-O(12)	1.474(2)
S(4)-C(64)	1.832(3)
F(4)-C(62)	1.328(5)
N(5)-C(44)	1.394(3)
F(5)-C(62)	1.340(5)
F(6)-C(62)	1.312(4)
F(7)-C(63)	1.325(4)
F(8)-C(63)	1.337(4)
F(9)-C(63)	1.317(4)
F(10)-C(64)	1.330(4)
F(11)-C(64)	1.324(4)
F(12)-C(64)	1.326(4)
O(15)-C(67)	1.448(4)
O(15)-C(66)	1.448(4)
C(44)-C(49)	1.398(4)
C(44)-C(45)	1.402(4)
C(45)-C(46)	1.389(4)
C(45)-H(45)	0.9500
C(46)-C(47)	1.393(4)
C(46)-C(50)	1.503(4)
C(47)-C(48)	1.397(4)
C(47)-H(47)	0.9500
C(48)-C(49)	1.388(4)
C(48)-C(51)	1.510(4)
C(49)-H(49)	0.9500
C(50)-H(50A)	0.9800
C(50)-H(50B)	0.9800
C(50)-H(50C)	0.9800
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800
C(52)-C(53)	1.520(4)
C(52)-H(52)	0.9500
C(53)-C(54)	1.536(4)
C(53)-C(55)	1.537(4)
C(53)-C(56)	1.542(4)
C(54)-H(54A)	0.9800
C(54)-H(54B)	0.9800
C(54)-H(54C)	0.9800
C(55)-H(55A)	0.9800

C(55)-H(55B)	0.9800
C(55)-H(55C)	0.9800
C(56)-C(61)	1.392(4)
C(56)-C(57)	1.400(4)
C(57)-C(58)	1.381(4)
C(57)-H(57)	0.9500
C(58)-C(59)	1.377(5)
C(58)-H(58)	0.9500
C(59)-C(60)	1.383(5)
C(59)-H(59)	0.9500
C(60)-C(61)	1.394(4)
C(60)-H(60)	0.9500
C(61)-H(61)	0.9500
C(65)-C(66)	1.503(5)
C(65)-H(65A)	0.9800
C(65)-H(65B)	0.9800
C(65)-H(65C)	0.9800
C(66)-H(66A)	0.9900
C(66)-H(66B)	0.9900
C(67)-C(68)	1.515(5)
C(67)-H(67A)	0.9900
C(67)-H(67B)	0.9900
C(68)-H(68A)	0.9800
C(68)-H(68B)	0.9800
C(68)-H(68C)	0.9800
O(1X)-C(1X)	1.390(5)
O(1X)-C(3X)	1.395(5)
C(1X)-C(2X)	1.486(7)
C(1X)-H(1X1)	0.9900
C(1X)-H(1X2)	0.9900
C(2X)-H(2X1)	0.9800
C(2X)-H(2X2)	0.9800
C(2X)-H(2X3)	0.9800
C(3X)-C(4X)	1.442(6)
C(3X)-H(3X1)	0.9900
C(3X)-H(3X2)	0.9900
C(4X)-H(4X1)	0.9800
C(4X)-H(4X2)	0.9800
C(4X)-H(4X3)	0.9800

N(4)-Mo(1)-C(29)	98.59(11)
N(4)-Mo(1)-O(3)	93.77(9)
C(29)-Mo(1)-O(3)	102.64(10)
N(4)-Mo(1)-C(1)	96.75(10)
C(29)-Mo(1)-C(1)	91.43(11)
O(3)-Mo(1)-C(1)	160.98(9)
N(4)-Mo(1)-O(1)	100.05(9)
C(29)-Mo(1)-O(1)	161.25(10)
O(3)-Mo(1)-O(1)	78.14(7)
C(1)-Mo(1)-O(1)	84.44(8)

N(4)-Mo(1)-O(2)	167.18(9)
C(29)-Mo(1)-O(2)	90.32(10)
O(3)-Mo(1)-O(2)	75.20(7)
C(1)-Mo(1)-O(2)	92.20(8)
O(1)-Mo(1)-O(2)	71.63(7)
C(1)-N(1)-N(3)	114.0(2)
C(1)-N(1)-C(3)	130.3(2)
N(3)-N(1)-C(3)	115.8(2)
C(40)-O(1)-C(41)	113.5(2)
C(40)-O(1)-Mo(1)	121.22(16)
C(41)-O(1)-Mo(1)	113.55(15)
N(1)-C(1)-N(2)	102.2(2)
N(1)-C(1)-Mo(1)	128.01(19)
N(2)-C(1)-Mo(1)	129.55(18)
C(42)-O(2)-C(43)	110.3(2)
C(42)-O(2)-Mo(1)	113.12(16)
C(43)-O(2)-Mo(1)	122.96(17)
C(1)-N(2)-C(2)	109.2(2)
C(1)-N(2)-C(9)	128.7(2)
C(2)-N(2)-C(9)	122.1(2)
N(3)-C(2)-N(2)	110.8(3)
N(3)-C(2)-C(15)	124.7(3)
N(2)-C(2)-C(15)	124.5(3)
C(2)-N(3)-N(1)	103.9(2)
C(4)-C(3)-C(8)	121.7(3)
C(4)-C(3)-N(1)	118.5(2)
C(8)-C(3)-N(1)	119.7(2)
C(21)-N(4)-Mo(1)	168.1(2)
C(3)-C(4)-C(5)	118.6(3)
C(3)-C(4)-H(4)	120.7
C(5)-C(4)-H(4)	120.7
C(4)-C(5)-C(6)	120.5(3)
C(4)-C(5)-H(5)	119.7
C(6)-C(5)-H(5)	119.7
C(7)-C(6)-C(5)	120.3(3)
C(7)-C(6)-H(6)	119.8
C(5)-C(6)-H(6)	119.8
C(6)-C(7)-C(8)	119.7(3)
C(6)-C(7)-H(7)	120.1
C(8)-C(7)-H(7)	120.1
C(3)-C(8)-C(7)	119.0(3)
C(3)-C(8)-H(8)	120.5
C(7)-C(8)-H(8)	120.5
C(14)-C(9)-C(10)	121.9(3)
C(14)-C(9)-N(2)	118.8(3)
C(10)-C(9)-N(2)	119.1(2)
C(11)-C(10)-C(9)	119.2(3)
C(11)-C(10)-H(10)	120.4
C(9)-C(10)-H(10)	120.4
C(10)-C(11)-C(12)	119.5(3)

C(10)-C(11)-H(11)	120.3
C(12)-C(11)-H(11)	120.3
C(13)-C(12)-C(11)	120.7(3)
C(13)-C(12)-H(12)	119.7
C(11)-C(12)-H(12)	119.7
C(14)-C(13)-C(12)	120.3(3)
C(14)-C(13)-H(13)	119.8
C(12)-C(13)-H(13)	119.8
C(13)-C(14)-C(9)	118.4(3)
C(13)-C(14)-H(14)	120.8
C(9)-C(14)-H(14)	120.8
C(20)-C(15)-C(16)	119.3(3)
C(20)-C(15)-C(2)	121.3(3)
C(16)-C(15)-C(2)	119.4(3)
C(15)-C(16)-C(17)	120.8(4)
C(15)-C(16)-H(16)	119.6
C(17)-C(16)-H(16)	119.6
C(18)-C(17)-C(16)	119.0(5)
C(18)-C(17)-H(17)	120.5
C(16)-C(17)-H(17)	120.5
C(19)-C(18)-C(17)	120.2(4)
C(19)-C(18)-H(18)	119.9
C(17)-C(18)-H(18)	119.9
C(18)-C(19)-C(20)	120.6(3)
C(18)-C(19)-H(19)	119.7
C(20)-C(19)-H(19)	119.7
C(15)-C(20)-C(19)	120.0(3)
C(15)-C(20)-H(20)	120.0
C(19)-C(20)-H(20)	120.0
C(22)-C(21)-C(26)	121.4(3)
C(22)-C(21)-N(4)	118.7(2)
C(26)-C(21)-N(4)	119.9(3)
C(21)-C(22)-C(23)	119.9(3)
C(21)-C(22)-H(22)	120.0
C(23)-C(22)-H(22)	120.0
C(22)-C(23)-C(24)	118.4(3)
C(22)-C(23)-C(27)	120.7(3)
C(24)-C(23)-C(27)	120.9(3)
C(25)-C(24)-C(23)	122.5(3)
C(25)-C(24)-H(24)	118.7
C(23)-C(24)-H(24)	118.7
C(24)-C(25)-C(26)	118.7(3)
C(24)-C(25)-C(28)	121.5(3)
C(26)-C(25)-C(28)	119.9(3)
C(21)-C(26)-C(25)	119.2(3)
C(21)-C(26)-H(26)	120.4
C(25)-C(26)-H(26)	120.4
C(23)-C(27)-H(27A)	109.5
C(23)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5

C(23)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(25)-C(28)-H(28A)	109.5
C(25)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(25)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(30)-C(29)-Mo(1)	143.1(2)
C(30)-C(29)-H(29)	108.5
Mo(1)-C(29)-H(29)	108.5
C(29)-C(30)-C(31)	113.2(2)
C(29)-C(30)-C(33)	106.0(2)
C(31)-C(30)-C(33)	109.8(2)
C(29)-C(30)-C(32)	107.3(2)
C(31)-C(30)-C(32)	108.1(2)
C(33)-C(30)-C(32)	112.4(2)
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(34)-C(33)-C(38)	117.7(3)
C(34)-C(33)-C(30)	123.5(3)
C(38)-C(33)-C(30)	118.8(3)
C(33)-C(34)-C(35)	121.1(3)
C(33)-C(34)-H(34)	119.4
C(35)-C(34)-H(34)	119.4
C(36)-C(35)-C(34)	120.7(3)
C(36)-C(35)-H(35)	119.6
C(34)-C(35)-H(35)	119.6
C(37)-C(36)-C(35)	119.0(3)
C(37)-C(36)-H(36)	120.5
C(35)-C(36)-H(36)	120.5
C(38)-C(37)-C(36)	120.3(3)
C(38)-C(37)-H(37)	119.8
C(36)-C(37)-H(37)	119.8
C(37)-C(38)-C(33)	121.1(3)
C(37)-C(38)-H(38)	119.4
C(33)-C(38)-H(38)	119.4
O(5A)-S(1)-O(4A)	117.0(6)
O(5A)-S(1)-O(5)	26.0(5)

O(4A)-S(1)-O(5)	132.9(5)
O(5A)-S(1)-O(4)	93.5(5)
O(4A)-S(1)-O(4)	28.7(3)
O(5)-S(1)-O(4)	116.1(4)
O(5A)-S(1)-O(3)	115.2(5)
O(4A)-S(1)-O(3)	112.6(4)
O(5)-S(1)-O(3)	112.5(3)
O(4)-S(1)-O(3)	113.9(3)
O(5A)-S(1)-C(39)	129.2(5)
O(4A)-S(1)-C(39)	77.1(4)
O(5)-S(1)-C(39)	107.7(4)
O(4)-S(1)-C(39)	104.9(3)
O(3)-S(1)-C(39)	99.8(2)
O(5A)-S(1)-C(39A)	106.1(5)
O(4A)-S(1)-C(39A)	104.1(5)
O(5)-S(1)-C(39A)	81.4(4)
O(4)-S(1)-C(39A)	129.3(4)
O(3)-S(1)-C(39A)	99.2(3)
C(39)-S(1)-C(39A)	29.0(3)
S(1)-O(3)-Mo(1)	132.52(12)
F(2)-C(39)-F(3)	107.4(5)
F(2)-C(39)-F(1)	106.7(5)
F(3)-C(39)-F(1)	110.3(6)
F(2)-C(39)-S(1)	111.2(4)
F(3)-C(39)-S(1)	110.0(5)
F(1)-C(39)-S(1)	111.2(5)
F(1A)-C(39A)-F(2A)	107.2(7)
F(1A)-C(39A)-F(3A)	107.3(9)
F(2A)-C(39A)-F(3A)	110.0(8)
F(1A)-C(39A)-S(1)	112.6(6)
F(2A)-C(39A)-S(1)	110.2(6)
F(3A)-C(39A)-S(1)	109.5(7)
O(1)-C(40)-H(40A)	109.5
O(1)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
O(1)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
O(1)-C(41)-C(42)	108.9(2)
O(1)-C(41)-H(41A)	109.9
C(42)-C(41)-H(41A)	109.9
O(1)-C(41)-H(41B)	109.9
C(42)-C(41)-H(41B)	109.9
H(41A)-C(41)-H(41B)	108.3
O(2)-C(42)-C(41)	106.1(2)
O(2)-C(42)-H(42A)	110.5
C(41)-C(42)-H(42A)	110.5
O(2)-C(42)-H(42B)	110.5
C(41)-C(42)-H(42B)	110.5
H(42A)-C(42)-H(42B)	108.7

O(2)-C(43)-H(43A)	109.5
O(2)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
O(2)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
N(5)-Mo(2)-C(52)	98.75(11)
N(5)-Mo(2)-O(9)	97.02(9)
C(52)-Mo(2)-O(9)	97.63(9)
N(5)-Mo(2)-O(6)	98.46(9)
C(52)-Mo(2)-O(6)	98.83(10)
O(9)-Mo(2)-O(6)	155.35(8)
N(5)-Mo(2)-O(12)	168.22(9)
C(52)-Mo(2)-O(12)	93.03(10)
O(9)-Mo(2)-O(12)	81.16(8)
O(6)-Mo(2)-O(12)	79.76(8)
N(5)-Mo(2)-O(15)	90.79(9)
C(52)-Mo(2)-O(15)	169.05(9)
O(9)-Mo(2)-O(15)	75.74(7)
O(6)-Mo(2)-O(15)	84.97(8)
O(12)-Mo(2)-O(15)	77.46(7)
O(8)-S(2)-O(7)	117.01(15)
O(8)-S(2)-O(6)	114.54(13)
O(7)-S(2)-O(6)	112.04(13)
O(8)-S(2)-C(62)	104.7(2)
O(7)-S(2)-C(62)	103.99(18)
O(6)-S(2)-C(62)	102.48(16)
O(10)-S(3)-O(11)	118.56(15)
O(10)-S(3)-O(9)	113.86(13)
O(11)-S(3)-O(9)	112.57(13)
O(10)-S(3)-C(63)	104.93(15)
O(11)-S(3)-C(63)	105.72(15)
O(9)-S(3)-C(63)	98.36(13)
O(13)-S(4)-O(14)	117.47(13)
O(13)-S(4)-O(12)	113.78(12)
O(14)-S(4)-O(12)	112.68(13)
O(13)-S(4)-C(64)	105.30(13)
O(14)-S(4)-C(64)	104.72(14)
O(12)-S(4)-C(64)	100.60(13)
C(44)-N(5)-Mo(2)	171.5(2)
S(2)-O(6)-Mo(2)	145.38(13)
S(3)-O(9)-Mo(2)	131.01(12)
S(4)-O(12)-Mo(2)	144.80(12)
C(67)-O(15)-C(66)	113.2(2)
C(67)-O(15)-Mo(2)	118.86(18)
C(66)-O(15)-Mo(2)	124.34(18)
N(5)-C(44)-C(49)	119.4(3)
N(5)-C(44)-C(45)	119.5(2)
C(49)-C(44)-C(45)	121.0(3)
C(46)-C(45)-C(44)	119.7(3)

C(46)-C(45)-H(45)	120.2
C(44)-C(45)-H(45)	120.2
C(45)-C(46)-C(47)	118.5(3)
C(45)-C(46)-C(50)	120.4(3)
C(47)-C(46)-C(50)	121.1(3)
C(46)-C(47)-C(48)	122.5(3)
C(46)-C(47)-H(47)	118.8
C(48)-C(47)-H(47)	118.8
C(49)-C(48)-C(47)	118.6(3)
C(49)-C(48)-C(51)	119.9(3)
C(47)-C(48)-C(51)	121.5(3)
C(48)-C(49)-C(44)	119.7(3)
C(48)-C(49)-H(49)	120.2
C(44)-C(49)-H(49)	120.2
C(46)-C(50)-H(50A)	109.5
C(46)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
C(46)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
C(48)-C(51)-H(51A)	109.5
C(48)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(48)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(53)-C(52)-Mo(2)	142.7(2)
C(53)-C(52)-H(52)	108.7
Mo(2)-C(52)-H(52)	108.7
C(52)-C(53)-C(54)	112.7(2)
C(52)-C(53)-C(55)	108.0(2)
C(54)-C(53)-C(55)	108.7(2)
C(52)-C(53)-C(56)	105.4(2)
C(54)-C(53)-C(56)	109.5(2)
C(55)-C(53)-C(56)	112.5(2)
C(53)-C(54)-H(54A)	109.5
C(53)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(53)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
C(53)-C(55)-H(55A)	109.5
C(53)-C(55)-H(55B)	109.5
H(55A)-C(55)-H(55B)	109.5
C(53)-C(55)-H(55C)	109.5
H(55A)-C(55)-H(55C)	109.5
H(55B)-C(55)-H(55C)	109.5
C(61)-C(56)-C(57)	118.0(3)
C(61)-C(56)-C(53)	122.9(3)
C(57)-C(56)-C(53)	119.1(3)

C(58)-C(57)-C(56)	120.9(3)
C(58)-C(57)-H(57)	119.5
C(56)-C(57)-H(57)	119.5
C(59)-C(58)-C(57)	120.8(3)
C(59)-C(58)-H(58)	119.6
C(57)-C(58)-H(58)	119.6
C(58)-C(59)-C(60)	119.2(3)
C(58)-C(59)-H(59)	120.4
C(60)-C(59)-H(59)	120.4
C(59)-C(60)-C(61)	120.5(3)
C(59)-C(60)-H(60)	119.7
C(61)-C(60)-H(60)	119.7
C(56)-C(61)-C(60)	120.6(3)
C(56)-C(61)-H(61)	119.7
C(60)-C(61)-H(61)	119.7
F(6)-C(62)-F(4)	108.7(4)
F(6)-C(62)-F(5)	107.3(4)
F(4)-C(62)-F(5)	108.0(4)
F(6)-C(62)-S(2)	110.8(3)
F(4)-C(62)-S(2)	111.9(3)
F(5)-C(62)-S(2)	110.1(3)
F(9)-C(63)-F(7)	108.4(3)
F(9)-C(63)-F(8)	109.1(3)
F(7)-C(63)-F(8)	107.6(3)
F(9)-C(63)-S(3)	111.1(2)
F(7)-C(63)-S(3)	111.5(2)
F(8)-C(63)-S(3)	109.0(2)
F(11)-C(64)-F(12)	108.6(2)
F(11)-C(64)-F(10)	108.3(3)
F(12)-C(64)-F(10)	108.1(3)
F(11)-C(64)-S(4)	110.1(2)
F(12)-C(64)-S(4)	110.9(2)
F(10)-C(64)-S(4)	110.7(2)
C(66)-C(65)-H(65A)	109.5
C(66)-C(65)-H(65B)	109.5
H(65A)-C(65)-H(65B)	109.5
C(66)-C(65)-H(65C)	109.5
H(65A)-C(65)-H(65C)	109.5
H(65B)-C(65)-H(65C)	109.5
O(15)-C(66)-C(65)	110.7(3)
O(15)-C(66)-H(66A)	109.5
C(65)-C(66)-H(66A)	109.5
O(15)-C(66)-H(66B)	109.5
C(65)-C(66)-H(66B)	109.5
H(66A)-C(66)-H(66B)	108.1
O(15)-C(67)-C(68)	113.3(3)
O(15)-C(67)-H(67A)	108.9
C(68)-C(67)-H(67A)	108.9
O(15)-C(67)-H(67B)	108.9
C(68)-C(67)-H(67B)	108.9

H(67A)-C(67)-H(67B)	107.7
C(67)-C(68)-H(68A)	109.5
C(67)-C(68)-H(68B)	109.5
H(68A)-C(68)-H(68B)	109.5
C(67)-C(68)-H(68C)	109.5
H(68A)-C(68)-H(68C)	109.5
H(68B)-C(68)-H(68C)	109.5
C(1X)-O(1X)-C(3X)	116.8(4)
O(1X)-C(1X)-C(2X)	111.4(4)
O(1X)-C(1X)-H(1X1)	109.4
C(2X)-C(1X)-H(1X1)	109.4
O(1X)-C(1X)-H(1X2)	109.4
C(2X)-C(1X)-H(1X2)	109.4
H(1X1)-C(1X)-H(1X2)	108.0
C(1X)-C(2X)-H(2X1)	109.5
C(1X)-C(2X)-H(2X2)	109.5
H(2X1)-C(2X)-H(2X2)	109.5
C(1X)-C(2X)-H(2X3)	109.5
H(2X1)-C(2X)-H(2X3)	109.5
H(2X2)-C(2X)-H(2X3)	109.5
O(1X)-C(3X)-C(4X)	113.2(4)
O(1X)-C(3X)-H(3X1)	108.9
C(4X)-C(3X)-H(3X1)	108.9
O(1X)-C(3X)-H(3X2)	108.9
C(4X)-C(3X)-H(3X2)	108.9
H(3X1)-C(3X)-H(3X2)	107.8
C(3X)-C(4X)-H(4X1)	109.5
C(3X)-C(4X)-H(4X2)	109.5
H(4X1)-C(4X)-H(4X2)	109.5
C(3X)-C(4X)-H(4X3)	109.5
H(4X1)-C(4X)-H(4X3)	109.5
H(4X2)-C(4X)-H(4X3)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 28.4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **28**.The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11}+ ... + 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	13(1)	17(1)	17(1)	6(1)	7(1)	6(1)
N(1)	16(1)	17(1)	21(1)	9(1)	10(1)	7(1)
O(1)	17(1)	20(1)	24(1)	5(1)	11(1)	6(1)
C(1)	14(1)	20(1)	16(1)	6(1)	8(1)	5(1)
O(2)	18(1)	23(1)	22(1)	4(1)	7(1)	7(1)
N(2)	21(1)	20(1)	19(1)	8(1)	12(1)	11(1)
C(2)	22(1)	25(2)	26(2)	11(1)	15(1)	13(1)
N(3)	24(1)	21(1)	25(1)	9(1)	12(1)	13(1)

C(3)	22(1)	17(1)	16(1)	7(1)	8(1)	7(1)
N(4)	14(1)	21(1)	22(1)	9(1)	9(1)	8(1)
C(4)	22(1)	24(2)	24(1)	11(1)	10(1)	12(1)
C(5)	24(2)	29(2)	22(1)	11(1)	4(1)	9(1)
C(6)	35(2)	22(2)	18(1)	8(1)	9(1)	7(1)
C(7)	30(2)	24(2)	25(2)	10(1)	16(1)	9(1)
C(8)	20(1)	24(2)	20(1)	9(1)	8(1)	9(1)
C(9)	25(2)	20(1)	16(1)	7(1)	9(1)	12(1)
C(10)	26(2)	27(2)	24(2)	7(1)	15(1)	6(1)
C(11)	27(2)	35(2)	24(2)	3(1)	9(1)	8(1)
C(12)	37(2)	41(2)	17(1)	6(1)	10(1)	16(2)
C(13)	29(2)	46(2)	25(2)	15(2)	17(1)	16(2)
C(14)	20(1)	33(2)	25(2)	9(1)	12(1)	10(1)
C(15)	29(2)	27(2)	26(2)	11(1)	14(1)	18(1)
C(16)	65(3)	35(2)	143(4)	-1(2)	75(3)	16(2)
C(17)	73(3)	40(2)	151(5)	-6(3)	69(3)	17(2)
C(18)	50(2)	34(2)	60(3)	-1(2)	24(2)	25(2)
C(19)	45(2)	46(2)	77(3)	-1(2)	34(2)	27(2)
C(20)	30(2)	34(2)	66(3)	-3(2)	23(2)	12(2)
C(21)	19(1)	19(1)	17(1)	8(1)	6(1)	2(1)
C(22)	24(2)	18(1)	23(1)	9(1)	12(1)	4(1)
C(23)	36(2)	15(1)	23(2)	6(1)	15(1)	1(1)
C(24)	40(2)	20(2)	19(1)	3(1)	7(1)	-5(1)
C(25)	24(2)	27(2)	25(2)	11(1)	2(1)	0(1)
C(26)	20(1)	24(2)	28(2)	13(1)	9(1)	8(1)
C(27)	54(2)	23(2)	36(2)	3(1)	29(2)	7(2)
C(28)	26(2)	44(2)	37(2)	7(2)	-4(2)	-3(2)
C(29)	19(1)	24(2)	21(1)	10(1)	8(1)	10(1)
C(30)	19(1)	26(2)	26(1)	13(1)	13(1)	10(1)
C(31)	24(2)	26(2)	38(2)	13(1)	17(1)	7(1)
C(32)	33(2)	40(2)	35(2)	23(2)	21(2)	18(2)
C(33)	16(1)	28(2)	28(2)	9(1)	10(1)	7(1)
C(34)	27(2)	44(2)	33(2)	16(2)	19(1)	15(2)
C(35)	32(2)	55(2)	42(2)	13(2)	23(2)	24(2)
C(36)	28(2)	44(2)	49(2)	14(2)	18(2)	21(2)
C(37)	22(2)	35(2)	38(2)	17(2)	13(1)	14(1)
C(38)	18(1)	30(2)	27(2)	11(1)	11(1)	11(1)
S(1)	30(1)	23(1)	29(1)	12(1)	13(1)	12(1)
O(3)	18(1)	20(1)	31(1)	9(1)	11(1)	8(1)
O(4)	36(3)	27(2)	60(3)	14(2)	17(2)	4(2)
O(5)	86(4)	48(3)	28(2)	18(2)	27(3)	35(3)
C(39)	43(3)	35(3)	49(3)	19(3)	26(3)	23(3)
F(1)	35(2)	53(3)	122(5)	40(3)	33(3)	30(2)
F(2)	73(3)	41(2)	52(2)	25(2)	31(2)	42(2)
F(3)	128(4)	71(3)	64(2)	41(2)	69(3)	70(3)
O(4A)	50(5)	35(4)	33(4)	5(3)	2(3)	8(4)
O(5A)	70(6)	58(5)	66(5)	38(4)	30(4)	23(4)
C(39A)	45(5)	35(5)	77(6)	20(5)	12(4)	18(4)
F(1A)	47(3)	55(4)	114(5)	36(4)	-23(3)	13(3)
F(2A)	61(4)	50(4)	103(5)	29(4)	4(4)	38(3)

F(3A)	76(5)	83(5)	130(6)	27(5)	61(5)	54(4)
C(40)	26(2)	27(2)	36(2)	5(1)	21(1)	10(1)
C(41)	14(1)	24(2)	26(2)	7(1)	5(1)	3(1)
C(42)	16(1)	25(2)	29(2)	9(1)	5(1)	7(1)
C(43)	26(2)	34(2)	20(1)	4(1)	5(1)	10(1)
Mo(2)	13(1)	16(1)	15(1)	2(1)	6(1)	4(1)
S(2)	27(1)	27(1)	19(1)	4(1)	11(1)	3(1)
S(3)	25(1)	23(1)	21(1)	9(1)	12(1)	12(1)
S(4)	14(1)	19(1)	22(1)	6(1)	9(1)	7(1)
F(4)	112(2)	29(1)	48(1)	3(1)	36(2)	3(1)
N(5)	21(1)	20(1)	16(1)	3(1)	7(1)	7(1)
F(5)	130(3)	76(2)	92(2)	26(2)	80(2)	67(2)
O(6)	24(1)	31(1)	18(1)	4(1)	11(1)	8(1)
F(6)	181(3)	58(2)	31(1)	6(1)	54(2)	32(2)
F(7)	72(2)	30(1)	54(1)	24(1)	36(1)	26(1)
O(7)	37(1)	35(1)	32(1)	10(1)	20(1)	4(1)
F(8)	108(2)	63(2)	35(1)	33(1)	44(1)	53(2)
O(8)	27(1)	51(2)	29(1)	14(1)	9(1)	7(1)
O(9)	26(1)	22(1)	20(1)	8(1)	12(1)	10(1)
F(9)	49(1)	73(2)	59(1)	35(1)	20(1)	43(1)
F(10)	41(1)	51(1)	28(1)	21(1)	14(1)	22(1)
O(10)	39(1)	27(1)	22(1)	0(1)	7(1)	8(1)
F(11)	20(1)	41(1)	46(1)	9(1)	-3(1)	9(1)
O(11)	34(1)	39(1)	48(1)	21(1)	26(1)	21(1)
O(12)	14(1)	18(1)	24(1)	3(1)	7(1)	5(1)
F(12)	38(1)	36(1)	47(1)	12(1)	13(1)	25(1)
O(13)	18(1)	18(1)	28(1)	4(1)	8(1)	5(1)
O(14)	29(1)	35(1)	35(1)	13(1)	23(1)	14(1)
O(15)	23(1)	16(1)	27(1)	1(1)	6(1)	7(1)
C(44)	13(1)	15(1)	22(1)	2(1)	6(1)	3(1)
C(45)	20(1)	21(1)	21(1)	4(1)	9(1)	5(1)
C(46)	22(2)	21(2)	25(2)	-1(1)	4(1)	7(1)
C(47)	17(1)	17(1)	37(2)	2(1)	9(1)	3(1)
C(48)	20(1)	21(2)	38(2)	11(1)	14(1)	7(1)
C(49)	26(2)	27(2)	24(2)	10(1)	10(1)	11(1)
C(50)	27(2)	40(2)	21(2)	0(1)	-1(1)	9(2)
C(51)	30(2)	44(2)	58(2)	28(2)	21(2)	6(2)
C(52)	16(1)	18(1)	15(1)	6(1)	7(1)	4(1)
C(53)	17(1)	22(1)	16(1)	5(1)	8(1)	8(1)
C(54)	15(1)	25(2)	26(1)	6(1)	9(1)	8(1)
C(55)	29(2)	31(2)	21(1)	8(1)	15(1)	16(1)
C(56)	14(1)	21(1)	26(1)	9(1)	10(1)	9(1)
C(57)	19(1)	28(2)	26(2)	9(1)	11(1)	10(1)
C(58)	23(2)	49(2)	28(2)	19(2)	13(1)	18(2)
C(59)	22(2)	39(2)	51(2)	29(2)	19(2)	14(2)
C(60)	24(2)	23(2)	50(2)	13(2)	15(2)	8(1)
C(61)	20(1)	23(2)	30(2)	7(1)	11(1)	8(1)
C(62)	85(3)	36(2)	36(2)	9(2)	33(2)	24(2)
C(63)	50(2)	35(2)	29(2)	18(2)	22(2)	25(2)
C(64)	22(2)	29(2)	28(2)	9(1)	8(1)	12(1)

C(65)	41(2)	51(3)	77(3)	3(2)	30(2)	23(2)
C(66)	28(2)	22(2)	48(2)	9(2)	13(2)	11(1)
C(67)	31(2)	20(2)	31(2)	-1(1)	9(1)	7(1)
C(68)	35(2)	25(2)	50(2)	11(2)	17(2)	7(2)
O(1X)	38(1)	48(2)	45(1)	8(1)	17(1)	20(1)
C(1X)	54(3)	105(4)	81(3)	-1(3)	29(3)	26(3)
C(2X)	54(3)	58(3)	102(4)	6(3)	19(3)	21(2)
C(3X)	62(3)	95(4)	47(2)	-15(2)	19(2)	27(3)
C(4X)	47(2)	75(3)	56(3)	-8(2)	6(2)	22(2)

Table 28.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **28**.

	x	y	z	U(eq)
H(4)	-429	4092	363	27
H(5)	-1040	3296	-911	32
H(6)	-38	2814	-1357	32
H(7)	1610	3186	-554	30
H(8)	2251	4039	712	25
H(10)	3871	6077	3506	31
H(11)	4657	6532	4839	38
H(12)	3754	6112	5547	39
H(13)	2088	5236	4936	37
H(14)	1281	4824	3603	30
H(16)	3045	7180	2849	91
H(17)	3185	8516	3501	104
H(18)	1806	8659	3614	57
H(19)	387	7464	3224	64
H(20)	258	6126	2599	53
H(22)	1807	1567	685	26
H(24)	-762	329	-1180	39
H(26)	-520	2237	471	29
H(27A)	1226	519	-994	57
H(27B)	545	-290	-849	57
H(27C)	1611	314	-197	57
H(28A)	-1974	1108	-1420	68
H(28B)	-1986	1626	-670	68
H(28C)	-2309	606	-870	68
H(29)	1881	3478	3348	24
H(31A)	-230	1918	1665	42
H(31B)	-687	1413	2163	42
H(31C)	322	1406	2148	42
H(32A)	1141	1948	3573	47
H(32B)	101	1906	3554	47
H(32C)	1054	2778	3999	47

H(34)	-311	3098	3743	38
H(35)	-1170	3997	3650	47
H(36)	-1482	4589	2633	46
H(37)	-954	4240	1688	36
H(38)	-77	3356	1785	29
H(40A)	4027	3799	1116	42
H(40B)	3027	3010	919	42
H(40C)	4025	3120	1597	42
H(41A)	4205	5147	2563	28
H(41B)	4874	4706	2335	28
H(42A)	4657	3796	3101	30
H(42B)	5082	4776	3611	30
H(43A)	3753	3392	4009	43
H(43B)	3313	4076	4222	43
H(43C)	4463	4381	4423	43
H(45)	8773	8113	4178	26
H(47)	11282	9801	4266	32
H(49)	8916	8634	2243	30
H(50A)	11236	9587	5417	52
H(50B)	10704	8580	5283	52
H(50C)	10182	9216	5438	52
H(51A)	10959	9355	2526	66
H(51B)	11357	10239	3173	66
H(51C)	10359	9968	2431	66
H(52)	5664	5854	1470	20
H(54A)	8183	6755	1804	33
H(54B)	8420	5922	1905	33
H(54C)	8285	6479	2567	33
H(55A)	5923	4989	550	37
H(55B)	6994	4993	707	37
H(55C)	6761	5818	564	37
H(57)	7321	5828	3110	28
H(58)	7050	4794	3740	37
H(59)	6328	3340	3077	40
H(60)	5848	2923	1762	38
H(61)	6091	3954	1113	29
H(65A)	4561	8091	2771	83
H(65B)	4197	8817	2505	83
H(65C)	5152	9072	3279	83
H(66A)	5024	8438	1795	40
H(66B)	5615	9421	2303	40
H(67A)	7646	9239	3485	36
H(67B)	6990	9800	3443	36
H(68A)	7754	9468	2350	57
H(68B)	8175	10365	2985	57
H(68C)	7101	10031	2310	57
H(1X1)	2376	7535	5155	102
H(1X2)	2327	6878	5659	102
H(2X1)	2572	8612	6158	117
H(2X2)	3421	8251	6434	117

H(2X3)	2510	7957	6660	117
H(3X1)	667	5918	4818	89
H(3X2)	756	6491	4251	89
H(4X1)	-645	6300	4853	102
H(4X2)	-860	5690	4054	102
H(4X3)	-609	6695	4167	102

Table 28.6. Torsion angles [°] for **28**.

N(4)-Mo(1)-O(1)-C(40)	-41.4(2)
C(29)-Mo(1)-O(1)-C(40)	144.8(3)
O(3)-Mo(1)-O(1)-C(40)	50.4(2)
C(1)-Mo(1)-O(1)-C(40)	-137.3(2)
O(2)-Mo(1)-O(1)-C(40)	128.5(2)
N(4)-Mo(1)-O(1)-C(41)	177.99(18)
C(29)-Mo(1)-O(1)-C(41)	4.2(4)
O(3)-Mo(1)-O(1)-C(41)	-90.23(18)
C(1)-Mo(1)-O(1)-C(41)	82.11(18)
O(2)-Mo(1)-O(1)-C(41)	-12.08(17)
N(3)-N(1)-C(1)-N(2)	-1.1(3)
C(3)-N(1)-C(1)-N(2)	177.7(2)
N(3)-N(1)-C(1)-Mo(1)	173.58(18)
C(3)-N(1)-C(1)-Mo(1)	-7.7(4)
N(4)-Mo(1)-C(1)-N(1)	-18.6(2)
C(29)-Mo(1)-C(1)-N(1)	-117.4(2)
O(3)-Mo(1)-C(1)-N(1)	104.5(3)
O(1)-Mo(1)-C(1)-N(1)	80.9(2)
O(2)-Mo(1)-C(1)-N(1)	152.2(2)
N(4)-Mo(1)-C(1)-N(2)	154.6(2)
C(29)-Mo(1)-C(1)-N(2)	55.8(2)
O(3)-Mo(1)-C(1)-N(2)	-82.3(4)
O(1)-Mo(1)-C(1)-N(2)	-105.9(2)
O(2)-Mo(1)-C(1)-N(2)	-34.6(2)
N(4)-Mo(1)-O(2)-C(42)	31.5(5)
C(29)-Mo(1)-O(2)-C(42)	165.73(19)
O(3)-Mo(1)-O(2)-C(42)	62.74(17)
C(1)-Mo(1)-O(2)-C(42)	-102.82(18)
O(1)-Mo(1)-O(2)-C(42)	-19.43(17)
N(4)-Mo(1)-O(2)-C(43)	-105.0(4)
C(29)-Mo(1)-O(2)-C(43)	29.2(2)
O(3)-Mo(1)-O(2)-C(43)	-73.8(2)
C(1)-Mo(1)-O(2)-C(43)	120.7(2)
O(1)-Mo(1)-O(2)-C(43)	-155.9(2)
N(1)-C(1)-N(2)-C(2)	0.7(3)
Mo(1)-C(1)-N(2)-C(2)	-173.79(19)
N(1)-C(1)-N(2)-C(9)	178.0(2)
Mo(1)-C(1)-N(2)-C(9)	3.5(4)
C(1)-N(2)-C(2)-N(3)	-0.2(3)
C(9)-N(2)-C(2)-N(3)	-177.7(2)

C(1)-N(2)-C(2)-C(15)	-177.2(3)
C(9)-N(2)-C(2)-C(15)	5.3(4)
N(2)-C(2)-N(3)-N(1)	-0.4(3)
C(15)-C(2)-N(3)-N(1)	176.6(3)
C(1)-N(1)-N(3)-C(2)	1.0(3)
C(3)-N(1)-N(3)-C(2)	-178.0(2)
C(1)-N(1)-C(3)-C(4)	131.7(3)
N(3)-N(1)-C(3)-C(4)	-49.6(3)
C(1)-N(1)-C(3)-C(8)	-51.6(4)
N(3)-N(1)-C(3)-C(8)	127.2(3)
C(29)-Mo(1)-N(4)-C(21)	-124.9(10)
O(3)-Mo(1)-N(4)-C(21)	-21.5(10)
C(1)-Mo(1)-N(4)-C(21)	142.6(10)
O(1)-Mo(1)-N(4)-C(21)	57.1(10)
O(2)-Mo(1)-N(4)-C(21)	8.6(13)
C(8)-C(3)-C(4)-C(5)	2.6(4)
N(1)-C(3)-C(4)-C(5)	179.2(2)
C(3)-C(4)-C(5)-C(6)	0.6(4)
C(4)-C(5)-C(6)-C(7)	-2.1(5)
C(5)-C(6)-C(7)-C(8)	0.5(4)
C(4)-C(3)-C(8)-C(7)	-4.1(4)
N(1)-C(3)-C(8)-C(7)	179.3(2)
C(6)-C(7)-C(8)-C(3)	2.5(4)
C(1)-N(2)-C(9)-C(14)	-92.4(4)
C(2)-N(2)-C(9)-C(14)	84.6(3)
C(1)-N(2)-C(9)-C(10)	92.9(4)
C(2)-N(2)-C(9)-C(10)	-90.1(3)
C(14)-C(9)-C(10)-C(11)	0.4(5)
N(2)-C(9)-C(10)-C(11)	175.0(3)
C(9)-C(10)-C(11)-C(12)	0.5(5)
C(10)-C(11)-C(12)-C(13)	0.1(5)
C(11)-C(12)-C(13)-C(14)	-1.5(5)
C(12)-C(13)-C(14)-C(9)	2.3(5)
C(10)-C(9)-C(14)-C(13)	-1.8(5)
N(2)-C(9)-C(14)-C(13)	-176.4(3)
N(3)-C(2)-C(15)-C(20)	77.4(4)
N(2)-C(2)-C(15)-C(20)	-106.0(4)
N(3)-C(2)-C(15)-C(16)	-102.0(5)
N(2)-C(2)-C(15)-C(16)	74.6(5)
C(20)-C(15)-C(16)-C(17)	0.6(8)
C(2)-C(15)-C(16)-C(17)	179.9(5)
C(15)-C(16)-C(17)-C(18)	-2.6(9)
C(16)-C(17)-C(18)-C(19)	3.8(9)
C(17)-C(18)-C(19)-C(20)	-3.1(8)
C(16)-C(15)-C(20)-C(19)	0.2(6)
C(2)-C(15)-C(20)-C(19)	-179.1(4)
C(18)-C(19)-C(20)-C(15)	1.0(7)
Mo(1)-N(4)-C(21)-C(22)	-2.4(11)
Mo(1)-N(4)-C(21)-C(26)	178.2(8)
C(26)-C(21)-C(22)-C(23)	0.4(4)

N(4)-C(21)-C(22)-C(23)	-179.0(2)
C(21)-C(22)-C(23)-C(24)	0.0(4)
C(21)-C(22)-C(23)-C(27)	179.5(3)
C(22)-C(23)-C(24)-C(25)	-0.1(4)
C(27)-C(23)-C(24)-C(25)	-179.6(3)
C(23)-C(24)-C(25)-C(26)	-0.3(5)
C(23)-C(24)-C(25)-C(28)	179.7(3)
C(22)-C(21)-C(26)-C(25)	-0.8(4)
N(4)-C(21)-C(26)-C(25)	178.6(3)
C(24)-C(25)-C(26)-C(21)	0.7(4)
C(28)-C(25)-C(26)-C(21)	-179.3(3)
N(4)-Mo(1)-C(29)-C(30)	2.4(4)
O(3)-Mo(1)-C(29)-C(30)	-93.5(3)
C(1)-Mo(1)-C(29)-C(30)	99.4(3)
O(1)-Mo(1)-C(29)-C(30)	176.2(2)
O(2)-Mo(1)-C(29)-C(30)	-168.4(3)
Mo(1)-C(29)-C(30)-C(31)	19.0(5)
Mo(1)-C(29)-C(30)-C(33)	-101.5(4)
Mo(1)-C(29)-C(30)-C(32)	138.2(3)
C(29)-C(30)-C(33)-C(34)	-120.0(3)
C(31)-C(30)-C(33)-C(34)	117.3(3)
C(32)-C(30)-C(33)-C(34)	-3.1(4)
C(29)-C(30)-C(33)-C(38)	59.3(3)
C(31)-C(30)-C(33)-C(38)	-63.4(3)
C(32)-C(30)-C(33)-C(38)	176.2(3)
C(38)-C(33)-C(34)-C(35)	-0.6(5)
C(30)-C(33)-C(34)-C(35)	178.6(3)
C(33)-C(34)-C(35)-C(36)	0.2(6)
C(34)-C(35)-C(36)-C(37)	0.8(6)
C(35)-C(36)-C(37)-C(38)	-1.2(5)
C(36)-C(37)-C(38)-C(33)	0.7(5)
C(34)-C(33)-C(38)-C(37)	0.2(5)
C(30)-C(33)-C(38)-C(37)	-179.1(3)
O(5A)-S(1)-O(3)-Mo(1)	-53.4(5)
O(4A)-S(1)-O(3)-Mo(1)	84.3(4)
O(5)-S(1)-O(3)-Mo(1)	-81.7(4)
O(4)-S(1)-O(3)-Mo(1)	53.1(3)
C(39)-S(1)-O(3)-Mo(1)	164.4(3)
C(39A)-S(1)-O(3)-Mo(1)	-166.2(3)
N(4)-Mo(1)-O(3)-S(1)	-70.33(18)
C(29)-Mo(1)-O(3)-S(1)	29.34(19)
C(1)-Mo(1)-O(3)-S(1)	166.1(2)
O(1)-Mo(1)-O(3)-S(1)	-169.83(18)
O(2)-Mo(1)-O(3)-S(1)	116.29(18)
O(5A)-S(1)-C(39)-F(2)	42.7(9)
O(4A)-S(1)-C(39)-F(2)	-71.9(6)
O(5)-S(1)-C(39)-F(2)	59.4(6)
O(4)-S(1)-C(39)-F(2)	-64.8(6)
O(3)-S(1)-C(39)-F(2)	177.0(4)
C(39A)-S(1)-C(39)-F(2)	85.8(8)

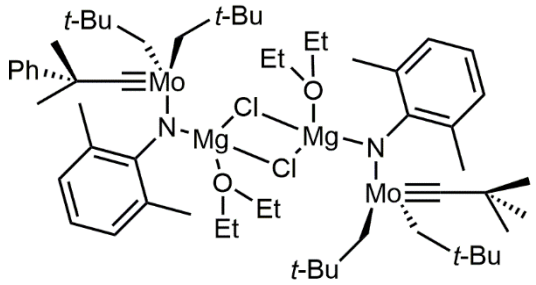
O(5A)-S(1)-C(39)-F(3)	161.5(7)
O(4A)-S(1)-C(39)-F(3)	47.0(6)
O(5)-S(1)-C(39)-F(3)	178.3(5)
O(4)-S(1)-C(39)-F(3)	54.0(5)
O(3)-S(1)-C(39)-F(3)	-64.2(5)
C(39A)-S(1)-C(39)-F(3)	-155.4(10)
O(5A)-S(1)-C(39)-F(1)	-76.1(8)
O(4A)-S(1)-C(39)-F(1)	169.4(7)
O(5)-S(1)-C(39)-F(1)	-59.3(6)
O(4)-S(1)-C(39)-F(1)	176.5(5)
O(3)-S(1)-C(39)-F(1)	58.3(5)
C(39A)-S(1)-C(39)-F(1)	-33.0(6)
O(5A)-S(1)-C(39A)-F(1A)	-55.2(9)
O(4A)-S(1)-C(39A)-F(1A)	-179.3(7)
O(5)-S(1)-C(39A)-F(1A)	-47.1(7)
O(4)-S(1)-C(39A)-F(1A)	-163.9(6)
O(3)-S(1)-C(39A)-F(1A)	64.5(7)
C(39)-S(1)-C(39A)-F(1A)	158.2(11)
O(5A)-S(1)-C(39A)-F(2A)	64.3(9)
O(4A)-S(1)-C(39A)-F(2A)	-59.8(8)
O(5)-S(1)-C(39A)-F(2A)	72.5(8)
O(4)-S(1)-C(39A)-F(2A)	-44.4(9)
O(3)-S(1)-C(39A)-F(2A)	-176.0(7)
C(39)-S(1)-C(39A)-F(2A)	-82.2(9)
O(5A)-S(1)-C(39A)-F(3A)	-174.6(8)
O(4A)-S(1)-C(39A)-F(3A)	61.3(8)
O(5)-S(1)-C(39A)-F(3A)	-166.4(8)
O(4)-S(1)-C(39A)-F(3A)	76.7(8)
O(3)-S(1)-C(39A)-F(3A)	-54.9(7)
C(39)-S(1)-C(39A)-F(3A)	38.9(7)
C(40)-O(1)-C(41)-C(42)	-102.5(3)
Mo(1)-O(1)-C(41)-C(42)	41.2(3)
C(43)-O(2)-C(42)-C(41)	-171.4(2)
Mo(1)-O(2)-C(42)-C(41)	46.6(3)
O(1)-C(41)-C(42)-O(2)	-56.7(3)
C(52)-Mo(2)-N(5)-C(44)	165.9(14)
O(9)-Mo(2)-N(5)-C(44)	67.0(14)
O(6)-Mo(2)-N(5)-C(44)	-93.8(14)
O(12)-Mo(2)-N(5)-C(44)	-13.4(17)
O(15)-Mo(2)-N(5)-C(44)	-8.7(14)
O(8)-S(2)-O(6)-Mo(2)	-14.8(3)
O(7)-S(2)-O(6)-Mo(2)	-151.1(2)
C(62)-S(2)-O(6)-Mo(2)	98.0(3)
N(5)-Mo(2)-O(6)-S(2)	-11.2(3)
C(52)-Mo(2)-O(6)-S(2)	89.1(2)
O(9)-Mo(2)-O(6)-S(2)	-139.5(2)
O(12)-Mo(2)-O(6)-S(2)	-179.4(3)
O(15)-Mo(2)-O(6)-S(2)	-101.2(2)
O(10)-S(3)-O(9)-Mo(2)	65.6(2)
O(11)-S(3)-O(9)-Mo(2)	-72.97(19)

C(63)-S(3)-O(9)-Mo(2)	176.08(17)
N(5)-Mo(2)-O(9)-S(3)	83.80(17)
C(52)-Mo(2)-O(9)-S(3)	-16.06(18)
O(6)-Mo(2)-O(9)-S(3)	-147.60(16)
O(12)-Mo(2)-O(9)-S(3)	-107.96(17)
O(15)-Mo(2)-O(9)-S(3)	172.83(18)
O(13)-S(4)-O(12)-Mo(2)	-34.7(2)
O(14)-S(4)-O(12)-Mo(2)	102.2(2)
C(64)-S(4)-O(12)-Mo(2)	-146.8(2)
N(5)-Mo(2)-O(12)-S(4)	-151.4(4)
C(52)-Mo(2)-O(12)-S(4)	29.4(2)
O(9)-Mo(2)-O(12)-S(4)	126.6(2)
O(6)-Mo(2)-O(12)-S(4)	-69.0(2)
O(15)-Mo(2)-O(12)-S(4)	-156.1(2)
N(5)-Mo(2)-O(15)-C(67)	3.3(2)
C(52)-Mo(2)-O(15)-C(67)	-147.4(5)
O(9)-Mo(2)-O(15)-C(67)	-93.7(2)
O(6)-Mo(2)-O(15)-C(67)	101.7(2)
O(12)-Mo(2)-O(15)-C(67)	-177.7(2)
N(5)-Mo(2)-O(15)-C(66)	160.3(2)
C(52)-Mo(2)-O(15)-C(66)	9.6(6)
O(9)-Mo(2)-O(15)-C(66)	63.2(2)
O(6)-Mo(2)-O(15)-C(66)	-101.3(2)
O(12)-Mo(2)-O(15)-C(66)	-20.7(2)
Mo(2)-N(5)-C(44)-C(49)	-82.1(14)
Mo(2)-N(5)-C(44)-C(45)	94.5(14)
N(5)-C(44)-C(45)-C(46)	-175.2(3)
C(49)-C(44)-C(45)-C(46)	1.3(4)
C(44)-C(45)-C(46)-C(47)	0.3(4)
C(44)-C(45)-C(46)-C(50)	-179.8(3)
C(45)-C(46)-C(47)-C(48)	-1.2(5)
C(50)-C(46)-C(47)-C(48)	178.9(3)
C(46)-C(47)-C(48)-C(49)	0.5(5)
C(46)-C(47)-C(48)-C(51)	-177.9(3)
C(47)-C(48)-C(49)-C(44)	1.1(4)
C(51)-C(48)-C(49)-C(44)	179.6(3)
N(5)-C(44)-C(49)-C(48)	174.5(3)
C(45)-C(44)-C(49)-C(48)	-2.0(4)
N(5)-Mo(2)-C(52)-C(53)	-1.8(3)
O(9)-Mo(2)-C(52)-C(53)	96.5(3)
O(6)-Mo(2)-C(52)-C(53)	-101.9(3)
O(12)-Mo(2)-C(52)-C(53)	178.0(3)
O(15)-Mo(2)-C(52)-C(53)	148.5(4)
Mo(2)-C(52)-C(53)-C(54)	-6.7(4)
Mo(2)-C(52)-C(53)-C(55)	-126.8(3)
Mo(2)-C(52)-C(53)-C(56)	112.7(3)
C(52)-C(53)-C(56)-C(61)	116.3(3)
C(54)-C(53)-C(56)-C(61)	-122.2(3)
C(55)-C(53)-C(56)-C(61)	-1.2(4)
C(52)-C(53)-C(56)-C(57)	-63.6(3)

C(54)-C(53)-C(56)-C(57)	57.9(3)
C(55)-C(53)-C(56)-C(57)	178.9(2)
C(61)-C(56)-C(57)-C(58)	1.0(4)
C(53)-C(56)-C(57)-C(58)	-179.2(3)
C(56)-C(57)-C(58)-C(59)	0.1(5)
C(57)-C(58)-C(59)-C(60)	-0.7(5)
C(58)-C(59)-C(60)-C(61)	0.2(5)
C(57)-C(56)-C(61)-C(60)	-1.5(4)
C(53)-C(56)-C(61)-C(60)	178.6(3)
C(59)-C(60)-C(61)-C(56)	1.0(5)
O(8)-S(2)-C(62)-F(6)	-64.8(4)
O(7)-S(2)-C(62)-F(6)	58.5(4)
O(6)-S(2)-C(62)-F(6)	175.3(3)
O(8)-S(2)-C(62)-F(4)	56.6(3)
O(7)-S(2)-C(62)-F(4)	179.9(3)
O(6)-S(2)-C(62)-F(4)	-63.2(3)
O(8)-S(2)-C(62)-F(5)	176.7(3)
O(7)-S(2)-C(62)-F(5)	-60.0(3)
O(6)-S(2)-C(62)-F(5)	56.9(3)
O(10)-S(3)-C(63)-F(9)	55.0(3)
O(11)-S(3)-C(63)-F(9)	-178.9(2)
O(9)-S(3)-C(63)-F(9)	-62.5(3)
O(10)-S(3)-C(63)-F(7)	176.1(2)
O(11)-S(3)-C(63)-F(7)	-57.9(3)
O(9)-S(3)-C(63)-F(7)	58.5(3)
O(10)-S(3)-C(63)-F(8)	-65.3(3)
O(11)-S(3)-C(63)-F(8)	60.8(3)
O(9)-S(3)-C(63)-F(8)	177.1(2)
O(13)-S(4)-C(64)-F(11)	57.4(2)
O(14)-S(4)-C(64)-F(11)	-67.1(2)
O(12)-S(4)-C(64)-F(11)	175.8(2)
O(13)-S(4)-C(64)-F(12)	177.6(2)
O(14)-S(4)-C(64)-F(12)	53.1(2)
O(12)-S(4)-C(64)-F(12)	-63.9(2)
O(13)-S(4)-C(64)-F(10)	-62.4(2)
O(14)-S(4)-C(64)-F(10)	173.1(2)
O(12)-S(4)-C(64)-F(10)	56.1(2)
C(67)-O(15)-C(66)-C(65)	-101.6(3)
Mo(2)-O(15)-C(66)-C(65)	100.3(3)
C(66)-O(15)-C(67)-C(68)	-76.3(3)
Mo(2)-O(15)-C(67)-C(68)	83.2(3)
C(3X)-O(1X)-C(1X)-C(2X)	-174.6(5)
C(1X)-O(1X)-C(3X)-C(4X)	-176.6(5)

Symmetry transformations used to generate equivalent atoms:

Complex 29


t-Bu
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Mo
N
Mg
Cl
Et
O
Et
Mg
Cl
Et
O
Et
N
Mo
t-Bu
t-Bu

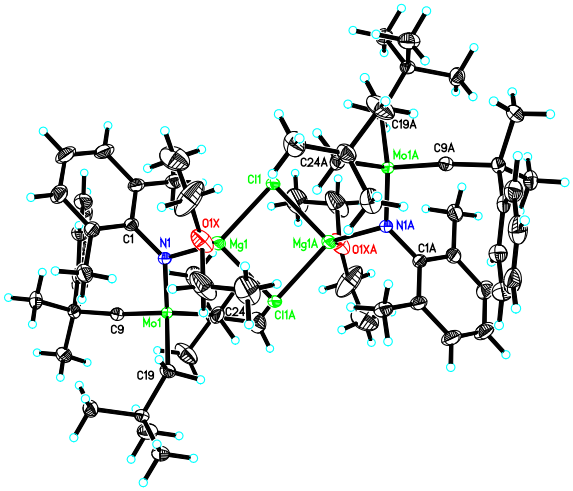

C19A
C24A
Mo1A
C9A
Cl1
O1X
N1
Mg1
Mg1A
O1XA
N1A
C1A
C1
C9
Mo1
C24
Cl1A
C19

Table 29.1. Crystal data and structure refinement for **29**.

Empirical formula	$C_{64}H_{104}Cl_2Mg_2Mo_2N_2O_2$
Formula weight	1244.89
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, $P2_1/n$
Unit cell dimensions	a = 17.1596(11) Å, α = 90°
	b = 10.2435(7) Å, β = 110.763(3)°
	c = 20.6639(13) Å, γ = 90°
Volume	3396.3(4) $Å^3$
Z, Calculated density	2, 1.217 Mg/m^3
Absorption coefficient	0.506 mm^{-1}
F(000)	1320
Crystal size	0.44 x 0.32 x 0.20 mm
Theta range for data collection	1.92 to 30.58 °
Limiting indices	-24<=h<=24, -14<=k<=14, -29<=l<=29
Reflections collected / unique	90088 / 10404 [R(int) = 0.0391]
Completeness to theta =	30.58 99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7461 and 0.6936
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10404 / 0 / 346
Goodness-of-fit on F^2	1.056
Final R indices [I>2σ(I)]	R1 = 0.0301, wR2 = 0.0745
R indices (all data)	R1 = 0.0465, wR2 = 0.0808
Largest diff. peak and hole	0.848 and -0.643 $e.Å^{-3}$

Table 29.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **29**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	7783(1)	752(1)	351(1)	15(1)
Cl(1)	10521(1)	1283(1)	-201(1)	26(1)
Mg(1)	9797(1)	917(1)	580(1)	23(1)
N(1)	8758(1)	1784(1)	579(1)	19(1)
C(1)	8926(1)	3095(2)	789(1)	19(1)
C(2)	9083(1)	3462(2)	1485(1)	23(1)
C(3)	9253(1)	4767(2)	1674(1)	31(1)
C(4)	9295(1)	5696(2)	1200(1)	37(1)
C(5)	9148(1)	5336(2)	523(1)	31(1)
C(6)	8955(1)	4050(2)	303(1)	23(1)
C(7)	8735(1)	3702(2)	-448(1)	28(1)
C(8)	9042(1)	2463(2)	2006(1)	27(1)
C(9)	7020(1)	1811(2)	429(1)	18(1)
C(10)	6426(1)	2831(2)	515(1)	20(1)
C(11)	6835(1)	3535(2)	1217(1)	25(1)
C(12)	5632(1)	2158(2)	530(1)	28(1)
C(13)	6244(1)	3830(2)	-74(1)	22(1)
C(14)	5471(1)	3923(2)	-606(1)	30(1)
C(15)	5337(1)	4836(2)	-1136(1)	38(1)
C(16)	5958(2)	5675(2)	-1140(1)	40(1)
C(17)	6730(2)	5596(2)	-613(1)	39(1)
C(18)	6872(1)	4682(2)	-90(1)	30(1)
C(19)	7946(1)	-789(2)	1100(1)	23(1)
C(20)	7330(1)	-1274(2)	1429(1)	21(1)
C(21)	7249(1)	-265(2)	1945(1)	30(1)
C(22)	6473(1)	-1492(2)	869(1)	35(1)
C(23)	7631(1)	-2569(2)	1805(1)	32(1)
C(24)	7316(1)	54(2)	-696(1)	26(1)
C(25)	6505(1)	357(2)	-1296(1)	27(1)
C(26)	5755(1)	92(3)	-1082(1)	48(1)
C(27)	6501(1)	1779(2)	-1512(1)	37(1)
C(28)	6435(1)	-524(2)	-1918(1)	40(1)
O(1X)	10670(1)	828(2)	1514(1)	38(1)
C(1X)	10646(2)	-253(3)	1956(1)	58(1)
C(2X)	11308(2)	-1248(3)	2018(1)	55(1)
C(3X)	11349(2)	1726(3)	1814(1)	69(1)
C(4X)	11236(2)	2983(3)	1469(1)	54(1)

Table 29.3. Bond lengths [Å] and angles [°] for **29**.

Mo(1)-C(9)	1.7500(16)
Mo(1)-N(1)	1.8930(13)
Mo(1)-C(24)	2.1455(16)
Mo(1)-C(19)	2.1592(16)
Mo(1)-Mg(1)	3.3228(6)
Cl(1)-Mg(1)#1	2.3838(7)
Cl(1)-Mg(1)	2.3884(7)
Mg(1)-O(1X)	1.9819(15)
Mg(1)-N(1)	1.9907(14)
Mg(1)-Cl(1)#1	2.3838(7)
Mg(1)-C(1)	2.8033(16)
Mg(1)-Mg(1)#1	3.3064(12)
N(1)-C(1)	1.409(2)
C(1)-C(6)	1.415(2)
C(1)-C(2)	1.418(2)
C(2)-C(3)	1.394(2)
C(2)-C(8)	1.505(2)
C(3)-C(4)	1.386(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.381(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.394(2)
C(5)-H(5)	0.9500
C(6)-C(7)	1.504(3)
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-C(10)	1.514(2)
C(10)-C(13)	1.536(2)
C(10)-C(12)	1.538(2)
C(10)-C(11)	1.548(2)
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.393(2)
C(13)-C(18)	1.395(3)
C(14)-C(15)	1.395(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.371(3)
C(15)-H(15)	0.9500
C(16)-C(17)	1.387(3)
C(16)-H(16)	0.9500

C(17)-C(18)	1.386(3)
C(17)-H(17)	0.9500
C(18)-H(18)	0.9500
C(19)-C(20)	1.529(2)
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-C(21)	1.527(2)
C(20)-C(22)	1.530(3)
C(20)-C(23)	1.531(2)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-C(25)	1.532(2)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-C(27)	1.522(3)
C(25)-C(26)	1.525(3)
C(25)-C(28)	1.540(3)
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
O(1X)-C(3X)	1.441(3)
O(1X)-C(1X)	1.445(3)
C(1X)-C(2X)	1.497(3)
C(1X)-H(1X1)	0.9900
C(1X)-H(1X2)	0.9900
C(2X)-H(2X1)	0.9800
C(2X)-H(2X2)	0.9800
C(2X)-H(2X3)	0.9800
C(3X)-C(4X)	1.451(4)
C(3X)-H(3X1)	0.9900
C(3X)-H(3X2)	0.9900
C(4X)-H(4X1)	0.9800
C(4X)-H(4X2)	0.9800
C(4X)-H(4X3)	0.9800

C(9)-Mo(1)-N(1)	104.80(7)
C(9)-Mo(1)-C(24)	105.98(7)

N(1)-Mo(1)-C(24)	114.71(6)
C(9)-Mo(1)-C(19)	107.34(7)
N(1)-Mo(1)-C(19)	110.57(6)
C(24)-Mo(1)-C(19)	112.74(7)
C(9)-Mo(1)-Mg(1)	136.84(5)
N(1)-Mo(1)-Mg(1)	32.06(4)
C(24)-Mo(1)-Mg(1)	99.11(5)
C(19)-Mo(1)-Mg(1)	94.06(5)
Mg(1)#1-Cl(1)-Mg(1)	87.71(2)
O(1X)-Mg(1)-N(1)	112.85(6)
O(1X)-Mg(1)-Cl(1)#1	106.43(5)
N(1)-Mg(1)-Cl(1)#1	108.72(5)
O(1X)-Mg(1)-Cl(1)	105.69(5)
N(1)-Mg(1)-Cl(1)	127.51(5)
Cl(1)#1-Mg(1)-Cl(1)	92.29(2)
O(1X)-Mg(1)-C(1)	98.40(6)
N(1)-Mg(1)-C(1)	28.21(5)
Cl(1)#1-Mg(1)-C(1)	136.92(4)
Cl(1)-Mg(1)-C(1)	114.37(4)
O(1X)-Mg(1)-Mg(1)#1	113.54(5)
N(1)-Mg(1)-Mg(1)#1	132.16(5)
Cl(1)#1-Mg(1)-Mg(1)#1	46.202(17)
Cl(1)-Mg(1)-Mg(1)#1	46.086(17)
C(1)-Mg(1)-Mg(1)#1	145.55(5)
O(1X)-Mg(1)-Mo(1)	121.66(5)
N(1)-Mg(1)-Mo(1)	30.31(4)
Cl(1)#1-Mg(1)-Mo(1)	78.461(19)
Cl(1)-Mg(1)-Mo(1)	132.51(3)
C(1)-Mg(1)-Mo(1)	58.51(3)
Mg(1)#1-Mg(1)-Mo(1)	110.12(3)
C(1)-N(1)-Mo(1)	132.40(11)
C(1)-N(1)-Mg(1)	109.90(10)
Mo(1)-N(1)-Mg(1)	117.63(7)
N(1)-C(1)-C(6)	119.65(14)
N(1)-C(1)-C(2)	120.70(14)
C(6)-C(1)-C(2)	119.64(15)
N(1)-C(1)-Mg(1)	41.89(7)
C(6)-C(1)-Mg(1)	106.63(11)
C(2)-C(1)-Mg(1)	116.62(11)
C(3)-C(2)-C(1)	118.92(16)
C(3)-C(2)-C(8)	120.74(16)
C(1)-C(2)-C(8)	120.32(15)
C(4)-C(3)-C(2)	121.28(18)
C(4)-C(3)-H(3)	119.4
C(2)-C(3)-H(3)	119.4
C(5)-C(4)-C(3)	119.74(17)
C(5)-C(4)-H(4)	120.1
C(3)-C(4)-H(4)	120.1
C(4)-C(5)-C(6)	121.26(18)
C(4)-C(5)-H(5)	119.4

C(6)-C(5)-H(5)	119.4
C(5)-C(6)-C(1)	119.13(17)
C(5)-C(6)-C(7)	120.23(16)
C(1)-C(6)-C(7)	120.55(14)
C(6)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(6)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(2)-C(8)-H(8A)	109.5
C(2)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(2)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(10)-C(9)-Mo(1)	174.33(12)
C(9)-C(10)-C(13)	108.88(12)
C(9)-C(10)-C(12)	109.35(14)
C(13)-C(10)-C(12)	112.48(14)
C(9)-C(10)-C(11)	109.37(13)
C(13)-C(10)-C(11)	109.25(13)
C(12)-C(10)-C(11)	107.46(13)
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(18)	117.74(17)
C(14)-C(13)-C(10)	122.73(16)
C(18)-C(13)-C(10)	119.53(15)
C(13)-C(14)-C(15)	120.74(19)
C(13)-C(14)-H(14)	119.6
C(15)-C(14)-H(14)	119.6
C(16)-C(15)-C(14)	120.8(2)
C(16)-C(15)-H(15)	119.6
C(14)-C(15)-H(15)	119.6
C(15)-C(16)-C(17)	119.17(19)
C(15)-C(16)-H(16)	120.4
C(17)-C(16)-H(16)	120.4
C(18)-C(17)-C(16)	120.4(2)
C(18)-C(17)-H(17)	119.8
C(16)-C(17)-H(17)	119.8

C(17)-C(18)-C(13)	121.14(19)
C(17)-C(18)-H(18)	119.4
C(13)-C(18)-H(18)	119.4
C(20)-C(19)-Mo(1)	128.45(12)
C(20)-C(19)-H(19A)	105.2
Mo(1)-C(19)-H(19A)	105.2
C(20)-C(19)-H(19B)	105.2
Mo(1)-C(19)-H(19B)	105.2
H(19A)-C(19)-H(19B)	105.9
C(21)-C(20)-C(19)	109.80(14)
C(21)-C(20)-C(22)	109.00(15)
C(19)-C(20)-C(22)	110.04(14)
C(21)-C(20)-C(23)	109.24(14)
C(19)-C(20)-C(23)	110.19(14)
C(22)-C(20)-C(23)	108.54(15)
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(20)-C(23)-H(23A)	109.5
C(20)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(20)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(25)-C(24)-Mo(1)	130.98(12)
C(25)-C(24)-H(24A)	104.5
Mo(1)-C(24)-H(24A)	104.5
C(25)-C(24)-H(24B)	104.5
Mo(1)-C(24)-H(24B)	104.5
H(24A)-C(24)-H(24B)	105.7
C(27)-C(25)-C(26)	109.80(19)
C(27)-C(25)-C(24)	109.80(15)
C(26)-C(25)-C(24)	110.32(15)
C(27)-C(25)-C(28)	108.99(15)
C(26)-C(25)-C(28)	108.27(17)
C(24)-C(25)-C(28)	109.61(16)
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5

H(26B)-C(26)-H(26C)	109.5
C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(25)-C(28)-H(28A)	109.5
C(25)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(25)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(3X)-O(1X)-C(1X)	114.6(2)
C(3X)-O(1X)-Mg(1)	127.38(14)
C(1X)-O(1X)-Mg(1)	118.03(16)
O(1X)-C(1X)-C(2X)	112.74(19)
O(1X)-C(1X)-H(1X1)	109.0
C(2X)-C(1X)-H(1X1)	109.0
O(1X)-C(1X)-H(1X2)	109.0
C(2X)-C(1X)-H(1X2)	109.0
H(1X1)-C(1X)-H(1X2)	107.8
C(1X)-C(2X)-H(2X1)	109.5
C(1X)-C(2X)-H(2X2)	109.5
H(2X1)-C(2X)-H(2X2)	109.5
C(1X)-C(2X)-H(2X3)	109.5
H(2X1)-C(2X)-H(2X3)	109.5
H(2X2)-C(2X)-H(2X3)	109.5
O(1X)-C(3X)-C(4X)	114.1(2)
O(1X)-C(3X)-H(3X1)	108.7
C(4X)-C(3X)-H(3X1)	108.7
O(1X)-C(3X)-H(3X2)	108.7
C(4X)-C(3X)-H(3X2)	108.7
H(3X1)-C(3X)-H(3X2)	107.6
C(3X)-C(4X)-H(4X1)	109.5
C(3X)-C(4X)-H(4X2)	109.5
H(4X1)-C(4X)-H(4X2)	109.5
C(3X)-C(4X)-H(4X3)	109.5
H(4X1)-C(4X)-H(4X3)	109.5
H(4X2)-C(4X)-H(4X3)	109.5

Symmetry transformations used to generate equivalent atoms: #1 -x+2,-y,-z

Table 29.4. Anisotropic displacement parameters ($Å^2$ x 10^3) for **29**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	19(1)	12(1)	17(1)	-1(1)	10(1)	-1(1)
Cl(1)	33(1)	13(1)	45(1)	2(1)	30(1)	0(1)

Mg(1)	23(1)	17(1)	36(1)	3(1)	18(1)	2(1)
N(1)	20(1)	14(1)	27(1)	0(1)	14(1)	-1(1)
C(1)	14(1)	15(1)	30(1)	-1(1)	10(1)	-1(1)
C(2)	17(1)	22(1)	32(1)	-4(1)	10(1)	-1(1)
C(3)	28(1)	28(1)	38(1)	-13(1)	11(1)	-7(1)
C(4)	38(1)	19(1)	52(1)	-9(1)	15(1)	-9(1)
C(5)	31(1)	17(1)	47(1)	1(1)	15(1)	-4(1)
C(6)	20(1)	16(1)	36(1)	1(1)	12(1)	-2(1)
C(7)	32(1)	20(1)	34(1)	5(1)	15(1)	0(1)
C(8)	26(1)	30(1)	27(1)	-3(1)	12(1)	1(1)
C(9)	20(1)	18(1)	20(1)	-1(1)	9(1)	-2(1)
C(10)	19(1)	20(1)	22(1)	-2(1)	10(1)	1(1)
C(11)	27(1)	26(1)	24(1)	-6(1)	11(1)	3(1)
C(12)	22(1)	29(1)	36(1)	-1(1)	16(1)	-1(1)
C(13)	23(1)	20(1)	25(1)	-3(1)	12(1)	5(1)
C(14)	27(1)	30(1)	33(1)	-1(1)	10(1)	6(1)
C(15)	41(1)	42(1)	32(1)	3(1)	12(1)	19(1)
C(16)	63(2)	30(1)	38(1)	9(1)	29(1)	21(1)
C(17)	50(1)	27(1)	50(1)	6(1)	30(1)	2(1)
C(18)	30(1)	25(1)	37(1)	2(1)	17(1)	2(1)
C(19)	26(1)	20(1)	27(1)	5(1)	15(1)	2(1)
C(20)	30(1)	17(1)	22(1)	0(1)	16(1)	-3(1)
C(21)	47(1)	23(1)	27(1)	2(1)	22(1)	3(1)
C(22)	32(1)	33(1)	41(1)	-2(1)	15(1)	-10(1)
C(23)	50(1)	21(1)	36(1)	7(1)	27(1)	2(1)
C(24)	35(1)	20(1)	22(1)	-5(1)	11(1)	0(1)
C(25)	28(1)	35(1)	21(1)	-2(1)	12(1)	-4(1)
C(26)	34(1)	84(2)	28(1)	-14(1)	15(1)	-23(1)
C(27)	38(1)	43(1)	28(1)	4(1)	11(1)	9(1)
C(28)	45(1)	50(1)	23(1)	-12(1)	11(1)	-7(1)
O(1X)	31(1)	54(1)	32(1)	14(1)	16(1)	12(1)
C(1X)	60(2)	75(2)	54(1)	39(1)	39(1)	36(1)
C(2X)	61(2)	61(2)	48(1)	26(1)	27(1)	29(1)
C(3X)	84(2)	43(1)	47(1)	-17(1)	-17(1)	5(1)
C(4X)	33(1)	79(2)	47(1)	4(1)	8(1)	-11(1)

Table 29.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **29**.

	x	y	z	U(eq)
H(3)	9343	5024	2136	38
H(4)	9424	6578	1340	44
H(5)	9179	5976	200	38
H(7A)	8773	4482	-709	42
H(7B)	8165	3359	-630	42
H(7C)	9122	3037	-494	42
H(8A)	9190	2874	2462	40
H(8B)	9435	1754	2029	40

H(8C)	8476	2109	1866	40
H(11A)	6944	2903	1595	38
H(11B)	6458	4215	1267	38
H(11C)	7360	3935	1234	38
H(12A)	5371	1669	100	41
H(12B)	5242	2818	577	41
H(12C)	5777	1556	924	41
H(14)	5031	3358	-609	36
H(15)	4808	4878	-1498	46
H(16)	5860	6302	-1498	48
H(17)	7164	6173	-611	46
H(18)	7405	4633	265	35
H(19A)	8095	-1572	887	27
H(19B)	8455	-551	1494	27
H(21A)	7792	-135	2311	45
H(21B)	6847	-575	2149	45
H(21C)	7054	564	1705	45
H(22A)	6083	-1805	1085	52
H(22B)	6520	-2144	538	52
H(22C)	6269	-668	628	52
H(23A)	8177	-2442	2169	48
H(23B)	7677	-3222	1474	48
H(23C)	7231	-2870	2013	48
H(24A)	7762	263	-879	31
H(24B)	7319	-908	-652	31
H(26A)	5776	670	-698	72
H(26B)	5766	-819	-935	72
H(26C)	5240	255	-1476	72
H(27A)	6546	2346	-1118	55
H(27B)	5980	1968	-1894	55
H(27C)	6975	1937	-1661	55
H(28A)	5911	-340	-2298	59
H(28B)	6445	-1442	-1781	59
H(28C)	6905	-352	-2070	59
H(1X1)	10093	-678	1768	70
H(1X2)	10717	84	2422	70
H(2X1)	11280	-1515	1555	82
H(2X2)	11219	-2011	2270	82
H(2X3)	11857	-870	2270	82
H(3X1)	11868	1324	1802	82
H(3X2)	11419	1867	2306	82
H(4X1)	11203	2861	990	82
H(4X2)	11709	3551	1712	82
H(4X3)	10719	3386	1473	82

Table 29.6. Torsion angles [°] for **29**.

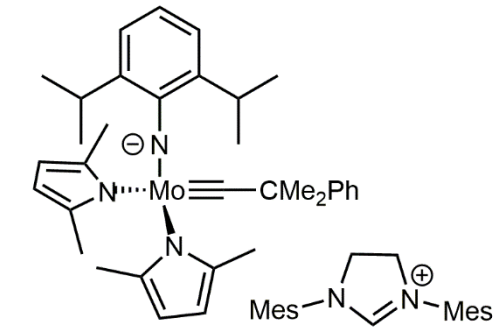
Mg(1)#1-Cl(1)-Mg(1)-O(1X)	107.78(6)
Mg(1)#1-Cl(1)-Mg(1)-N(1)	-115.82(6)
Mg(1)#1-Cl(1)-Mg(1)-Cl(1)#1	0.000(2)
Mg(1)#1-Cl(1)-Mg(1)-C(1)	-145.14(5)
Mg(1)#1-Cl(1)-Mg(1)-Mo(1)	-76.41(3)
C(9)-Mo(1)-Mg(1)-O(1X)	78.77(9)
N(1)-Mo(1)-Mg(1)-O(1X)	81.32(10)
C(24)-Mo(1)-Mg(1)-O(1X)	-155.88(8)
C(19)-Mo(1)-Mg(1)-O(1X)	-42.06(8)
C(9)-Mo(1)-Mg(1)-N(1)	-2.55(11)
C(24)-Mo(1)-Mg(1)-N(1)	122.80(9)
C(19)-Mo(1)-Mg(1)-N(1)	-123.39(9)
C(9)-Mo(1)-Mg(1)-Cl(1)#1	-178.92(7)
N(1)-Mo(1)-Mg(1)-Cl(1)#1	-176.36(8)
C(24)-Mo(1)-Mg(1)-Cl(1)#1	-53.56(5)
C(19)-Mo(1)-Mg(1)-Cl(1)#1	60.25(5)
C(9)-Mo(1)-Mg(1)-Cl(1)	-96.49(8)
N(1)-Mo(1)-Mg(1)-Cl(1)	-93.94(8)
C(24)-Mo(1)-Mg(1)-Cl(1)	28.86(6)
C(19)-Mo(1)-Mg(1)-Cl(1)	142.67(5)
C(9)-Mo(1)-Mg(1)-C(1)	-1.05(8)
N(1)-Mo(1)-Mg(1)-C(1)	1.50(8)
C(24)-Mo(1)-Mg(1)-C(1)	124.30(6)
C(19)-Mo(1)-Mg(1)-C(1)	-121.89(6)
C(9)-Mo(1)-Mg(1)-Mg(1)#1	-144.71(7)
N(1)-Mo(1)-Mg(1)-Mg(1)#1	-142.16(8)
C(24)-Mo(1)-Mg(1)-Mg(1)#1	-19.36(5)
C(19)-Mo(1)-Mg(1)-Mg(1)#1	94.45(5)
C(9)-Mo(1)-N(1)-C(1)	1.64(16)
C(24)-Mo(1)-N(1)-C(1)	117.43(14)
C(19)-Mo(1)-N(1)-C(1)	-113.73(14)
Mg(1)-Mo(1)-N(1)-C(1)	-176.55(19)
C(9)-Mo(1)-N(1)-Mg(1)	178.19(8)
C(24)-Mo(1)-N(1)-Mg(1)	-66.02(9)
C(19)-Mo(1)-N(1)-Mg(1)	62.82(9)
O(1X)-Mg(1)-N(1)-C(1)	63.23(12)
Cl(1)#1-Mg(1)-N(1)-C(1)	-178.94(9)
Cl(1)-Mg(1)-N(1)-C(1)	-70.69(12)
Mg(1)#1-Mg(1)-N(1)-C(1)	-131.71(10)
Mo(1)-Mg(1)-N(1)-C(1)	177.29(15)
O(1X)-Mg(1)-N(1)-Mo(1)	-114.07(8)
Cl(1)#1-Mg(1)-N(1)-Mo(1)	3.76(8)
Cl(1)-Mg(1)-N(1)-Mo(1)	112.02(7)
C(1)-Mg(1)-N(1)-Mo(1)	-177.29(15)
Mg(1)#1-Mg(1)-N(1)-Mo(1)	51.00(10)
Mo(1)-N(1)-C(1)-C(6)	-101.38(17)
Mg(1)-N(1)-C(1)-C(6)	81.87(16)
Mo(1)-N(1)-C(1)-C(2)	79.94(19)

Mg(1)-N(1)-C(1)-C(2)	-96.81(15)
Mo(1)-N(1)-C(1)-Mg(1)	176.75(18)
O(1X)-Mg(1)-C(1)-N(1)	-123.73(11)
Cl(1)#1-Mg(1)-C(1)-N(1)	1.47(13)
Cl(1)-Mg(1)-C(1)-N(1)	124.73(10)
Mg(1)#1-Mg(1)-C(1)-N(1)	78.02(13)
Mo(1)-Mg(1)-C(1)-N(1)	-1.60(9)
O(1X)-Mg(1)-C(1)-C(6)	120.15(11)
N(1)-Mg(1)-C(1)-C(6)	-116.12(16)
Cl(1)#1-Mg(1)-C(1)-C(6)	-114.65(11)
Cl(1)-Mg(1)-C(1)-C(6)	8.62(12)
Mg(1)#1-Mg(1)-C(1)-C(6)	-38.10(15)
Mo(1)-Mg(1)-C(1)-C(6)	-117.72(11)
O(1X)-Mg(1)-C(1)-C(2)	-16.50(13)
N(1)-Mg(1)-C(1)-C(2)	107.24(16)
Cl(1)#1-Mg(1)-C(1)-C(2)	108.70(12)
Cl(1)-Mg(1)-C(1)-C(2)	-128.03(11)
Mg(1)#1-Mg(1)-C(1)-C(2)	-174.74(10)
Mo(1)-Mg(1)-C(1)-C(2)	105.63(12)
N(1)-C(1)-C(2)-C(3)	179.42(15)
C(6)-C(1)-C(2)-C(3)	0.7(2)
Mg(1)-C(1)-C(2)-C(3)	131.55(14)
N(1)-C(1)-C(2)-C(8)	-2.2(2)
C(6)-C(1)-C(2)-C(8)	179.14(15)
Mg(1)-C(1)-C(2)-C(8)	-50.05(18)
C(1)-C(2)-C(3)-C(4)	-1.8(3)
C(8)-C(2)-C(3)-C(4)	179.77(18)
C(3)-C(4)-C(5)-C(6)	0.2(3)
C(4)-C(5)-C(6)-C(1)	-1.2(3)
C(4)-C(5)-C(6)-C(7)	175.39(18)
N(1)-C(1)-C(6)-C(5)	-177.93(15)
C(2)-C(1)-C(6)-C(5)	0.8(2)
Mg(1)-C(1)-C(6)-C(5)	-134.31(15)
N(1)-C(1)-C(6)-C(7)	5.4(2)
C(2)-C(1)-C(6)-C(7)	-175.86(15)
Mg(1)-C(1)-C(6)-C(7)	49.06(18)
N(1)-Mo(1)-C(9)-C(10)	1.5(12)
C(24)-Mo(1)-C(9)-C(10)	-120.2(12)
C(19)-Mo(1)-C(9)-C(10)	119.1(12)
Mg(1)-Mo(1)-C(9)-C(10)	2.9(12)
Mo(1)-C(9)-C(10)-C(13)	69.0(12)
Mo(1)-C(9)-C(10)-C(12)	-167.7(11)
C(9)-C(10)-C(13)-C(14)	109.92(17)
C(12)-C(10)-C(13)-C(14)	-11.4(2)
C(11)-C(10)-C(13)-C(14)	-130.69(17)
C(9)-C(10)-C(13)-C(18)	-69.49(19)
C(12)-C(10)-C(13)-C(18)	169.14(15)
C(11)-C(10)-C(13)-C(18)	49.9(2)
C(18)-C(13)-C(14)-C(15)	0.2(3)
C(10)-C(13)-C(14)-C(15)	-179.26(16)

C(13)-C(14)-C(15)-C(16)	-0.8(3)
C(14)-C(15)-C(16)-C(17)	0.8(3)
C(15)-C(16)-C(17)-C(18)	0.0(3)
C(16)-C(17)-C(18)-C(13)	-0.7(3)
C(14)-C(13)-C(18)-C(17)	0.6(3)
C(10)-C(13)-C(18)-C(17)	-179.99(17)
C(9)-Mo(1)-C(19)-C(20)	24.03(16)
N(1)-Mo(1)-C(19)-C(20)	137.80(14)
C(24)-Mo(1)-C(19)-C(20)	-92.31(15)
Mg(1)-Mo(1)-C(19)-C(20)	166.05(14)
Mo(1)-C(19)-C(20)-C(21)	-72.14(19)
Mo(1)-C(19)-C(20)-C(22)	47.8(2)
Mo(1)-C(19)-C(20)-C(23)	167.49(13)
C(9)-Mo(1)-C(24)-C(25)	0.66(18)
N(1)-Mo(1)-C(24)-C(25)	-114.45(16)
C(19)-Mo(1)-C(24)-C(25)	117.81(16)
Mg(1)-Mo(1)-C(24)-C(25)	-143.86(16)
Mo(1)-C(24)-C(25)-C(27)	66.4(2)
Mo(1)-C(24)-C(25)-C(26)	-54.8(2)
Mo(1)-C(24)-C(25)-C(28)	-173.91(14)
N(1)-Mg(1)-O(1X)-C(3X)	-95.2(2)
Cl(1)#1-Mg(1)-O(1X)-C(3X)	145.6(2)
Cl(1)-Mg(1)-O(1X)-C(3X)	48.4(2)
C(1)-Mg(1)-O(1X)-C(3X)	-70.0(2)
Mg(1)#1-Mg(1)-O(1X)-C(3X)	96.8(2)
Mo(1)-Mg(1)-O(1X)-C(3X)	-128.02(19)
N(1)-Mg(1)-O(1X)-C(1X)	85.43(15)
Cl(1)#1-Mg(1)-O(1X)-C(1X)	-33.73(15)
Cl(1)-Mg(1)-O(1X)-C(1X)	-130.97(14)
C(1)-Mg(1)-O(1X)-C(1X)	110.69(15)
Mg(1)#1-Mg(1)-O(1X)-C(1X)	-82.54(15)
Mo(1)-Mg(1)-O(1X)-C(1X)	52.65(16)
C(3X)-O(1X)-C(1X)-C(2X)	-73.7(3)
Mg(1)-O(1X)-C(1X)-C(2X)	105.8(2)
C(1X)-O(1X)-C(3X)-C(4X)	-162.6(2)
Mg(1)-O(1X)-C(3X)-C(4X)	18.1(4)

Symmetry transformations used to generate

Complex 30



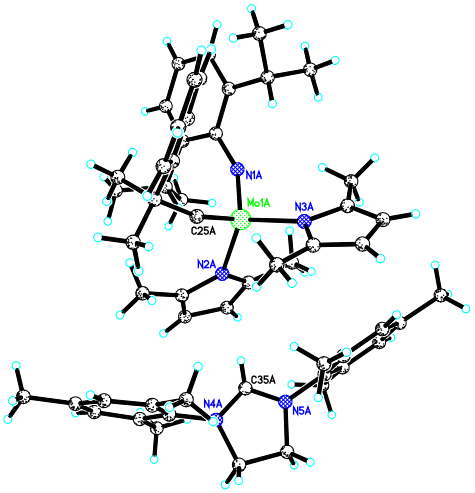


Table 30.1. Crystal data and structure refinement for **30**.

Empirical formula	$C_{55}H_{71}MoN_5$
Formula weight	898.11
Temperature	100(2) K
Wavelength	0.71073Å
Crystal system, space group	Monoclinic, *P*c
Unit cell dimensions	a = 19.9397(13) Å, α = 90°
	b = 12.3206(8) Å, β = 92.843(3)°
	c = 21.1394(12) Å, γ = 90°
Volume	5186.9(6) $Å^3$
Z, Calculated density	4, 1.150 Mg/m^3
Absorption coefficient	0.291 mm^{-1}
F(000)	1912
Crystal size	0.18 x 0.18 x 0.16 mm
Theta range for data collection	1.65 to 25.26°
Limiting indices	-23<=h<=23, -12<=k<=14, -25<=l<=22
Reflections collected / unique	36461 / 15727 [R(int) = 0.0458]
Completeness to theta = 25.26	98.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7452 and 0.6676
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	15727 / 86 / 1139
Goodness-of-fit on F^2	1.041
Final R indices [I>2σ(I)]	R1 = 0.0548, wR2 = 0.1259
R indices (all data)	R1 = 0.0694, wR2 = 0.1326
Absolute structure parameter	0.00(5)
Largest diff. peak and hole	1.297 and -0.491 $e.Å^{-3}$

****
REMARK: Disordered solvent electron density squeezed by PLATON !
****

Table 30.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **30**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1A)	994(1)	7609(1)	2177(1)	29(1)
N(1A)	1522(3)	6703(4)	1761(2)	28(1)
C(1A)	1653(3)	5757(4)	1446(3)	26(2)
N(2A)	1101(3)	7225(4)	3155(3)	31(1)
C(2A)	1686(3)	4750(5)	1784(3)	27(2)
C(3A)	1886(4)	3834(5)	1474(3)	34(2)
N(3A)	1108(4)	9250(5)	1859(3)	52(2)
N(4A)	196(3)	8726(3)	4789(2)	23(1)
C(4A)	2050(3)	3840(5)	847(3)	31(2)
N(5A)	1113(3)	9653(4)	4600(2)	23(1)
C(5A)	1992(4)	4798(5)	511(3)	34(2)
C(6A)	1807(3)	5757(5)	799(3)	28(2)
C(7A)	1482(4)	4688(5)	2473(3)	42(2)
C(8A)	2097(5)	4508(8)	2899(4)	72(3)
C(9A)	962(5)	3787(7)	2592(4)	63(2)
C(10A)	1819(4)	6806(5)	422(3)	37(2)
C(11A)	2525(5)	7237(6)	379(5)	69(3)
C(12A)	1546(5)	6666(7)	-248(4)	72(2)
C(13A)	741(4)	6545(5)	3553(4)	38(2)
C(14A)	1107(4)	6315(5)	4086(3)	42(2)
C(15A)	1736(4)	6841(5)	4021(3)	39(2)
C(16A)	1722(4)	7371(4)	3465(3)	30(2)
C(17A)	47(5)	6186(6)	3372(4)	63(3)
C(18A)	2260(3)	7991(5)	3164(3)	29(2)
C(19A)	644(7)	10054(9)	1879(4)	86(4)
C(20A)	974(5)	11002(6)	1739(4)	52(2)
C(21A)	1646(6)	10799(7)	1632(4)	70(3)
C(22A)	1773(5)	9688(6)	1719(4)	51(2)
C(23A)	-49(6)	9887(8)	1987(5)	81(3)
C(24A)	2378(5)	9096(7)	1652(4)	67(3)
C(25A)	162(4)	7288(6)	1959(4)	44(2)
C(26A)	-459(4)	6762(9)	1644(4)	67(3)
C(27A)	-1057(6)	7067(11)	2022(6)	105(4)
C(28A)	-376(5)	5513(8)	1625(4)	74(3)
C(29A)	-536(5)	7192(10)	975(5)	87(4)
C(30A)	-95(4)	6910(8)	545(4)	68(2)
C(31A)	-200(5)	7197(7)	-92(4)	70(2)
C(32A)	-761(5)	7734(7)	-303(5)	71(2)
C(33A)	-1217(5)	8037(9)	158(4)	82(3)
C(34A)	-1127(5)	7687(9)	783(4)	94(3)
C(35A)	723(4)	8851(4)	4446(3)	26(2)
C(36A)	193(3)	9600(5)	5271(3)	28(2)
C(37A)	842(4)	10228(5)	5152(3)	30(2)

C(38A)	-293(3)	7900(5)	4735(3)	30(2)
C(39A)	-207(4)	6956(5)	5117(3)	34(2)
C(40A)	-678(4)	6122(5)	5046(3)	39(2)
C(41A)	-1238(4)	6246(6)	4646(3)	45(2)
C(42A)	-1317(4)	7181(6)	4300(4)	44(2)
C(43A)	-847(4)	8015(5)	4326(3)	41(2)
C(44A)	387(4)	6812(6)	5563(3)	47(2)
C(45A)	-1754(4)	5334(6)	4583(4)	64(2)
C(46A)	-925(5)	9025(6)	3921(4)	62(2)
C(47A)	1631(3)	10103(4)	4225(3)	25(2)
C(48A)	2311(3)	9955(4)	4414(3)	24(2)
C(49A)	2777(3)	10416(4)	4040(3)	26(2)
C(50A)	2599(3)	11003(4)	3502(3)	30(2)
C(51A)	1928(3)	11136(4)	3325(3)	26(2)
C(52A)	1431(3)	10690(4)	3691(3)	24(2)
C(53A)	2517(4)	9300(5)	4981(3)	35(2)
C(54A)	3109(4)	11520(5)	3100(4)	41(2)
C(55A)	706(4)	10872(5)	3489(3)	36(2)
Mo(1B)	5509(1)	2810(1)	3070(1)	22(1)
N(1B)	4994(3)	1808(3)	3440(2)	23(1)
C(1B)	4873(3)	839(4)	3760(3)	24(2)
N(2B)	5514(3)	2373(3)	2125(3)	21(1)
C(2B)	4783(4)	-115(5)	3414(3)	33(2)
N(3B)	5287(2)	4421(3)	3366(2)	21(1)
C(3B)	4611(4)	-1069(5)	3714(3)	34(2)
N(4B)	5405(3)	4664(4)	628(3)	27(1)
C(4B)	4529(4)	-1073(5)	4361(4)	44(2)
N(5B)	6335(3)	3822(4)	456(2)	30(1)
C(5B)	4621(4)	-132(5)	4703(3)	37(2)
C(6B)	4795(3)	846(4)	4421(3)	29(2)
C(7B)	4860(4)	-145(5)	2687(3)	42(2)
C(8B)	4267(5)	-655(7)	2320(4)	66(3)
C(9B)	5495(4)	-721(7)	2546(4)	62(2)
C(10B)	4870(4)	1863(5)	4818(3)	34(2)
C(11B)	5356(4)	1707(6)	5389(3)	52(2)
C(12B)	4207(4)	2241(5)	5029(4)	52(2)
C(13B)	4903(4)	2372(4)	1769(3)	26(2)
C(14B)	4972(4)	1791(5)	1212(3)	33(2)
C(15B)	5639(4)	1408(5)	1227(3)	37(2)
C(16B)	5969(3)	1759(4)	1772(3)	26(1)
C(17B)	4289(3)	2906(5)	1999(3)	29(2)
C(18B)	6666(3)	1583(5)	2003(3)	38(2)
C(19B)	4665(4)	4796(5)	3514(3)	30(2)
C(20B)	4683(4)	5896(5)	3606(3)	30(2)
C(21B)	5353(3)	6212(5)	3525(3)	28(1)
C(22B)	5712(3)	5299(4)	3382(3)	24(1)
C(23B)	4058(3)	4081(5)	3531(4)	38(2)
C(24B)	6444(3)	5245(5)	3269(3)	32(2)
C(25B)	6317(4)	2597(4)	3331(3)	33(2)
C(26B)	6927(3)	2105(5)	3745(3)	32(2)

C(27B)	6756(4)	946(5)	3903(3)	47(2)
C(28B)	6996(4)	2741(6)	4369(4)	47(2)
C(29B)	7586(4)	2209(5)	3400(4)	45(2)
C(30B)	7815(3)	3186(5)	3200(3)	38(2)
C(31B)	8430(4)	3318(6)	2923(3)	50(2)
C(32B)	8812(4)	2433(7)	2805(4)	64(2)
C(33B)	8572(4)	1420(8)	2972(4)	78(3)
C(34B)	7962(4)	1315(6)	3273(4)	56(2)
C(35B)	5827(3)	3917(4)	827(3)	21(1)
C(36B)	5596(4)	5156(5)	29(3)	29(2)
C(37B)	6269(4)	4610(5)	-67(3)	35(2)
C(38B)	4877(3)	5084(4)	1008(3)	24(2)
C(39B)	4217(3)	4878(4)	830(3)	26(2)
C(40B)	3725(3)	5314(4)	1205(3)	29(2)
C(41B)	3895(3)	5945(4)	1733(3)	26(2)
C(42B)	4568(3)	6128(5)	1891(3)	28(2)
C(43B)	5065(3)	5722(5)	1533(3)	27(2)
C(44B)	4011(4)	4182(5)	253(3)	34(2)
C(45B)	3343(4)	6425(5)	2138(3)	37(2)
C(46B)	5798(4)	5936(6)	1707(3)	41(2)
C(47B)	6910(4)	3077(6)	540(3)	39(2)
C(48B)	6917(4)	2167(6)	190(3)	43(2)
C(49B)	7467(4)	1474(7)	286(4)	61(3)
C(50B)	7992(4)	1763(9)	735(4)	67(3)
C(51B)	7967(4)	2709(8)	1077(4)	62(3)
C(52B)	7416(3)	3412(7)	982(4)	48(2)
C(53B)	6357(4)	1871(6)	-288(3)	58(2)
C(54B)	8578(4)	989(8)	873(5)	84(3)
C(55B)	7397(4)	4416(7)	1370(4)	65(2)

Table 30.3. Bond lengths [Å] and angles [°] for **30**.

Mo(1A)-C(25A)	1.745(8)
Mo(1A)-N(1A)	1.795(5)
Mo(1A)-N(2A)	2.121(6)
Mo(1A)-N(3A)	2.146(6)
N(1A)-C(1A)	1.374(7)
C(1A)-C(6A)	1.415(9)
C(1A)-C(2A)	1.432(8)
N(2A)-C(16A)	1.383(10)
N(2A)-C(13A)	1.410(8)
C(2A)-C(3A)	1.373(9)
C(2A)-C(7A)	1.535(9)
C(3A)-C(4A)	1.380(9)
C(3A)-H(3A)	0.9500
N(3A)-C(19A)	1.357(12)
N(3A)-C(22A)	1.476(11)
N(4A)-C(35A)	1.313(8)

N(4A)-C(38A)	1.411(8)
N(4A)-C(36A)	1.483(8)
C(4A)-C(5A)	1.379(9)
C(4A)-H(4A)	0.9500
N(5A)-C(35A)	1.290(7)
N(5A)-C(47A)	1.444(8)
N(5A)-C(37A)	1.488(8)
C(5A)-C(6A)	1.387(9)
C(5A)-H(5A)	0.9500
C(6A)-C(10A)	1.520(8)
C(7A)-C(8A)	1.502(12)
C(7A)-C(9A)	1.548(11)
C(7A)-H(7A)	1.0000
C(8A)-H(8A1)	0.9800
C(8A)-H(8A2)	0.9800
C(8A)-H(8A3)	0.9800
C(9A)-H(9A1)	0.9800
C(9A)-H(9A2)	0.9800
C(9A)-H(9A3)	0.9800
C(10A)-C(12A)	1.503(10)
C(10A)-C(11A)	1.511(11)
C(10A)-H(10A)	1.0000
C(11A)-H(11A)	0.9800
C(11A)-H(11B)	0.9800
C(11A)-H(11C)	0.9800
C(12A)-H(12A)	0.9800
C(12A)-H(12B)	0.9800
C(12A)-H(12C)	0.9800
C(13A)-C(14A)	1.342(10)
C(13A)-C(17A)	1.484(10)
C(14A)-C(15A)	1.424(11)
C(14A)-H(14A)	0.9500
C(15A)-C(16A)	1.344(9)
C(15A)-H(15A)	0.9500
C(16A)-C(18A)	1.486(10)
C(17A)-H(17A)	0.9800
C(17A)-H(17B)	0.9800
C(17A)-H(17C)	0.9800
C(18A)-H(18A)	0.9800
C(18A)-H(18B)	0.9800
C(18A)-H(18C)	0.9800
C(19A)-C(20A)	1.379(14)
C(19A)-C(23A)	1.426(15)
C(20A)-C(21A)	1.394(13)
C(20A)-H(20A)	0.9500
C(21A)-C(22A)	1.401(12)
C(21A)-H(21A)	0.9500
C(22A)-C(24A)	1.423(13)
C(23A)-H(23A)	0.9800
C(23A)-H(23B)	0.9800

C(23A)-H(23C)	0.9800
C(24A)-H(24A)	0.9800
C(24A)-H(24B)	0.9800
C(24A)-H(24C)	0.9800
C(25A)-C(26A)	1.522(11)
C(26A)-C(29A)	1.509(14)
C(26A)-C(27A)	1.515(13)
C(26A)-C(28A)	1.549(13)
C(27A)-H(27A)	0.9800
C(27A)-H(27B)	0.9800
C(27A)-H(27C)	0.9800
C(28A)-H(28A)	0.9800
C(28A)-H(28B)	0.9800
C(28A)-H(28C)	0.9800
C(29A)-C(30A)	1.342(12)
C(29A)-C(34A)	1.371(13)
C(30A)-C(31A)	1.399(11)
C(30A)-H(30A)	0.9500
C(31A)-C(32A)	1.355(12)
C(31A)-H(31A)	0.9500
C(32A)-C(33A)	1.417(12)
C(32A)-H(32A)	0.9500
C(33A)-C(34A)	1.393(12)
C(33A)-H(33A)	0.9500
C(34A)-H(34A)	0.9500
C(35A)-H(35A)	0.83(7)
C(36A)-C(37A)	1.538(9)
C(36A)-H(36A)	0.9900
C(36A)-H(36B)	0.9900
C(37A)-H(37A)	0.9900
C(37A)-H(37B)	0.9900
C(38A)-C(43A)	1.376(10)
C(38A)-C(39A)	1.422(10)
C(39A)-C(40A)	1.395(9)
C(39A)-C(44A)	1.487(10)
C(40A)-C(41A)	1.376(10)
C(40A)-H(40A)	0.9500
C(41A)-C(42A)	1.369(11)
C(41A)-C(45A)	1.526(10)
C(42A)-C(43A)	1.390(10)
C(42A)-H(42A)	0.9500
C(43A)-C(46A)	1.514(10)
C(44A)-H(44A)	0.9800
C(44A)-H(44B)	0.9800
C(44A)-H(44C)	0.9800
C(45A)-H(45A)	0.9800
C(45A)-H(45B)	0.9800
C(45A)-H(45C)	0.9800
C(46A)-H(46A)	0.9800
C(46A)-H(46B)	0.9800

C(46A)-H(46C)	0.9800
C(47A)-C(52A)	1.382(9)
C(47A)-C(48A)	1.408(9)
C(48A)-C(49A)	1.372(9)
C(48A)-C(53A)	1.485(9)
C(49A)-C(50A)	1.378(9)
C(49A)-H(49A)	0.9500
C(50A)-C(51A)	1.382(9)
C(50A)-C(54A)	1.499(9)
C(51A)-C(52A)	1.398(9)
C(51A)-H(51A)	0.9500
C(52A)-C(55A)	1.504(9)
C(53A)-H(53A)	0.9800
C(53A)-H(53B)	0.9800
C(53A)-H(53C)	0.9800
C(54A)-H(54A)	0.9800
C(54A)-H(54B)	0.9800
C(54A)-H(54C)	0.9800
C(55A)-H(55A)	0.9800
C(55A)-H(55B)	0.9800
C(55A)-H(55C)	0.9800
Mo(1B)-C(25B)	1.698(8)
Mo(1B)-N(1B)	1.809(4)
Mo(1B)-N(2B)	2.069(6)
Mo(1B)-N(3B)	2.135(4)
N(1B)-C(1B)	1.400(7)
C(1B)-C(2B)	1.390(9)
C(1B)-C(6B)	1.413(9)
N(2B)-C(13B)	1.400(9)
N(2B)-C(16B)	1.420(7)
C(2B)-C(3B)	1.387(9)
C(2B)-C(7B)	1.554(10)
N(3B)-C(19B)	1.375(8)
N(3B)-C(22B)	1.374(7)
C(3B)-C(4B)	1.384(10)
C(3B)-H(3B)	0.9500
N(4B)-C(35B)	1.302(8)
N(4B)-C(38B)	1.451(8)
N(4B)-C(36B)	1.471(8)
C(4B)-C(5B)	1.375(9)
C(4B)-H(4B)	0.9500
N(5B)-C(35B)	1.315(8)
N(5B)-C(37B)	1.473(7)
N(5B)-C(47B)	1.473(8)
C(5B)-C(6B)	1.396(8)
C(5B)-H(5B)	0.9500
C(6B)-C(10B)	1.512(8)
C(7B)-C(9B)	1.494(11)
C(7B)-C(8B)	1.516(11)
C(7B)-H(7B)	1.0000

C(8B)-H(8B1)	0.9800
C(8B)-H(8B2)	0.9800
C(8B)-H(8B3)	0.9800
C(9B)-H(9B1)	0.9800
C(9B)-H(9B2)	0.9800
C(9B)-H(9B3)	0.9800
C(10B)-C(12B)	1.491(10)
C(10B)-C(11B)	1.523(10)
C(10B)-H(10B)	1.0000
C(11B)-H(11D)	0.9800
C(11B)-H(11E)	0.9800
C(11B)-H(11F)	0.9800
C(12B)-H(12D)	0.9800
C(12B)-H(12E)	0.9800
C(12B)-H(12F)	0.9800
C(13B)-C(14B)	1.390(9)
C(13B)-C(17B)	1.493(9)
C(14B)-C(15B)	1.410(10)
C(14B)-H(14B)	0.9500
C(15B)-C(16B)	1.370(9)
C(15B)-H(15B)	0.9500
C(16B)-C(18B)	1.465(9)
C(17B)-H(17D)	0.9800
C(17B)-H(17E)	0.9800
C(17B)-H(17F)	0.9800
C(18B)-H(18D)	0.9800
C(18B)-H(18E)	0.9800
C(18B)-H(18F)	0.9800
C(19B)-C(20B)	1.370(8)
C(19B)-C(23B)	1.499(9)
C(20B)-C(21B)	1.409(9)
C(20B)-H(20B)	0.9500
C(21B)-C(22B)	1.376(8)
C(21B)-H(21B)	0.9500
C(22B)-C(24B)	1.492(9)
C(23B)-H(23D)	0.9800
C(23B)-H(23E)	0.9800
C(23B)-H(23F)	0.9800
C(24B)-H(24D)	0.9800
C(24B)-H(24E)	0.9800
C(24B)-H(24F)	0.9800
C(25B)-C(26B)	1.582(10)
C(26B)-C(27B)	1.510(9)
C(26B)-C(28B)	1.533(10)
C(26B)-C(29B)	1.540(10)
C(27B)-H(27D)	0.9800
C(27B)-H(27E)	0.9800
C(27B)-H(27F)	0.9800
C(28B)-H(28D)	0.9800
C(28B)-H(28E)	0.9800

C(28B)-H(28F)	0.9800
C(29B)-C(30B)	1.363(9)
C(29B)-C(34B)	1.367(10)
C(30B)-C(31B)	1.393(9)
C(30B)-H(30B)	0.9500
C(31B)-C(32B)	1.361(10)
C(31B)-H(31B)	0.9500
C(32B)-C(33B)	1.388(12)
C(32B)-H(32B)	0.9500
C(33B)-C(34B)	1.406(11)
C(33B)-H(33B)	0.9500
C(34B)-H(34B)	0.9500
C(35B)-H(35B)	0.99(5)
C(36B)-C(37B)	1.525(9)
C(36B)-H(36C)	0.9900
C(36B)-H(36D)	0.9900
C(37B)-H(37C)	0.9900
C(37B)-H(37D)	0.9900
C(38B)-C(39B)	1.374(9)
C(38B)-C(43B)	1.397(9)
C(39B)-C(40B)	1.397(9)
C(39B)-C(44B)	1.531(8)
C(40B)-C(41B)	1.388(9)
C(40B)-H(40B)	0.9500
C(41B)-C(42B)	1.386(9)
C(41B)-C(45B)	1.546(9)
C(42B)-C(43B)	1.371(9)
C(42B)-H(42B)	0.9500
C(43B)-C(46B)	1.512(9)
C(44B)-H(44D)	0.9800
C(44B)-H(44E)	0.9800
C(44B)-H(44F)	0.9800
C(45B)-H(45D)	0.9800
C(45B)-H(45E)	0.9800
C(45B)-H(45F)	0.9800
C(46B)-H(46D)	0.9800
C(46B)-H(46E)	0.9800
C(46B)-H(46F)	0.9800
C(47B)-C(48B)	1.344(11)
C(47B)-C(52B)	1.403(11)
C(48B)-C(49B)	1.397(10)
C(48B)-C(53B)	1.512(11)
C(49B)-C(50B)	1.424(13)
C(49B)-H(49B)	0.9500
C(50B)-C(51B)	1.374(14)
C(50B)-C(54B)	1.525(11)
C(51B)-C(52B)	1.406(11)
C(51B)-H(51B)	0.9500
C(52B)-C(55B)	1.486(12)
C(53B)-H(53D)	0.9800

C(53B)-H(53E)	0.9800
C(53B)-H(53F)	0.9800
C(54B)-H(54D)	0.9800
C(54B)-H(54E)	0.9800
C(54B)-H(54F)	0.9800
C(55B)-H(55D)	0.9800
C(55B)-H(55E)	0.9800
C(55B)-H(55F)	0.9800

C(25A)-Mo(1A)-N(1A)	107.6(3)
C(25A)-Mo(1A)-N(2A)	104.9(3)
N(1A)-Mo(1A)-N(2A)	107.7(2)
C(25A)-Mo(1A)-N(3A)	104.2(3)
N(1A)-Mo(1A)-N(3A)	111.0(2)
N(2A)-Mo(1A)-N(3A)	120.5(2)
C(1A)-N(1A)-Mo(1A)	153.6(5)
N(1A)-C(1A)-C(6A)	121.6(5)
N(1A)-C(1A)-C(2A)	119.9(5)
C(6A)-C(1A)-C(2A)	118.3(5)
C(16A)-N(2A)-C(13A)	105.4(6)
C(16A)-N(2A)-Mo(1A)	118.6(4)
C(13A)-N(2A)-Mo(1A)	133.2(5)
C(3A)-C(2A)-C(1A)	118.8(6)
C(3A)-C(2A)-C(7A)	120.6(5)
C(1A)-C(2A)-C(7A)	120.6(5)
C(2A)-C(3A)-C(4A)	122.8(6)
C(2A)-C(3A)-H(3A)	118.6
C(4A)-C(3A)-H(3A)	118.6
C(19A)-N(3A)-C(22A)	111.1(8)
C(19A)-N(3A)-Mo(1A)	126.5(8)
C(22A)-N(3A)-Mo(1A)	121.2(5)
C(35A)-N(4A)-C(38A)	127.4(5)
C(35A)-N(4A)-C(36A)	108.9(5)
C(38A)-N(4A)-C(36A)	123.7(5)
C(5A)-C(4A)-C(3A)	118.7(6)
C(5A)-C(4A)-H(4A)	120.6
C(3A)-C(4A)-H(4A)	120.6
C(35A)-N(5A)-C(47A)	126.5(5)
C(35A)-N(5A)-C(37A)	108.9(5)
C(47A)-N(5A)-C(37A)	123.0(4)
C(4A)-C(5A)-C(6A)	121.3(6)
C(4A)-C(5A)-H(5A)	119.3
C(6A)-C(5A)-H(5A)	119.3
C(5A)-C(6A)-C(1A)	120.0(5)
C(5A)-C(6A)-C(10A)	118.9(6)
C(1A)-C(6A)-C(10A)	121.0(5)
C(8A)-C(7A)-C(2A)	109.2(7)
C(8A)-C(7A)-C(9A)	109.2(6)
C(2A)-C(7A)-C(9A)	113.6(6)
C(8A)-C(7A)-H(7A)	108.2

C(2A)-C(7A)-H(7A)	108.2
C(9A)-C(7A)-H(7A)	108.2
C(7A)-C(8A)-H(8A1)	109.5
C(7A)-C(8A)-H(8A2)	109.5
H(8A1)-C(8A)-H(8A2)	109.5
C(7A)-C(8A)-H(8A3)	109.5
H(8A1)-C(8A)-H(8A3)	109.5
H(8A2)-C(8A)-H(8A3)	109.5
C(7A)-C(9A)-H(9A1)	109.5
C(7A)-C(9A)-H(9A2)	109.5
H(9A1)-C(9A)-H(9A2)	109.5
C(7A)-C(9A)-H(9A3)	109.5
H(9A1)-C(9A)-H(9A3)	109.5
H(9A2)-C(9A)-H(9A3)	109.5
C(12A)-C(10A)-C(11A)	106.1(7)
C(12A)-C(10A)-C(6A)	112.5(6)
C(11A)-C(10A)-C(6A)	111.6(6)
C(12A)-C(10A)-H(10A)	108.8
C(11A)-C(10A)-H(10A)	108.8
C(6A)-C(10A)-H(10A)	108.8
C(10A)-C(11A)-H(11A)	109.5
C(10A)-C(11A)-H(11B)	109.5
H(11A)-C(11A)-H(11B)	109.5
C(10A)-C(11A)-H(11C)	109.5
H(11A)-C(11A)-H(11C)	109.5
H(11B)-C(11A)-H(11C)	109.5
C(10A)-C(12A)-H(12A)	109.5
C(10A)-C(12A)-H(12B)	109.5
H(12A)-C(12A)-H(12B)	109.5
C(10A)-C(12A)-H(12C)	109.5
H(12A)-C(12A)-H(12C)	109.5
H(12B)-C(12A)-H(12C)	109.5
C(14A)-C(13A)-N(2A)	110.7(6)
C(14A)-C(13A)-C(17A)	128.0(7)
N(2A)-C(13A)-C(17A)	121.3(7)
C(13A)-C(14A)-C(15A)	105.6(6)
C(13A)-C(14A)-H(14A)	127.2
C(15A)-C(14A)-H(14A)	127.2
C(16A)-C(15A)-C(14A)	108.9(7)
C(16A)-C(15A)-H(15A)	125.5
C(14A)-C(15A)-H(15A)	125.5
C(15A)-C(16A)-N(2A)	109.3(7)
C(15A)-C(16A)-C(18A)	129.8(7)
N(2A)-C(16A)-C(18A)	120.8(6)
C(13A)-C(17A)-H(17A)	109.5
C(13A)-C(17A)-H(17B)	109.5
H(17A)-C(17A)-H(17B)	109.5
C(13A)-C(17A)-H(17C)	109.5
H(17A)-C(17A)-H(17C)	109.5
H(17B)-C(17A)-H(17C)	109.5

C(16A)-C(18A)-H(18A)	109.5
C(16A)-C(18A)-H(18B)	109.5
H(18A)-C(18A)-H(18B)	109.5
C(16A)-C(18A)-H(18C)	109.5
H(18A)-C(18A)-H(18C)	109.5
H(18B)-C(18A)-H(18C)	109.5
N(3A)-C(19A)-C(20A)	106.2(11)
N(3A)-C(19A)-C(23A)	124.5(10)
C(20A)-C(19A)-C(23A)	129.3(10)
C(19A)-C(20A)-C(21A)	110.9(8)
C(19A)-C(20A)-H(20A)	124.6
C(21A)-C(20A)-H(20A)	124.6
C(20A)-C(21A)-C(22A)	108.8(8)
C(20A)-C(21A)-H(21A)	125.6
C(22A)-C(21A)-H(21A)	125.6
C(21A)-C(22A)-C(24A)	129.4(9)
C(21A)-C(22A)-N(3A)	103.1(8)
C(24A)-C(22A)-N(3A)	127.4(7)
C(19A)-C(23A)-H(23A)	109.5
C(19A)-C(23A)-H(23B)	109.5
H(23A)-C(23A)-H(23B)	109.5
C(19A)-C(23A)-H(23C)	109.5
H(23A)-C(23A)-H(23C)	109.5
H(23B)-C(23A)-H(23C)	109.5
C(22A)-C(24A)-H(24A)	109.5
C(22A)-C(24A)-H(24B)	109.5
H(24A)-C(24A)-H(24B)	109.5
C(22A)-C(24A)-H(24C)	109.5
H(24A)-C(24A)-H(24C)	109.5
H(24B)-C(24A)-H(24C)	109.5
C(26A)-C(25A)-Mo(1A)	162.7(5)
C(29A)-C(26A)-C(27A)	111.2(9)
C(29A)-C(26A)-C(25A)	107.6(8)
C(27A)-C(26A)-C(25A)	107.9(8)
C(29A)-C(26A)-C(28A)	109.3(7)
C(27A)-C(26A)-C(28A)	110.3(9)
C(25A)-C(26A)-C(28A)	110.4(7)
C(26A)-C(27A)-H(27A)	109.5
C(26A)-C(27A)-H(27B)	109.5
H(27A)-C(27A)-H(27B)	109.5
C(26A)-C(27A)-H(27C)	109.5
H(27A)-C(27A)-H(27C)	109.5
H(27B)-C(27A)-H(27C)	109.5
C(26A)-C(28A)-H(28A)	109.5
C(26A)-C(28A)-H(28B)	109.5
H(28A)-C(28A)-H(28B)	109.5
C(26A)-C(28A)-H(28C)	109.5
H(28A)-C(28A)-H(28C)	109.5
H(28B)-C(28A)-H(28C)	109.5
C(30A)-C(29A)-C(34A)	119.8(10)

C(30A)-C(29A)-C(26A)	120.3(9)
C(34A)-C(29A)-C(26A)	118.7(9)
C(29A)-C(30A)-C(31A)	121.0(9)
C(29A)-C(30A)-H(30A)	119.5
C(31A)-C(30A)-H(30A)	119.5
C(32A)-C(31A)-C(30A)	121.4(9)
C(32A)-C(31A)-H(31A)	119.3
C(30A)-C(31A)-H(31A)	119.3
C(31A)-C(32A)-C(33A)	116.7(9)
C(31A)-C(32A)-H(32A)	121.6
C(33A)-C(32A)-H(32A)	121.6
C(34A)-C(33A)-C(32A)	121.0(9)
C(34A)-C(33A)-H(33A)	119.5
C(32A)-C(33A)-H(33A)	119.5
C(29A)-C(34A)-C(33A)	119.2(10)
C(29A)-C(34A)-H(34A)	120.4
C(33A)-C(34A)-H(34A)	120.4
N(5A)-C(35A)-N(4A)	116.0(6)
N(5A)-C(35A)-H(35A)	118(5)
N(4A)-C(35A)-H(35A)	125(5)
N(4A)-C(36A)-C(37A)	102.7(5)
N(4A)-C(36A)-H(36A)	111.2
C(37A)-C(36A)-H(36A)	111.2
N(4A)-C(36A)-H(36B)	111.2
C(37A)-C(36A)-H(36B)	111.2
H(36A)-C(36A)-H(36B)	109.1
N(5A)-C(37A)-C(36A)	103.3(5)
N(5A)-C(37A)-H(37A)	111.1
C(36A)-C(37A)-H(37A)	111.1
N(5A)-C(37A)-H(37B)	111.1
C(36A)-C(37A)-H(37B)	111.1
H(37A)-C(37A)-H(37B)	109.1
C(43A)-C(38A)-N(4A)	120.5(6)
C(43A)-C(38A)-C(39A)	120.8(6)
N(4A)-C(38A)-C(39A)	118.7(6)
C(40A)-C(39A)-C(38A)	118.7(7)
C(40A)-C(39A)-C(44A)	119.4(6)
C(38A)-C(39A)-C(44A)	121.8(6)
C(41A)-C(40A)-C(39A)	120.4(7)
C(41A)-C(40A)-H(40A)	119.8
C(39A)-C(40A)-H(40A)	119.8
C(42A)-C(41A)-C(40A)	119.4(7)
C(42A)-C(41A)-C(45A)	120.9(8)
C(40A)-C(41A)-C(45A)	119.7(7)
C(41A)-C(42A)-C(43A)	122.7(7)
C(41A)-C(42A)-H(42A)	118.6
C(43A)-C(42A)-H(42A)	118.6
C(38A)-C(43A)-C(42A)	117.9(7)
C(38A)-C(43A)-C(46A)	119.8(6)
C(42A)-C(43A)-C(46A)	122.3(7)

C(39A)-C(44A)-H(44A)	109.5
C(39A)-C(44A)-H(44B)	109.5
H(44A)-C(44A)-H(44B)	109.5
C(39A)-C(44A)-H(44C)	109.5
H(44A)-C(44A)-H(44C)	109.5
H(44B)-C(44A)-H(44C)	109.5
C(41A)-C(45A)-H(45A)	109.5
C(41A)-C(45A)-H(45B)	109.5
H(45A)-C(45A)-H(45B)	109.5
C(41A)-C(45A)-H(45C)	109.5
H(45A)-C(45A)-H(45C)	109.5
H(45B)-C(45A)-H(45C)	109.5
C(43A)-C(46A)-H(46A)	109.5
C(43A)-C(46A)-H(46B)	109.5
H(46A)-C(46A)-H(46B)	109.5
C(43A)-C(46A)-H(46C)	109.5
H(46A)-C(46A)-H(46C)	109.5
H(46B)-C(46A)-H(46C)	109.5
C(52A)-C(47A)-C(48A)	122.3(6)
C(52A)-C(47A)-N(5A)	117.7(6)
C(48A)-C(47A)-N(5A)	119.9(6)
C(49A)-C(48A)-C(47A)	116.9(6)
C(49A)-C(48A)-C(53A)	121.5(6)
C(47A)-C(48A)-C(53A)	121.6(5)
C(48A)-C(49A)-C(50A)	122.6(6)
C(48A)-C(49A)-H(49A)	118.7
C(50A)-C(49A)-H(49A)	118.7
C(49A)-C(50A)-C(51A)	119.4(6)
C(49A)-C(50A)-C(54A)	122.5(6)
C(51A)-C(50A)-C(54A)	118.1(6)
C(50A)-C(51A)-C(52A)	120.5(6)
C(50A)-C(51A)-H(51A)	119.8
C(52A)-C(51A)-H(51A)	119.8
C(47A)-C(52A)-C(51A)	118.3(6)
C(47A)-C(52A)-C(55A)	122.9(6)
C(51A)-C(52A)-C(55A)	118.8(6)
C(48A)-C(53A)-H(53A)	109.5
C(48A)-C(53A)-H(53B)	109.5
H(53A)-C(53A)-H(53B)	109.5
C(48A)-C(53A)-H(53C)	109.5
H(53A)-C(53A)-H(53C)	109.5
H(53B)-C(53A)-H(53C)	109.5
C(50A)-C(54A)-H(54A)	109.5
C(50A)-C(54A)-H(54B)	109.5
H(54A)-C(54A)-H(54B)	109.5
C(50A)-C(54A)-H(54C)	109.5
H(54A)-C(54A)-H(54C)	109.5
H(54B)-C(54A)-H(54C)	109.5
C(52A)-C(55A)-H(55A)	109.5
C(52A)-C(55A)-H(55B)	109.5

H(55A)-C(55A)-H(55B)	109.5
C(52A)-C(55A)-H(55C)	109.5
H(55A)-C(55A)-H(55C)	109.5
H(55B)-C(55A)-H(55C)	109.5
C(25B)-Mo(1B)-N(1B)	107.7(2)
C(25B)-Mo(1B)-N(2B)	103.0(3)
N(1B)-Mo(1B)-N(2B)	105.7(2)
C(25B)-Mo(1B)-N(3B)	104.8(2)
N(1B)-Mo(1B)-N(3B)	112.1(2)
N(2B)-Mo(1B)-N(3B)	122.44(17)
C(1B)-N(1B)-Mo(1B)	155.0(4)
C(2B)-C(1B)-N(1B)	119.2(6)
C(2B)-C(1B)-C(6B)	120.5(5)
N(1B)-C(1B)-C(6B)	120.2(5)
C(13B)-N(2B)-C(16B)	106.2(5)
C(13B)-N(2B)-Mo(1B)	118.2(4)
C(16B)-N(2B)-Mo(1B)	132.8(4)
C(3B)-C(2B)-C(1B)	120.3(6)
C(3B)-C(2B)-C(7B)	118.1(6)
C(1B)-C(2B)-C(7B)	121.6(5)
C(19B)-N(3B)-C(22B)	107.0(5)
C(19B)-N(3B)-Mo(1B)	125.6(4)
C(22B)-N(3B)-Mo(1B)	127.1(4)
C(4B)-C(3B)-C(2B)	119.9(6)
C(4B)-C(3B)-H(3B)	120.0
C(2B)-C(3B)-H(3B)	120.0
C(35B)-N(4B)-C(38B)	123.3(5)
C(35B)-N(4B)-C(36B)	112.2(5)
C(38B)-N(4B)-C(36B)	123.7(5)
C(5B)-C(4B)-C(3B)	119.8(6)
C(5B)-C(4B)-H(4B)	120.1
C(3B)-C(4B)-H(4B)	120.1
C(35B)-N(5B)-C(37B)	110.3(5)
C(35B)-N(5B)-C(47B)	127.0(5)
C(37B)-N(5B)-C(47B)	122.7(5)
C(4B)-C(5B)-C(6B)	122.2(6)
C(4B)-C(5B)-H(5B)	118.9
C(6B)-C(5B)-H(5B)	118.9
C(5B)-C(6B)-C(1B)	117.4(5)
C(5B)-C(6B)-C(10B)	119.9(6)
C(1B)-C(6B)-C(10B)	122.7(5)
C(9B)-C(7B)-C(8B)	110.4(6)
C(9B)-C(7B)-C(2B)	109.5(6)
C(8B)-C(7B)-C(2B)	113.8(7)
C(9B)-C(7B)-H(7B)	107.7
C(8B)-C(7B)-H(7B)	107.7
C(2B)-C(7B)-H(7B)	107.7
C(7B)-C(8B)-H(8B1)	109.5
C(7B)-C(8B)-H(8B2)	109.5
H(8B1)-C(8B)-H(8B2)	109.5

C(7B)-C(8B)-H(8B3)	109.5
H(8B1)-C(8B)-H(8B3)	109.5
H(8B2)-C(8B)-H(8B3)	109.5
C(7B)-C(9B)-H(9B1)	109.5
C(7B)-C(9B)-H(9B2)	109.5
H(9B1)-C(9B)-H(9B2)	109.5
C(7B)-C(9B)-H(9B3)	109.5
H(9B1)-C(9B)-H(9B3)	109.5
H(9B2)-C(9B)-H(9B3)	109.5
C(12B)-C(10B)-C(6B)	111.1(6)
C(12B)-C(10B)-C(11B)	109.9(6)
C(6B)-C(10B)-C(11B)	112.2(5)
C(12B)-C(10B)-H(10B)	107.8
C(6B)-C(10B)-H(10B)	107.8
C(11B)-C(10B)-H(10B)	107.8
C(10B)-C(11B)-H(11D)	109.5
C(10B)-C(11B)-H(11E)	109.5
H(11D)-C(11B)-H(11E)	109.5
C(10B)-C(11B)-H(11F)	109.5
H(11D)-C(11B)-H(11F)	109.5
H(11E)-C(11B)-H(11F)	109.5
C(10B)-C(12B)-H(12D)	109.5
C(10B)-C(12B)-H(12E)	109.5
H(12D)-C(12B)-H(12E)	109.5
C(10B)-C(12B)-H(12F)	109.5
H(12D)-C(12B)-H(12F)	109.5
H(12E)-C(12B)-H(12F)	109.5
C(14B)-C(13B)-N(2B)	109.6(6)
C(14B)-C(13B)-C(17B)	128.3(7)
N(2B)-C(13B)-C(17B)	122.0(6)
C(13B)-C(14B)-C(15B)	106.6(6)
C(13B)-C(14B)-H(14B)	126.7
C(15B)-C(14B)-H(14B)	126.7
C(16B)-C(15B)-C(14B)	109.1(5)
C(16B)-C(15B)-H(15B)	125.5
C(14B)-C(15B)-H(15B)	125.5
C(15B)-C(16B)-N(2B)	108.5(6)
C(15B)-C(16B)-C(18B)	129.9(6)
N(2B)-C(16B)-C(18B)	121.6(5)
C(13B)-C(17B)-H(17D)	109.5
C(13B)-C(17B)-H(17E)	109.5
H(17D)-C(17B)-H(17E)	109.5
C(13B)-C(17B)-H(17F)	109.5
H(17D)-C(17B)-H(17F)	109.5
H(17E)-C(17B)-H(17F)	109.5
C(16B)-C(18B)-H(18D)	109.5
C(16B)-C(18B)-H(18E)	109.5
H(18D)-C(18B)-H(18E)	109.5
C(16B)-C(18B)-H(18F)	109.5
H(18D)-C(18B)-H(18F)	109.5

H(18E)-C(18B)-H(18F)	109.5
C(20B)-C(19B)-N(3B)	110.3(6)
C(20B)-C(19B)-C(23B)	126.5(6)
N(3B)-C(19B)-C(23B)	123.2(5)
C(19B)-C(20B)-C(21B)	106.0(6)
C(19B)-C(20B)-H(20B)	127.0
C(21B)-C(20B)-H(20B)	127.0
C(22B)-C(21B)-C(20B)	107.9(5)
C(22B)-C(21B)-H(21B)	126.0
C(20B)-C(21B)-H(21B)	126.0
N(3B)-C(22B)-C(21B)	108.8(5)
N(3B)-C(22B)-C(24B)	124.6(5)
C(21B)-C(22B)-C(24B)	126.6(5)
C(19B)-C(23B)-H(23D)	109.5
C(19B)-C(23B)-H(23E)	109.5
H(23D)-C(23B)-H(23E)	109.5
C(19B)-C(23B)-H(23F)	109.5
H(23D)-C(23B)-H(23F)	109.5
H(23E)-C(23B)-H(23F)	109.5
C(22B)-C(24B)-H(24D)	109.5
C(22B)-C(24B)-H(24E)	109.5
H(24D)-C(24B)-H(24E)	109.5
C(22B)-C(24B)-H(24F)	109.5
H(24D)-C(24B)-H(24F)	109.5
H(24E)-C(24B)-H(24F)	109.5
C(26B)-C(25B)-Mo(1B)	158.4(5)
C(27B)-C(26B)-C(28B)	107.8(6)
C(27B)-C(26B)-C(29B)	113.0(5)
C(28B)-C(26B)-C(29B)	108.7(6)
C(27B)-C(26B)-C(25B)	108.0(5)
C(28B)-C(26B)-C(25B)	108.3(5)
C(29B)-C(26B)-C(25B)	110.9(5)
C(26B)-C(27B)-H(27D)	109.5
C(26B)-C(27B)-H(27E)	109.5
H(27D)-C(27B)-H(27E)	109.5
C(26B)-C(27B)-H(27F)	109.5
H(27D)-C(27B)-H(27F)	109.5
H(27E)-C(27B)-H(27F)	109.5
C(26B)-C(28B)-H(28D)	109.5
C(26B)-C(28B)-H(28E)	109.5
H(28D)-C(28B)-H(28E)	109.5
C(26B)-C(28B)-H(28F)	109.5
H(28D)-C(28B)-H(28F)	109.5
H(28E)-C(28B)-H(28F)	109.5
C(30B)-C(29B)-C(34B)	117.0(7)
C(30B)-C(29B)-C(26B)	121.9(6)
C(34B)-C(29B)-C(26B)	121.1(6)
C(29B)-C(30B)-C(31B)	123.3(6)
C(29B)-C(30B)-H(30B)	118.3
C(31B)-C(30B)-H(30B)	118.3

C(32B)-C(31B)-C(30B)	119.7(7)
C(32B)-C(31B)-H(31B)	120.1
C(30B)-C(31B)-H(31B)	120.1
C(31B)-C(32B)-C(33B)	118.1(7)
C(31B)-C(32B)-H(32B)	121.0
C(33B)-C(32B)-H(32B)	121.0
C(32B)-C(33B)-C(34B)	120.9(7)
C(32B)-C(33B)-H(33B)	119.5
C(34B)-C(33B)-H(33B)	119.5
C(29B)-C(34B)-C(33B)	120.7(7)
C(29B)-C(34B)-H(34B)	119.6
C(33B)-C(34B)-H(34B)	119.6
N(4B)-C(35B)-N(5B)	112.0(5)
N(4B)-C(35B)-H(35B)	123(3)
N(5B)-C(35B)-H(35B)	124(3)
N(4B)-C(36B)-C(37B)	101.6(5)
N(4B)-C(36B)-H(36C)	111.5
C(37B)-C(36B)-H(36C)	111.5
N(4B)-C(36B)-H(36D)	111.5
C(37B)-C(36B)-H(36D)	111.5
H(36C)-C(36B)-H(36D)	109.3
N(5B)-C(37B)-C(36B)	103.7(5)
N(5B)-C(37B)-H(37C)	111.0
C(36B)-C(37B)-H(37C)	111.0
N(5B)-C(37B)-H(37D)	111.0
C(36B)-C(37B)-H(37D)	111.0
H(37C)-C(37B)-H(37D)	109.0
C(39B)-C(38B)-C(43B)	122.5(6)
C(39B)-C(38B)-N(4B)	119.7(5)
C(43B)-C(38B)-N(4B)	117.8(6)
C(38B)-C(39B)-C(40B)	117.6(6)
C(38B)-C(39B)-C(44B)	122.5(5)
C(40B)-C(39B)-C(44B)	119.9(6)
C(41B)-C(40B)-C(39B)	121.4(6)
C(41B)-C(40B)-H(40B)	119.3
C(39B)-C(40B)-H(40B)	119.3
C(42B)-C(41B)-C(40B)	118.6(6)
C(42B)-C(41B)-C(45B)	120.8(5)
C(40B)-C(41B)-C(45B)	120.6(6)
C(43B)-C(42B)-C(41B)	121.7(6)
C(43B)-C(42B)-H(42B)	119.1
C(41B)-C(42B)-H(42B)	119.1
C(42B)-C(43B)-C(38B)	118.1(6)
C(42B)-C(43B)-C(46B)	121.3(6)
C(38B)-C(43B)-C(46B)	120.6(6)
C(39B)-C(44B)-H(44D)	109.5
C(39B)-C(44B)-H(44E)	109.5
H(44D)-C(44B)-H(44E)	109.5
C(39B)-C(44B)-H(44F)	109.5
H(44D)-C(44B)-H(44F)	109.5

H(44E)-C(44B)-H(44F)	109.5
C(41B)-C(45B)-H(45D)	109.5
C(41B)-C(45B)-H(45E)	109.5
H(45D)-C(45B)-H(45E)	109.5
C(41B)-C(45B)-H(45F)	109.5
H(45D)-C(45B)-H(45F)	109.5
H(45E)-C(45B)-H(45F)	109.5
C(43B)-C(46B)-H(46D)	109.5
C(43B)-C(46B)-H(46E)	109.5
H(46D)-C(46B)-H(46E)	109.5
C(43B)-C(46B)-H(46F)	109.5
H(46D)-C(46B)-H(46F)	109.5
H(46E)-C(46B)-H(46F)	109.5
C(48B)-C(47B)-C(52B)	125.8(7)
C(48B)-C(47B)-N(5B)	118.9(7)
C(52B)-C(47B)-N(5B)	115.2(7)
C(47B)-C(48B)-C(49B)	117.3(8)
C(47B)-C(48B)-C(53B)	122.8(6)
C(49B)-C(48B)-C(53B)	119.9(7)
C(48B)-C(49B)-C(50B)	119.4(8)
C(48B)-C(49B)-H(49B)	120.3
C(50B)-C(49B)-H(49B)	120.3
C(51B)-C(50B)-C(49B)	121.2(7)
C(51B)-C(50B)-C(54B)	118.5(10)
C(49B)-C(50B)-C(54B)	120.2(10)
C(50B)-C(51B)-C(52B)	119.7(8)
C(50B)-C(51B)-H(51B)	120.1
C(52B)-C(51B)-H(51B)	120.1
C(47B)-C(52B)-C(51B)	116.5(8)
C(47B)-C(52B)-C(55B)	125.1(7)
C(51B)-C(52B)-C(55B)	118.3(8)
C(48B)-C(53B)-H(53D)	109.5
C(48B)-C(53B)-H(53E)	109.5
H(53D)-C(53B)-H(53E)	109.5
C(48B)-C(53B)-H(53F)	109.5
H(53D)-C(53B)-H(53F)	109.5
H(53E)-C(53B)-H(53F)	109.5
C(50B)-C(54B)-H(54D)	109.5
C(50B)-C(54B)-H(54E)	109.5
H(54D)-C(54B)-H(54E)	109.5
C(50B)-C(54B)-H(54F)	109.5
H(54D)-C(54B)-H(54F)	109.5
H(54E)-C(54B)-H(54F)	109.5
C(52B)-C(55B)-H(55D)	109.5
C(52B)-C(55B)-H(55E)	109.5
H(55D)-C(55B)-H(55E)	109.5
C(52B)-C(55B)-H(55F)	109.5
H(55D)-C(55B)-H(55F)	109.5
H(55E)-C(55B)-H(55F)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 30.4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **30**. The anisotropic displacement factor exponent takes the form: $-2\ \pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1A)	42(1)	25(1)	20(1)	-5(1)	0(1)	4(1)
N(1A)	43(4)	21(2)	20(3)	11(2)	0(3)	-6(2)
C(1A)	35(4)	20(3)	22(4)	-3(2)	5(3)	-10(3)
N(2A)	46(4)	30(3)	16(3)	-7(2)	9(3)	-7(2)
C(2A)	35(4)	23(3)	24(4)	2(3)	-3(3)	-2(3)
C(3A)	44(5)	21(3)	36(4)	-2(3)	0(3)	3(3)
N(3A)	88(5)	40(3)	26(3)	-7(2)	-13(3)	31(3)
N(4A)	27(3)	24(2)	17(3)	4(2)	3(3)	-6(2)
C(4A)	35(4)	26(3)	33(4)	-9(3)	3(3)	-3(3)
N(5A)	32(3)	26(3)	12(3)	-4(2)	8(2)	-10(2)
C(5A)	43(4)	30(3)	30(4)	-9(3)	10(3)	-7(3)
C(6A)	35(4)	26(3)	22(4)	0(3)	3(3)	-3(3)
C(7A)	80(6)	20(3)	27(4)	0(3)	5(4)	3(3)
C(8A)	96(6)	78(5)	44(4)	13(4)	2(4)	-31(4)
C(9A)	72(6)	70(5)	47(5)	24(4)	16(4)	-2(4)
C(10A)	56(5)	30(3)	25(4)	-1(3)	6(3)	7(3)
C(11A)	70(5)	51(4)	88(5)	30(4)	26(4)	-9(4)
C(12A)	99(5)	69(4)	49(4)	8(3)	2(4)	16(4)
C(13A)	44(4)	23(3)	48(5)	-16(3)	16(4)	-13(3)
C(14A)	68(5)	31(3)	28(3)	3(3)	12(3)	6(3)
C(15A)	59(5)	28(3)	30(4)	0(3)	0(3)	12(3)
C(16A)	50(5)	15(3)	24(4)	-6(2)	-5(3)	7(3)
C(17A)	96(7)	49(4)	46(5)	-22(4)	39(5)	-31(4)
C(18A)	38(4)	18(3)	31(4)	3(3)	0(3)	0(3)
C(19A)	144(11)	94(8)	17(4)	-14(4)	-20(6)	35(7)
C(20A)	86(5)	26(3)	41(4)	5(3)	-14(4)	11(3)
C(21A)	100(6)	49(4)	59(5)	6(4)	-5(4)	-14(4)
C(22A)	94(6)	29(3)	29(4)	1(3)	-5(4)	-13(4)
C(23A)	94(6)	78(5)	69(5)	-16(4)	-20(5)	51(5)
C(24A)	97(8)	49(5)	55(6)	-2(4)	10(5)	-22(5)
C(25A)	36(4)	60(4)	36(4)	-18(3)	4(3)	10(3)
C(26A)	35(5)	130(8)	37(5)	-30(5)	4(4)	14(5)
C(27A)	83(6)	128(7)	107(6)	-22(5)	24(5)	2(5)
C(28A)	71(6)	90(7)	60(6)	-33(5)	9(5)	-20(5)
C(29A)	37(6)	147(10)	77(8)	-45(7)	-7(5)	30(6)
C(30A)	57(5)	89(6)	57(5)	12(5)	-6(4)	-13(5)
C(31A)	65(6)	91(7)	56(5)	-1(5)	11(5)	-16(5)
C(32A)	57(6)	76(6)	80(6)	17(5)	-5(5)	-14(5)
C(33A)	55(6)	116(8)	73(6)	9(6)	-15(5)	8(5)
C(34A)	62(7)	165(11)	53(6)	1(6)	-5(5)	15(6)
C(35A)	41(5)	19(3)	18(4)	-3(2)	-4(3)	-2(3)

C(36A)	27(4)	33(3)	24(4)	-1(3)	0(3)	-1(3)
C(37A)	39(4)	28(3)	24(4)	-10(3)	5(3)	0(3)
C(38A)	24(4)	33(3)	31(4)	-9(3)	-1(3)	-3(3)
C(39A)	43(4)	28(3)	31(4)	3(3)	10(3)	-10(3)
C(40A)	46(5)	36(4)	36(4)	0(3)	12(4)	-7(3)
C(41A)	49(5)	43(4)	44(4)	-9(3)	28(4)	-6(3)
C(42A)	27(4)	65(5)	40(5)	-21(4)	-7(3)	-3(3)
C(43A)	52(5)	29(3)	43(4)	-10(3)	-2(4)	-1(3)
C(44A)	67(5)	37(4)	36(4)	9(3)	-9(4)	0(3)
C(45A)	58(5)	60(5)	75(6)	-22(4)	28(4)	-32(4)
C(46A)	59(6)	56(5)	67(6)	-2(4)	-27(5)	-2(4)
C(47A)	32(4)	17(3)	25(4)	-4(2)	2(3)	-9(3)
C(48A)	31(4)	14(3)	28(4)	-4(2)	0(3)	-3(2)
C(49A)	24(4)	21(3)	32(4)	-7(3)	3(3)	0(2)
C(50A)	32(4)	21(3)	36(4)	-5(3)	11(4)	-9(3)
C(51A)	43(5)	13(3)	23(4)	-2(2)	0(3)	-3(3)
C(52A)	28(4)	22(3)	24(4)	-8(2)	1(3)	2(2)
C(53A)	33(4)	32(3)	41(5)	7(3)	7(4)	4(3)
C(54A)	40(5)	22(3)	61(5)	4(3)	20(4)	-5(3)
C(55A)	38(5)	46(4)	25(4)	9(3)	7(3)	-3(3)
Mo(1B)	28(1)	17(1)	21(1)	0(1)	5(1)	-2(1)
N(1B)	30(3)	15(2)	23(3)	4(2)	7(2)	-7(2)
C(1B)	20(4)	24(3)	29(4)	2(3)	0(3)	-3(2)
N(2B)	26(3)	13(2)	25(3)	1(2)	1(2)	3(2)
C(2B)	40(4)	19(3)	41(4)	-3(3)	4(4)	2(3)
N(3B)	25(3)	20(2)	18(3)	2(2)	1(2)	-7(2)
C(3B)	45(5)	16(3)	42(5)	2(3)	0(4)	-1(3)
N(4B)	28(3)	25(3)	27(3)	2(2)	-4(3)	4(2)
C(4B)	52(5)	18(3)	61(5)	17(3)	12(4)	0(3)
N(5B)	33(4)	33(3)	24(3)	13(2)	7(3)	8(2)
C(5B)	59(5)	28(3)	24(4)	10(3)	10(3)	6(3)
C(6B)	38(4)	16(3)	33(4)	0(2)	6(3)	6(3)
C(7B)	72(6)	20(3)	35(4)	0(3)	7(4)	-7(3)
C(8B)	70(6)	78(6)	47(5)	-34(4)	-26(4)	27(5)
C(9B)	60(6)	75(6)	53(5)	-2(4)	16(4)	-20(5)
C(10B)	56(5)	25(3)	22(3)	3(2)	3(3)	-1(3)
C(11B)	70(6)	53(4)	31(4)	4(3)	-5(4)	-15(4)
C(12B)	58(5)	35(4)	65(5)	-6(3)	28(4)	9(3)
C(13B)	34(4)	21(3)	24(4)	3(2)	13(3)	0(2)
C(14B)	44(4)	30(3)	22(3)	-3(3)	-5(3)	-3(3)
C(15B)	65(5)	26(3)	21(4)	-10(3)	6(3)	6(3)
C(16B)	41(4)	24(3)	15(3)	4(2)	13(3)	8(3)
C(17B)	35(4)	27(3)	24(4)	8(3)	6(3)	-9(3)
C(18B)	44(4)	43(4)	26(3)	7(3)	14(3)	11(3)
C(19B)	45(4)	24(3)	23(4)	-4(3)	11(3)	1(3)
C(20B)	49(4)	14(3)	26(3)	-1(2)	-1(3)	0(3)
C(21B)	35(4)	26(3)	22(3)	0(2)	0(3)	-7(3)
C(22B)	24(3)	26(3)	22(3)	1(2)	-4(3)	-3(2)
C(23B)	38(4)	23(3)	55(5)	-5(3)	17(4)	-2(3)
C(24B)	39(4)	38(3)	21(3)	4(3)	1(3)	-7(3)

C(25B)	59(4)	12(3)	29(3)	4(2)	23(3)	1(3)
C(26B)	32(4)	30(3)	36(4)	7(3)	13(3)	1(3)
C(27B)	44(4)	42(4)	54(5)	21(3)	-3(4)	7(3)
C(28B)	42(5)	59(5)	39(4)	8(3)	-5(4)	-5(4)
C(29B)	30(4)	39(4)	67(5)	13(3)	4(4)	14(3)
C(30B)	42(4)	31(3)	42(4)	4(3)	12(3)	-2(3)
C(31B)	47(5)	46(4)	56(4)	12(3)	-5(4)	10(3)
C(32B)	41(5)	89(6)	62(5)	4(4)	8(4)	5(4)
C(33B)	63(6)	92(7)	82(6)	13(5)	22(5)	42(5)
C(34B)	61(5)	43(4)	65(5)	10(4)	25(4)	3(4)
C(35B)	18(3)	24(3)	21(4)	-4(2)	3(3)	1(2)
C(36B)	37(4)	33(3)	19(3)	8(2)	4(3)	7(3)
C(37B)	46(5)	36(3)	22(4)	14(3)	9(4)	8(3)
C(38B)	35(4)	16(3)	20(4)	2(2)	7(3)	3(3)
C(39B)	38(4)	13(3)	29(4)	2(2)	8(3)	1(3)
C(40B)	33(4)	18(3)	33(4)	5(2)	-2(3)	6(3)
C(41B)	36(4)	19(3)	22(4)	2(2)	-1(3)	0(3)
C(42B)	35(4)	29(3)	20(4)	-4(2)	1(3)	-2(3)
C(43B)	30(4)	30(3)	21(4)	6(3)	3(3)	-1(3)
C(44B)	34(4)	36(3)	31(4)	-13(3)	-1(3)	4(3)
C(45B)	35(4)	44(4)	33(4)	-6(3)	9(3)	7(3)
C(46B)	35(5)	58(4)	28(4)	-1(3)	-2(3)	-2(3)
C(47B)	31(4)	59(4)	29(4)	21(4)	11(3)	22(3)
C(48B)	50(5)	61(5)	17(3)	8(3)	8(3)	30(4)
C(49B)	73(6)	77(5)	35(4)	15(4)	31(5)	43(5)
C(50B)	31(5)	129(8)	44(5)	51(6)	24(4)	43(5)
C(51B)	17(4)	126(8)	44(5)	22(5)	7(4)	5(4)
C(52B)	17(4)	89(6)	38(4)	36(4)	0(3)	-3(4)
C(53B)	96(7)	52(4)	27(4)	-5(3)	13(4)	35(4)
C(54B)	64(5)	104(5)	84(5)	31(4)	18(4)	40(4)
C(55B)	45(5)	78(6)	70(6)	8(5)	-25(4)	-21(4)

Table 30.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **30**.

	x	y	z	U(eq)
H(3A)	1913	3169	1700	40
H(4A)	2200	3197	651	38
H(5A)	2080	4801	74	41
H(7A)	1281	5402	2586	51
H(8A1)	2343	3875	2751	109
H(8A2)	1964	4379	3333	109
H(8A3)	2386	5151	2891	109
H(9A1)	1182	3076	2580	94
H(9A2)	599	3819	2263	94
H(9A3)	777	3894	3008	94

H(10A)	1543	7362	636	44
H(11A)	2806	6682	191	103
H(11B)	2710	7418	804	103
H(11C)	2516	7889	113	103
H(12A)	1784	6071	-448	108
H(12B)	1611	7339	-485	108
H(12C)	1066	6496	-249	108
H(14A)	975	5890	4433	50
H(15A)	2106	6820	4322	47
H(17A)	-152	5846	3737	94
H(17B)	59	5661	3025	94
H(17C)	-224	6815	3235	94
H(18A)	2662	8010	3450	44
H(18B)	2106	8733	3077	44
H(18C)	2368	7638	2766	44
H(20A)	770	11698	1718	62
H(21A)	1967	11326	1519	84
H(23A)	-255	9448	1643	122
H(23B)	-278	10590	2002	122
H(23C)	-91	9508	2391	122
H(24A)	2614	9385	1293	101
H(24B)	2272	8329	1577	101
H(24C)	2664	9166	2040	101
H(27A)	-1396	6491	1983	158
H(27B)	-1251	7748	1859	158
H(27C)	-911	7157	2468	158
H(28A)	-340	5229	2059	110
H(28B)	31	5329	1407	110
H(28C)	-768	5189	1398	110
H(30A)	295	6510	676	82
H(31A)	129	7012	-384	85
H(32A)	-844	7899	-739	86
H(33A)	-1590	8485	39	98
H(34A)	-1471	7790	1072	113
H(35A)	790(30)	8520(50)	4110(30)	31
H(36A)	204	9297	5705	34
H(36B)	-207	10071	5207	34
H(37A)	744	10998	5049	36
H(37B)	1161	10194	5525	36
H(40A)	-612	5465	5276	47
H(42A)	-1710	7263	4031	53
H(44A)	755	7273	5430	71
H(44B)	529	6051	5562	71
H(44C)	268	7018	5991	71
H(45A)	-2177	5621	4396	95
H(45B)	-1830	5034	5003	95
H(45C)	-1587	4762	4310	95
H(46A)	-743	9652	4157	92
H(46B)	-1402	9146	3809	92
H(46C)	-681	8931	3533	92

H(49A)	3240	10328	4156	31
H(51A)	1802	11533	2953	32
H(53A)	2976	9032	4940	53
H(53B)	2211	8683	5016	53
H(53C)	2501	9753	5361	53
H(54A)	3056	11235	2667	61
H(54B)	3561	11354	3276	61
H(54C)	3042	12308	3093	61
H(55A)	509	10190	3331	54
H(55B)	675	11420	3153	54
H(55C)	462	11125	3852	54
H(3B)	4549	-1719	3476	41
H(4B)	4409	-1725	4567	52
H(5B)	4565	-148	5147	44
H(7B)	4900	622	2537	51
H(8B1)	4337	-611	1865	99
H(8B2)	3855	-265	2414	99
H(8B3)	4226	-1417	2444	99
H(9B1)	5468	-1478	2686	93
H(9B2)	5875	-364	2772	93
H(9B3)	5558	-699	2090	93
H(10B)	5056	2445	4547	41
H(11D)	5390	2384	5632	78
H(11E)	5799	1510	5246	78
H(11F)	5191	1127	5658	78
H(12D)	3899	2350	4658	78
H(12E)	4265	2928	5259	78
H(12F)	4021	1695	5307	78
H(14B)	4635	1675	885	39
H(15B)	5828	975	909	44
H(17D)	4170	2572	2399	43
H(17E)	3917	2816	1683	43
H(17F)	4377	3682	2066	43
H(18D)	6674	1096	2370	56
H(18E)	6870	2279	2127	56
H(18F)	6919	1254	1667	56
H(20B)	4319	6353	3705	36
H(21B)	5525	6929	3562	33
H(23D)	3885	3932	3098	58
H(23E)	3710	4447	3765	58
H(23F)	4180	3396	3743	58
H(24D)	6614	5978	3196	49
H(24E)	6514	4793	2896	49
H(24F)	6685	4928	3639	49
H(27D)	6761	502	3519	71
H(27E)	6309	918	4074	71
H(27F)	7088	665	4219	71
H(28D)	7368	2442	4634	71
H(28E)	6579	2682	4592	71
H(28F)	7086	3506	4278	71

H(30B)	7543	3809	3252	46
H(31B)	8581	4023	2817	60
H(32B)	9231	2506	2615	77
H(33B)	8824	789	2882	94
H(34B)	7810	616	3388	67
H(35B)	5730(30)	3400(40)	1170(30)	15(13)
H(36C)	5644	5953	67	35
H(36D)	5265	4985	-322	35
H(37C)	6268	4239	-483	42
H(37D)	6640	5145	-41	42
H(40B)	3266	5175	1096	34
H(42B)	4688	6546	2257	34
H(44D)	4105	4577	-135	51
H(44E)	3529	4021	256	51
H(44F)	4266	3502	269	51
H(45D)	2909	6097	2011	56
H(45E)	3319	7212	2075	56
H(45F)	3451	6269	2587	56
H(46D)	5839	6587	1972	61
H(46E)	6041	6046	1320	61
H(46F)	5989	5313	1941	61
H(49B)	7490	816	54	73
H(51B)	8321	2888	1377	74
H(53D)	5936	2195	-161	87
H(53E)	6310	1080	-306	87
H(53F)	6464	2146	-706	87
H(54D)	8978	1265	674	126
H(54E)	8464	270	701	126
H(54F)	8669	935	1332	126
H(55D)	7259	5030	1099	98
H(55E)	7844	4557	1566	98
H(55F)	7075	4324	1701	98

Table 30.6. Torsion angles [°] for **30**.

C(25A)-Mo(1A)-N(1A)-C(1A)	-22.9(10)
N(2A)-Mo(1A)-N(1A)-C(1A)	89.7(10)
N(3A)-Mo(1A)-N(1A)-C(1A)	-136.3(9)
Mo(1A)-N(1A)-C(1A)-C(6A)	115.7(9)
Mo(1A)-N(1A)-C(1A)-C(2A)	-69.1(12)
C(25A)-Mo(1A)-N(2A)-C(16A)	178.5(4)
N(1A)-Mo(1A)-N(2A)-C(16A)	64.1(4)
N(3A)-Mo(1A)-N(2A)-C(16A)	-64.7(5)
C(25A)-Mo(1A)-N(2A)-C(13A)	20.8(6)
N(1A)-Mo(1A)-N(2A)-C(13A)	-93.7(6)
N(3A)-Mo(1A)-N(2A)-C(13A)	137.6(5)
N(1A)-C(1A)-C(2A)-C(3A)	-173.3(6)
C(6A)-C(1A)-C(2A)-C(3A)	2.0(10)
N(1A)-C(1A)-C(2A)-C(7A)	8.5(10)

C(6A)-C(1A)-C(2A)-C(7A)	-176.2(7)
C(1A)-C(2A)-C(3A)-C(4A)	-0.7(11)
C(7A)-C(2A)-C(3A)-C(4A)	177.5(7)
C(25A)-Mo(1A)-N(3A)-C(19A)	38.2(7)
N(1A)-Mo(1A)-N(3A)-C(19A)	153.8(6)
N(2A)-Mo(1A)-N(3A)-C(19A)	-78.9(7)
C(25A)-Mo(1A)-N(3A)-C(22A)	-155.5(5)
N(1A)-Mo(1A)-N(3A)-C(22A)	-39.9(6)
N(2A)-Mo(1A)-N(3A)-C(22A)	87.4(6)
C(2A)-C(3A)-C(4A)-C(5A)	-2.0(11)
C(3A)-C(4A)-C(5A)-C(6A)	3.4(11)
C(4A)-C(5A)-C(6A)-C(1A)	-2.1(11)
C(4A)-C(5A)-C(6A)-C(10A)	174.0(6)
N(1A)-C(1A)-C(6A)-C(5A)	174.6(6)
C(2A)-C(1A)-C(6A)-C(5A)	-0.6(10)
N(1A)-C(1A)-C(6A)-C(10A)	-1.4(10)
C(2A)-C(1A)-C(6A)-C(10A)	-176.7(6)
C(3A)-C(2A)-C(7A)-C(8A)	72.0(8)
C(1A)-C(2A)-C(7A)-C(8A)	-109.9(7)
C(3A)-C(2A)-C(7A)-C(9A)	-50.3(10)
C(1A)-C(2A)-C(7A)-C(9A)	127.9(7)
C(5A)-C(6A)-C(10A)-C(12A)	41.5(9)
C(1A)-C(6A)-C(10A)-C(12A)	-142.4(7)
C(5A)-C(6A)-C(10A)-C(11A)	-77.6(8)
C(1A)-C(6A)-C(10A)-C(11A)	98.4(8)
C(16A)-N(2A)-C(13A)-C(14A)	1.9(7)
Mo(1A)-N(2A)-C(13A)-C(14A)	161.7(5)
C(16A)-N(2A)-C(13A)-C(17A)	-178.9(6)
Mo(1A)-N(2A)-C(13A)-C(17A)	-19.0(9)
N(2A)-C(13A)-C(14A)-C(15A)	-1.6(7)
C(17A)-C(13A)-C(14A)-C(15A)	179.2(6)
C(13A)-C(14A)-C(15A)-C(16A)	0.8(7)
C(14A)-C(15A)-C(16A)-N(2A)	0.4(7)
C(14A)-C(15A)-C(16A)-C(18A)	-176.5(6)
C(13A)-N(2A)-C(16A)-C(15A)	-1.4(6)
Mo(1A)-N(2A)-C(16A)-C(15A)	-164.7(4)
C(13A)-N(2A)-C(16A)-C(18A)	175.9(5)
Mo(1A)-N(2A)-C(16A)-C(18A)	12.5(7)
C(22A)-N(3A)-C(19A)-C(20A)	1.7(9)
Mo(1A)-N(3A)-C(19A)-C(20A)	169.1(5)
C(22A)-N(3A)-C(19A)-C(23A)	178.2(8)
Mo(1A)-N(3A)-C(19A)-C(23A)	-14.3(12)
N(3A)-C(19A)-C(20A)-C(21A)	-0.1(10)
C(23A)-C(19A)-C(20A)-C(21A)	-176.5(9)
C(19A)-C(20A)-C(21A)-C(22A)	-1.5(10)
C(20A)-C(21A)-C(22A)-C(24A)	178.8(9)
C(20A)-C(21A)-C(22A)-N(3A)	2.3(9)
C(19A)-N(3A)-C(22A)-C(21A)	-2.5(9)
Mo(1A)-N(3A)-C(22A)-C(21A)	-170.8(5)
C(19A)-N(3A)-C(22A)-C(24A)	-179.1(8)

Mo(1A)-N(3A)-C(22A)-C(24A)	12.7(11)
N(1A)-Mo(1A)-C(25A)-C(26A)	-2(2)
N(2A)-Mo(1A)-C(25A)-C(26A)	-116(2)
N(3A)-Mo(1A)-C(25A)-C(26A)	116(2)
Mo(1A)-C(25A)-C(26A)-C(29A)	-76(3)
Mo(1A)-C(25A)-C(26A)-C(27A)	164(2)
Mo(1A)-C(25A)-C(26A)-C(28A)	44(3)
C(27A)-C(26A)-C(29A)-C(30A)	-172.8(10)
C(25A)-C(26A)-C(29A)-C(30A)	69.2(12)
C(28A)-C(26A)-C(29A)-C(30A)	-50.8(12)
C(27A)-C(26A)-C(29A)-C(34A)	-5.7(15)
C(25A)-C(26A)-C(29A)-C(34A)	-123.7(10)
C(28A)-C(26A)-C(29A)-C(34A)	116.3(11)
C(34A)-C(29A)-C(30A)-C(31A)	5.6(16)
C(26A)-C(29A)-C(30A)-C(31A)	172.6(9)
C(29A)-C(30A)-C(31A)-C(32A)	-2.4(14)
C(30A)-C(31A)-C(32A)-C(33A)	3.1(13)
C(31A)-C(32A)-C(33A)-C(34A)	-7.1(14)
C(30A)-C(29A)-C(34A)-C(33A)	-9.5(17)
C(26A)-C(29A)-C(34A)-C(33A)	-176.7(10)
C(32A)-C(33A)-C(34A)-C(29A)	10.5(16)
C(47A)-N(5A)-C(35A)-N(4A)	-165.6(6)
C(37A)-N(5A)-C(35A)-N(4A)	0.3(8)
C(38A)-N(4A)-C(35A)-N(5A)	-177.6(6)
C(36A)-N(4A)-C(35A)-N(5A)	1.2(7)
C(35A)-N(4A)-C(36A)-C(37A)	-2.1(7)
C(38A)-N(4A)-C(36A)-C(37A)	176.8(6)
C(35A)-N(5A)-C(37A)-C(36A)	-1.6(7)
C(47A)-N(5A)-C(37A)-C(36A)	164.9(6)
N(4A)-C(36A)-C(37A)-N(5A)	2.1(6)
C(35A)-N(4A)-C(38A)-C(43A)	-87.7(8)
C(36A)-N(4A)-C(38A)-C(43A)	93.6(8)
C(35A)-N(4A)-C(38A)-C(39A)	93.3(8)
C(36A)-N(4A)-C(38A)-C(39A)	-85.4(7)
C(43A)-C(38A)-C(39A)-C(40A)	3.2(10)
N(4A)-C(38A)-C(39A)-C(40A)	-177.7(6)
C(43A)-C(38A)-C(39A)-C(44A)	-179.9(6)
N(4A)-C(38A)-C(39A)-C(44A)	-0.9(10)
C(38A)-C(39A)-C(40A)-C(41A)	-4.4(10)
C(44A)-C(39A)-C(40A)-C(41A)	178.7(6)
C(39A)-C(40A)-C(41A)-C(42A)	2.2(10)
C(39A)-C(40A)-C(41A)-C(45A)	-178.9(6)
C(40A)-C(41A)-C(42A)-C(43A)	1.2(10)
C(45A)-C(41A)-C(42A)-C(43A)	-177.7(7)
N(4A)-C(38A)-C(43A)-C(42A)	-179.0(6)
C(39A)-C(38A)-C(43A)-C(42A)	0.0(10)
N(4A)-C(38A)-C(43A)-C(46A)	1.3(10)
C(39A)-C(38A)-C(43A)-C(46A)	-179.6(7)
C(41A)-C(42A)-C(43A)-C(38A)	-2.3(11)
C(41A)-C(42A)-C(43A)-C(46A)	177.4(7)

C(35A)-N(5A)-C(47A)-C(52A)	71.4(8)
C(37A)-N(5A)-C(47A)-C(52A)	-92.7(7)
C(35A)-N(5A)-C(47A)-C(48A)	-109.9(7)
C(37A)-N(5A)-C(47A)-C(48A)	86.0(7)
C(52A)-C(47A)-C(48A)-C(49A)	-0.4(8)
N(5A)-C(47A)-C(48A)-C(49A)	-179.1(5)
C(52A)-C(47A)-C(48A)-C(53A)	-178.6(5)
N(5A)-C(47A)-C(48A)-C(53A)	2.7(8)
C(47A)-C(48A)-C(49A)-C(50A)	0.1(8)
C(53A)-C(48A)-C(49A)-C(50A)	178.2(5)
C(48A)-C(49A)-C(50A)-C(51A)	-0.2(9)
C(48A)-C(49A)-C(50A)-C(54A)	179.0(6)
C(49A)-C(50A)-C(51A)-C(52A)	0.6(8)
C(54A)-C(50A)-C(51A)-C(52A)	-178.7(5)
C(48A)-C(47A)-C(52A)-C(51A)	0.9(8)
N(5A)-C(47A)-C(52A)-C(51A)	179.6(5)
C(48A)-C(47A)-C(52A)-C(55A)	-178.9(5)
N(5A)-C(47A)-C(52A)-C(55A)	-0.1(8)
C(50A)-C(51A)-C(52A)-C(47A)	-0.9(8)
C(50A)-C(51A)-C(52A)-C(55A)	178.8(5)
C(25B)-Mo(1B)-N(1B)-C(1B)	-18.2(11)
N(2B)-Mo(1B)-N(1B)-C(1B)	91.3(10)
N(3B)-Mo(1B)-N(1B)-C(1B)	-132.9(10)
Mo(1B)-N(1B)-C(1B)-C(2B)	-85.1(12)
Mo(1B)-N(1B)-C(1B)-C(6B)	99.5(11)
C(25B)-Mo(1B)-N(2B)-C(13B)	175.2(4)
N(1B)-Mo(1B)-N(2B)-C(13B)	62.3(4)
N(3B)-Mo(1B)-N(2B)-C(13B)	-67.7(4)
C(25B)-Mo(1B)-N(2B)-C(16B)	17.1(5)
N(1B)-Mo(1B)-N(2B)-C(16B)	-95.8(5)
N(3B)-Mo(1B)-N(2B)-C(16B)	134.2(5)
N(1B)-C(1B)-C(2B)-C(3B)	-174.9(6)
C(6B)-C(1B)-C(2B)-C(3B)	0.5(10)
N(1B)-C(1B)-C(2B)-C(7B)	4.0(10)
C(6B)-C(1B)-C(2B)-C(7B)	179.5(7)
C(25B)-Mo(1B)-N(3B)-C(19B)	-150.2(5)
N(1B)-Mo(1B)-N(3B)-C(19B)	-33.7(6)
N(2B)-Mo(1B)-N(3B)-C(19B)	93.5(5)
C(25B)-Mo(1B)-N(3B)-C(22B)	37.2(5)
N(1B)-Mo(1B)-N(3B)-C(22B)	153.8(5)
N(2B)-Mo(1B)-N(3B)-C(22B)	-79.0(5)
C(1B)-C(2B)-C(3B)-C(4B)	-0.1(11)
C(7B)-C(2B)-C(3B)-C(4B)	-179.1(7)
C(2B)-C(3B)-C(4B)-C(5B)	-0.3(11)
C(3B)-C(4B)-C(5B)-C(6B)	0.3(11)
C(4B)-C(5B)-C(6B)-C(1B)	0.1(11)
C(4B)-C(5B)-C(6B)-C(10B)	178.2(7)
C(2B)-C(1B)-C(6B)-C(5B)	-0.5(10)
N(1B)-C(1B)-C(6B)-C(5B)	174.9(6)
C(2B)-C(1B)-C(6B)-C(10B)	-178.5(6)

N(1B)-C(1B)-C(6B)-C(10B)	-3.1(10)
C(3B)-C(2B)-C(7B)-C(9B)	-73.4(8)
C(1B)-C(2B)-C(7B)-C(9B)	107.6(7)
C(3B)-C(2B)-C(7B)-C(8B)	50.6(9)
C(1B)-C(2B)-C(7B)-C(8B)	-128.4(7)
C(5B)-C(6B)-C(10B)-C(12B)	-69.8(8)
C(1B)-C(6B)-C(10B)-C(12B)	108.2(7)
C(5B)-C(6B)-C(10B)-C(11B)	53.7(9)
C(1B)-C(6B)-C(10B)-C(11B)	-128.3(7)
C(16B)-N(2B)-C(13B)-C(14B)	-0.6(6)
Mo(1B)-N(2B)-C(13B)-C(14B)	-164.0(4)
C(16B)-N(2B)-C(13B)-C(17B)	177.7(5)
Mo(1B)-N(2B)-C(13B)-C(17B)	14.3(7)
N(2B)-C(13B)-C(14B)-C(15B)	0.9(7)
C(17B)-C(13B)-C(14B)-C(15B)	-177.2(6)
C(13B)-C(14B)-C(15B)-C(16B)	-0.9(7)
C(14B)-C(15B)-C(16B)-N(2B)	0.5(7)
C(14B)-C(15B)-C(16B)-C(18B)	-179.7(6)
C(13B)-N(2B)-C(16B)-C(15B)	0.0(6)
Mo(1B)-N(2B)-C(16B)-C(15B)	160.0(4)
C(13B)-N(2B)-C(16B)-C(18B)	-179.8(5)
Mo(1B)-N(2B)-C(16B)-C(18B)	-19.8(8)
C(22B)-N(3B)-C(19B)-C(20B)	1.6(7)
Mo(1B)-N(3B)-C(19B)-C(20B)	-172.2(4)
C(22B)-N(3B)-C(19B)-C(23B)	178.6(6)
Mo(1B)-N(3B)-C(19B)-C(23B)	4.8(9)
N(3B)-C(19B)-C(20B)-C(21B)	-1.3(7)
C(23B)-C(19B)-C(20B)-C(21B)	-178.1(7)
C(19B)-C(20B)-C(21B)-C(22B)	0.5(7)
C(19B)-N(3B)-C(22B)-C(21B)	-1.3(7)
Mo(1B)-N(3B)-C(22B)-C(21B)	172.4(4)
C(19B)-N(3B)-C(22B)-C(24B)	178.1(6)
Mo(1B)-N(3B)-C(22B)-C(24B)	-8.2(9)
C(20B)-C(21B)-C(22B)-N(3B)	0.5(7)
C(20B)-C(21B)-C(22B)-C(24B)	-178.8(6)
N(1B)-Mo(1B)-C(25B)-C(26B)	-9.7(13)
N(2B)-Mo(1B)-C(25B)-C(26B)	-121.1(13)
N(3B)-Mo(1B)-C(25B)-C(26B)	109.8(13)
Mo(1B)-C(25B)-C(26B)-C(27B)	34.2(15)
Mo(1B)-C(25B)-C(26B)-C(28B)	-82.3(14)
Mo(1B)-C(25B)-C(26B)-C(29B)	158.5(11)
C(27B)-C(26B)-C(29B)-C(30B)	177.9(7)
C(28B)-C(26B)-C(29B)-C(30B)	-62.5(9)
C(25B)-C(26B)-C(29B)-C(30B)	56.5(9)
C(27B)-C(26B)-C(29B)-C(34B)	-1.0(11)
C(28B)-C(26B)-C(29B)-C(34B)	118.6(8)
C(25B)-C(26B)-C(29B)-C(34B)	-122.4(8)
C(34B)-C(29B)-C(30B)-C(31B)	-5.3(12)
C(26B)-C(29B)-C(30B)-C(31B)	175.8(7)
C(29B)-C(30B)-C(31B)-C(32B)	4.2(11)

C(30B)-C(31B)-C(32B)-C(33B)	-0.4(12)
C(31B)-C(32B)-C(33B)-C(34B)	-2.0(13)
C(30B)-C(29B)-C(34B)-C(33B)	2.7(13)
C(26B)-C(29B)-C(34B)-C(33B)	-178.3(8)
C(32B)-C(33B)-C(34B)-C(29B)	0.8(14)
C(38B)-N(4B)-C(35B)-N(5B)	-167.5(5)
C(36B)-N(4B)-C(35B)-N(5B)	2.7(7)
C(37B)-N(5B)-C(35B)-N(4B)	0.8(7)
C(47B)-N(5B)-C(35B)-N(4B)	179.0(6)
C(35B)-N(4B)-C(36B)-C(37B)	-4.8(7)
C(38B)-N(4B)-C(36B)-C(37B)	165.3(6)
C(35B)-N(5B)-C(37B)-C(36B)	-3.8(7)
C(47B)-N(5B)-C(37B)-C(36B)	178.0(6)
N(4B)-C(36B)-C(37B)-N(5B)	4.8(7)
C(35B)-N(4B)-C(38B)-C(39B)	-112.8(7)
C(36B)-N(4B)-C(38B)-C(39B)	78.2(7)
C(35B)-N(4B)-C(38B)-C(43B)	69.5(7)
C(36B)-N(4B)-C(38B)-C(43B)	-99.6(7)
C(43B)-C(38B)-C(39B)-C(40B)	-1.3(8)
N(4B)-C(38B)-C(39B)-C(40B)	-179.0(5)
C(43B)-C(38B)-C(39B)-C(44B)	179.8(5)
N(4B)-C(38B)-C(39B)-C(44B)	2.1(8)
C(38B)-C(39B)-C(40B)-C(41B)	0.8(8)
C(44B)-C(39B)-C(40B)-C(41B)	179.7(5)
C(39B)-C(40B)-C(41B)-C(42B)	-0.9(8)
C(39B)-C(40B)-C(41B)-C(45B)	179.6(5)
C(40B)-C(41B)-C(42B)-C(43B)	1.4(8)
C(45B)-C(41B)-C(42B)-C(43B)	-179.1(6)
C(41B)-C(42B)-C(43B)-C(38B)	-1.8(9)
C(41B)-C(42B)-C(43B)-C(46B)	179.4(6)
C(39B)-C(38B)-C(43B)-C(42B)	1.8(9)
N(4B)-C(38B)-C(43B)-C(42B)	179.5(5)
C(39B)-C(38B)-C(43B)-C(46B)	-179.4(6)
N(4B)-C(38B)-C(43B)-C(46B)	-1.7(8)
C(35B)-N(5B)-C(47B)-C(48B)	101.6(8)
C(37B)-N(5B)-C(47B)-C(48B)	-80.4(8)
C(35B)-N(5B)-C(47B)-C(52B)	-79.6(8)
C(37B)-N(5B)-C(47B)-C(52B)	98.3(7)
C(52B)-C(47B)-C(48B)-C(49B)	2.0(11)
N(5B)-C(47B)-C(48B)-C(49B)	-179.4(6)
C(52B)-C(47B)-C(48B)-C(53B)	-178.7(7)
N(5B)-C(47B)-C(48B)-C(53B)	-0.1(10)
C(47B)-C(48B)-C(49B)-C(50B)	-1.0(11)
C(53B)-C(48B)-C(49B)-C(50B)	179.8(7)
C(48B)-C(49B)-C(50B)-C(51B)	0.2(11)
C(48B)-C(49B)-C(50B)-C(54B)	176.7(7)
C(49B)-C(50B)-C(51B)-C(52B)	-0.4(11)
C(54B)-C(50B)-C(51B)-C(52B)	-176.9(7)
C(48B)-C(47B)-C(52B)-C(51B)	-2.2(10)
N(5B)-C(47B)-C(52B)-C(51B)	179.2(6)

C(48B)-C(47B)-C(52B)-C(55B)	-179.4(7)
N(5B)-C(47B)-C(52B)-C(55B)	2.0(10)
C(50B)-C(51B)-C(52B)-C(47B)	1.2(10)
C(50B)-C(51B)-C(52B)-C(55B)	178.6(7)

Symmetry transformations used to generate equivalent atoms: