

Anhang zur Dissertation Gernot Volker Bauer
Kristallographische Daten und Messparameter

***cis-Bis[3-{(Diphenylphosphanyl-*kP*)methyl}benzol-1,2-diolato-*kO*¹]
palladium(II) (5)***

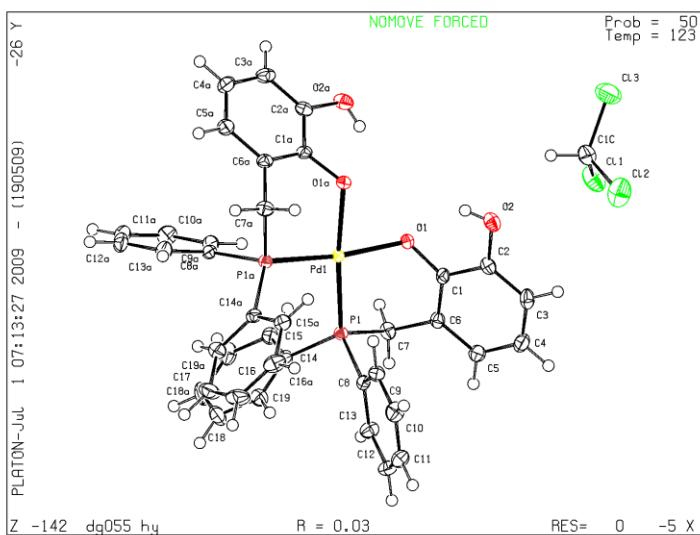
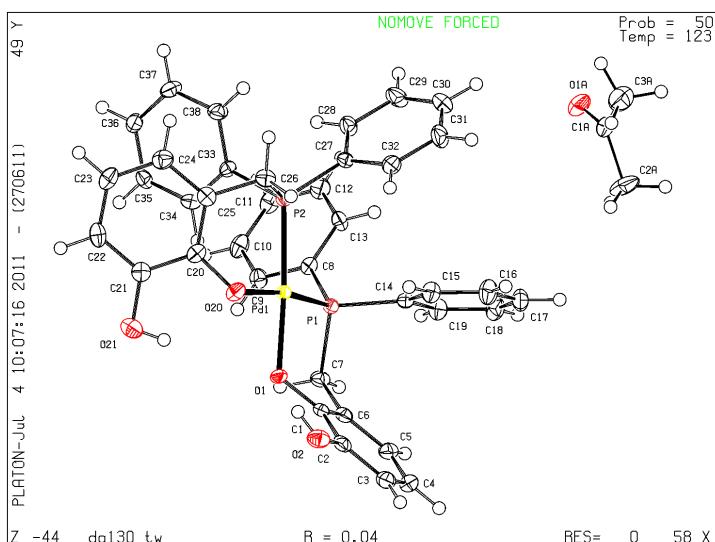


Table 1. Crystal data and structure refinement for dg055_hy.

Identification code	dg055_hy			
Empirical formula	C ₄₀ H ₃₄ Cl ₁₆ O ₄ P ₂ Pd C ₃₈ H ₃₂ O ₄ P ₂ Pd - 2 CHCl ₃			
Formula weight	959.71			
Temperature	123(2) K			
Wavelength	0.71073 Å			
Crystal system, space group	Monoclinic, C2/c (No.15)			
Unit cell dimensions	a = 13.848(1) Å	alpha = 90 deg. b = 28.665(2) Å	beta = 116.05(1) deg. c = 11.434(1) Å	gamma = 90 deg.
Volume	4077.7(5) Å ³			
Z, Calculated density	4, 1.563 Mg/m ³			
Absorption coefficient	0.967 mm ⁻¹			
F(000)	1936			
Crystal size	0.35 x 0.20 x 0.10 mm			
Theta range for data collection	3.16 to 27.48 deg.			
Limiting indices	-17<=h<=17, -37<=k<=37, -14<=l<=14			
Reflections collected / unique	47694 / 4678 [R(int) = 0.0384]			
Completeness to theta = 27.48	99.8 %			
Absorption correction	Semi-empirical from equivalents			
Max. and min. transmission	0.9010 and 0.7415			
Refinement method	Full-matrix least-squares on F ²			
Data / restraints / parameters	4678 / 1 / 243			
Goodness-of-fit on F ²	1.043			
Final R indices [I>2sigma(I)]	R1 = 0.0258, wR2 = 0.0560			
R indices (all data)	R1 = 0.0331, wR2 = 0.0587			
Largest diff. peak and hole	0.663 and -0.603 e.Å ⁻³			



DG130_HY K-289

G. Bauer

non-merohedral twin
BASF 0.0962(15)

solved by
Patterson Methods

See also:
DG055_HY
DG129_HY

Crystal data and structure refinement for dg130_hy.

Identification code	dg130_tw
Empirical formula	C39.50 H35 O4.50 P2 Pd C38 H32 O4 P2 Pd - 1/2 aceton
Formula weight	750.02
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1 (No.2)
Unit cell dimensions	a = 11.447(1) Å alpha = 68.51(1) deg. b = 12.559(2) Å beta = 68.15(1) deg. c = 13.501(2) Å gamma = 88.13(1) deg.
Volume	1664.1(4) Å^3
Z, Calculated density	2, 1.497 Mg/m^3
Absorption coefficient	0.697 mm^-1
F(000)	768
Crystal size	0.24 x 0.16 x 0.08 mm
Theta range for data collection	2.92 to 27.48 deg.
Limiting indices	-14<=h<=14, -15<=k<=16, -17<=l<=17
Reflections collected / unique	7617 / 7617 [R(int) = 0.0000]
non-merohedral twin	BASF = 0.0962(15)
Completeness to theta = 27.48	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9422 and 0.6498
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7617 / 41 / 451
Goodness-of-fit on F^2	1.189
Final R indices [I>2sigma(I)]	R1 = 0.0400, wR2 = 0.0919
R indices (all data)	R1 = 0.0468, wR2 = 0.0942
Largest diff. peak and hole	0.931 and -0.878 e.Å^-3

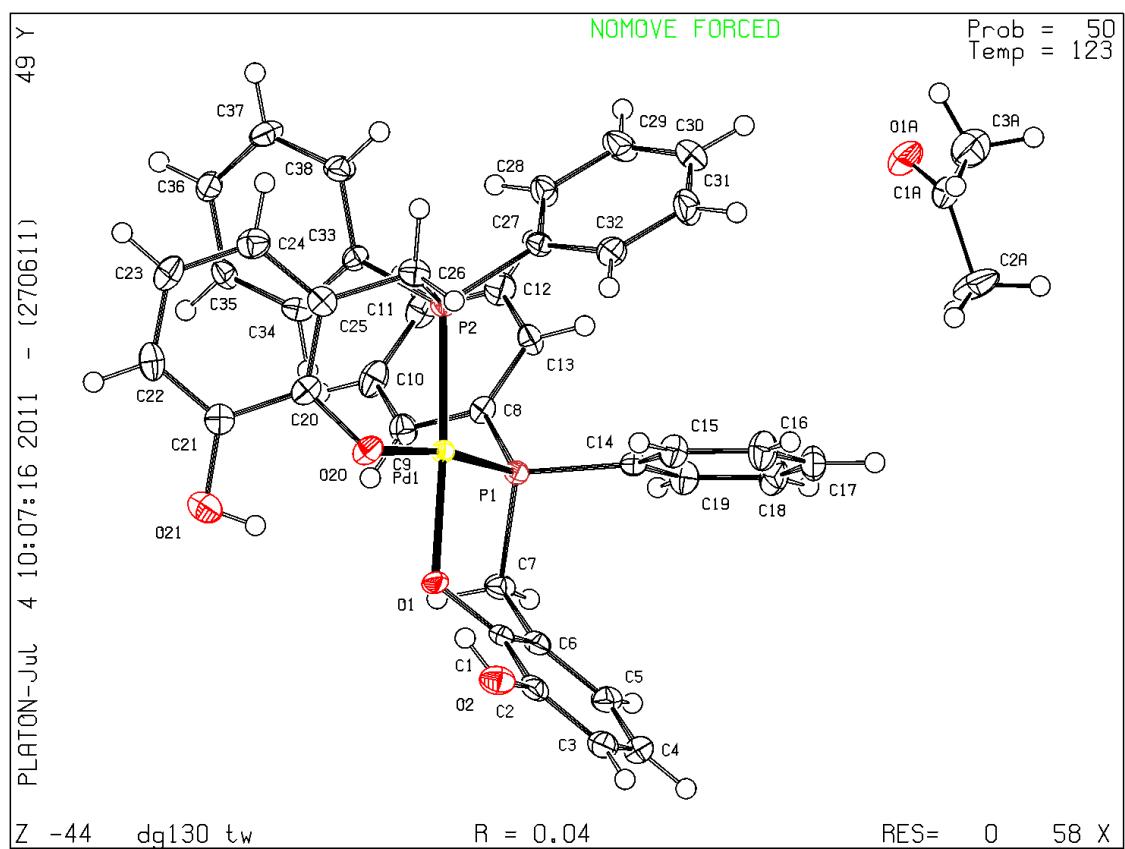
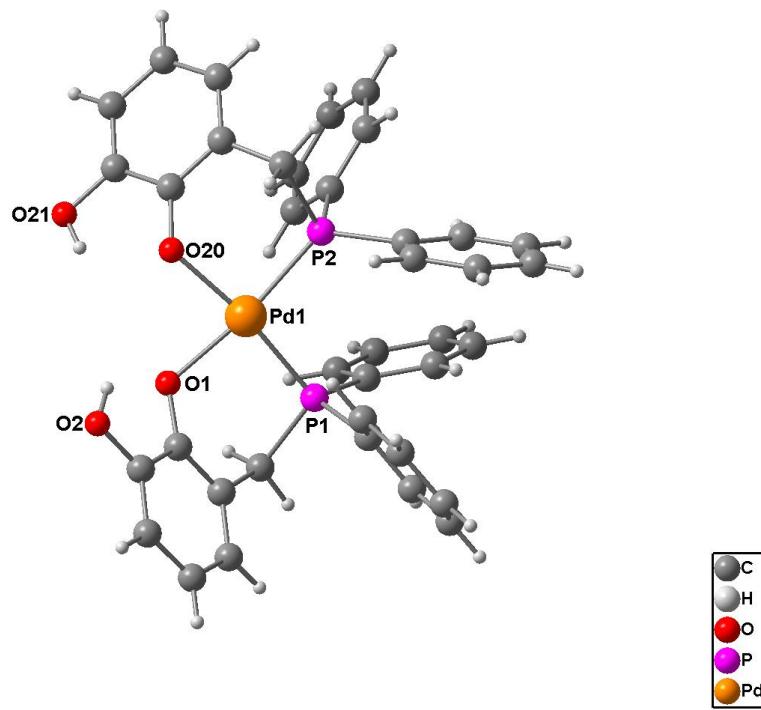


Table 1. Crystal data and structure refinement for dg130_hy.

Identification code	dg130_tw
Empirical formula	C39.50 H35 O4.50 P2 Pd C38 H32 O4 P2 Pd - 1/2 aceton
Formula weight	750.02
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1 (No.2)
Unit cell dimensions	a = 11.447(1) Å alpha = 68.51(1) deg. b = 12.559(2) Å beta = 68.15(1) deg. c = 13.501(2) Å gamma = 88.13(1) deg.
Volume	1664.1(4) Å^3
Z, Calculated density	2, 1.497 Mg/m^3
Absorption coefficient	0.697 mm^-1
F(000)	768
Crystal size	0.24 x 0.16 x 0.08 mm
Theta range for data collection	2.92 to 27.48 deg.
Limiting indices	-14<=h<=14, -15<=k<=16, -17<=l<=17
Reflections collected / unique	7617 / 7617 [R(int) = 0.0000]
non-merohedral twin	BASF = 0.0962(15)
Completeness to theta = 27.48	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9422 and 0.6498
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7617 / 41 / 451
Goodness-of-fit on F^2	1.189
Final R indices [I>2sigma(I)]	R1 = 0.0400, wR2 = 0.0919
R indices (all data)	R1 = 0.0468, wR2 = 0.0942
Largest diff. peak and hole	0.931 and -0.878 e.Å^-3

***cis*-Bis[3-{(Diphenylphosphanyl-*kP*)methyl}benzol-1,2-diolato-
*kO*¹]platin(II) (6)**

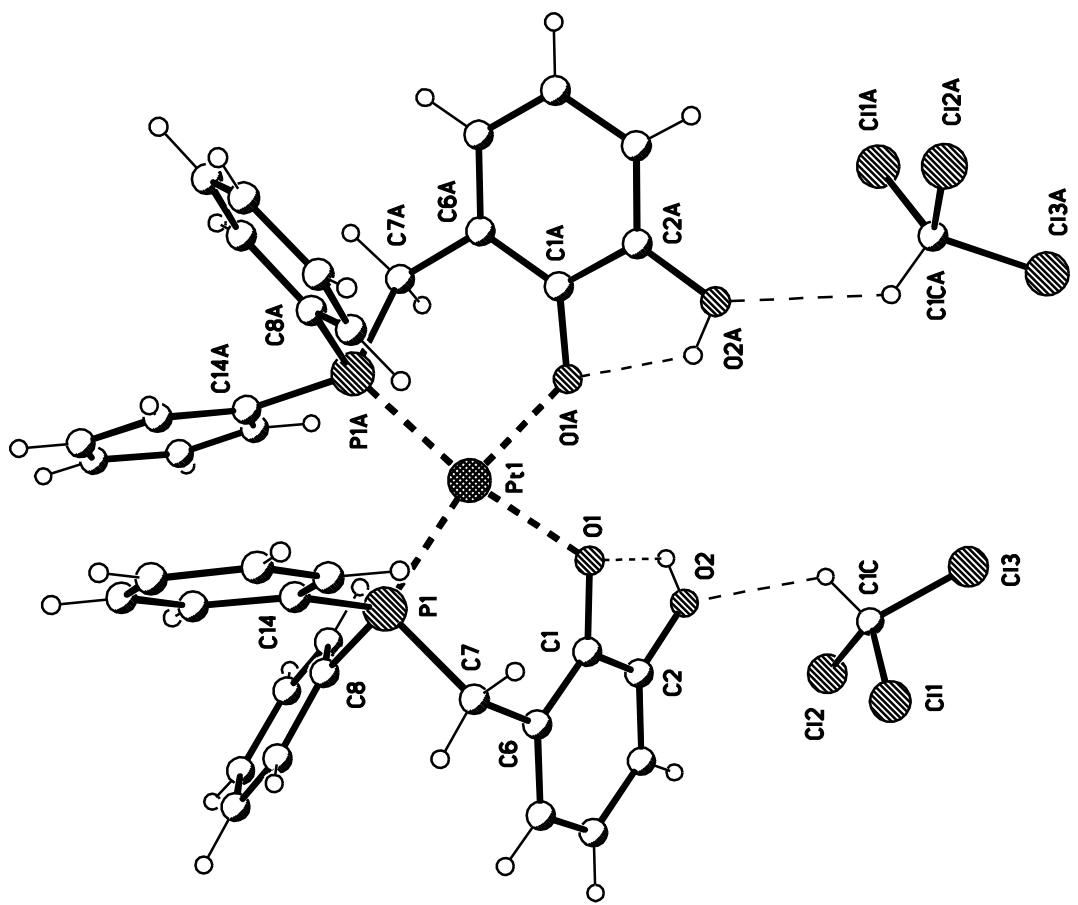


Table 1. Crystal data and structure refinement for gbau02.

Identification code	gbau02
Empirical formula	C40 H34 Cl6 O4 P2 Pt
Formula weight	1048.40
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, C 2/c (No. 15)
Unit cell dimensions	a = 13.864(2) Å alpha = 90 deg. b = 28.702(4) Å beta = 116.210(10) deg. c = 11.4290(10) Å gamma = 90 deg.
Volume	4080.3(9) Å^3
Z, Calculated density	4, 1.707 Mg/m^3
Absorption coefficient	3.951 mm^-1
F(000)	2064
Crystal size	0.30 x 0.10 x 0.05 mm
Theta range for data collection	3.16 to 27.48 deg.
Limiting indices	-17<=h<=17, -37<=k<=37, -14<=l<=14
Reflections collected / unique	46840 / 4671 [R(int) = 0.0535]
Completeness to theta = 27.48	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8372 and 0.4616
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4671 / 1 / 243
Goodness-of-fit on F^2	1.076
Final R indices [I>2sigma(I)]	R1 = 0.0256, wR2 = 0.0636
R indices (all data)	R1 = 0.0282, wR2 = 0.0649
Largest diff. peak and hole	2.285 and -0.974 e.Å^-3

2,2'-Bis(ethoxymethoxy)biphenyl (18)

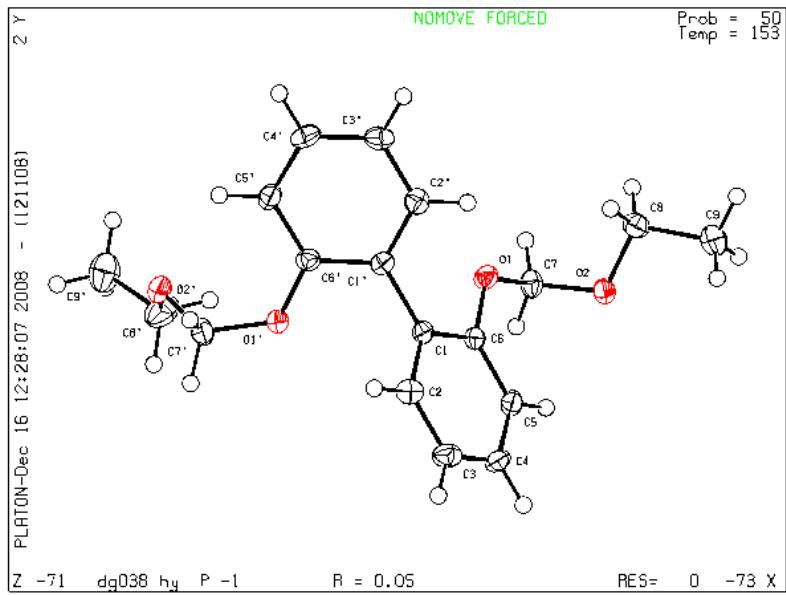


Table 1. Crystal data and structure refinement for dg038_hy.

Identification code	dg038_hy
Empirical formula	C18 H22 O4
Formula weight	302.36
Temperature	153(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1 (No.2)
Unit cell dimensions	a = 7.895(1) Å alpha = 78.17(1) deg. b = 10.347(1) Å beta = 74.08(1) deg. c = 10.530(1) Å gamma = 86.21(1) deg.
Volume	809.59(15) Å^3
Z, Calculated density	2, 1.240 Mg/m^3
Absorption coefficient	0.087 mm^-1
F(000)	324
Crystal size	0.30 x 0.10 x 0.10 mm
Theta range for data collection	3.14 to 27.48 deg.
Limiting indices	-10<=h<=10, -13<=k<=12, -12<=l<=13
Reflections collected / unique	8422 / 3697 [R(int) = 0.0319]
Completeness to theta = 25.00	99.7 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3697 / 0 / 199
Goodness-of-fit on F^2	1.016
Final R indices [I>2sigma(I)]	R1 = 0.0491, wR2 = 0.0977
R indices (all data)	R1 = 0.0858, wR2 = 0.1110
Largest diff. peak and hole	0.248 and -0.216 e.Å^-3

3-[(Diphenylphosphorothioyl)methyl]benzol-1,2-diol (23)

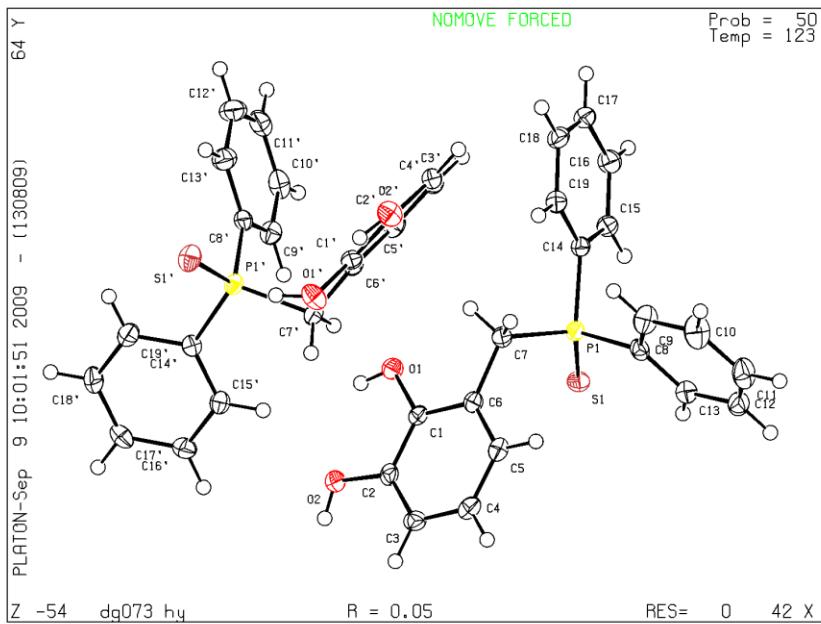


Table 1. Crystal data and structure refinement for dg073_hy.

Identification code	dg073_hy
Empirical formula	C19 H17 O2 P S
Formula weight	340.36
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 9.493(2) Å alpha = 89.55(2) deg. b = 13.293(3) Å beta = 72.32(2) deg. c = 13.863(3) Å gamma = 81.28(2) deg.
Volume	1646.1(6) Å^3
Z, Calculated density	4, 1.373 Mg/m^3
Absorption coefficient	0.300 mm^-1
F(000)	712
Crystal size	0.35 x 0.30 x 0.25 mm
Theta range for data collection	3.10 to 27.48 deg.
Limiting indices	-12<=h<=11, -17<=k<=16, -17<=l<=17
Reflections collected / unique	16589 / 7394 [R(int) = 0.0398]
Completeness to theta = 25.00	98.4 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7394 / 4 / 427
Goodness-of-fit on F^2	1.119
Final R indices [I>2sigma(I)]	R1 = 0.0541, wR2 = 0.1184
R indices (all data)	R1 = 0.0788, wR2 = 0.1298
Largest diff. peak and hole	0.571 and -0.383 e.Å^-3

[Diphenyl-(benzo-[1,3]-4-ylmethyl)-phosphan-*kP*]chlorogold(I) (24)

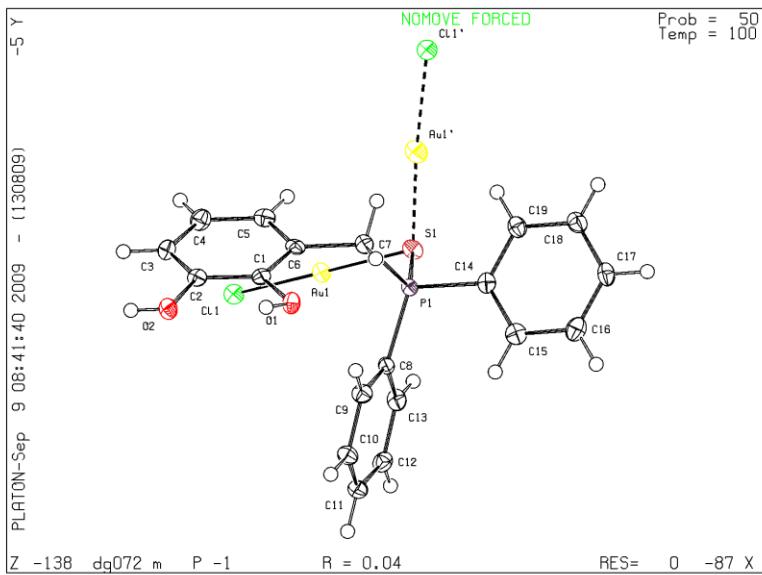


Table 1. Crystal data and structure refinement for dg072_m.

Identification code	dg072_m
Empirical formula	C19 H17 Au Cl O2 P S
Formula weight	572.77
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1 (No.2)
Unit cell dimensions	a = 9.4738(3) Å alpha = 108.527(2) deg. b = 10.0651(3) Å beta = 105.608(2) deg. c = 10.8564(3) Å gamma = 98.982(2) deg.
Volume	911.67(5) Å^3
Z, Calculated density	2, 2.087 Mg/m^3
Absorption coefficient	8.427 mm^-1
F(000)	548
Crystal size	0.20 x 0.15 x 0.10 mm
Theta range for data collection	3.25 to 27.42 deg.
Limiting indices	-12<=h<=12, -13<=k<=13, -14<=l<=14
Reflections collected / unique	16429 / 4131 [R(int) = 0.0610]
Completeness to theta = 27.42	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.48526 and 0.28698
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4131 / 5 / 242
Goodness-of-fit on F^2	1.064
Final R indices [I>2sigma(I)]	R1 = 0.0378, wR2 = 0.0960
R indices (all data)	R1 = 0.0400, wR2 = 0.0981
Largest diff. peak and hole	3.905 and -3.174 e.Å^-3

**μ -(η^2 ; η^6 -3-[(Diphenylphosphorothioyl)-methyl]-benzol-1,2-diolato-
 kO, kO')-di-[(cycloocta-1,5-dien)rhodium(I)] (25)**

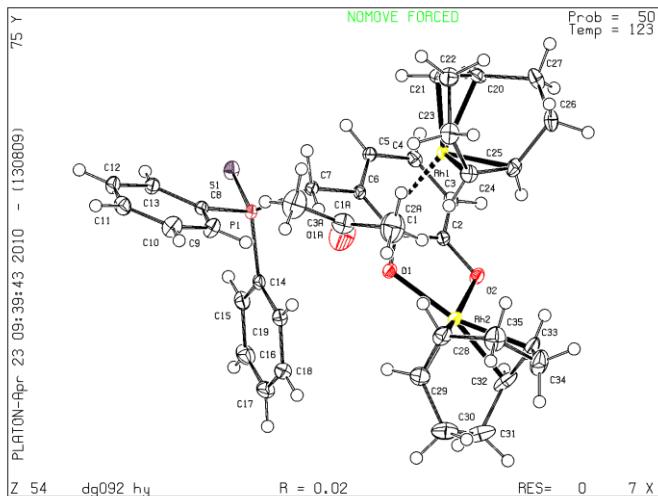


Table 1. Crystal data and structure refinement for dg092_hy.

Identification code	dg092_hy
Empirical formula	C ₃₈ H ₄₅ O ₃ P Rh ₂ S C ₃₅ H ₃₉ O ₂ P Rh ₂ S - aceton
Formula weight	818.59
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1 (No.2)
Unit cell dimensions	a = 11.383(1) Å alpha = 72.45(1) deg. b = 12.220(1) Å beta = 89.12(1) deg. c = 13.029(1) Å gamma = 82.82(1) deg.
Volume	1714.0(2) Å ³
Z, Calculated density	2, 1.586 Mg/m ³
Absorption coefficient	1.107 mm ⁻¹
F(000)	836
Crystal size	0.40 x 0.16 x 0.08 mm
Theta range for data collection	3.14 to 27.48 deg.
Limiting indices	-14<=h<=14, -15<=k<=15, -16<=l<=16
Reflections collected / unique	41778 / 7843 [R(int) = 0.0282]
Completeness to theta = 27.48	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9144 and 0.7262
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	7843 / 0 / 408
Goodness-of-fit on F ²	1.051
Final R indices [I>2sigma(I)]	R1 = 0.0197, wR2 = 0.0471
R indices (all data)	R1 = 0.0250, wR2 = 0.0499
Largest diff. peak and hole	0.516 and -0.529 e.Å ⁻³

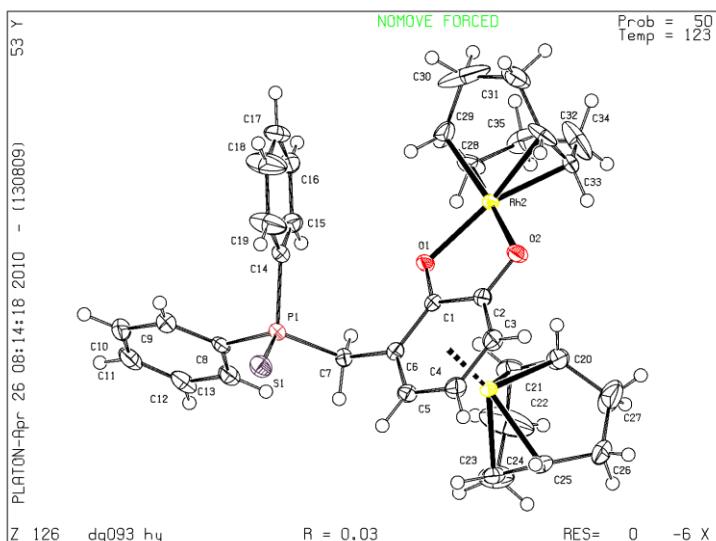
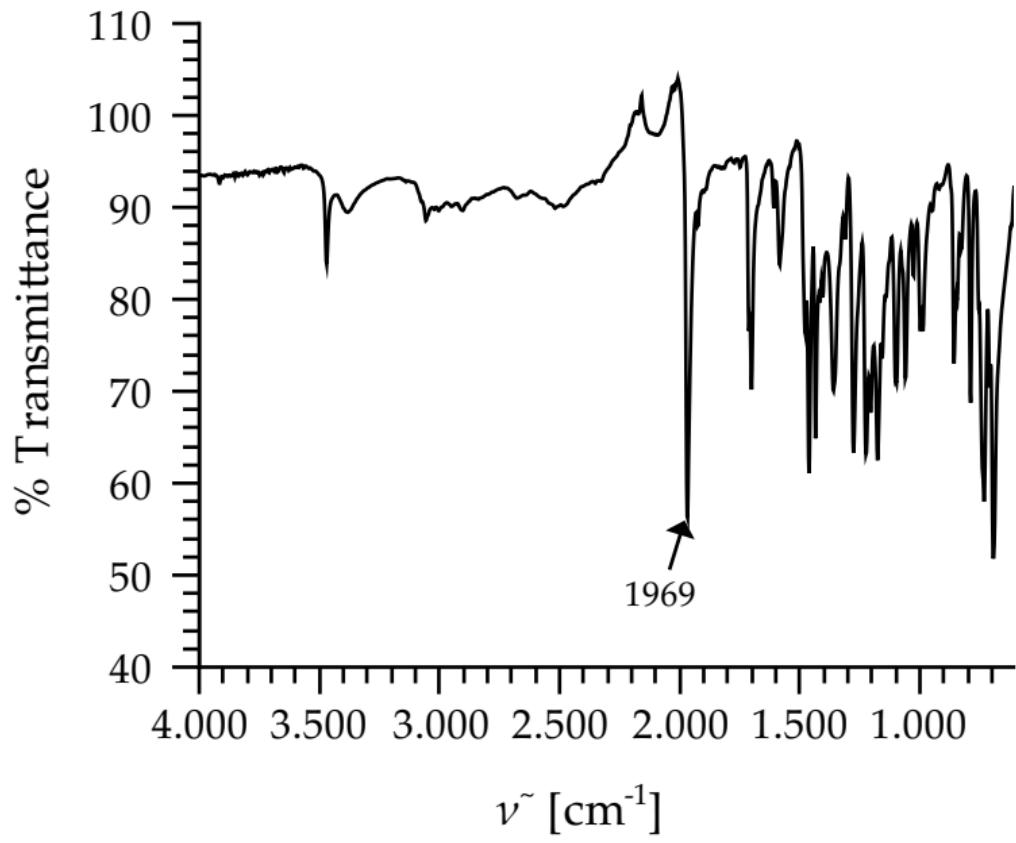


Table 1. Crystal data and structure refinement for dg093_hy.

Identification code	dg093_hy	
Empirical formula	C35 H39 O2 P Rh2 S	
Formula weight	760.51	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Triclinic, P-1 (No.2)	
Unit cell dimensions	$a = 10.482(1)$ Å $\alpha = 110.91(1)$ deg. $b = 12.689(1)$ Å $\beta = 111.70(1)$ deg. $c = 13.314(1)$ Å $\gamma = 90.77(1)$ deg.	
Volume	1515.3(2) Å ³	
Z, Calculated density	2, 1.667 Mg/m ³	
Absorption coefficient	1.243 mm ⁻¹	
F(000)	772	
Crystal size	0.40 x 0.30 x 0.25 mm	
Theta range for data collection	2.94 to 27.48 deg.	
Limiting indices	-13<=h<=10, -16<=k<=16, -17<=l<=17	
Reflections collected / unique	22746 / 6923 [R(int) = 0.0309]	
Completeness to theta = 27.48	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6403	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	6923 / 0 / 370	
Goodness-of-fit on F ²	1.075	
Final R indices [I>2sigma(I)]	R1 = 0.0312, wR2 = 0.0730	
R indices (all data)	R1 = 0.0399, wR2 = 0.0780	
Largest diff. peak and hole	0.890 and -0.680 e.Å ⁻³	



trans-[3-{(Diphenylphosphanyl-*kP*)methyl}benzol-1,2-diolato-*kO*¹]-
[3-{(Diphenylphosphanyl-*kP*)methyl}benzol-1,2-
diol](carbonyl)rhodium(I) (26)

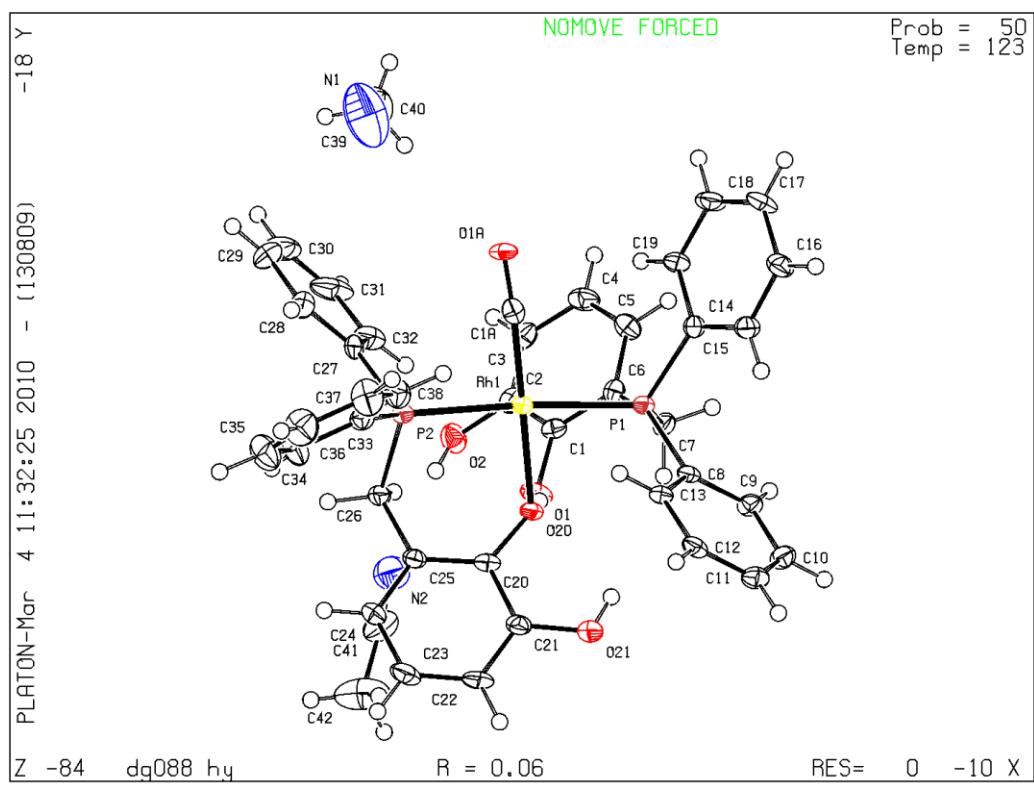
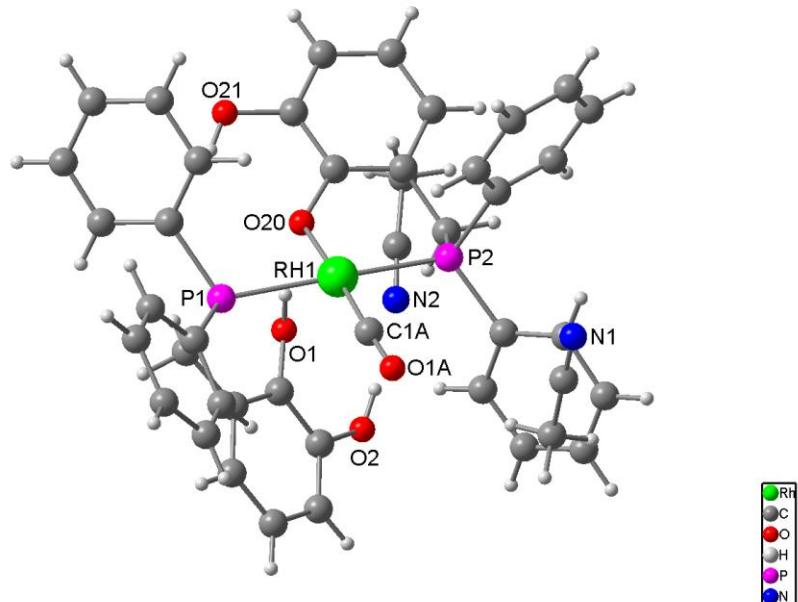


Table 1. Crystal data and structure refinement for dg088_hy.

Identification code	dg088_hy
Empirical formula	C43 H39 N2 O5 P2 Rh C39 H33 N2 O5 P2 Rh - 2 CH3CN
Formula weight	828.61
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c (No.14)
Unit cell dimensions	a = 10.624(1) Å alpha = 90 deg. b = 15.477(2) Å beta = 95.53(1) deg. c = 23.849(4) Å gamma = 90 deg.
Volume	3903.2(9) Å^3
Z, Calculated density	4, 1.410 Mg/m^3
Absorption coefficient	0.567 mm^-1
F(000)	1704
Crystal size	0.24 x 0.08 x 0.04 mm
Theta range for data collection	3.00 to 27.48 deg.
Limiting indices	-13<=h<=13, -20<=k<=20, -30<=l<=30
Reflections collected / unique	58886 / 8934 [R(int) = 0.0992]
Completeness to theta = 27.48	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9703 and 0.7118
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8934 / 3 / 489
Goodness-of-fit on F^2	1.072
Final R indices [I>2sigma(I)]	R1 = 0.0640, wR2 = 0.1461
R indices (all data)	R1 = 0.0995, wR2 = 0.1642
Largest diff. peak and hole	2.563 and -1.051 e.Å^-3

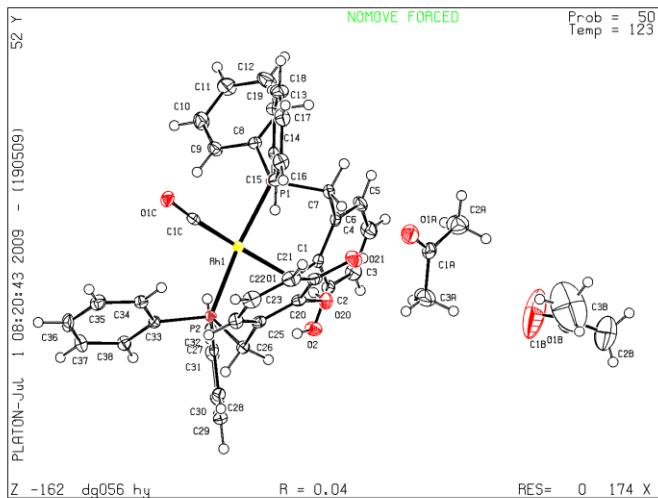


Table 1. Crystal data and structure refinement for dg056_hy.

Identification code	dg056_hy
Empirical formula	C45 H45 O7 P2 Rh C39 H33 O5 P2 Rh - 2 aceton
Formula weight	862.66
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c (No.14)
Unit cell dimensions	a = 10.593(1) Å alpha = 90 deg. b = 16.620(2) Å beta = 93.03(1) deg. c = 23.179(3) Å gamma = 90 deg.
Volume	4075.1(8) Å ³
Z, Calculated density	4, 1.406 Mg/m ³
Absorption coefficient	0.548 mm ⁻¹
F(000)	1784
Crystal size	0.30 x 0.15 x 0.10 mm
Theta range for data collection	2.91 to 27.48 deg.
Limiting indices	-13<=h<=13, -21<=k<=21, -30<=l<=29
Reflections collected / unique	61872 / 9325 [R(int) = 0.0676]
Completeness to theta = 27.48	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9472 and 0.7068
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	9325 / 9 / 509
Goodness-of-fit on F ²	1.046
Final R indices [I>2sigma(I)]	R1 = 0.0398, wR2 = 0.0749
R indices (all data)	R1 = 0.0600, wR2 = 0.0812
Largest diff. peak and hole	0.607 and -0.418 e.Å ⁻³

Palladium(II)-bis{diphenyl-(benzo-[1,3]- μ -oxo-*k*-oxo-4-ylmethyl)-phosphan}-aluminium(III)-2,4-pentandionat (27)

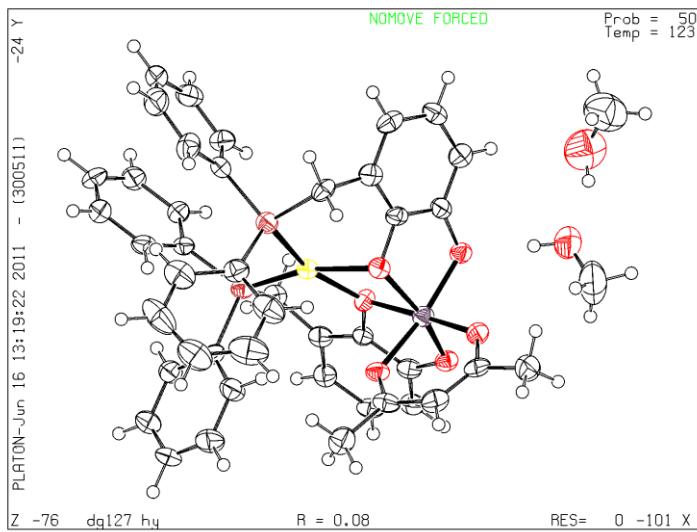


Table 1. Crystal data and structure refinement for dg127_hy.

Identification code	dg127_hy	
Empirical formula	C45 H45 Al O8 P2 Pd C43 H37 Al O6 P2 Pd - 2 MeOH	
Formula weight	909.13	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Triclinic, P -1	
Unit cell dimensions	a = 12.393(2) Å	alpha = 96.11(1) deg.
	b = 13.325(2) Å	beta = 112.09(1) deg.
	c = 13.465(2) Å	gamma = 97.42(1) deg.
Volume	2013.8(5) Å^3	
Z, Calculated density	2, 1.499 Mg/m^3	
Absorption coefficient	0.617 mm^-1	
F(000)	936	
Crystal size	0.16 x 0.08 x 0.04 mm	
Theta range for data collection	2.98 to 25.00 deg.	
Limiting indices	-14<=h<=14, -15<=k<=15, -15<=l<=15	
Reflections collected / unique	28365 / 7058 [R(int) = 0.1239]	
Completeness to theta = 25.00	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9801 and 0.6572	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7058 / 37 / 520	
Goodness-of-fit on F^2	1.041	
Final R indices [I>2sigma(I)]	R1 = 0.0759, wR2 = 0.1556	
R indices (all data)	R1 = 0.1322, wR2 = 0.1802	
Largest diff. peak and hole	1.125 and -0.724 e.Å^-3	

Bis-[palladium(II)-bis{diphenyl-(benzo-[1,3]- μ -oxo-*k*-oxo-4- γ lmethyl)-phosphan)}]aluminium(III) (28)

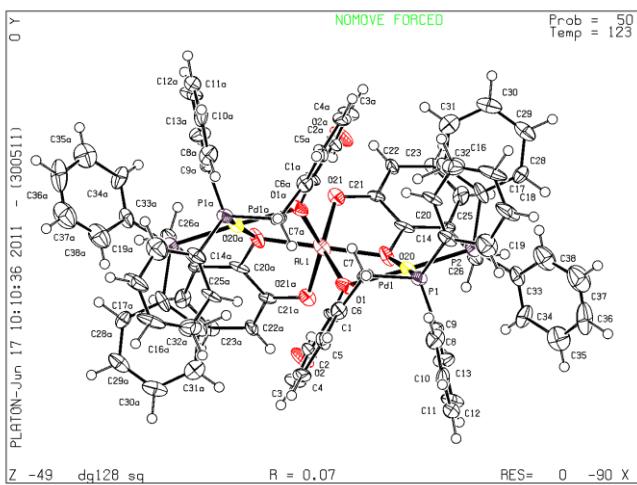
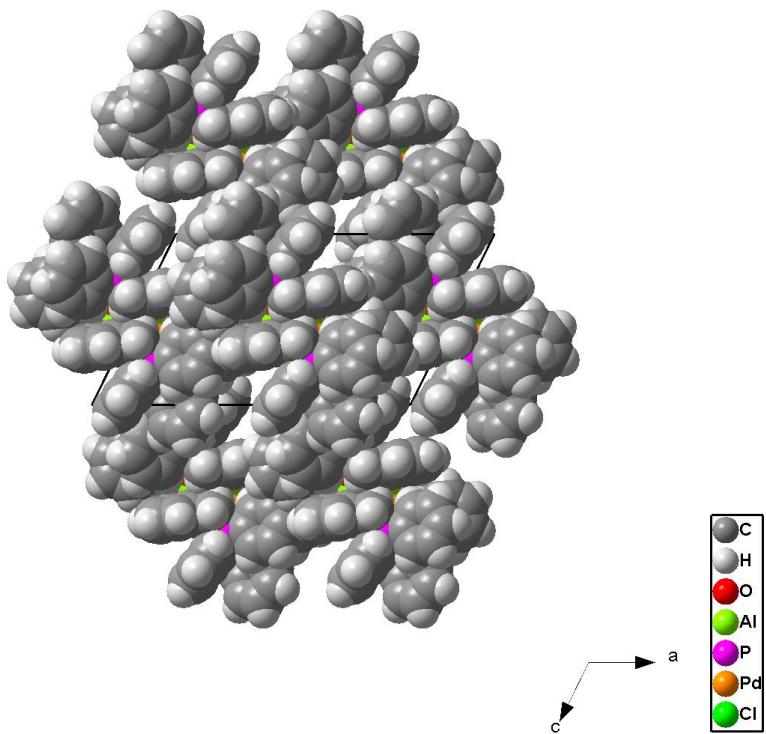


Table 1. Crystal data and structure refinement for dg128_sq.

Identification code	dg128_sq - SQUEEZE data			
Empirical formula	C78 H65 Al C14 O8 P4 Pd2 C76 H61 Al O8 P4 Pd2 - 2 CH2Cl2			
Formula weight	1635.76			
Temperature	123(2) K			
Wavelength	0.71073 Å			
Crystal system, space group	Monoclinic, C2 (No. 5)			
Unit cell dimensions	a = 22.608(2) Å	alpha = 90 deg. b = 13.568(1) Å	beta = 116.15(1) deg. c = 13.497(1) Å	gamma = 90 deg.

Volume	3716.4 (5) Å^3
Z, Calculated density	2, 1.462 Mg/m^3
Absorption coefficient	0.780 mm^-1
F(000)	1660
Crystal size	0.12 x 0.06 x 0.02 mm
Theta range for data collection	3.00 to 25.02 deg.
Limiting indices	-26<=h<=24, -16<=k<=16, 0<=l<=16
Reflections collected / unique	6509 / 6509 [R(int) = 0.0000]
Completeness to theta = 25.02	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9801 and 0.7985
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6509 / 1 / 412
Goodness-of-fit on F^2	0.947
Final R indices [I>2sigma(I)]	R1 = 0.0700, wR2 = 0.1309
R indices (all data)	R1 = 0.1300, wR2 = 0.1475
Absolute structure parameter	-0.10 (5)
Largest diff. peak and hole	0.759 and -0.661 e.Å^-3

Palladium(II)-bis{diphenyl-(benzo-[1,3]- μ -oxo-*k*-oxo-4-ylmethyl)-phosphan}-chloro(dimethylformamid-*O*)gallium(III) (33)

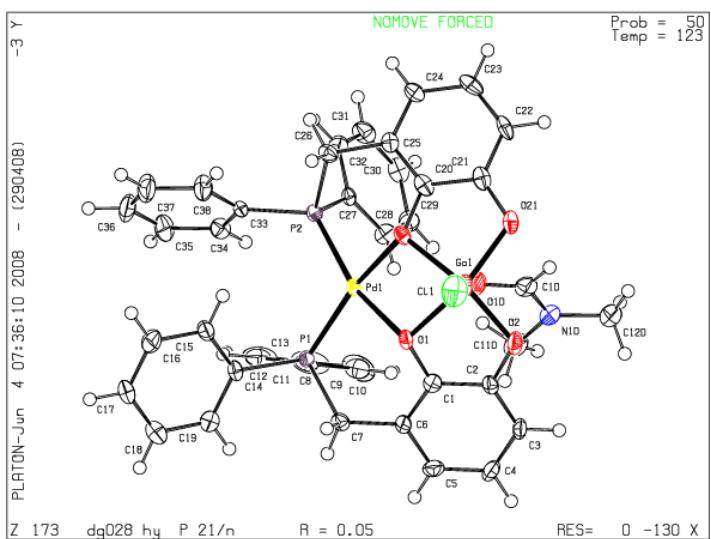


Table 1. Crystal data and structure refinement for dg028_hy.

Identification code	dg028_hy
Empirical formula	C41 H37 Cl Ga N O5 P2 Pd
Formula weight	897.23
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n (No.14)
Unit cell dimensions	a = 12.644(1) Å alpha = 90 deg. b = 16.798(2) Å beta = 104.01(1) deg. c = 17.833(2) Å gamma = 90 deg.
Volume	3675.0(7) Å^3
Z, Calculated density	4, 1.622 Mg/m^3
Absorption coefficient	1.430 mm^-1
F(000)	1816
Crystal size	0.20 x 0.12 x 0.08 mm
Theta range for data collection	2.94 to 25.02 deg.
Limiting indices	-15<=h<=14, -18<=k<=19, -21<=l<=21
Reflections collected / unique	26201 / 6417 [R(int) = 0.0865]
Completeness to theta = 25.02	99.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8620 and 0.7504
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6417 / 0 / 471
Goodness-of-fit on F^2	1.069
Final R indices [I>2sigma(I)]	R1 = 0.0531, wR2 = 0.0776
R indices (all data)	R1 = 0.0978, wR2 = 0.0877
Largest diff. peak and hole	0.586 and -0.550 e.Å^-3

Dichloro-[bis{bis(diphenyl-{benzo-[1,3]- μO^1 - kO^2 -4-ylmethyl}-phosphan- kP)palladium(II)}- μO^1 - kO^2 - μO^2 -diindium(III)] (34)

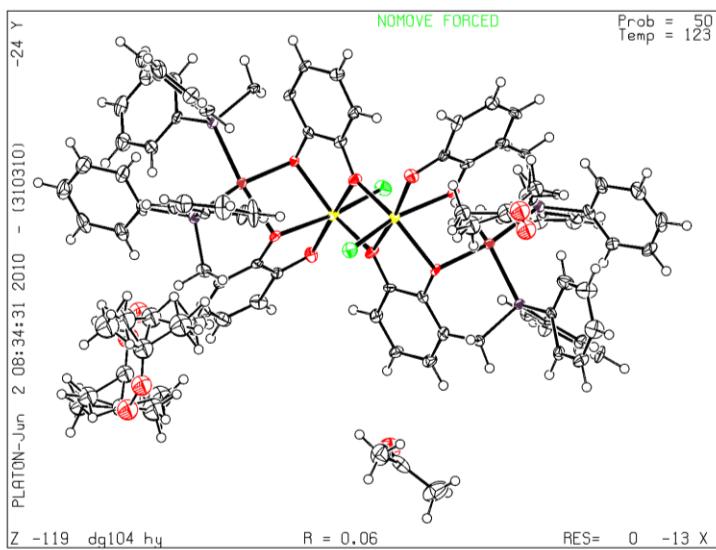


Table 1. Crystal data and structure refinement for dg104_hy.

Identification code	dg104_hy	
Empirical formula	C ₈₈ H ₈₄ Cl ₂ In ₂ O ₁₂ P ₄ Pd ₂ C ₇₆ H ₆₀ Cl ₂ In ₂ O ₈ P ₄ Pd ₂ - 4 aceton	
Formula weight	1970.77	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Triclinic, P-1 (No.2)	
Unit cell dimensions	a = 11.116(1) Å alpha = 100.09(1) deg. b = 19.005(2) Å beta = 103.19(1) deg. c = 20.826(2) Å gamma = 99.94(1) deg.	
Volume	4112.3(7) Å ³	
Z, Calculated density	2, 1.592 Mg/m ³	
Absorption coefficient	1.188 mm ⁻¹	
F(000)	1984	
Crystal size	0.18 x 0.09 x 0.03 mm	
Theta range for data collection	2.93 to 25.03 deg.	
Limiting indices	-13<=h<=13, -22<=k<=22, -24<=l<=24	
Reflections collected / unique	43026 / 14483 [R(int) = 0.0717]	
Completeness to theta = 25.03	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9703 and 0.8188	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	14483 / 224 / 981	
Goodness-of-fit on F ²	1.019	
Final R indices [I>2sigma(I)]	R1 = 0.0571, wR2 = 0.1048	
R indices (all data)	R1 = 0.1140, wR2 = 0.1238	
Largest diff. peak and hole	1.637 and -1.016 e.Å ⁻³	

Palladium(II)-bis{diphenyl-(benzo-[1,3]- μ -oxo-*k*-oxo-4-ylmethyl)-phosphan}-dimethoxytitan(IV) (36)

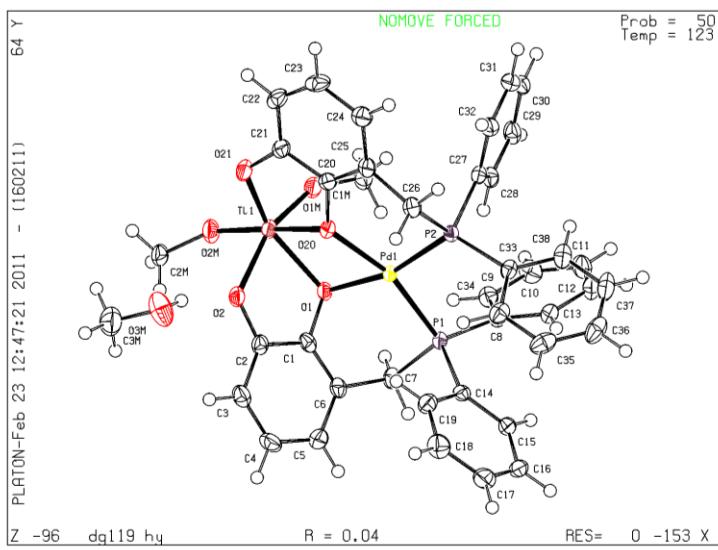
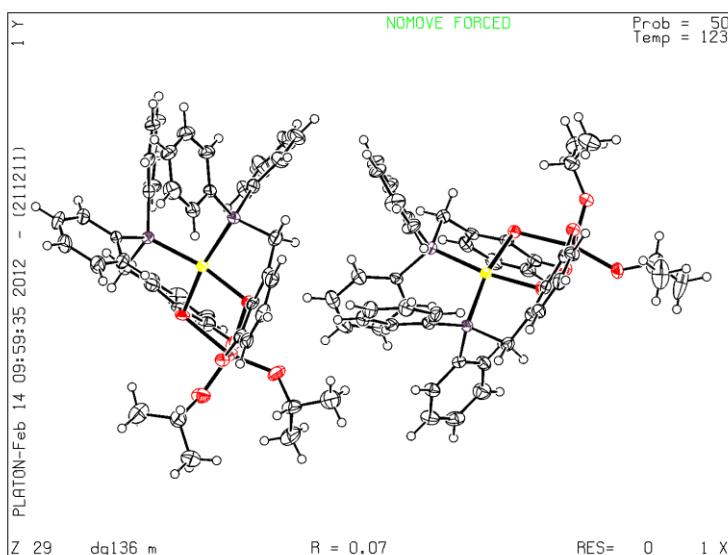


Table 1. Crystal data and structure refinement for dg119_hy.

Identification code	dg119_hy
Empirical formula	C ₄₁ H ₄₀ O ₇ Pd Ti C ₄₀ H ₃₆ O ₆ Pd Ti - MeOH
Formula weight	860.97
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n (No.14)
Unit cell dimensions	a = 14.598(1) Å alpha = 90 deg. b = 12.951(1) Å beta = 97.28(1) deg. c = 19.652(2) Å gamma = 90 deg.
Volume	3685.4(5) Å ³
Z, Calculated density	4, 1.552 Mg/m ³
Absorption coefficient	0.843 mm ⁻¹
F(000)	1760
Crystal size	0.18 x 0.09 x 0.03 mm
Theta range for data collection	3.09 to 27.48 deg.
Limiting indices	-18<=h<=18, -16<=k<=16, -25<=l<=25
Reflections collected / unique	36654 / 8431 [R(int) = 0.0506]
Completeness to theta = 27.48	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9703 and 0.8632
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	8431 / 1 / 475
Goodness-of-fit on F ²	1.041
Final R indices [I>2sigma(I)]	R1 = 0.0394, wR2 = 0.0740
R indices (all data)	R1 = 0.0705, wR2 = 0.0828
Largest diff. peak and hole	1.087 and -0.402 e.Å ⁻³

Palladium(II)-bis{diphenyl-(benzo-[1,3]- μ -oxo-*k*-oxo-4-ylmethyl)-phosphan}-diisopropoxytitan(IV) (37)



DG136 HY

A-304

G. Bauer

Crystal data and structure refinement for dg136.m.

Identification code	dg136_m
Empirical formula	C44 H44 O6 P2 Pd Ti
Formula weight	885.03
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n (no.14)
Unit cell dimensions	a = 17.7428(6) Å alpha = 90 deg. b = 20.2475(9) Å beta = 95.659(3) deg. c = 22.5638(9) Å gamma = 90 deg.
Volume	8066.5(6) Å^3
Z, Calculated density	8, 1.458 Mg/m^3
Absorption coefficient	0.770 mm^-1
F(000)	3632
Crystal size	0.24 x 0.06 x 0.03 mm
Theta range for data collection	3.63 to 25.03 deg.
Limiting indices	-21<=h<=21, -22<=k<=24, -21<=l<=26
Reflections collected / unique	36717 / 14106 [R(int) = 0.0894]
Completeness to theta = 25.03	99.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.96554 and 0.84633
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	14106 / 0 / 973
Goodness-of-fit on F^2	1.111
Final R indices [I>2sigma(I)]	R1 = 0.0657, wR2 = 0.1041
R indices (all data)	R1 = 0.1301, wR2 = 0.1258
Largest diff. peak and hole	0.626 and -0.531 e.Å^-3

[*SP*-4-2]-[{Bis-(diphenyl-{benzo-[1,3]- $\mu O^1:kO^2$ -4-ylmethyl}-phosphan- kP)palladium(II)}-[*OC*-6-33]- $\mu O^1:kO^2$ -dioxiomolybdän(VI)]
(38)

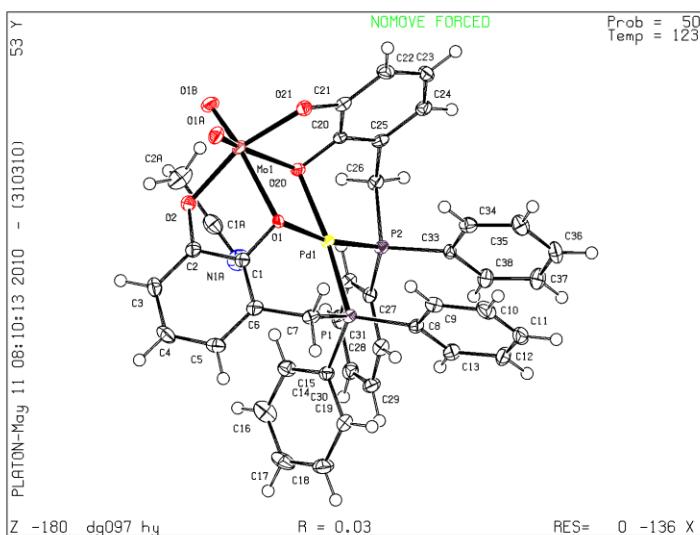


Table 1. Crystal data and structure refinement for dg097_hy.

Identification code	dg097_hy
Empirical formula	C ₄₀ H ₃₃ Mo N O ₆ P ₂ Pd C ₃₈ H ₃₀ Mo O ₆ P ₂ Pd - CH ₃ CN
Formula weight	887.95
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n (No.14)
Unit cell dimensions	a = 18.725(1) Å alpha = 90 deg. b = 10.391(1) Å beta = 114.46(1) deg. c = 19.739(1) Å gamma = 90 deg.
Volume	3495.9(4) Å ³
Z, Calculated density	4, 1.687 Mg/m ³
Absorption coefficient	1.015 mm ⁻¹
F(000)	1784
Crystal size	0.18 x 0.12 x 0.06 mm
Theta range for data collection	2.93 to 27.48 deg.
Limiting indices	-20<=h<=24, -12<=k<=13, -25<=l<=20
Reflections collected / unique	22097 / 7985 [R(int) = 0.0390]
Completeness to theta = 27.48	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9422 and 0.8218
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	7985 / 0 / 461
Goodness-of-fit on F ²	1.042
Final R indices [I>2sigma(I)]	R1 = 0.0346, wR2 = 0.0603
R indices (all data)	R1 = 0.0562, wR2 = 0.0659
Largest diff. peak and hole	0.576 and -0.487 e.Å ⁻³

[*SP*-4-2]-[{Bis-(diphenyl-{benzo-[1,3]- $\mu O^1:kO^2$ -4-ylmethyl}-phosphan- kP)platin(II)}-[OC-6-33]- $\mu O^1:kO^2$ -dioxiomolybdän(VI)] (39)

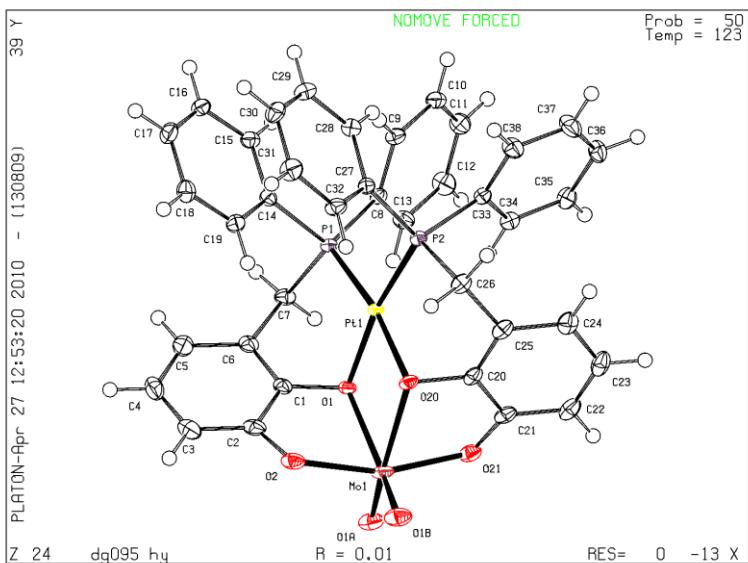


Table 1. Crystal data and structure refinement for dg095_hy.

Identification code	dg095_hy	
Empirical formula	C38 H30 Mo O6 P2 Pt	
Formula weight	935.59	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Triclinic, P-1 (No.2)	
Unit cell dimensions	a = 10.434(1) Å	alpha = 82.00(1) deg.
	b = 10.784(1) Å	beta = 77.33(1) deg.
	c = 16.890(1) Å	gamma = 62.81(1) deg.
Volume	1647.6(2) Å^3	
Z, Calculated density	2, 1.886 Mg/m^3	
Absorption coefficient	4.767 mm^-1	
F(000)	912	
Crystal size	0.30 x 0.15 x 0.10 mm	
Theta range for data collection	3.02 to 27.48 deg.	
Limiting indices	-13<=h<=13, -14<=k<=14, -21<=l<=21	
Reflections collected / unique	38161 / 7533 [R(int) = 0.0199]	
Completeness to theta = 27.48	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.6468 and 0.4225	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7533 / 0 / 433	
Goodness-of-fit on F^2	1.056	
Final R indices [I>2sigma(I)]	R1 = 0.0129, wR2 = 0.0306	
R indices (all data)	R1 = 0.0148, wR2 = 0.0314	
Largest diff. peak and hole	0.492 and -0.511 e.Å^-3	

[*SP*-4-2]-[{Bis-(diphenyl-{benzo-[1,3]- $\mu O^1:kO^2$ -4-ylmethyl}-phosphan- kP)platin(II)}-[OC-6-33]- $\mu O^1:kO^2$ -dioxowolfram(VI)] (41)

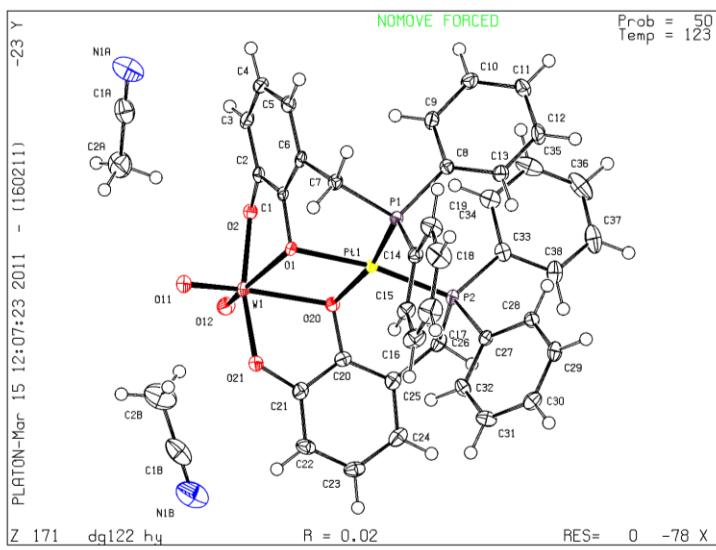
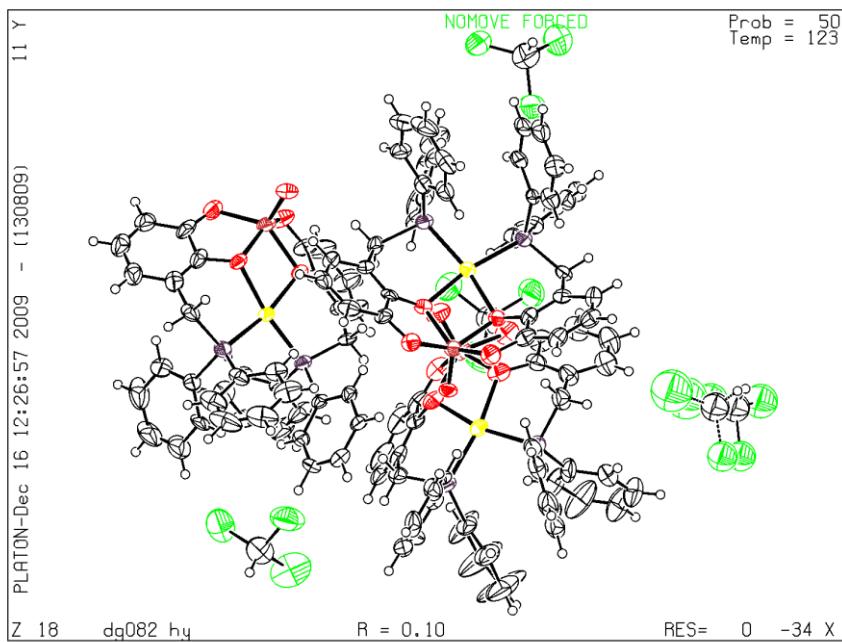


Table 1. Crystal data and structure refinement for dg122_hy.

Identification code	dg122_hy
Empirical formula	C ₄₂ H ₃₆ N ₂ O ₆ P ₂ Pt W C ₃₈ H ₃₀ O ₆ P ₂ Pt W - 2 CH ₃ CN
Formula weight	1105.61
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n (No.14)
Unit cell dimensions	a = 11.2931(7) Å alpha = 90 deg. b = 17.2776(3) Å beta = 100.306(6) deg. c = 19.4364(15) Å gamma = 90 deg.
Volume	3731.2(4) Å ³
Z, Calculated density	4, 1.968 Mg/m ³
Absorption coefficient	6.964 mm ⁻¹
F(000)	2128
Crystal size	0.16 x 0.10 x 0.08 mm
Theta range for data collection	3.06 to 27.48 deg.
Limiting indices	-14<=h<=14, -22<=k<=22, -25<=l<=25
Reflections collected / unique	53995 / 8540 [R(int) = 0.0290]
Completeness to theta = 27.48	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.5949 and 0.4539
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	8540 / 0 / 489
Goodness-of-fit on F ²	1.070
Final R indices [I>2sigma(I)]	R1 = 0.0178, wR2 = 0.0362
R indices (all data)	R1 = 0.0235, wR2 = 0.0378
Largest diff. peak and hole	0.530 and -0.487 e.Å ⁻³

[*SP*-4-2]-[{Bis-(diphenyl-{benzo-[1,3]- μO^1 - kO^2 -4-ylmethyl}-phosphan- kP)palladium(II)}-[*SPY*-5-32]- μO^1 - kO^2 -oxovanadium(IV)]
(42)



DG082_HY
PdVO1
G. Bauer
AK Gudat

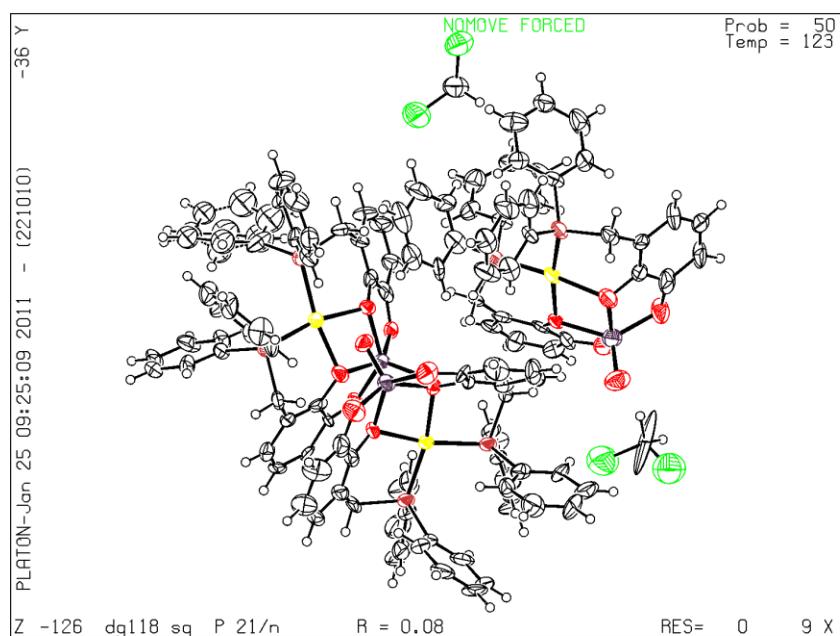
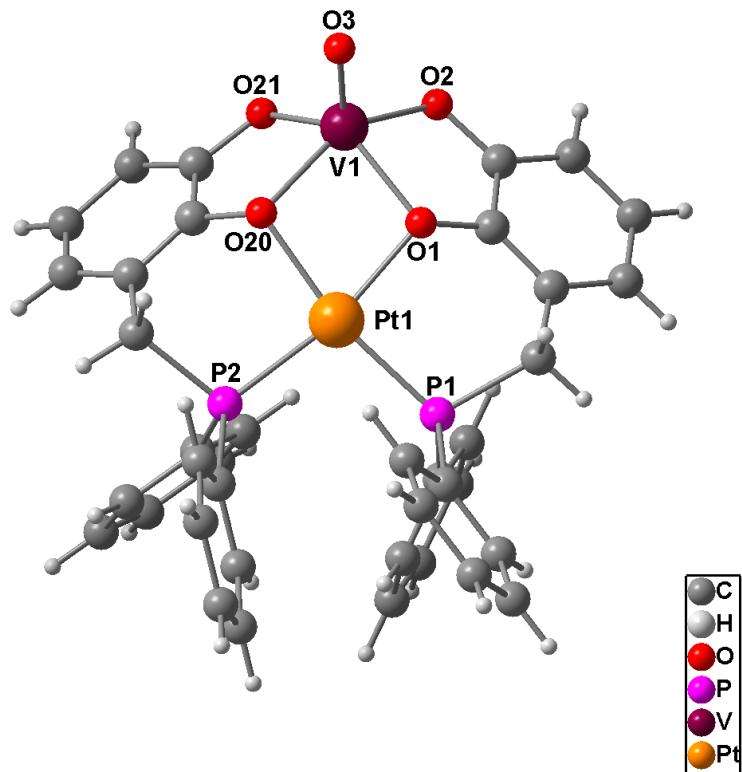
Crystal data and structure refinement for dg082_hy.
 G.Bauer (AK Gudat, Stuttgart) 16.12.2009

Identification code	dg082_hy	
Empirical formula	C ₃₉ . ³³ H ₃₁ . ³³ Cl ₄ O ₅ P ₂ Pd V	
	C ₃₈ H ₃₀ O ₅ P ₂ Pd V - 4/3 CHCl ₃	
Formula weight	945.06	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, P2(1)/n (No.14)	
Unit cell dimensions	$a = 18.945(1)$ Å $\alpha = 90$ deg. $b = 22.082(2)$ Å $\beta = 97.47(1)$ deg. $c = 28.081(3)$ Å $\gamma = 90$ deg.	
Volume	11647.8(17) Å ³	
Z, Calculated density	12, 1.617 Mg/m ³	
Absorption coefficient	1.105 mm ⁻¹	
F(000)	5692	
Crystal size	0.50 x 0.08 x 0.04 mm	
Theta range for data collection	2.92 to 25.00 deg.	
Limiting indices	-22<=h<=22, -25<=k<=26, -31<=l<=33	
Reflections collected / unique	69656 / 20428 [R(int) = 0.1291]	
Completeness to theta = 25.00	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9280 and 0.3917	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	20428 / 396 / 1407	
Goodness-of-fit on F ²	1.037	
Final R indices [I>2sigma(I)]	R1 = 0.0955, wR2 = 0.2286	
R indices (all data)	R1 = 0.1785, wR2 = 0.2824	
Largest diff. peak and hole	1.666 and -2.068 e.Å ⁻³	

[*SP*-4-2]-[{Bis-(diphenyl-{benzo-[1,3]- $\mu O^1:kO^2$ -4-ylmethyl}-phosphan- kP)platin(II)}-[*SPY*-5-32]- $\mu O^1:kO^2$ -oxovanadium(IV)] (43)

DG118_HY
K237

SQUEEZE data: 4 CH₂Cl₂ 'squeezed out'



2 methylenchloride / molecule, but only 2 in the asymmetric unit reasonable refined

Crystal data and structure refinement for dg118_sq.
SWQUEEZE-data

Identification code	dg118_sq
Empirical formula	C40 H34 C14 O5 P2 Pt V C38 H30 O5 P2 Pt V - 2 CH2Cl2
Formula weight	1044.44
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P 21/n
Unit cell dimensions	a = 23.423(2) Å alpha = 90 deg. b = 18.647(1) Å beta = 98.84(1) deg. c = 28.122(2) Å gamma = 90 deg.
Volume	12136.9(15) Å^3
Z, Calculated density	12, 1.715 Mg/m^3
Absorption coefficient	4.071 mm^-1
F(000)	6156
Crystal size	0.16 x 0.12 x 0.04 mm
Theta range for data collection	2.93 to 25.03 deg.
Limiting indices	-27<=h<=27, 0<=k<=22, 0<=l<=33
Reflections collected / unique	20683 / 20683 [R(int) = 0.0000]
Completeness to theta = 25.03	96.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8621 and 0.4500
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	20683 / 51 / 1183
Goodness-of-fit on F^2	0.951
Final R indices [I>2sigma(I)]	R1 = 0.0781, wR2 = 0.1903
R indices (all data)	R1 = 0.1451, wR2 = 0.2154
Largest diff. peak and hole	4.809 and -2.481 e.Å^-3

[*SP*-4-2]-Chloro[$\{\text{bis}-(\text{diphenyl}-\{\text{benzo-[1,3]-}\mu O^1:\text{k}O^2\text{-4-ylmethyl}\}\text{-}$
 $\text{phosphan-}kP\text{)}\text{palladium(II)}\}-[\text{SPY-5-13}]\text{-}\mu O^1:\text{k}O^2\text{-eisen(III)}]$] (44)

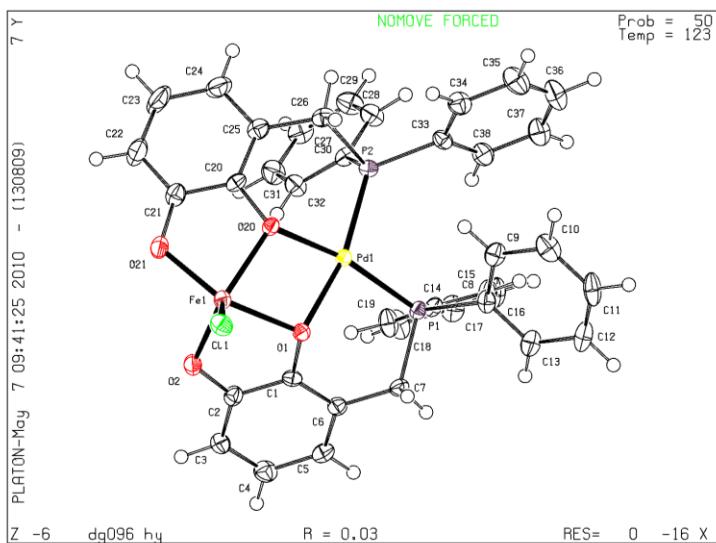


Table 1. Crystal data and structure refinement for dg096_hy.

Identification code	dg096_hy
Empirical formula	C38 H30 Cl Fe O4 P2 Pd
Formula weight	810.26
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 12.623(1) Å alpha = 90 deg. b = 13.212(1) Å beta = 90 deg. c = 20.098(1) Å gamma = 90 deg.
Volume	3351.8(4) Å ³
Z, Calculated density	4, 1.606 Mg/m ³
Absorption coefficient	1.185 mm ⁻¹
F(000)	1636
Crystal size	0.36 x 0.12 x 0.06 mm
Theta range for data collection	3.02 to 27.48 deg.
Limiting indices	-16<=h<=16, -17<=k<=17, -26<=l<=26
Reflections collected / unique	45337 / 7673 [R(int) = 0.0562]
Completeness to theta = 27.48	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9281 and 0.6162
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	7673 / 0 / 424
Goodness-of-fit on F ²	1.061
Final R indices [I>2sigma(I)]	R1 = 0.0257, wR2 = 0.0579
R indices (all data)	R1 = 0.0301, wR2 = 0.0598
Absolute structure parameter	-0.006(13)
Largest diff. peak and hole	0.793 and -0.413 e.Å ⁻³

Bis-[SP-4-2]-[{bis-(diphenyl-{benzo-[1,3]- μO^1 : kO^2 -4-ylmethyl}-phosphan- kP)platin(II)}-[SPY-5-32]- μO^1 : kO^2 -eisen(III)]-oxid (45)

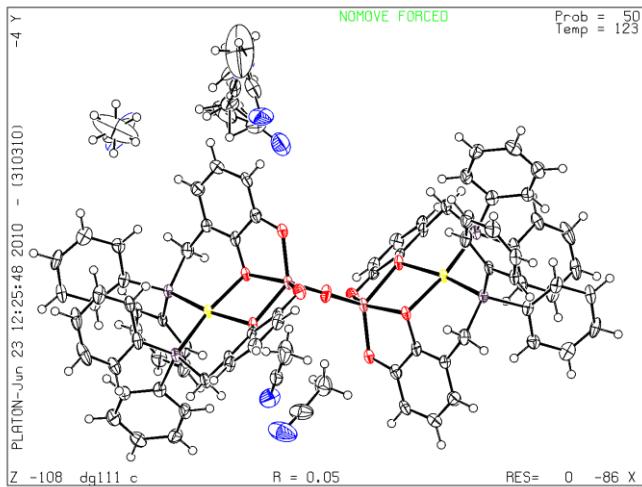


Table 1. Crystal data and structure refinement for dg111_hy.

Identification code	dg111_hy
Empirical formula	C94 H87 Fe2 N9 O9 P4 Pt2 C76 H60 Fe2 O9 P4 Pt2 - 9 CH3CN
Formula weight	2112.49
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, C2/c (No.15)
Unit cell dimensions	a = 24.856(2) Å alpha = 90 deg. b = 16.089(1) Å beta = 109.92(1) deg. c = 23.260(2) Å gamma = 90 deg.
Volume	8745.3(12) Å^3
Z, Calculated density	4, 1.604 Mg/m^3
Absorption coefficient	3.651 mm^-1
F(000)	4216
Crystal size	0.18 x 0.09 x 0.03 mm
Theta range for data collection	2.92 to 27.48 deg.
Limiting indices	-32<=h<=32, -20<=k<=20, -30<=l<=29
Reflections collected / unique	60538 / 10008 [R(int) = 0.1044]
Completeness to theta = 27.48	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8940 and 0.6023
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10008 / 90 / 598
Goodness-of-fit on F^2	1.039
Final R indices [I>2sigma(I)]	R1 = 0.0538, wR2 = 0.1082
R indices (all data)	R1 = 0.0889, wR2 = 0.1214
Largest diff. peak and hole	2.612 and -1.461 e.Å^-3

Bis-[*SP*-4-2]-[{(diphenyl-{benzo-[1,3]- μO^1 : kO^2 -4-ylmethyl}-phosphan-*kP*)(diphenyl-{benzo-[1,3]- μO^1 -4-ylmethyl}-phosphan-*kP*-palladium(II)}-[*SPY*-5-13]- μO^1 : μO^1 : kO^2 -chlorocobalt(II)] (48)

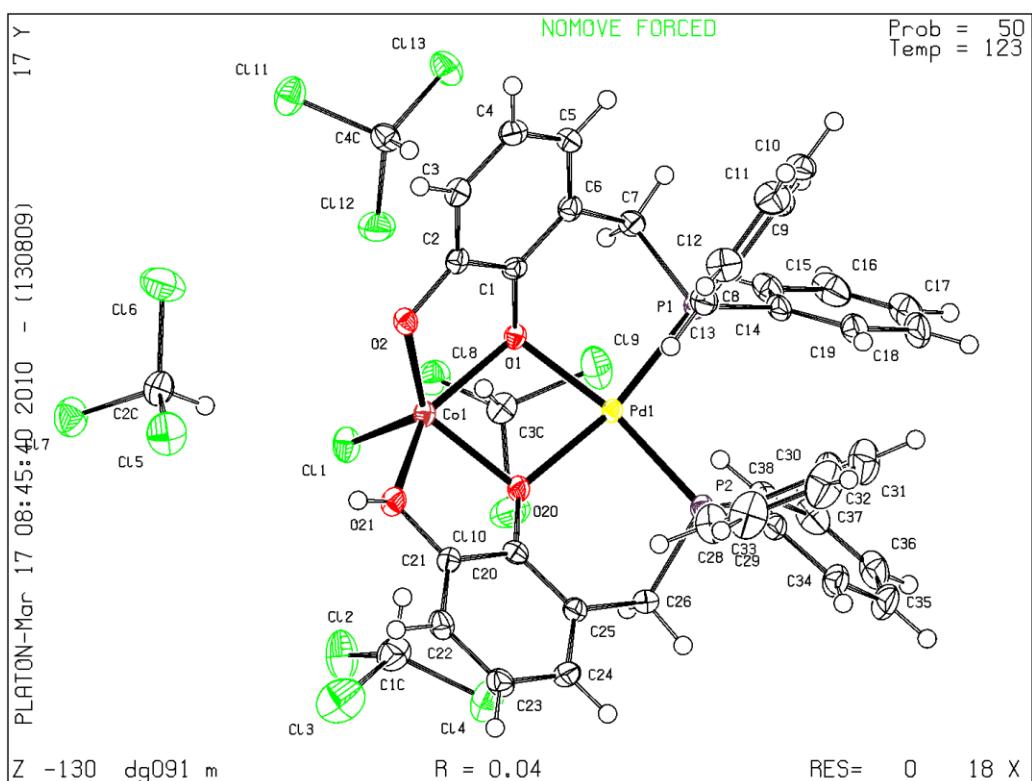
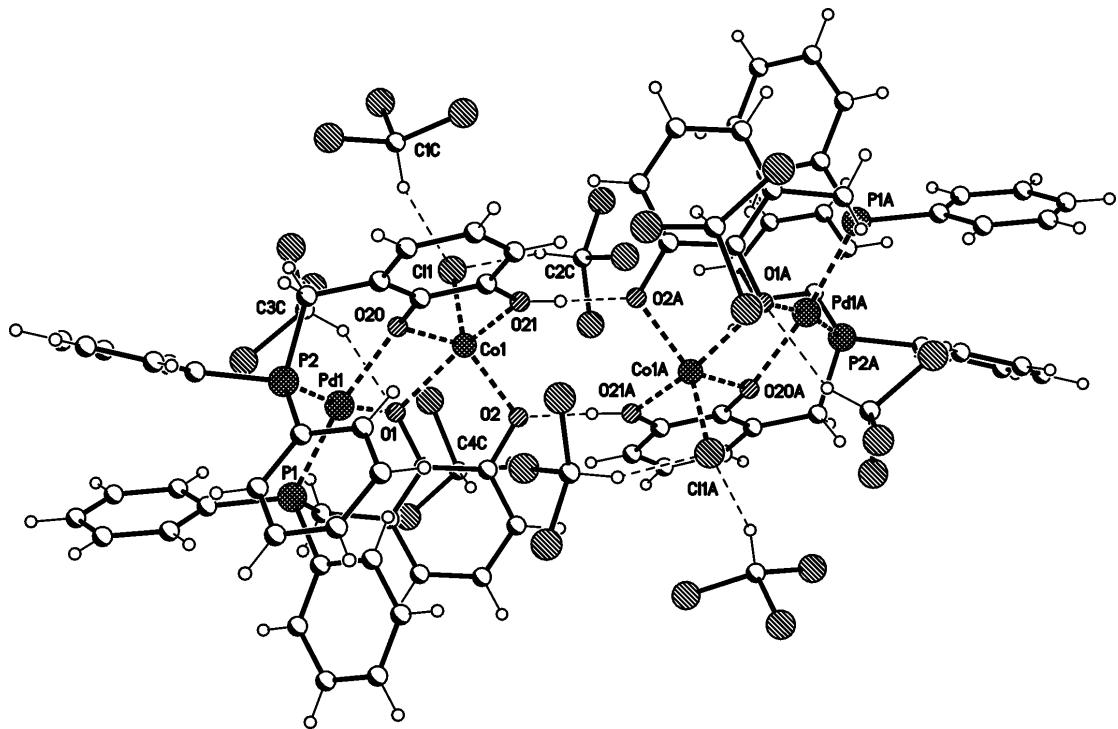


Table 1. Crystal data and structure refinement for dg091_hy.

Identification code	dg091_m
Empirical formula	C42 H35 Cl13 Co O4 P2 Pd C38 H31 Cl Co O4 P2 Pd - 4 CHCl3
Formula weight	1291.82
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c (No.14)
Unit cell dimensions	a = 15.009(1) Å alpha = 90 deg. b = 13.892(1) Å beta = 92.52(1) deg. c = 23.974(2) Å gamma = 90 deg.
Volume	4993.9(6) Å^3
Z, Calculated density	4, 1.718 Mg/m^3
Absorption coefficient	1.493 mm^-1
F(000)	2572
Crystal size	0.12 x 0.08 x 0.04 mm
Theta range for data collection	2.93 to 27.48 deg.
Limiting indices	-19<=h<=19, -18<=k<=18, -31<=l<=31
Reflections collected / unique	66297 / 11432 [R(int) = 0.0581]
Completeness to theta = 27.48	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9422 and 0.7916
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11432 / 1 / 571
Goodness-of-fit on F^2	1.034
Final R indices [I>2sigma(I)]	R1 = 0.0387, wR2 = 0.0725
R indices (all data)	R1 = 0.0680, wR2 = 0.0817
Largest diff. peak and hole	0.553 and -0.535 e.Å^-3

Zink-Komplex von 5 (49)

Table 1. Crystal data and structure refinement for gud17_sq.

Identification code	gud17_sq
Empirical formula	C318.50 H332.50 Cl8 N17.50 O45.50 P14 Pd7 Zn11
Formula weight	7314.57
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	$a = 21.4475(12)$ Å $\alpha = 88.469(3)$ deg. $b = 25.3152(12)$ Å $\beta = 85.014(3)$ deg. $c = 27.7107(13)$ Å $\gamma = 88.086(3)$ deg.
Volume	14975.9(13) Å ³
Z, Calculated density	2, 1.622 Mg/m ³
Absorption coefficient	1.494 mm ⁻¹
F(000)	7456
Crystal size	0.52 x 0.20 x 0.09 mm
Theta range for data collection	2.94 to 25.03 deg.

Limiting indices $-25 \leq h \leq 25, -30 \leq k \leq 30, 0 \leq l \leq 32$

Reflections collected / unique 51709 / 51709 [R(int) = 0.0000]

Completeness to theta = 25.03 97.8 %

Absorption correction Semi-empirical from equivalents

Max. and min. transmission 0.7516 and 0.6518

Refinement method Full-matrix least-squares on F^2

Data / restraints / parameters 51709 / 6099 / 3168

Goodness-of-fit on F^2 1.004

Final R indices [$I > 2\sigma(I)$] R1 = 0.1059, wR2 = 0.2649

R indices (all data) R1 = 0.2317, wR2 = 0.3268

Largest diff. peak and hole 3.704 and -1.193 e. \AA^{-3}

Table 3. Bond lengths [Å] and angles [deg] for gud17_sq.

Zn(1)-O(2B)	1.972(10)
Zn(1)-O(21A)	1.982(9)
Zn(1)-O(21C)	1.987(9)
Zn(1)-Cl(1)	2.220(4)
Pd(1A)-O(20A)	2.076(9)
Pd(1A)-O(1A)	2.079(9)
Pd(1A)-P(2A)	2.240(4)
Pd(1A)-P(1A)	2.265(4)
Pd(1A)-Zn(1A)	3.1640(17)
Zn(1A)-O(2C)	1.930(9)
Zn(1A)-O(20A)	2.033(9)
Zn(1A)-O(2A)	2.044(9)
Zn(1A)-O(21A)	2.045(9)
Zn(1A)-O(1A)	2.099(9)
P(1A)-C(14A)	1.788(7)
P(1A)-C(8A)	1.805(7)
P(1A)-C(7A)	1.867(13)
P(2A)-C(33A)	1.824(7)
P(2A)-C(27A)	1.834(9)
P(2A)-C(26A)	1.836(15)
O(1A)-C(1A)	1.318(16)
O(2A)-C(2A)	1.342(15)
O(2A)-Zn(1B)	1.959(9)
O(20A)-C(20A)	1.357(16)
O(21A)-C(21A)	1.364(16)
C(1A)-C(6A)	1.356(18)

C(1A)-C(2A)	1.463(18)
C(2A)-C(3A)	1.322(18)
C(3A)-C(4A)	1.400(19)
C(3A)-H(3A)	0.9500
C(4A)-C(5A)	1.387(19)
C(4A)-H(4A)	0.9500
C(5A)-C(6A)	1.380(19)
C(5A)-H(5A)	0.9500
C(6A)-C(7A)	1.539(18)
C(7A)-H(7A1)	0.9900
C(7A)-H(7A2)	0.9900
C(8A)-C(9A)	1.3900
C(8A)-C(13A)	1.3900
C(9A)-C(10A)	1.3900
C(9A)-H(9A)	0.9500
C(10A)-C(11A)	1.3900
C(10A)-H(10A)	0.9500
C(11A)-C(12A)	1.3900
C(11A)-H(11A)	0.9500
C(12A)-C(13A)	1.3900
C(12A)-H(12A)	0.9500
C(13A)-H(13A)	0.9500
C(14A)-C(15A)	1.3900
C(14A)-C(19A)	1.3900
C(15A)-C(16A)	1.3900
C(15A)-H(15A)	0.9500
C(16A)-C(17A)	1.3900
C(16A)-H(16A)	0.9500
C(17A)-C(18A)	1.3900
C(17A)-H(17A)	0.9500

C(18A)-C(19A)	1.3900
C(18A)-H(18A)	0.9500
C(19A)-H(19A)	0.9500
C(20A)-C(25A)	1.406(19)
C(20A)-C(21A)	1.407(19)
C(21A)-C(22A)	1.377(19)
C(22A)-C(23A)	1.38(2)
C(22A)-H(22A)	0.9500
C(23A)-C(24A)	1.35(2)
C(23A)-H(23A)	0.9500
C(24A)-C(25A)	1.378(19)
C(24A)-H(24A)	0.9500
C(25A)-C(26A)	1.55(2)
C(26A)-H(26A)	0.9900
C(26A)-H(26B)	0.9900
C(27A)-C(28A)	1.3900
C(27A)-C(32A)	1.3900
C(28A)-C(29A)	1.3900
C(28A)-H(28A)	0.9500
C(29A)-C(30A)	1.3900
C(29A)-H(29A)	0.9500
C(30A)-C(31A)	1.3900
C(30A)-H(30A)	0.9500
C(31A)-C(32A)	1.3900
C(31A)-H(31A)	0.9500
C(32A)-H(32A)	0.9500
C(33A)-C(34A)	1.3900
C(33A)-C(38A)	1.3900
C(34A)-C(35A)	1.3900
C(34A)-H(34A)	0.9500

C(35A)-C(36A)	1.3900
C(35A)-H(35A)	0.9500
C(36A)-C(37A)	1.3900
C(36A)-H(36A)	0.9500
C(37A)-C(38A)	1.3900
C(37A)-H(37A)	0.9500
C(38A)-H(38A)	0.9500
Pd(1B)-O(20B)	2.063(8)
Pd(1B)-O(1B)	2.077(9)
Pd(1B)-P(2B)	2.237(4)
Pd(1B)-P(1B)	2.249(4)
Pd(1B)-Zn(1B)	3.152(2)
Zn(1B)-O(2B)	2.019(9)
Zn(1B)-O(21B)	2.022(9)
Zn(1B)-O(1B)	2.063(9)
Zn(1B)-O(20B)	2.081(9)
P(1B)-C(8B)	1.804(7)
P(1B)-C(14B)	1.807(9)
P(1B)-C(7B)	1.839(14)
P(2B)-C(33B)	1.774(12)
P(2B)-C(27B)	1.799(9)
P(2B)-C(26B)	1.862(14)
O(1B)-C(1B)	1.358(15)
O(2B)-C(2B)	1.397(16)
O(20B)-C(20B)	1.373(15)
O(21B)-C(21B)	1.397(16)
O(21B)-Zn(1C)	1.957(10)
C(1B)-C(6B)	1.371(18)
C(1B)-C(2B)	1.384(19)
C(2B)-C(3B)	1.433(18)

C(3B)-C(4B)	1.407(19)
C(3B)-H(3B)	0.9500
C(4B)-C(5B)	1.37(2)
C(4B)-H(4B)	0.9500
C(5B)-C(6B)	1.396(19)
C(5B)-H(5B)	0.9500
C(6B)-C(7B)	1.47(2)
C(7B)-H(7B1)	0.9900
C(7B)-H(7B2)	0.9900
C(8B)-C(9B)	1.3900
C(8B)-C(13B)	1.3900
C(9B)-C(10B)	1.3900
C(9B)-H(9B)	0.9500
C(10B)-C(11B)	1.3900
C(10B)-H(10B)	0.9500
C(11B)-C(12B)	1.3900
C(11B)-H(11B)	0.9500
C(12B)-C(13B)	1.3900
C(12B)-H(12B)	0.9500
C(13B)-H(13B)	0.9500
C(14B)-C(15B)	1.3900
C(14B)-C(19B)	1.3900
C(15B)-C(16B)	1.3900
C(15B)-H(15B)	0.9500
C(16B)-C(17B)	1.3900
C(16B)-H(16B)	0.9500
C(17B)-C(18B)	1.3900
C(17B)-H(17B)	0.9500
C(18B)-C(19B)	1.3900
C(18B)-H(18B)	0.9500

C(19B)-H(19B)	0.9500
C(20B)-C(21B)	1.384(19)
C(20B)-C(25B)	1.389(19)
C(21B)-C(22B)	1.375(18)
C(22B)-C(23B)	1.424(19)
C(22B)-H(22B)	0.9500
C(23B)-C(24B)	1.30(2)
C(23B)-H(23B)	0.9500
C(24B)-C(25B)	1.45(2)
C(24B)-H(24B)	0.9500
C(25B)-C(26B)	1.43(2)
C(26B)-H(26C)	0.9900
C(26B)-H(26D)	0.9900
C(27B)-C(28B)	1.3900
C(27B)-C(32B)	1.3900
C(28B)-C(29B)	1.3900
C(28B)-H(28B)	0.9500
C(29B)-C(30B)	1.3900
C(29B)-H(29B)	0.9500
C(30B)-C(31B)	1.3900
C(30B)-H(30B)	0.9500
C(31B)-C(32B)	1.3900
C(31B)-H(31B)	0.9500
C(32B)-H(32B)	0.9500
C(33B)-C(34B)	1.3900
C(33B)-C(38B)	1.3900
C(34B)-C(35B)	1.3900
C(34B)-H(34B)	0.9500
C(35B)-C(36B)	1.3900
C(35B)-H(35B)	0.9500

C(36B)-C(37B)	1.3900
C(36B)-H(36B)	0.9500
C(37B)-C(38B)	1.3900
C(37B)-H(37B)	0.9500
C(38B)-H(38B)	0.9500
Pd(1C)-O(20C)	2.040(9)
Pd(1C)-O(1C)	2.061(9)
Pd(1C)-P(1C)	2.221(4)
Pd(1C)-P(2C)	2.257(4)
Pd(1C)-Zn(1C)	3.1334(19)
Zn(1C)-O(2C)	1.999(8)
Zn(1C)-O(21C)	2.046(9)
Zn(1C)-O(20C)	2.047(9)
Zn(1C)-O(1C)	2.120(9)
P(1C)-C(14C)	1.764(10)
P(1C)-C(8C)	1.810(9)
P(1C)-C(7C)	1.861(15)
P(2C)-C(33C)	1.784(12)
P(2C)-C(26C)	1.836(16)
P(2C)-C(27C)	1.837(9)
O(1C)-C(1C)	1.328(16)
O(2C)-C(2C)	1.375(16)
O(20C)-C(20C)	1.344(16)
O(21C)-C(21C)	1.359(17)
C(1C)-C(6C)	1.320(19)
C(1C)-C(2C)	1.402(19)
C(2C)-C(3C)	1.444(19)
C(3C)-C(4C)	1.39(2)
C(3C)-H(3C)	0.9500
C(4C)-C(5C)	1.40(2)

C(4C)-H(4C)	0.9500
C(5C)-C(6C)	1.42(2)
C(5C)-H(5C)	0.9500
C(6C)-C(7C)	1.494(19)
C(7C)-H(7C1)	0.9900
C(7C)-H(7C2)	0.9900
C(8C)-C(9C)	1.3900
C(8C)-C(13C)	1.3900
C(9C)-C(10C)	1.3900
C(9C)-H(9C)	0.9500
C(10C)-C(11C)	1.3900
C(10C)-H(10C)	0.9500
C(11C)-C(12C)	1.3900
C(11C)-H(11C)	0.9500
C(12C)-C(13C)	1.3900
C(12C)-H(12C)	0.9500
C(13C)-H(13C)	0.9500
C(14C)-C(15C)	1.3900
C(14C)-C(19C)	1.3900
C(15C)-C(16C)	1.3900
C(15C)-H(15C)	0.9500
C(16C)-C(17C)	1.3900
C(16C)-H(16C)	0.9500
C(17C)-C(18C)	1.3900
C(17C)-H(17C)	0.9500
C(18C)-C(19C)	1.3900
C(18C)-H(18C)	0.9500
C(19C)-H(19C)	0.9500
C(20C)-C(25C)	1.40(2)
C(20C)-C(21C)	1.407(19)

C(21C)-C(22C)	1.38(2)
C(22C)-C(23C)	1.42(2)
C(22C)-H(22C)	0.9500
C(23C)-C(24C)	1.39(2)
C(23C)-H(23C)	0.9500
C(24C)-C(25C)	1.42(2)
C(24C)-H(24C)	0.9500
C(25C)-C(26C)	1.50(2)
C(26C)-H(26E)	0.9900
C(26C)-H(26F)	0.9900
C(27C)-C(28C)	1.3900
C(27C)-C(32C)	1.3900
C(28C)-C(29C)	1.3900
C(28C)-H(28C)	0.9500
C(29C)-C(30C)	1.3900
C(29C)-H(29C)	0.9500
C(30C)-C(31C)	1.3900
C(30C)-H(30C)	0.9500
C(31C)-C(32C)	1.3900
C(31C)-H(31C)	0.9500
C(32C)-H(32C)	0.9500
C(33C)-C(34C)	1.3900
C(33C)-C(38C)	1.3900
C(34C)-C(35C)	1.3900
C(34C)-H(34C)	0.9500
C(35C)-C(36C)	1.3900
C(35C)-H(35C)	0.9500
C(36C)-C(37C)	1.3900
C(36C)-H(36C)	0.9500
C(37C)-C(38C)	1.3900

C(37C)-H(37C)	0.9500
C(38C)-H(38C)	0.9500
Zn(2)-O(2D)	1.966(9)
Zn(2)-O(21F)	1.969(10)
Zn(2)-O(21E)	1.973(9)
Zn(2)-Cl(2)	2.239(4)
Pd(1D)-O(1D)	2.050(9)
Pd(1D)-O(20D)	2.065(9)
Pd(1D)-P(2D)	2.239(4)
Pd(1D)-P(1D)	2.243(4)
Pd(1D)-Zn(1D)	3.165(2)
Zn(1D)-O(2F)	1.941(10)
Zn(1D)-O(21D)	1.982(9)
Zn(1D)-O(1D)	2.026(9)
Zn(1D)-O(2D)	2.070(9)
Zn(1D)-O(20D)	2.115(9)
P(1D)-C(8D)	1.799(6)
P(1D)-C(14D)	1.805(7)
P(1D)-C(7D)	1.846(15)
P(2D)-C(33D)	1.807(8)
P(2D)-C(27D)	1.811(7)
P(2D)-C(26D)	1.872(14)
O(1D)-C(1D)	1.339(16)
O(2D)-C(2D)	1.377(15)
O(20D)-C(20D)	1.322(16)
O(21D)-C(21D)	1.335(17)
O(21D)-Zn(1E)	1.967(9)
C(1D)-C(6D)	1.389(18)
C(1D)-C(2D)	1.394(18)
C(2D)-C(3D)	1.391(19)

C(3D)-C(4D)	1.354(19)
C(3D)-H(3D)	0.9500
C(4D)-C(5D)	1.422(19)
C(4D)-H(4D)	0.9500
C(5D)-C(6D)	1.368(19)
C(5D)-H(5D)	0.9500
C(6D)-C(7D)	1.503(19)
C(7D)-H(7D1)	0.9900
C(7D)-H(7D2)	0.9900
C(8D)-C(9D)	1.3900
C(8D)-C(13D)	1.3900
C(9D)-C(10D)	1.3900
C(9D)-H(9D)	0.9500
C(10D)-C(11D)	1.3900
C(10D)-H(10D)	0.9500
C(11D)-C(12D)	1.3900
C(11D)-H(11D)	0.9500
C(12D)-C(13D)	1.3900
C(12D)-H(12D)	0.9500
C(13D)-H(13D)	0.9500
C(14D)-C(15D)	1.3900
C(14D)-C(19D)	1.3900
C(15D)-C(16D)	1.3900
C(15D)-H(15D)	0.9500
C(16D)-C(17D)	1.3900
C(16D)-H(16D)	0.9500
C(17D)-C(18D)	1.3900
C(17D)-H(17D)	0.9500
C(18D)-C(19D)	1.3900
C(18D)-H(18D)	0.9500

C(19D)-H(19D)	0.9500
C(20D)-C(25D)	1.418(19)
C(20D)-C(21D)	1.436(19)
C(21D)-C(22D)	1.43(2)
C(22D)-C(23D)	1.37(2)
C(22D)-H(22D)	0.9500
C(23D)-C(24D)	1.39(2)
C(23D)-H(23D)	0.9500
C(24D)-C(25D)	1.403(19)
C(24D)-H(24D)	0.9500
C(25D)-C(26D)	1.458(19)
C(26D)-H(26G)	0.9900
C(26D)-H(26H)	0.9900
C(27D)-C(28D)	1.3900
C(27D)-C(32D)	1.3900
C(28D)-C(29D)	1.3900
C(28D)-H(28D)	0.9500
C(29D)-C(30D)	1.3900
C(29D)-H(29D)	0.9500
C(30D)-C(31D)	1.3900
C(30D)-H(30D)	0.9500
C(31D)-C(32D)	1.3900
C(31D)-H(31D)	0.9500
C(32D)-H(32D)	0.9500
C(33D)-C(34D)	1.3900
C(33D)-C(38D)	1.3900
C(34D)-C(35D)	1.3900
C(34D)-H(34D)	0.9500
C(35D)-C(36D)	1.3900
C(35D)-H(35D)	0.9500

C(36D)-C(37D)	1.3900
C(36D)-H(36D)	0.9500
C(37D)-C(38D)	1.3900
C(37D)-H(37D)	0.9500
C(38D)-H(38D)	0.9500
Pd(1E)-O(20E)	2.004(9)
Pd(1E)-O(1E)	2.036(9)
Pd(1E)-P(2E)	2.231(4)
Pd(1E)-P(1E)	2.249(4)
Pd(1E)-Zn(1E)	3.1685(18)
Zn(1E)-O(2E)	1.978(10)
Zn(1E)-O(20E)	1.989(9)
Zn(1E)-O(21E)	2.073(9)
Zn(1E)-O(1E)	2.142(9)
P(1E)-C(14E)	1.792(8)
P(1E)-C(8E)	1.822(8)
P(1E)-C(7E)	1.841(14)
P(2E)-C(33E)	1.804(7)
P(2E)-C(27E)	1.822(8)
P(2E)-C(26E)	1.859(14)
O(1E)-C(1E)	1.351(17)
O(2E)-C(2E)	1.352(16)
O(2E)-Zn(1F)	1.989(9)
O(20E)-C(20E)	1.364(16)
O(21E)-C(21E)	1.364(16)
C(1E)-C(6E)	1.439(19)
C(1E)-C(2E)	1.46(2)
C(2E)-C(3E)	1.36(2)
C(3E)-C(4E)	1.37(2)
C(3E)-H(3E)	0.9500

C(4E)-C(5E)	1.37(2)
C(4E)-H(4E)	0.9500
C(5E)-C(6E)	1.24(2)
C(5E)-H(5E)	0.9500
C(6E)-C(7E)	1.52(2)
C(7E)-H(7E1)	0.9900
C(7E)-H(7E2)	0.9900
C(8E)-C(9E)	1.3900
C(8E)-C(13E)	1.3900
C(9E)-C(10E)	1.3900
C(9E)-H(9E)	0.9500
C(10E)-C(11E)	1.3900
C(10E)-H(10E)	0.9500
C(11E)-C(12E)	1.3900
C(11E)-H(11E)	0.9500
C(12E)-C(13E)	1.3900
C(12E)-H(12E)	0.9500
C(13E)-H(13E)	0.9500
C(14E)-C(15E)	1.3900
C(14E)-C(19E)	1.3900
C(15E)-C(16E)	1.3900
C(15E)-H(15E)	0.9500
C(16E)-C(17E)	1.3900
C(16E)-H(16E)	0.9500
C(17E)-C(18E)	1.3900
C(17E)-H(17E)	0.9500
C(18E)-C(19E)	1.3900
C(18E)-H(18E)	0.9500
C(19E)-H(19E)	0.9500
C(20E)-C(25E)	1.390(19)

C(20E)-C(21E)	1.415(19)
C(21E)-C(22E)	1.391(19)
C(22E)-C(23E)	1.38(2)
C(22E)-H(22E)	0.9500
C(23E)-C(24E)	1.35(2)
C(23E)-H(23E)	0.9500
C(24E)-C(25E)	1.403(19)
C(24E)-H(24E)	0.9500
C(25E)-C(26E)	1.48(2)
C(26E)-H(26I)	0.9900
C(26E)-H(26J)	0.9900
C(27E)-C(28E)	1.3900
C(27E)-C(32E)	1.3900
C(28E)-C(29E)	1.3900
C(28E)-H(28E)	0.9500
C(29E)-C(30E)	1.3900
C(29E)-H(29E)	0.9500
C(30E)-C(31E)	1.3900
C(30E)-H(30E)	0.9500
C(31E)-C(32E)	1.3900
C(31E)-H(31E)	0.9500
C(32E)-H(32E)	0.9500
C(33E)-C(34E)	1.3900
C(33E)-C(38E)	1.3900
C(34E)-C(35E)	1.3900
C(34E)-H(34E)	0.9500
C(35E)-C(36E)	1.3900
C(35E)-H(35E)	0.9500
C(36E)-C(37E)	1.3900
C(36E)-H(36E)	0.9500

C(37E)-C(38E)	1.3900
C(37E)-H(37E)	0.9500
C(38E)-H(38E)	0.9500
Pd(1F)-O(20F)	2.057(10)
Pd(1F)-O(1F)	2.070(11)
Pd(1F)-P(1F)	2.238(4)
Pd(1F)-P(2F)	2.267(5)
Pd(1F)-Zn(1F)	3.150(2)
Zn(1F)-O(2F)	2.030(10)
Zn(1F)-O(20F)	2.032(11)
Zn(1F)-O(21F)	2.079(9)
Zn(1F)-O(1F)	2.085(10)
P(1F)-C(14F)	1.777(11)
P(1F)-C(8F)	1.818(9)
P(1F)-C(7F)	1.859(18)
P(2F)-C(27F)	1.785(10)
P(2F)-C(33F)	1.789(9)
P(2F)-C(26F)	1.799(15)
O(1F)-C(1F)	1.377(18)
O(2F)-C(2F)	1.375(16)
O(20F)-C(20F)	1.362(17)
O(21F)-C(21F)	1.349(17)
C(1F)-C(6F)	1.36(2)
C(1F)-C(2F)	1.39(2)
C(2F)-C(3F)	1.38(2)
C(3F)-C(4F)	1.40(2)
C(3F)-H(3F)	0.9500
C(4F)-C(5F)	1.43(2)
C(4F)-H(4F)	0.9500
C(5F)-C(6F)	1.36(2)

C(5F)-H(5F)	0.9500
C(6F)-C(7F)	1.50(2)
C(7F)-H(7F1)	0.9900
C(7F)-H(7F2)	0.9900
C(8F)-C(9F)	1.3900
C(8F)-C(13F)	1.3900
C(9F)-C(10F)	1.3900
C(9F)-H(9F)	0.9500
C(10F)-C(11F)	1.3900
C(10F)-H(10F)	0.9500
C(11F)-C(12F)	1.3900
C(11F)-H(11F)	0.9500
C(12F)-C(13F)	1.3900
C(12F)-H(12F)	0.9500
C(13F)-H(13F)	0.9500
C(14F)-C(15F)	1.3900
C(14F)-C(19F)	1.3900
C(15F)-C(16F)	1.3900
C(15F)-H(15F)	0.9500
C(16F)-C(17F)	1.3900
C(16F)-H(16F)	0.9500
C(17F)-C(18F)	1.3900
C(17F)-H(17F)	0.9500
C(18F)-C(19F)	1.3900
C(18F)-H(18F)	0.9500
C(19F)-H(19F)	0.9500
C(20F)-C(25F)	1.40(2)
C(20F)-C(21F)	1.42(2)
C(21F)-C(22F)	1.37(2)
C(22F)-C(23F)	1.37(2)

C(22F)-H(22F)	0.9500
C(23F)-C(24F)	1.38(2)
C(23F)-H(23F)	0.9500
C(24F)-C(25F)	1.37(2)
C(24F)-H(24F)	0.9500
C(25F)-C(26F)	1.56(2)
C(26F)-H(26K)	0.9900
C(26F)-H(26L)	0.9900
C(27F)-C(28F)	1.3900
C(27F)-C(32F)	1.3900
C(28F)-C(29F)	1.3900
C(28F)-H(28F)	0.9500
C(29F)-C(30F)	1.3900
C(29F)-H(29F)	0.9500
C(30F)-C(31F)	1.3900
C(30F)-H(30F)	0.9500
C(31F)-C(32F)	1.3900
C(31F)-H(31F)	0.9500
C(32F)-H(32F)	0.9500
C(33F)-C(34F)	1.3900
C(33F)-C(38F)	1.3900
C(34F)-C(35F)	1.3900
C(34F)-H(34F)	0.9500
C(35F)-C(36F)	1.3900
C(35F)-H(35F)	0.9500
C(36F)-C(37F)	1.3900
C(36F)-H(36F)	0.9500
C(37F)-C(38F)	1.3900
C(37F)-H(37F)	0.9500
C(38F)-H(38F)	0.9500

Pd(1G)-O(20G)	2.079(11)
Pd(1G)-O(1G)	2.085(11)
Pd(1G)-P(1G)	2.233(5)
Pd(1G)-P(2G)	2.243(5)
Pd(1G)-Zn(1G)	3.175(2)
Zn(1G)-O(2G)	2.037(13)
Zn(1G)-O(20G)	2.070(11)
Zn(1G)-O(21G)	2.088(12)
Zn(1G)-O(1G)	2.154(12)
Zn(1G)-Cl(1G)	2.197(6)
Zn(1G)-Zn(3)	3.058(3)
P(1G)-C(8G)	1.799(10)
P(1G)-C(14G)	1.835(11)
P(1G)-C(7G)	1.853(19)
P(2G)-C(33G)	1.780(9)
P(2G)-C(27G)	1.815(9)
P(2G)-C(26G)	1.833(16)
O(1G)-C(1G)	1.33(2)
O(2G)-C(2G)	1.39(2)
O(2G)-Zn(3)	2.055(13)
O(20G)-C(20G)	1.376(19)
O(21G)-C(21G)	1.326(19)
O(21G)-Zn(3)	2.035(12)
C(1G)-C(2G)	1.39(3)
C(1G)-C(6G)	1.40(2)
C(2G)-C(3G)	1.37(3)
C(3G)-C(4G)	1.39(3)
C(3G)-H(3G)	0.9500
C(4G)-C(5G)	1.35(3)
C(4G)-H(4G)	0.9500

C(5G)-C(6G)	1.39(3)
C(5G)-H(5G)	0.9500
C(6G)-C(7G)	1.53(3)
C(7G)-H(7G1)	0.9900
C(7G)-H(7G2)	0.9900
C(8G)-C(9G)	1.3900
C(8G)-C(13G)	1.3900
C(9G)-C(10G)	1.3900
C(9G)-H(9G)	0.9500
C(10G)-C(11G)	1.3900
C(10G)-H(10G)	0.9500
C(11G)-C(12G)	1.3900
C(11G)-H(11G)	0.9500
C(12G)-C(13G)	1.3900
C(12G)-H(12G)	0.9500
C(13G)-H(13G)	0.9500
C(14G)-C(15G)	1.3900
C(14G)-C(19G)	1.3900
C(15G)-C(16G)	1.3900
C(15G)-H(15G)	0.9500
C(16G)-C(17G)	1.3900
C(16G)-H(16G)	0.9500
C(17G)-C(18G)	1.3900
C(17G)-H(17G)	0.9500
C(18G)-C(19G)	1.3900
C(18G)-H(18G)	0.9500
C(19G)-H(19G)	0.9500
C(20G)-C(21G)	1.36(2)
C(20G)-C(25G)	1.36(2)
C(21G)-C(22G)	1.43(2)

C(22G)-C(23G)	1.38(2)
C(22G)-H(22G)	0.9500
C(23G)-C(24G)	1.38(2)
C(23G)-H(23G)	0.9500
C(24G)-C(25G)	1.41(2)
C(24G)-H(24G)	0.9500
C(25G)-C(26G)	1.53(2)
C(26G)-H(26M)	0.9900
C(26G)-H(26N)	0.9900
C(27G)-C(28G)	1.3900
C(27G)-C(32G)	1.3900
C(28G)-C(29G)	1.3900
C(28G)-H(28G)	0.9500
C(29G)-C(30G)	1.3900
C(29G)-H(29G)	0.9500
C(30G)-C(31G)	1.3900
C(30G)-H(30G)	0.9500
C(31G)-C(32G)	1.3900
C(31G)-H(31G)	0.9500
C(32G)-H(32G)	0.9500
C(33G)-C(34G)	1.3900
C(33G)-C(38G)	1.3900
C(34G)-C(35G)	1.3900
C(34G)-H(34G)	0.9500
C(35G)-C(36G)	1.3900
C(35G)-H(35G)	0.9500
C(36G)-C(37G)	1.3900
C(36G)-H(36G)	0.9500
C(37G)-C(38G)	1.3900
C(37G)-H(37G)	0.9500

C(38G)-H(38G)	0.9500
Zn(3)-Cl(5)	2.192(6)
Zn(3)-Cl(4)	2.195(6)
Zn(4)-O(11)	1.994(12)
Zn(4)-Cl(7)	2.224(10)
Zn(4)-Cl(6)	2.258(8)
Zn(4)-Cl(8)	2.265(8)
O(11)-C(11)	1.281(10)
C(11)-N(11)	1.354(11)
C(11)-H(11)	0.9500
N(11)-C(112)	1.472(9)
N(11)-C(111)	1.476(9)
C(111)-H(11H)	0.9800
C(111)-H(11I)	0.9800
C(111)-H(11J)	0.9800
C(112)-H(11K)	0.9800
C(112)-H(11L)	0.9800
C(112)-H(11M)	0.9800
O(21)-C(21)	1.275(10)
C(21)-N(21)	1.348(11)
C(21)-H(21)	0.9500
N(21)-C(211)	1.466(9)
N(21)-C(212)	1.469(9)
C(211)-H(21A)	0.9800
C(211)-H(21B)	0.9800
C(211)-H(21C)	0.9800
C(212)-H(21D)	0.9800
C(212)-H(21E)	0.9800
C(212)-H(21F)	0.9800
O(31)-C(31)	1.284(10)

C(31)-N(31)	1.351(11)
C(31)-H(31)	0.9500
N(31)-C(312)	1.470(9)
N(31)-C(311)	1.473(9)
C(311)-H(31H)	0.9800
C(311)-H(31I)	0.9800
C(311)-H(31J)	0.9800
C(312)-H(31K)	0.9800
C(312)-H(31L)	0.9800
C(312)-H(31M)	0.9800
O(41)-C(41)	1.280(10)
C(41)-N(41)	1.353(11)
C(41)-H(41)	0.9500
N(41)-C(412)	1.468(9)
N(41)-C(411)	1.468(9)
C(411)-H(41A)	0.9800
C(411)-H(41B)	0.9800
C(411)-H(41C)	0.9800
C(412)-H(41D)	0.9800
C(412)-H(41E)	0.9800
C(412)-H(41F)	0.9800
O(51)-C(51)	1.279(10)
C(51)-N(51)	1.352(11)
C(51)-H(51)	0.9500
N(51)-C(511)	1.471(9)
N(51)-C(512)	1.472(9)
C(511)-H(51A)	0.9800
C(511)-H(51B)	0.9800
C(511)-H(51C)	0.9800
C(512)-H(51D)	0.9800

C(512)-H(51E)	0.9800
C(512)-H(51F)	0.9800
O(61)-C(61)	1.283(10)
C(61)-N(61)	1.347(11)
C(61)-H(61)	0.9500
N(61)-C(611)	1.468(9)
N(61)-C(612)	1.474(9)
C(611)-H(61A)	0.9800
C(611)-H(61B)	0.9800
C(611)-H(61C)	0.9800
C(612)-H(61D)	0.9800
C(612)-H(61E)	0.9800
C(612)-H(61F)	0.9800
O(71)-C(71)	1.287(11)
C(71)-N(71)	1.354(11)
C(71)-H(71)	0.9500
N(71)-C(711)	1.470(9)
N(71)-C(712)	1.471(9)
C(711)-H(71A)	0.9800
C(711)-H(71B)	0.9800
C(711)-H(71C)	0.9800
C(712)-H(71D)	0.9800
C(712)-H(71E)	0.9800
C(712)-H(71F)	0.9800
O(81)-C(81)	1.284(11)
C(81)-N(81)	1.360(12)
C(81)-H(81)	0.9500
N(81)-C(812)	1.469(9)
N(81)-C(811)	1.470(9)
C(811)-H(81A)	0.9800

C(811)-H(81B)	0.9800
C(811)-H(81C)	0.9800
C(812)-H(81D)	0.9800
C(812)-H(81E)	0.9800
C(812)-H(81F)	0.9800
O(91)-C(91)	1.284(11)
C(91)-N(91)	1.357(12)
C(91)-H(91)	0.9500
N(91)-C(912)	1.472(9)
N(91)-C(911)	1.475(9)
C(911)-H(91A)	0.9800
C(911)-H(91B)	0.9800
C(911)-H(91C)	0.9800
C(912)-H(91D)	0.9800
C(912)-H(91E)	0.9800
C(912)-H(91F)	0.9800
O(22)-C(22)	1.279(11)
C(22)-N(22)	1.349(12)
C(22)-H(22)	0.9500
N(22)-C(221)	1.469(9)
N(22)-C(222)	1.470(9)
C(221)-H(22H)	0.9800
C(221)-H(22I)	0.9800
C(221)-H(22J)	0.9800
C(222)-H(22K)	0.9800
C(222)-H(22L)	0.9800
C(222)-H(22M)	0.9800
O(32)-C(32)	1.284(11)
C(32)-N(32)	1.358(12)
C(32)-H(32)	0.9500

N(32)-C(322)	1.472(9)
N(32)-C(321)	1.475(9)
C(321)-H(32H)	0.9800
C(321)-H(32I)	0.9800
C(321)-H(32J)	0.9800
C(322)-H(32K)	0.9800
C(322)-H(32L)	0.9800
C(322)-H(32M)	0.9800
O(2B)-Zn(1)-O(21A)	102.4(4)
O(2B)-Zn(1)-O(21C)	94.7(4)
O(21A)-Zn(1)-O(21C)	107.2(4)
O(2B)-Zn(1)-Cl(1)	117.9(3)
O(21A)-Zn(1)-Cl(1)	112.0(3)
O(21C)-Zn(1)-Cl(1)	120.0(3)
O(20A)-Pd(1A)-O(1A)	79.8(3)
O(20A)-Pd(1A)-P(2A)	90.3(3)
O(1A)-Pd(1A)-P(2A)	170.1(3)
O(20A)-Pd(1A)-P(1A)	167.4(3)
O(1A)-Pd(1A)-P(1A)	88.6(3)
P(2A)-Pd(1A)-P(1A)	101.25(14)
O(20A)-Pd(1A)-Zn(1A)	39.2(2)
O(1A)-Pd(1A)-Zn(1A)	41.0(2)
P(2A)-Pd(1A)-Zn(1A)	129.17(11)
P(1A)-Pd(1A)-Zn(1A)	129.58(10)
O(2C)-Zn(1A)-O(20A)	109.5(4)
O(2C)-Zn(1A)-O(2A)	112.0(4)
O(20A)-Zn(1A)-O(2A)	137.9(4)
O(2C)-Zn(1A)-O(21A)	106.4(4)
O(20A)-Zn(1A)-O(21A)	82.1(4)

O(2A)-Zn(1A)-O(21A)	93.3(4)
O(2C)-Zn(1A)-O(1A)	108.2(3)
O(20A)-Zn(1A)-O(1A)	80.3(4)
O(2A)-Zn(1A)-O(1A)	80.0(4)
O(21A)-Zn(1A)-O(1A)	144.7(3)
O(2C)-Zn(1A)-Pd(1A)	119.1(3)
O(20A)-Zn(1A)-Pd(1A)	40.1(3)
O(2A)-Zn(1A)-Pd(1A)	109.4(3)
O(21A)-Zn(1A)-Pd(1A)	113.9(2)
O(1A)-Zn(1A)-Pd(1A)	40.5(2)
C(14A)-P(1A)-C(8A)	106.6(4)
C(14A)-P(1A)-C(7A)	105.7(5)
C(8A)-P(1A)-C(7A)	103.4(5)
C(14A)-P(1A)-Pd(1A)	118.7(3)
C(8A)-P(1A)-Pd(1A)	113.8(3)
C(7A)-P(1A)-Pd(1A)	107.2(4)
C(33A)-P(2A)-C(27A)	105.6(5)
C(33A)-P(2A)-C(26A)	102.5(6)
C(27A)-P(2A)-C(26A)	102.5(6)
C(33A)-P(2A)-Pd(1A)	118.7(4)
C(27A)-P(2A)-Pd(1A)	116.5(4)
C(26A)-P(2A)-Pd(1A)	109.0(5)
C(1A)-O(1A)-Pd(1A)	120.0(7)
C(1A)-O(1A)-Zn(1A)	111.9(7)
Pd(1A)-O(1A)-Zn(1A)	98.5(4)
C(2A)-O(2A)-Zn(1B)	121.8(8)
C(2A)-O(2A)-Zn(1A)	113.3(8)
Zn(1B)-O(2A)-Zn(1A)	117.8(4)
C(20A)-O(20A)-Zn(1A)	110.6(8)
C(20A)-O(20A)-Pd(1A)	122.4(8)

Zn(1A)-O(20A)-Pd(1A)	100.7(4)
C(21A)-O(21A)-Zn(1)	130.1(8)
C(21A)-O(21A)-Zn(1A)	109.3(8)
Zn(1)-O(21A)-Zn(1A)	118.5(4)
O(1A)-C(1A)-C(6A)	124.1(12)
O(1A)-C(1A)-C(2A)	117.3(11)
C(6A)-C(1A)-C(2A)	118.3(13)
C(3A)-C(2A)-O(2A)	126.3(12)
C(3A)-C(2A)-C(1A)	117.2(12)
O(2A)-C(2A)-C(1A)	116.4(12)
C(2A)-C(3A)-C(4A)	123.7(13)
C(2A)-C(3A)-H(3A)	118.2
C(4A)-C(3A)-H(3A)	118.2
C(5A)-C(4A)-C(3A)	119.5(14)
C(5A)-C(4A)-H(4A)	120.3
C(3A)-C(4A)-H(4A)	120.3
C(6A)-C(5A)-C(4A)	117.6(13)
C(6A)-C(5A)-H(5A)	121.2
C(4A)-C(5A)-H(5A)	121.2
C(1A)-C(6A)-C(5A)	123.4(13)
C(1A)-C(6A)-C(7A)	116.2(13)
C(5A)-C(6A)-C(7A)	120.3(12)
C(6A)-C(7A)-P(1A)	116.5(9)
C(6A)-C(7A)-H(7A1)	108.2
P(1A)-C(7A)-H(7A1)	108.2
C(6A)-C(7A)-H(7A2)	108.2
P(1A)-C(7A)-H(7A2)	108.2
H(7A1)-C(7A)-H(7A2)	107.3
C(9A)-C(8A)-C(13A)	120.0
C(9A)-C(8A)-P(1A)	120.3(5)

C(13A)-C(8A)-P(1A)	119.7(5)
C(10A)-C(9A)-C(8A)	120.0
C(10A)-C(9A)-H(9A)	120.0
C(8A)-C(9A)-H(9A)	120.0
C(9A)-C(10A)-C(11A)	120.0
C(9A)-C(10A)-H(10A)	120.0
C(11A)-C(10A)-H(10A)	120.0
C(12A)-C(11A)-C(10A)	120.0
C(12A)-C(11A)-H(11A)	120.0
C(10A)-C(11A)-H(11A)	120.0
C(11A)-C(12A)-C(13A)	120.0
C(11A)-C(12A)-H(12A)	120.0
C(13A)-C(12A)-H(12A)	120.0
C(12A)-C(13A)-C(8A)	120.0
C(12A)-C(13A)-H(13A)	120.0
C(8A)-C(13A)-H(13A)	120.0
C(15A)-C(14A)-C(19A)	120.0
C(15A)-C(14A)-P(1A)	117.8(5)
C(19A)-C(14A)-P(1A)	122.1(5)
C(16A)-C(15A)-C(14A)	120.0
C(16A)-C(15A)-H(15A)	120.0
C(14A)-C(15A)-H(15A)	120.0
C(15A)-C(16A)-C(17A)	120.0
C(15A)-C(16A)-H(16A)	120.0
C(17A)-C(16A)-H(16A)	120.0
C(18A)-C(17A)-C(16A)	120.0
C(18A)-C(17A)-H(17A)	120.0
C(16A)-C(17A)-H(17A)	120.0
C(17A)-C(18A)-C(19A)	120.0
C(17A)-C(18A)-H(18A)	120.0

C(19A)-C(18A)-H(18A)	120.0
C(18A)-C(19A)-C(14A)	120.0
C(18A)-C(19A)-H(19A)	120.0
C(14A)-C(19A)-H(19A)	120.0
O(20A)-C(20A)-C(25A)	122.0(12)
O(20A)-C(20A)-C(21A)	117.5(12)
C(25A)-C(20A)-C(21A)	120.5(12)
O(21A)-C(21A)-C(22A)	123.9(12)
O(21A)-C(21A)-C(20A)	118.1(12)
C(22A)-C(21A)-C(20A)	118.0(13)
C(21A)-C(22A)-C(23A)	121.5(13)
C(21A)-C(22A)-H(22A)	119.3
C(23A)-C(22A)-H(22A)	119.3
C(24A)-C(23A)-C(22A)	119.4(14)
C(24A)-C(23A)-H(23A)	120.3
C(22A)-C(23A)-H(23A)	120.3
C(23A)-C(24A)-C(25A)	122.5(14)
C(23A)-C(24A)-H(24A)	118.7
C(25A)-C(24A)-H(24A)	118.7
C(24A)-C(25A)-C(20A)	117.7(13)
C(24A)-C(25A)-C(26A)	124.2(12)
C(20A)-C(25A)-C(26A)	118.1(12)
C(25A)-C(26A)-P(2A)	113.9(10)
C(25A)-C(26A)-H(26A)	108.8
P(2A)-C(26A)-H(26A)	108.8
C(25A)-C(26A)-H(26B)	108.8
H(26A)-C(26A)-H(26B)	107.7
C(28A)-C(27A)-C(32A)	120.0
C(28A)-C(27A)-P(2A)	121.2(6)

C(32A)-C(27A)-P(2A)	118.7(6)
C(27A)-C(28A)-C(29A)	120.0
C(27A)-C(28A)-H(28A)	120.0
C(29A)-C(28A)-H(28A)	120.0
C(30A)-C(29A)-C(28A)	120.0
C(30A)-C(29A)-H(29A)	120.0
C(28A)-C(29A)-H(29A)	120.0
C(31A)-C(30A)-C(29A)	120.0
C(31A)-C(30A)-H(30A)	120.0
C(29A)-C(30A)-H(30A)	120.0
C(30A)-C(31A)-C(32A)	120.0
C(30A)-C(31A)-H(31A)	120.0
C(32A)-C(31A)-H(31A)	120.0
C(31A)-C(32A)-C(27A)	120.0
C(31A)-C(32A)-H(32A)	120.0
C(27A)-C(32A)-H(32A)	120.0
C(34A)-C(33A)-C(38A)	120.0
C(34A)-C(33A)-P(2A)	120.3(5)
C(38A)-C(33A)-P(2A)	119.6(5)
C(33A)-C(34A)-C(35A)	120.0
C(33A)-C(34A)-H(34A)	120.0
C(35A)-C(34A)-H(34A)	120.0
C(34A)-C(35A)-C(36A)	120.0
C(34A)-C(35A)-H(35A)	120.0
C(36A)-C(35A)-H(35A)	120.0
C(37A)-C(36A)-C(35A)	120.0
C(37A)-C(36A)-H(36A)	120.0
C(35A)-C(36A)-H(36A)	120.0
C(38A)-C(37A)-C(36A)	120.0
C(38A)-C(37A)-H(37A)	120.0

C(36A)-C(37A)-H(37A)	120.0
C(37A)-C(38A)-C(33A)	120.0
C(37A)-C(38A)-H(38A)	120.0
C(33A)-C(38A)-H(38A)	120.0
O(20B)-Pd(1B)-O(1B)	79.6(3)
O(20B)-Pd(1B)-P(2B)	90.6(3)
O(1B)-Pd(1B)-P(2B)	168.7(3)
O(20B)-Pd(1B)-P(1B)	168.6(3)
O(1B)-Pd(1B)-P(1B)	90.8(3)
P(2B)-Pd(1B)-P(1B)	99.51(15)
O(20B)-Pd(1B)-Zn(1B)	40.7(2)
O(1B)-Pd(1B)-Zn(1B)	40.3(2)
P(2B)-Pd(1B)-Zn(1B)	130.90(12)
P(1B)-Pd(1B)-Zn(1B)	128.51(11)
O(2A)-Zn(1B)-O(2B)	102.1(4)
O(2A)-Zn(1B)-O(21B)	107.9(4)
O(2B)-Zn(1B)-O(21B)	96.4(4)
O(2A)-Zn(1B)-O(1B)	116.8(4)
O(2B)-Zn(1B)-O(1B)	81.9(4)
O(21B)-Zn(1B)-O(1B)	134.6(4)
O(2A)-Zn(1B)-O(20B)	105.6(4)
O(2B)-Zn(1B)-O(20B)	151.4(3)
O(21B)-Zn(1B)-O(20B)	81.8(4)
O(1B)-Zn(1B)-O(20B)	79.5(3)
O(2A)-Zn(1B)-Pd(1B)	125.9(3)
O(2B)-Zn(1B)-Pd(1B)	115.1(3)
O(21B)-Zn(1B)-Pd(1B)	105.5(3)
O(1B)-Zn(1B)-Pd(1B)	40.6(2)
O(20B)-Zn(1B)-Pd(1B)	40.3(2)
C(8B)-P(1B)-C(14B)	108.7(5)

C(8B)-P(1B)-C(7B)	104.2(6)
C(14B)-P(1B)-C(7B)	103.0(6)
C(8B)-P(1B)-Pd(1B)	112.5(3)
C(14B)-P(1B)-Pd(1B)	122.3(4)
C(7B)-P(1B)-Pd(1B)	104.1(5)
C(33B)-P(2B)-C(27B)	105.2(7)
C(33B)-P(2B)-C(26B)	103.2(7)
C(27B)-P(2B)-C(26B)	107.9(6)
C(33B)-P(2B)-Pd(1B)	116.7(5)
C(27B)-P(2B)-Pd(1B)	116.8(4)
C(26B)-P(2B)-Pd(1B)	105.9(5)
C(1B)-O(1B)-Zn(1B)	110.0(8)
C(1B)-O(1B)-Pd(1B)	123.0(7)
Zn(1B)-O(1B)-Pd(1B)	99.2(3)
C(2B)-O(2B)-Zn(1)	125.8(8)
C(2B)-O(2B)-Zn(1B)	107.9(8)
Zn(1)-O(2B)-Zn(1B)	126.1(4)
C(20B)-O(20B)-Pd(1B)	117.2(8)
C(20B)-O(20B)-Zn(1B)	110.0(8)
Pd(1B)-O(20B)-Zn(1B)	99.0(3)
C(21B)-O(21B)-Zn(1C)	124.9(8)
C(21B)-O(21B)-Zn(1B)	112.0(8)
Zn(1C)-O(21B)-Zn(1B)	120.0(4)
O(1B)-C(1B)-C(6B)	123.1(13)
O(1B)-C(1B)-C(2B)	116.7(11)
C(6B)-C(1B)-C(2B)	120.2(12)
C(1B)-C(2B)-O(2B)	118.9(11)
C(1B)-C(2B)-C(3B)	120.4(12)
O(2B)-C(2B)-C(3B)	120.7(12)
C(4B)-C(3B)-C(2B)	117.5(13)

C(4B)-C(3B)-H(3B)	121.2
C(2B)-C(3B)-H(3B)	121.2
C(5B)-C(4B)-C(3B)	120.8(13)
C(5B)-C(4B)-H(4B)	119.6
C(3B)-C(4B)-H(4B)	119.6
C(4B)-C(5B)-C(6B)	120.6(14)
C(4B)-C(5B)-H(5B)	119.7
C(6B)-C(5B)-H(5B)	119.7
C(1B)-C(6B)-C(5B)	120.2(14)
C(1B)-C(6B)-C(7B)	116.4(12)
C(5B)-C(6B)-C(7B)	123.4(13)
C(6B)-C(7B)-P(1B)	113.9(9)
C(6B)-C(7B)-H(7B1)	108.8
P(1B)-C(7B)-H(7B1)	108.8
C(6B)-C(7B)-H(7B2)	108.8
P(1B)-C(7B)-H(7B2)	108.8
H(7B1)-C(7B)-H(7B2)	107.7
C(9B)-C(8B)-C(13B)	120.0
C(9B)-C(8B)-P(1B)	119.0(5)
C(13B)-C(8B)-P(1B)	121.0(5)
C(8B)-C(9B)-C(10B)	120.0
C(8B)-C(9B)-H(9B)	120.0
C(10B)-C(9B)-H(9B)	120.0
C(11B)-C(10B)-C(9B)	120.0
C(11B)-C(10B)-H(10B)	120.0
C(9B)-C(10B)-H(10B)	120.0
C(12B)-C(11B)-C(10B)	120.0
C(12B)-C(11B)-H(11B)	120.0
C(10B)-C(11B)-H(11B)	120.0
C(11B)-C(12B)-C(13B)	120.0

C(11B)-C(12B)-H(12B)	120.0
C(13B)-C(12B)-H(12B)	120.0
C(12B)-C(13B)-C(8B)	120.0
C(12B)-C(13B)-H(13B)	120.0
C(8B)-C(13B)-H(13B)	120.0
C(15B)-C(14B)-C(19B)	120.0
C(15B)-C(14B)-P(1B)	123.0(6)
C(19B)-C(14B)-P(1B)	116.8(6)
C(16B)-C(15B)-C(14B)	120.0
C(16B)-C(15B)-H(15B)	120.0
C(14B)-C(15B)-H(15B)	120.0
C(15B)-C(16B)-C(17B)	120.0
C(15B)-C(16B)-H(16B)	120.0
C(17B)-C(16B)-H(16B)	120.0
C(18B)-C(17B)-C(16B)	120.0
C(18B)-C(17B)-H(17B)	120.0
C(16B)-C(17B)-H(17B)	120.0
C(17B)-C(18B)-C(19B)	120.0
C(17B)-C(18B)-H(18B)	120.0
C(19B)-C(18B)-H(18B)	120.0
C(18B)-C(19B)-C(14B)	120.0
C(18B)-C(19B)-H(19B)	120.0
C(14B)-C(19B)-H(19B)	120.0
O(20B)-C(20B)-C(21B)	119.0(12)
O(20B)-C(20B)-C(25B)	119.3(13)
C(21B)-C(20B)-C(25B)	121.7(12)
C(22B)-C(21B)-C(20B)	121.4(13)
C(22B)-C(21B)-O(21B)	121.5(13)
C(20B)-C(21B)-O(21B)	117.1(11)
C(21B)-C(22B)-C(23B)	117.0(14)

C(21B)-C(22B)-H(22B)	121.5
C(23B)-C(22B)-H(22B)	121.5
C(24B)-C(23B)-C(22B)	122.5(13)
C(24B)-C(23B)-H(23B)	118.8
C(22B)-C(23B)-H(23B)	118.8
C(23B)-C(24B)-C(25B)	121.6(14)
C(23B)-C(24B)-H(24B)	119.2
C(25B)-C(24B)-H(24B)	119.2
C(20B)-C(25B)-C(26B)	120.2(13)
C(20B)-C(25B)-C(24B)	115.8(14)
C(26B)-C(25B)-C(24B)	124.0(13)
C(25B)-C(26B)-P(2B)	116.5(9)
C(25B)-C(26B)-H(26C)	108.2
P(2B)-C(26B)-H(26C)	108.2
C(25B)-C(26B)-H(26D)	108.2
P(2B)-C(26B)-H(26D)	108.2
H(26C)-C(26B)-H(26D)	107.3
C(28B)-C(27B)-C(32B)	120.0
C(28B)-C(27B)-P(2B)	120.5(7)
C(32B)-C(27B)-P(2B)	119.3(7)
C(27B)-C(28B)-C(29B)	120.0
C(27B)-C(28B)-H(28B)	120.0
C(29B)-C(28B)-H(28B)	120.0
C(30B)-C(29B)-C(28B)	120.0
C(30B)-C(29B)-H(29B)	120.0
C(28B)-C(29B)-H(29B)	120.0
C(29B)-C(30B)-C(31B)	120.0
C(29B)-C(30B)-H(30B)	120.0
C(31B)-C(30B)-H(30B)	120.0
C(32B)-C(31B)-C(30B)	120.0

C(32B)-C(31B)-H(31B)	120.0
C(30B)-C(31B)-H(31B)	120.0
C(31B)-C(32B)-C(27B)	120.0
C(31B)-C(32B)-H(32B)	120.0
C(27B)-C(32B)-H(32B)	120.0
C(34B)-C(33B)-C(38B)	120.0
C(34B)-C(33B)-P(2B)	120.2(9)
C(38B)-C(33B)-P(2B)	119.6(9)
C(35B)-C(34B)-C(33B)	120.0
C(35B)-C(34B)-H(34B)	120.0
C(33B)-C(34B)-H(34B)	120.0
C(34B)-C(35B)-C(36B)	120.0
C(34B)-C(35B)-H(35B)	120.0
C(36B)-C(35B)-H(35B)	120.0
C(37B)-C(36B)-C(35B)	120.0
C(37B)-C(36B)-H(36B)	120.0
C(35B)-C(36B)-H(36B)	120.0
C(38B)-C(37B)-C(36B)	120.0
C(38B)-C(37B)-H(37B)	120.0
C(36B)-C(37B)-H(37B)	120.0
C(37B)-C(38B)-C(33B)	120.0
C(37B)-C(38B)-H(38B)	120.0
C(33B)-C(38B)-H(38B)	120.0
O(20C)-Pd(1C)-O(1C)	80.9(4)
O(20C)-Pd(1C)-P(1C)	166.9(3)
O(1C)-Pd(1C)-P(1C)	89.6(3)
O(20C)-Pd(1C)-P(2C)	90.1(3)
O(1C)-Pd(1C)-P(2C)	170.9(3)
P(1C)-Pd(1C)-P(2C)	99.55(15)
O(20C)-Pd(1C)-Zn(1C)	40.0(2)

O(1C)-Pd(1C)-Zn(1C)	42.2(3)
P(1C)-Pd(1C)-Zn(1C)	131.68(12)
P(2C)-Pd(1C)-Zn(1C)	128.70(11)
O(21B)-Zn(1C)-O(2C)	103.5(4)
O(21B)-Zn(1C)-O(21C)	108.9(4)
O(2C)-Zn(1C)-O(21C)	96.7(4)
O(21B)-Zn(1C)-O(20C)	110.9(4)
O(2C)-Zn(1C)-O(20C)	143.8(4)
O(21C)-Zn(1C)-O(20C)	82.7(4)
O(21B)-Zn(1C)-O(1C)	107.8(4)
O(2C)-Zn(1C)-O(1C)	79.9(3)
O(21C)-Zn(1C)-O(1C)	142.9(4)
O(20C)-Zn(1C)-O(1C)	79.4(3)
O(21B)-Zn(1C)-Pd(1C)	123.2(3)
O(2C)-Zn(1C)-Pd(1C)	110.3(3)
O(21C)-Zn(1C)-Pd(1C)	110.8(3)
O(20C)-Zn(1C)-Pd(1C)	39.9(3)
O(1C)-Zn(1C)-Pd(1C)	40.8(2)
C(14C)-P(1C)-C(8C)	110.2(5)
C(14C)-P(1C)-C(7C)	107.4(7)
C(8C)-P(1C)-C(7C)	101.3(6)
C(14C)-P(1C)-Pd(1C)	116.3(4)
C(8C)-P(1C)-Pd(1C)	112.6(4)
C(7C)-P(1C)-Pd(1C)	107.7(5)
C(33C)-P(2C)-C(26C)	106.6(7)
C(33C)-P(2C)-C(27C)	106.3(6)
C(26C)-P(2C)-C(27C)	107.3(6)
C(33C)-P(2C)-Pd(1C)	114.1(5)
C(26C)-P(2C)-Pd(1C)	103.5(5)
C(27C)-P(2C)-Pd(1C)	118.2(4)

C(1C)-O(1C)-Pd(1C)	119.6(9)
C(1C)-O(1C)-Zn(1C)	112.4(8)
Pd(1C)-O(1C)-Zn(1C)	97.1(4)
C(2C)-O(2C)-Zn(1A)	125.6(8)
C(2C)-O(2C)-Zn(1C)	111.0(8)
Zn(1A)-O(2C)-Zn(1C)	121.7(4)
C(20C)-O(20C)-Pd(1C)	123.2(9)
C(20C)-O(20C)-Zn(1C)	109.9(8)
Pd(1C)-O(20C)-Zn(1C)	100.1(4)
C(21C)-O(21C)-Zn(1)	125.8(9)
C(21C)-O(21C)-Zn(1C)	109.9(8)
Zn(1)-O(21C)-Zn(1C)	121.3(5)
C(6C)-C(1C)-O(1C)	124.7(13)
C(6C)-C(1C)-C(2C)	121.4(13)
O(1C)-C(1C)-C(2C)	114.0(12)
O(2C)-C(2C)-C(1C)	120.8(12)
O(2C)-C(2C)-C(3C)	120.6(12)
C(1C)-C(2C)-C(3C)	118.6(13)
C(4C)-C(3C)-C(2C)	119.3(13)
C(4C)-C(3C)-H(3C)	120.3
C(2C)-C(3C)-H(3C)	120.3
C(3C)-C(4C)-C(5C)	119.9(14)
C(3C)-C(4C)-H(4C)	120.1
C(5C)-C(4C)-H(4C)	120.1
C(4C)-C(5C)-C(6C)	119.2(14)
C(4C)-C(5C)-H(5C)	120.4
C(6C)-C(5C)-H(5C)	120.4
C(1C)-C(6C)-C(5C)	121.7(14)
C(1C)-C(6C)-C(7C)	118.8(13)
C(5C)-C(6C)-C(7C)	119.0(13)

C(6C)-C(7C)-P(1C)	117.0(10)
C(6C)-C(7C)-H(7C1)	108.0
P(1C)-C(7C)-H(7C1)	108.0
C(6C)-C(7C)-H(7C2)	108.0
P(1C)-C(7C)-H(7C2)	108.0
H(7C1)-C(7C)-H(7C2)	107.3
C(9C)-C(8C)-C(13C)	120.0
C(9C)-C(8C)-P(1C)	122.7(6)
C(13C)-C(8C)-P(1C)	116.8(6)
C(10C)-C(9C)-C(8C)	120.0
C(10C)-C(9C)-H(9C)	120.0
C(8C)-C(9C)-H(9C)	120.0
C(9C)-C(10C)-C(11C)	120.0
C(9C)-C(10C)-H(10C)	120.0
C(11C)-C(10C)-H(10C)	120.0
C(12C)-C(11C)-C(10C)	120.0
C(12C)-C(11C)-H(11C)	120.0
C(10C)-C(11C)-H(11C)	120.0
C(11C)-C(12C)-C(13C)	120.0
C(11C)-C(12C)-H(12C)	120.0
C(13C)-C(12C)-H(12C)	120.0
C(12C)-C(13C)-C(8C)	120.0
C(12C)-C(13C)-H(13C)	120.0
C(8C)-C(13C)-H(13C)	120.0
C(15C)-C(14C)-C(19C)	120.0
C(15C)-C(14C)-P(1C)	120.7(7)
C(19C)-C(14C)-P(1C)	118.3(7)
C(14C)-C(15C)-C(16C)	120.0
C(14C)-C(15C)-H(15C)	120.0
C(16C)-C(15C)-H(15C)	120.0

C(15C)-C(16C)-C(17C)	120.0
C(15C)-C(16C)-H(16C)	120.0
C(17C)-C(16C)-H(16C)	120.0
C(18C)-C(17C)-C(16C)	120.0
C(18C)-C(17C)-H(17C)	120.0
C(16C)-C(17C)-H(17C)	120.0
C(19C)-C(18C)-C(17C)	120.0
C(19C)-C(18C)-H(18C)	120.0
C(17C)-C(18C)-H(18C)	120.0
C(18C)-C(19C)-C(14C)	120.0
C(18C)-C(19C)-H(19C)	120.0
C(14C)-C(19C)-H(19C)	120.0
O(20C)-C(20C)-C(25C)	119.4(12)
O(20C)-C(20C)-C(21C)	119.1(13)
C(25C)-C(20C)-C(21C)	121.2(14)
O(21C)-C(21C)-C(22C)	122.5(13)
O(21C)-C(21C)-C(20C)	118.2(13)
C(22C)-C(21C)-C(20C)	119.3(14)
C(21C)-C(22C)-C(23C)	120.5(14)
C(21C)-C(22C)-H(22C)	119.8
C(23C)-C(22C)-H(22C)	119.8
C(24C)-C(23C)-C(22C)	119.8(15)
C(24C)-C(23C)-H(23C)	120.1
C(22C)-C(23C)-H(23C)	120.1
C(23C)-C(24C)-C(25C)	120.4(14)
C(23C)-C(24C)-H(24C)	119.8
C(25C)-C(24C)-H(24C)	119.8
C(20C)-C(25C)-C(24C)	118.6(13)
C(20C)-C(25C)-C(26C)	116.7(13)
C(24C)-C(25C)-C(26C)	124.6(13)

C(25C)-C(26C)-P(2C)	112.1(11)
C(25C)-C(26C)-H(26E)	109.2
P(2C)-C(26C)-H(26E)	109.2
C(25C)-C(26C)-H(26F)	109.2
P(2C)-C(26C)-H(26F)	109.2
H(26E)-C(26C)-H(26F)	107.9
C(28C)-C(27C)-C(32C)	120.0
C(28C)-C(27C)-P(2C)	115.8(7)
C(32C)-C(27C)-P(2C)	124.0(7)
C(27C)-C(28C)-C(29C)	120.0
C(27C)-C(28C)-H(28C)	120.0
C(29C)-C(28C)-H(28C)	120.0
C(30C)-C(29C)-C(28C)	120.0
C(30C)-C(29C)-H(29C)	120.0
C(28C)-C(29C)-H(29C)	120.0
C(29C)-C(30C)-C(31C)	120.0
C(29C)-C(30C)-H(30C)	120.0
C(31C)-C(30C)-H(30C)	120.0
C(32C)-C(31C)-C(30C)	120.0
C(32C)-C(31C)-H(31C)	120.0
C(30C)-C(31C)-H(31C)	120.0
C(31C)-C(32C)-C(27C)	120.0
C(31C)-C(32C)-H(32C)	120.0
C(27C)-C(32C)-H(32C)	120.0
C(34C)-C(33C)-C(38C)	120.0
C(34C)-C(33C)-P(2C)	117.2(8)
C(38C)-C(33C)-P(2C)	122.8(8)
C(33C)-C(34C)-C(35C)	120.0
C(33C)-C(34C)-H(34C)	120.0
C(35C)-C(34C)-H(34C)	120.0

C(36C)-C(35C)-C(34C)	120.0
C(36C)-C(35C)-H(35C)	120.0
C(34C)-C(35C)-H(35C)	120.0
C(35C)-C(36C)-C(37C)	120.0
C(35C)-C(36C)-H(36C)	120.0
C(37C)-C(36C)-H(36C)	120.0
C(38C)-C(37C)-C(36C)	120.0
C(38C)-C(37C)-H(37C)	120.0
C(36C)-C(37C)-H(37C)	120.0
C(37C)-C(38C)-C(33C)	120.0
C(37C)-C(38C)-H(38C)	120.0
C(33C)-C(38C)-H(38C)	120.0
O(2D)-Zn(2)-O(21F)	97.6(4)
O(2D)-Zn(2)-O(21E)	101.5(4)
O(21F)-Zn(2)-O(21E)	108.6(4)
O(2D)-Zn(2)-Cl(2)	122.6(3)
O(21F)-Zn(2)-Cl(2)	114.1(3)
O(21E)-Zn(2)-Cl(2)	110.8(3)
O(1D)-Pd(1D)-O(20D)	78.6(4)
O(1D)-Pd(1D)-P(2D)	170.4(3)
O(20D)-Pd(1D)-P(2D)	92.1(3)
O(1D)-Pd(1D)-P(1D)	90.5(3)
O(20D)-Pd(1D)-P(1D)	169.1(3)
P(2D)-Pd(1D)-P(1D)	98.78(14)
O(1D)-Pd(1D)-Zn(1D)	38.8(2)
O(20D)-Pd(1D)-Zn(1D)	41.4(3)
P(2D)-Pd(1D)-Zn(1D)	132.58(10)
P(1D)-Pd(1D)-Zn(1D)	127.96(11)
O(2F)-Zn(1D)-O(21D)	106.0(4)
O(2F)-Zn(1D)-O(1D)	109.5(4)

O(21D)-Zn(1D)-O(1D)	143.0(4)
O(2F)-Zn(1D)-O(2D)	101.4(4)
O(21D)-Zn(1D)-O(2D)	101.1(4)
O(1D)-Zn(1D)-O(2D)	82.0(3)
O(2F)-Zn(1D)-O(20D)	111.4(4)
O(21D)-Zn(1D)-O(20D)	79.6(4)
O(1D)-Zn(1D)-O(20D)	78.0(3)
O(2D)-Zn(1D)-O(20D)	145.7(4)
O(2F)-Zn(1D)-Pd(1D)	125.2(3)
O(21D)-Zn(1D)-Pd(1D)	109.1(3)
O(1D)-Zn(1D)-Pd(1D)	39.3(3)
O(2D)-Zn(1D)-Pd(1D)	111.3(3)
O(20D)-Zn(1D)-Pd(1D)	40.2(2)
C(8D)-P(1D)-C(14D)	108.5(4)
C(8D)-P(1D)-C(7D)	103.5(5)
C(14D)-P(1D)-C(7D)	108.1(6)
C(8D)-P(1D)-Pd(1D)	118.5(3)
C(14D)-P(1D)-Pd(1D)	111.9(3)
C(7D)-P(1D)-Pd(1D)	105.5(5)
C(33D)-P(2D)-C(27D)	110.9(5)
C(33D)-P(2D)-C(26D)	107.5(6)
C(27D)-P(2D)-C(26D)	103.4(6)
C(33D)-P(2D)-Pd(1D)	115.9(4)
C(27D)-P(2D)-Pd(1D)	112.8(4)
C(26D)-P(2D)-Pd(1D)	105.2(5)
C(1D)-O(1D)-Zn(1D)	111.8(8)
C(1D)-O(1D)-Pd(1D)	126.6(8)
Zn(1D)-O(1D)-Pd(1D)	101.9(4)
C(2D)-O(2D)-Zn(2)	126.0(8)
C(2D)-O(2D)-Zn(1D)	109.1(7)

Zn(2)-O(2D)-Zn(1D)	122.6(4)
C(20D)-O(20D)-Pd(1D)	120.7(9)
C(20D)-O(20D)-Zn(1D)	111.0(8)
Pd(1D)-O(20D)-Zn(1D)	98.4(4)
C(21D)-O(21D)-Zn(1E)	125.3(8)
C(21D)-O(21D)-Zn(1D)	114.7(8)
Zn(1E)-O(21D)-Zn(1D)	118.3(5)
O(1D)-C(1D)-C(6D)	120.7(12)
O(1D)-C(1D)-C(2D)	118.6(12)
C(6D)-C(1D)-C(2D)	120.6(13)
O(2D)-C(2D)-C(3D)	123.5(12)
O(2D)-C(2D)-C(1D)	118.2(12)
C(3D)-C(2D)-C(1D)	118.2(13)
C(4D)-C(3D)-C(2D)	121.9(14)
C(4D)-C(3D)-H(3D)	119.1
C(2D)-C(3D)-H(3D)	119.1
C(3D)-C(4D)-C(5D)	119.6(14)
C(3D)-C(4D)-H(4D)	120.2
C(5D)-C(4D)-H(4D)	120.2
C(6D)-C(5D)-C(4D)	119.2(14)
C(6D)-C(5D)-H(5D)	120.4
C(4D)-C(5D)-H(5D)	120.4
C(5D)-C(6D)-C(1D)	120.5(13)
C(5D)-C(6D)-C(7D)	119.9(13)
C(1D)-C(6D)-C(7D)	119.6(12)
C(6D)-C(7D)-P(1D)	112.5(10)
C(6D)-C(7D)-H(7D1)	109.1
P(1D)-C(7D)-H(7D1)	109.1
C(6D)-C(7D)-H(7D2)	109.1
P(1D)-C(7D)-H(7D2)	109.1

H(7D1)-C(7D)-H(7D2)	107.8
C(9D)-C(8D)-C(13D)	120.0
C(9D)-C(8D)-P(1D)	122.2(5)
C(13D)-C(8D)-P(1D)	117.7(5)
C(10D)-C(9D)-C(8D)	120.0
C(10D)-C(9D)-H(9D)	120.0
C(8D)-C(9D)-H(9D)	120.0
C(9D)-C(10D)-C(11D)	120.0
C(9D)-C(10D)-H(10D)	120.0
C(11D)-C(10D)-H(10D)	120.0
C(12D)-C(11D)-C(10D)	120.0
C(12D)-C(11D)-H(11D)	120.0
C(10D)-C(11D)-H(11D)	120.0
C(11D)-C(12D)-C(13D)	120.0
C(11D)-C(12D)-H(12D)	120.0
C(13D)-C(12D)-H(12D)	120.0
C(12D)-C(13D)-C(8D)	120.0
C(12D)-C(13D)-H(13D)	120.0
C(8D)-C(13D)-H(13D)	120.0
C(15D)-C(14D)-C(19D)	120.0
C(15D)-C(14D)-P(1D)	122.2(5)
C(19D)-C(14D)-P(1D)	117.7(5)
C(14D)-C(15D)-C(16D)	120.0
C(14D)-C(15D)-H(15D)	120.0
C(16D)-C(15D)-H(15D)	120.0
C(17D)-C(16D)-C(15D)	120.0
C(17D)-C(16D)-H(16D)	120.0
C(15D)-C(16D)-H(16D)	120.0
C(16D)-C(17D)-C(18D)	120.0
C(16D)-C(17D)-H(17D)	120.0

C(18D)-C(17D)-H(17D)	120.0
C(19D)-C(18D)-C(17D)	120.0
C(19D)-C(18D)-H(18D)	120.0
C(17D)-C(18D)-H(18D)	120.0
C(18D)-C(19D)-C(14D)	120.0
C(18D)-C(19D)-H(19D)	120.0
C(14D)-C(19D)-H(19D)	120.0
O(20D)-C(20D)-C(25D)	123.9(12)
O(20D)-C(20D)-C(21D)	116.6(13)
C(25D)-C(20D)-C(21D)	119.5(13)
O(21D)-C(21D)-C(22D)	124.6(13)
O(21D)-C(21D)-C(20D)	116.6(13)
C(22D)-C(21D)-C(20D)	118.7(13)
C(23D)-C(22D)-C(21D)	119.9(14)
C(23D)-C(22D)-H(22D)	120.0
C(21D)-C(22D)-H(22D)	120.0
C(22D)-C(23D)-C(24D)	122.1(14)
C(22D)-C(23D)-H(23D)	118.9
C(24D)-C(23D)-H(23D)	118.9
C(23D)-C(24D)-C(25D)	120.0(15)
C(23D)-C(24D)-H(24D)	120.0
C(25D)-C(24D)-H(24D)	120.0
C(24D)-C(25D)-C(20D)	119.7(13)
C(24D)-C(25D)-C(26D)	123.6(13)
C(20D)-C(25D)-C(26D)	116.6(12)
C(25D)-C(26D)-P(2D)	116.4(10)
C(25D)-C(26D)-H(26G)	108.2
P(2D)-C(26D)-H(26G)	108.2
C(25D)-C(26D)-H(26H)	108.2
P(2D)-C(26D)-H(26H)	108.2

H(26G)-C(26D)-H(26H)	107.3
C(28D)-C(27D)-C(32D)	120.0
C(28D)-C(27D)-P(2D)	124.1(6)
C(32D)-C(27D)-P(2D)	115.8(6)
C(27D)-C(28D)-C(29D)	120.0
C(27D)-C(28D)-H(28D)	120.0
C(29D)-C(28D)-H(28D)	120.0
C(28D)-C(29D)-C(30D)	120.0
C(28D)-C(29D)-H(29D)	120.0
C(30D)-C(29D)-H(29D)	120.0
C(31D)-C(30D)-C(29D)	120.0
C(31D)-C(30D)-H(30D)	120.0
C(29D)-C(30D)-H(30D)	120.0
C(30D)-C(31D)-C(32D)	120.0
C(30D)-C(31D)-H(31D)	120.0
C(32D)-C(31D)-H(31D)	120.0
C(31D)-C(32D)-C(27D)	120.0
C(31D)-C(32D)-H(32D)	120.0
C(27D)-C(32D)-H(32D)	120.0
C(34D)-C(33D)-C(38D)	120.0
C(34D)-C(33D)-P(2D)	122.1(6)
C(38D)-C(33D)-P(2D)	117.9(6)
C(33D)-C(34D)-C(35D)	120.0
C(33D)-C(34D)-H(34D)	120.0
C(35D)-C(34D)-H(34D)	120.0
C(34D)-C(35D)-C(36D)	120.0
C(34D)-C(35D)-H(35D)	120.0
C(36D)-C(35D)-H(35D)	120.0
C(35D)-C(36D)-C(37D)	120.0
C(35D)-C(36D)-H(36D)	120.0

C(37D)-C(36D)-H(36D)	120.0
C(38D)-C(37D)-C(36D)	120.0
C(38D)-C(37D)-H(37D)	120.0
C(36D)-C(37D)-H(37D)	120.0
C(37D)-C(38D)-C(33D)	120.0
C(37D)-C(38D)-H(38D)	120.0
C(33D)-C(38D)-H(38D)	120.0
O(20E)-Pd(1E)-O(1E)	78.8(4)
O(20E)-Pd(1E)-P(2E)	89.9(3)
O(1E)-Pd(1E)-P(2E)	168.7(3)
O(20E)-Pd(1E)-P(1E)	166.5(3)
O(1E)-Pd(1E)-P(1E)	88.3(3)
P(2E)-Pd(1E)-P(1E)	102.96(14)
O(20E)-Pd(1E)-Zn(1E)	37.3(3)
O(1E)-Pd(1E)-Zn(1E)	41.9(2)
P(2E)-Pd(1E)-Zn(1E)	126.80(10)
P(1E)-Pd(1E)-Zn(1E)	130.21(11)
O(21D)-Zn(1E)-O(2E)	115.1(4)
O(21D)-Zn(1E)-O(20E)	111.3(4)
O(2E)-Zn(1E)-O(20E)	132.4(4)
O(21D)-Zn(1E)-O(21E)	97.8(4)
O(2E)-Zn(1E)-O(21E)	102.0(4)
O(20E)-Zn(1E)-O(21E)	81.5(4)
O(21D)-Zn(1E)-O(1E)	104.0(4)
O(2E)-Zn(1E)-O(1E)	82.4(4)
O(20E)-Zn(1E)-O(1E)	76.7(4)
O(21E)-Zn(1E)-O(1E)	153.5(3)
O(21D)-Zn(1E)-Pd(1E)	117.0(3)
O(2E)-Zn(1E)-Pd(1E)	107.8(3)
O(20E)-Zn(1E)-Pd(1E)	37.6(3)

O(21E)-Zn(1E)-Pd(1E)	116.2(2)
O(1E)-Zn(1E)-Pd(1E)	39.4(2)
C(14E)-P(1E)-C(8E)	106.9(5)
C(14E)-P(1E)-C(7E)	104.9(5)
C(8E)-P(1E)-C(7E)	106.1(6)
C(14E)-P(1E)-Pd(1E)	113.2(3)
C(8E)-P(1E)-Pd(1E)	119.1(4)
C(7E)-P(1E)-Pd(1E)	105.7(4)
C(33E)-P(2E)-C(27E)	104.8(5)
C(33E)-P(2E)-C(26E)	107.5(6)
C(27E)-P(2E)-C(26E)	101.6(6)
C(33E)-P(2E)-Pd(1E)	112.3(4)
C(27E)-P(2E)-Pd(1E)	122.4(4)
C(26E)-P(2E)-Pd(1E)	107.0(5)
C(1E)-O(1E)-Pd(1E)	116.8(8)
C(1E)-O(1E)-Zn(1E)	105.7(8)
Pd(1E)-O(1E)-Zn(1E)	98.6(4)
C(2E)-O(2E)-Zn(1E)	115.5(8)
C(2E)-O(2E)-Zn(1F)	118.1(8)
Zn(1E)-O(2E)-Zn(1F)	118.8(5)
C(20E)-O(20E)-Zn(1E)	114.1(8)
C(20E)-O(20E)-Pd(1E)	138.4(8)
Zn(1E)-O(20E)-Pd(1E)	105.0(4)
C(21E)-O(21E)-Zn(2)	130.1(8)
C(21E)-O(21E)-Zn(1E)	109.4(8)
Zn(2)-O(21E)-Zn(1E)	118.8(4)
O(1E)-C(1E)-C(6E)	122.0(12)
O(1E)-C(1E)-C(2E)	121.9(12)
C(6E)-C(1E)-C(2E)	116.0(13)
O(2E)-C(2E)-C(3E)	128.4(14)

O(2E)-C(2E)-C(1E)	113.4(13)
C(3E)-C(2E)-C(1E)	118.1(14)
C(2E)-C(3E)-C(4E)	121.8(15)
C(2E)-C(3E)-H(3E)	119.1
C(4E)-C(3E)-H(3E)	119.1
C(3E)-C(4E)-C(5E)	117.5(16)
C(3E)-C(4E)-H(4E)	121.2
C(5E)-C(4E)-H(4E)	121.2
C(6E)-C(5E)-C(4E)	125.6(16)
C(6E)-C(5E)-H(5E)	117.2
C(4E)-C(5E)-H(5E)	117.2
C(5E)-C(6E)-C(1E)	120.9(15)
C(5E)-C(6E)-C(7E)	127.1(14)
C(1E)-C(6E)-C(7E)	111.4(13)
C(6E)-C(7E)-P(1E)	118.7(10)
C(6E)-C(7E)-H(7E1)	107.6
P(1E)-C(7E)-H(7E1)	107.6
C(6E)-C(7E)-H(7E2)	107.6
P(1E)-C(7E)-H(7E2)	107.6
H(7E1)-C(7E)-H(7E2)	107.1
C(9E)-C(8E)-C(13E)	120.0
C(9E)-C(8E)-P(1E)	119.6(6)
C(13E)-C(8E)-P(1E)	120.2(6)
C(10E)-C(9E)-C(8E)	120.0
C(10E)-C(9E)-H(9E)	120.0
C(8E)-C(9E)-H(9E)	120.0
C(9E)-C(10E)-C(11E)	120.0
C(9E)-C(10E)-H(10E)	120.0
C(11E)-C(10E)-H(10E)	120.0
C(12E)-C(11E)-C(10E)	120.0

C(12E)-C(11E)-H(11E)	120.0
C(10E)-C(11E)-H(11E)	120.0
C(11E)-C(12E)-C(13E)	120.0
C(11E)-C(12E)-H(12E)	120.0
C(13E)-C(12E)-H(12E)	120.0
C(12E)-C(13E)-C(8E)	120.0
C(12E)-C(13E)-H(13E)	120.0
C(8E)-C(13E)-H(13E)	120.0
C(15E)-C(14E)-C(19E)	120.0
C(15E)-C(14E)-P(1E)	120.1(5)
C(19E)-C(14E)-P(1E)	119.9(5)
C(16E)-C(15E)-C(14E)	120.0
C(16E)-C(15E)-H(15E)	120.0
C(14E)-C(15E)-H(15E)	120.0
C(17E)-C(16E)-C(15E)	120.0
C(17E)-C(16E)-H(16E)	120.0
C(15E)-C(16E)-H(16E)	120.0
C(18E)-C(17E)-C(16E)	120.0
C(18E)-C(17E)-H(17E)	120.0
C(16E)-C(17E)-H(17E)	120.0
C(17E)-C(18E)-C(19E)	120.0
C(17E)-C(18E)-H(18E)	120.0
C(19E)-C(18E)-H(18E)	120.0
C(18E)-C(19E)-C(14E)	120.0
C(18E)-C(19E)-H(19E)	120.0
C(14E)-C(19E)-H(19E)	120.0
O(20E)-C(20E)-C(25E)	120.7(13)
O(20E)-C(20E)-C(21E)	115.3(12)
C(25E)-C(20E)-C(21E)	123.9(13)
O(21E)-C(21E)-C(22E)	124.5(13)

O(21E)-C(21E)-C(20E)	118.5(12)
C(22E)-C(21E)-C(20E)	116.9(13)
C(23E)-C(22E)-C(21E)	120.2(15)
C(23E)-C(22E)-H(22E)	119.9
C(21E)-C(22E)-H(22E)	119.9
C(24E)-C(23E)-C(22E)	120.8(15)
C(24E)-C(23E)-H(23E)	119.6
C(22E)-C(23E)-H(23E)	119.6
C(23E)-C(24E)-C(25E)	122.9(14)
C(23E)-C(24E)-H(24E)	118.5
C(25E)-C(24E)-H(24E)	118.5
C(20E)-C(25E)-C(24E)	114.7(13)
C(20E)-C(25E)-C(26E)	123.0(13)
C(24E)-C(25E)-C(26E)	122.3(13)
C(25E)-C(26E)-P(2E)	117.5(11)
C(25E)-C(26E)-H(26I)	107.9
P(2E)-C(26E)-H(26I)	107.9
C(25E)-C(26E)-H(26J)	107.9
P(2E)-C(26E)-H(26J)	107.9
H(26I)-C(26E)-H(26J)	107.2
C(28E)-C(27E)-C(32E)	120.0
C(28E)-C(27E)-P(2E)	119.5(5)
C(32E)-C(27E)-P(2E)	120.4(5)
C(29E)-C(28E)-C(27E)	120.0
C(29E)-C(28E)-H(28E)	120.0
C(27E)-C(28E)-H(28E)	120.0
C(30E)-C(29E)-C(28E)	120.0
C(30E)-C(29E)-H(29E)	120.0
C(28E)-C(29E)-H(29E)	120.0
C(29E)-C(30E)-C(31E)	120.0

C(29E)-C(30E)-H(30E)	120.0
C(31E)-C(30E)-H(30E)	120.0
C(32E)-C(31E)-C(30E)	120.0
C(32E)-C(31E)-H(31E)	120.0
C(30E)-C(31E)-H(31E)	120.0
C(31E)-C(32E)-C(27E)	120.0
C(31E)-C(32E)-H(32E)	120.0
C(27E)-C(32E)-H(32E)	120.0
C(34E)-C(33E)-C(38E)	120.0
C(34E)-C(33E)-P(2E)	120.7(5)
C(38E)-C(33E)-P(2E)	119.1(5)
C(35E)-C(34E)-C(33E)	120.0
C(35E)-C(34E)-H(34E)	120.0
C(33E)-C(34E)-H(34E)	120.0
C(36E)-C(35E)-C(34E)	120.0
C(36E)-C(35E)-H(35E)	120.0
C(34E)-C(35E)-H(35E)	120.0
C(35E)-C(36E)-C(37E)	120.0
C(35E)-C(36E)-H(36E)	120.0
C(37E)-C(36E)-H(36E)	120.0
C(36E)-C(37E)-C(38E)	120.0
C(36E)-C(37E)-H(37E)	120.0
C(38E)-C(37E)-H(37E)	120.0
C(37E)-C(38E)-C(33E)	120.0
C(37E)-C(38E)-H(38E)	120.0
C(33E)-C(38E)-H(38E)	120.0
O(20F)-Pd(1F)-O(1F)	77.8(4)
O(20F)-Pd(1F)-P(1F)	168.4(3)
O(1F)-Pd(1F)-P(1F)	91.4(3)
O(20F)-Pd(1F)-P(2F)	91.4(3)

O(1F)-Pd(1F)-P(2F)	168.4(3)
P(1F)-Pd(1F)-P(2F)	99.67(18)
O(20F)-Pd(1F)-Zn(1F)	39.3(3)
O(1F)-Pd(1F)-Zn(1F)	40.9(3)
P(1F)-Pd(1F)-Zn(1F)	131.09(15)
P(2F)-Pd(1F)-Zn(1F)	127.56(12)
O(2E)-Zn(1F)-O(2F)	105.6(4)
O(2E)-Zn(1F)-O(20F)	118.6(4)
O(2F)-Zn(1F)-O(20F)	134.9(4)
O(2E)-Zn(1F)-O(21F)	99.4(3)
O(2F)-Zn(1F)-O(21F)	100.3(4)
O(20F)-Zn(1F)-O(21F)	81.9(4)
O(2E)-Zn(1F)-O(1F)	106.4(4)
O(2F)-Zn(1F)-O(1F)	81.5(4)
O(20F)-Zn(1F)-O(1F)	78.0(4)
O(21F)-Zn(1F)-O(1F)	152.6(4)
O(2E)-Zn(1F)-Pd(1F)	130.0(3)
O(2F)-Zn(1F)-Pd(1F)	103.6(3)
O(20F)-Zn(1F)-Pd(1F)	39.9(3)
O(21F)-Zn(1F)-Pd(1F)	114.1(3)
O(1F)-Zn(1F)-Pd(1F)	40.5(3)
C(14F)-P(1F)-C(8F)	110.9(6)
C(14F)-P(1F)-C(7F)	102.8(7)
C(8F)-P(1F)-C(7F)	105.7(7)
C(14F)-P(1F)-Pd(1F)	115.2(5)
C(8F)-P(1F)-Pd(1F)	115.8(4)
C(7F)-P(1F)-Pd(1F)	104.9(5)
C(27F)-P(2F)-C(33F)	103.7(6)
C(27F)-P(2F)-C(26F)	105.3(7)
C(33F)-P(2F)-C(26F)	106.9(7)

C(27F)-P(2F)-Pd(1F)	122.8(4)
C(33F)-P(2F)-Pd(1F)	112.4(5)
C(26F)-P(2F)-Pd(1F)	104.7(6)
C(1F)-O(1F)-Pd(1F)	115.8(9)
C(1F)-O(1F)-Zn(1F)	111.2(9)
Pd(1F)-O(1F)-Zn(1F)	98.6(4)
C(2F)-O(2F)-Zn(1D)	120.9(9)
C(2F)-O(2F)-Zn(1F)	111.2(8)
Zn(1D)-O(2F)-Zn(1F)	122.8(4)
C(20F)-O(20F)-Zn(1F)	110.7(9)
C(20F)-O(20F)-Pd(1F)	126.3(9)
Zn(1F)-O(20F)-Pd(1F)	100.8(4)
C(21F)-O(21F)-Zn(2)	127.9(9)
C(21F)-O(21F)-Zn(1F)	109.9(8)
Zn(2)-O(21F)-Zn(1F)	122.2(5)
C(6F)-C(1F)-O(1F)	121.9(14)
C(6F)-C(1F)-C(2F)	121.7(15)
O(1F)-C(1F)-C(2F)	116.2(13)
O(2F)-C(2F)-C(3F)	121.4(14)
O(2F)-C(2F)-C(1F)	119.9(13)
C(3F)-C(2F)-C(1F)	118.6(14)
C(2F)-C(3F)-C(4F)	119.1(15)
C(2F)-C(3F)-H(3F)	120.5
C(4F)-C(3F)-H(3F)	120.5
C(3F)-C(4F)-C(5F)	121.8(15)
C(3F)-C(4F)-H(4F)	119.1
C(5F)-C(4F)-H(4F)	119.1
C(6F)-C(5F)-C(4F)	116.0(15)
C(6F)-C(5F)-H(5F)	122.0
C(4F)-C(5F)-H(5F)	122.0

C(1F)-C(6F)-C(5F)	122.5(16)
C(1F)-C(6F)-C(7F)	117.2(15)
C(5F)-C(6F)-C(7F)	119.6(14)
C(6F)-C(7F)-P(1F)	113.1(12)
C(6F)-C(7F)-H(7F1)	109.0
P(1F)-C(7F)-H(7F1)	109.0
C(6F)-C(7F)-H(7F2)	109.0
P(1F)-C(7F)-H(7F2)	109.0
H(7F1)-C(7F)-H(7F2)	107.8
C(9F)-C(8F)-C(13F)	120.0
C(9F)-C(8F)-P(1F)	122.2(7)
C(13F)-C(8F)-P(1F)	117.8(7)
C(10F)-C(9F)-C(8F)	120.0
C(10F)-C(9F)-H(9F)	120.0
C(8F)-C(9F)-H(9F)	120.0
C(9F)-C(10F)-C(11F)	120.0
C(9F)-C(10F)-H(10F)	120.0
C(11F)-C(10F)-H(10F)	120.0
C(12F)-C(11F)-C(10F)	120.0
C(12F)-C(11F)-H(11F)	120.0
C(10F)-C(11F)-H(11F)	120.0
C(11F)-C(12F)-C(13F)	120.0
C(11F)-C(12F)-H(12F)	120.0
C(13F)-C(12F)-H(12F)	120.0
C(12F)-C(13F)-C(8F)	120.0
C(12F)-C(13F)-H(13F)	120.0
C(8F)-C(13F)-H(13F)	120.0
C(15F)-C(14F)-C(19F)	120.0
C(15F)-C(14F)-P(1F)	121.3(8)
C(19F)-C(14F)-P(1F)	118.6(8)

C(16F)-C(15F)-C(14F)	120.0
C(16F)-C(15F)-H(15F)	120.0
C(14F)-C(15F)-H(15F)	120.0
C(15F)-C(16F)-C(17F)	120.0
C(15F)-C(16F)-H(16F)	120.0
C(17F)-C(16F)-H(16F)	120.0
C(16F)-C(17F)-C(18F)	120.0
C(16F)-C(17F)-H(17F)	120.0
C(18F)-C(17F)-H(17F)	120.0
C(17F)-C(18F)-C(19F)	120.0
C(17F)-C(18F)-H(18F)	120.0
C(19F)-C(18F)-H(18F)	120.0
C(18F)-C(19F)-C(14F)	120.0
C(18F)-C(19F)-H(19F)	120.0
C(14F)-C(19F)-H(19F)	120.0
O(20F)-C(20F)-C(25F)	121.7(14)
O(20F)-C(20F)-C(21F)	118.4(14)
C(25F)-C(20F)-C(21F)	119.9(14)
O(21F)-C(21F)-C(22F)	126.5(14)
O(21F)-C(21F)-C(20F)	117.9(13)
C(22F)-C(21F)-C(20F)	115.5(15)
C(23F)-C(22F)-C(21F)	124.8(16)
C(23F)-C(22F)-H(22F)	117.6
C(21F)-C(22F)-H(22F)	117.6
C(22F)-C(23F)-C(24F)	119.1(16)
C(22F)-C(23F)-H(23F)	120.5
C(24F)-C(23F)-H(23F)	120.5
C(25F)-C(24F)-C(23F)	118.7(16)
C(25F)-C(24F)-H(24F)	120.7
C(23F)-C(24F)-H(24F)	120.7

C(24F)-C(25F)-C(20F)	121.9(15)
C(24F)-C(25F)-C(26F)	119.4(15)
C(20F)-C(25F)-C(26F)	118.5(14)
C(25F)-C(26F)-P(2F)	111.4(11)
C(25F)-C(26F)-H(26K)	109.3
P(2F)-C(26F)-H(26K)	109.3
C(25F)-C(26F)-H(26L)	109.3
P(2F)-C(26F)-H(26L)	109.3
H(26K)-C(26F)-H(26L)	108.0
C(28F)-C(27F)-C(32F)	120.0
C(28F)-C(27F)-P(2F)	121.3(7)
C(32F)-C(27F)-P(2F)	118.7(7)
C(29F)-C(28F)-C(27F)	120.0
C(29F)-C(28F)-H(28F)	120.0
C(27F)-C(28F)-H(28F)	120.0
C(28F)-C(29F)-C(30F)	120.0
C(28F)-C(29F)-H(29F)	120.0
C(30F)-C(29F)-H(29F)	120.0
C(31F)-C(30F)-C(29F)	120.0
C(31F)-C(30F)-H(30F)	120.0
C(29F)-C(30F)-H(30F)	120.0
C(32F)-C(31F)-C(30F)	120.0
C(32F)-C(31F)-H(31F)	120.0
C(30F)-C(31F)-H(31F)	120.0
C(31F)-C(32F)-C(27F)	120.0
C(31F)-C(32F)-H(32F)	120.0
C(27F)-C(32F)-H(32F)	120.0
C(34F)-C(33F)-C(38F)	120.0
C(34F)-C(33F)-P(2F)	122.7(7)
C(38F)-C(33F)-P(2F)	117.1(7)

C(35F)-C(34F)-C(33F)	120.0
C(35F)-C(34F)-H(34F)	120.0
C(33F)-C(34F)-H(34F)	120.0
C(34F)-C(35F)-C(36F)	120.0
C(34F)-C(35F)-H(35F)	120.0
C(36F)-C(35F)-H(35F)	120.0
C(35F)-C(36F)-C(37F)	120.0
C(35F)-C(36F)-H(36F)	120.0
C(37F)-C(36F)-H(36F)	120.0
C(38F)-C(37F)-C(36F)	120.0
C(38F)-C(37F)-H(37F)	120.0
C(36F)-C(37F)-H(37F)	120.0
C(37F)-C(38F)-C(33F)	120.0
C(37F)-C(38F)-H(38F)	120.0
C(33F)-C(38F)-H(38F)	120.0
O(20G)-Pd(1G)-O(1G)	81.6(4)
O(20G)-Pd(1G)-P(1G)	172.4(3)
O(1G)-Pd(1G)-P(1G)	90.9(3)
O(20G)-Pd(1G)-P(2G)	90.4(3)
O(1G)-Pd(1G)-P(2G)	170.0(4)
P(1G)-Pd(1G)-P(2G)	97.23(17)
O(20G)-Pd(1G)-Zn(1G)	40.0(3)
O(1G)-Pd(1G)-Zn(1G)	42.3(3)
P(1G)-Pd(1G)-Zn(1G)	132.67(14)
P(2G)-Pd(1G)-Zn(1G)	128.67(13)
O(2G)-Zn(1G)-O(20G)	129.3(5)
O(2G)-Zn(1G)-O(21G)	83.3(5)
O(20G)-Zn(1G)-O(21G)	80.1(4)
O(2G)-Zn(1G)-O(1G)	79.8(5)
O(20G)-Zn(1G)-O(1G)	80.2(4)

O(21G)-Zn(1G)-O(1G)	136.2(5)
O(2G)-Zn(1G)-Cl(1G)	121.8(4)
O(20G)-Zn(1G)-Cl(1G)	108.9(4)
O(21G)-Zn(1G)-Cl(1G)	111.4(4)
O(1G)-Zn(1G)-Cl(1G)	111.8(4)
O(2G)-Zn(1G)-Zn(3)	41.9(4)
O(20G)-Zn(1G)-Zn(3)	106.5(3)
O(21G)-Zn(1G)-Zn(3)	41.5(3)
O(1G)-Zn(1G)-Zn(3)	110.3(3)
Cl(1G)-Zn(1G)-Zn(3)	128.3(2)
O(2G)-Zn(1G)-Pd(1G)	103.1(3)
O(20G)-Zn(1G)-Pd(1G)	40.2(3)
O(21G)-Zn(1G)-Pd(1G)	107.0(3)
O(1G)-Zn(1G)-Pd(1G)	40.7(3)
Cl(1G)-Zn(1G)-Pd(1G)	122.8(2)
Zn(3)-Zn(1G)-Pd(1G)	108.59(8)
C(8G)-P(1G)-C(14G)	109.3(6)
C(8G)-P(1G)-C(7G)	105.1(8)
C(14G)-P(1G)-C(7G)	101.6(8)
C(8G)-P(1G)-Pd(1G)	115.8(5)
C(14G)-P(1G)-Pd(1G)	117.8(5)
C(7G)-P(1G)-Pd(1G)	105.4(6)
C(33G)-P(2G)-C(27G)	109.2(6)
C(33G)-P(2G)-C(26G)	105.9(7)
C(27G)-P(2G)-C(26G)	101.6(7)
C(33G)-P(2G)-Pd(1G)	122.9(5)
C(27G)-P(2G)-Pd(1G)	109.5(4)
C(26G)-P(2G)-Pd(1G)	105.6(6)
C(1G)-O(1G)-Pd(1G)	115.3(11)
C(1G)-O(1G)-Zn(1G)	108.3(11)

Pd(1G)-O(1G)-Zn(1G)	97.0(5)
C(2G)-O(2G)-Zn(1G)	113.9(11)
C(2G)-O(2G)-Zn(3)	120.0(12)
Zn(1G)-O(2G)-Zn(3)	96.7(5)
C(20G)-O(20G)-Zn(1G)	111.7(9)
C(20G)-O(20G)-Pd(1G)	121.4(9)
Zn(1G)-O(20G)-Pd(1G)	99.8(5)
C(21G)-O(21G)-Zn(3)	121.7(11)
C(21G)-O(21G)-Zn(1G)	109.8(10)
Zn(3)-O(21G)-Zn(1G)	95.7(5)
O(1G)-C(1G)-C(2G)	122.5(17)
O(1G)-C(1G)-C(6G)	121.4(17)
C(2G)-C(1G)-C(6G)	115.2(18)
C(3G)-C(2G)-O(2G)	120.6(17)
C(3G)-C(2G)-C(1G)	125.3(18)
O(2G)-C(2G)-C(1G)	114.1(17)
C(2G)-C(3G)-C(4G)	117(2)
C(2G)-C(3G)-H(3G)	121.6
C(4G)-C(3G)-H(3G)	121.6
C(5G)-C(4G)-C(3G)	120(2)
C(5G)-C(4G)-H(4G)	119.8
C(3G)-C(4G)-H(4G)	119.8
C(4G)-C(5G)-C(6G)	121.7(19)
C(4G)-C(5G)-H(5G)	119.2
C(6G)-C(5G)-H(5G)	119.2
C(5G)-C(6G)-C(1G)	120.4(18)
C(5G)-C(6G)-C(7G)	124.1(17)
C(1G)-C(6G)-C(7G)	115.4(17)
C(6G)-C(7G)-P(1G)	110.6(13)
C(6G)-C(7G)-H(7G1)	109.5

P(1G)-C(7G)-H(7G1)	109.5
C(6G)-C(7G)-H(7G2)	109.5
P(1G)-C(7G)-H(7G2)	109.5
H(7G1)-C(7G)-H(7G2)	108.1
C(9G)-C(8G)-C(13G)	120.0
C(9G)-C(8G)-P(1G)	121.6(7)
C(13G)-C(8G)-P(1G)	118.4(7)
C(10G)-C(9G)-C(8G)	120.0
C(10G)-C(9G)-H(9G)	120.0
C(8G)-C(9G)-H(9G)	120.0
C(9G)-C(10G)-C(11G)	120.0
C(9G)-C(10G)-H(10G)	120.0
C(11G)-C(10G)-H(10G)	120.0
C(12G)-C(11G)-C(10G)	120.0
C(12G)-C(11G)-H(11G)	120.0
C(10G)-C(11G)-H(11G)	120.0
C(13G)-C(12G)-C(11G)	120.0
C(13G)-C(12G)-H(12G)	120.0
C(11G)-C(12G)-H(12G)	120.0
C(12G)-C(13G)-C(8G)	120.0
C(12G)-C(13G)-H(13G)	120.0
C(8G)-C(13G)-H(13G)	120.0
C(15G)-C(14G)-C(19G)	120.0
C(15G)-C(14G)-P(1G)	121.7(8)
C(19G)-C(14G)-P(1G)	118.3(8)
C(16G)-C(15G)-C(14G)	120.0
C(16G)-C(15G)-H(15G)	120.0
C(14G)-C(15G)-H(15G)	120.0
C(15G)-C(16G)-C(17G)	120.0
C(15G)-C(16G)-H(16G)	120.0

C(17G)-C(16G)-H(16G)	120.0
C(18G)-C(17G)-C(16G)	120.0
C(18G)-C(17G)-H(17G)	120.0
C(16G)-C(17G)-H(17G)	120.0
C(17G)-C(18G)-C(19G)	120.0
C(17G)-C(18G)-H(18G)	120.0
C(19G)-C(18G)-H(18G)	120.0
C(18G)-C(19G)-C(14G)	120.0
C(18G)-C(19G)-H(19G)	120.0
C(14G)-C(19G)-H(19G)	120.0
C(21G)-C(20G)-C(25G)	124.3(17)
C(21G)-C(20G)-O(20G)	116.0(15)
C(25G)-C(20G)-O(20G)	119.8(15)
O(21G)-C(21G)-C(20G)	122.4(17)
O(21G)-C(21G)-C(22G)	121.2(15)
C(20G)-C(21G)-C(22G)	116.4(16)
C(23G)-C(22G)-C(21G)	121.4(16)
C(23G)-C(22G)-H(22G)	119.3
C(21G)-C(22G)-H(22G)	119.3
C(24G)-C(23G)-C(22G)	119.0(17)
C(24G)-C(23G)-H(23G)	120.5
C(22G)-C(23G)-H(23G)	120.5
C(23G)-C(24G)-C(25G)	120.2(16)
C(23G)-C(24G)-H(24G)	119.9
C(25G)-C(24G)-H(24G)	119.9
C(20G)-C(25G)-C(24G)	118.5(15)
C(20G)-C(25G)-C(26G)	120.0(15)
C(24G)-C(25G)-C(26G)	121.5(15)
C(25G)-C(26G)-P(2G)	108.7(11)
C(25G)-C(26G)-H(26M)	109.9

P(2G)-C(26G)-H(26M)	109.9
C(25G)-C(26G)-H(26N)	109.9
P(2G)-C(26G)-H(26N)	109.9
H(26M)-C(26G)-H(26N)	108.3
C(28G)-C(27G)-C(32G)	120.0
C(28G)-C(27G)-P(2G)	118.6(6)
C(32G)-C(27G)-P(2G)	121.0(6)
C(27G)-C(28G)-C(29G)	120.0
C(27G)-C(28G)-H(28G)	120.0
C(29G)-C(28G)-H(28G)	120.0
C(28G)-C(29G)-C(30G)	120.0
C(28G)-C(29G)-H(29G)	120.0
C(30G)-C(29G)-H(29G)	120.0
C(31G)-C(30G)-C(29G)	120.0
C(31G)-C(30G)-H(30G)	120.0
C(29G)-C(30G)-H(30G)	120.0
C(32G)-C(31G)-C(30G)	120.0
C(32G)-C(31G)-H(31G)	120.0
C(30G)-C(31G)-H(31G)	120.0
C(31G)-C(32G)-C(27G)	120.0
C(31G)-C(32G)-H(32G)	120.0
C(27G)-C(32G)-H(32G)	120.0
C(34G)-C(33G)-C(38G)	120.0
C(34G)-C(33G)-P(2G)	121.8(7)
C(38G)-C(33G)-P(2G)	118.1(7)
C(33G)-C(34G)-C(35G)	120.0
C(33G)-C(34G)-H(34G)	120.0
C(35G)-C(34G)-H(34G)	120.0
C(34G)-C(35G)-C(36G)	120.0
C(34G)-C(35G)-H(35G)	120.0

C(36G)-C(35G)-H(35G)	120.0
C(35G)-C(36G)-C(37G)	120.0
C(35G)-C(36G)-H(36G)	120.0
C(37G)-C(36G)-H(36G)	120.0
C(38G)-C(37G)-C(36G)	120.0
C(38G)-C(37G)-H(37G)	120.0
C(36G)-C(37G)-H(37G)	120.0
C(37G)-C(38G)-C(33G)	120.0
C(37G)-C(38G)-H(38G)	120.0
C(33G)-C(38G)-H(38G)	120.0
O(21G)-Zn(3)-O(2G)	84.2(5)
O(21G)-Zn(3)-Cl(5)	113.9(4)
O(2G)-Zn(3)-Cl(5)	112.8(4)
O(21G)-Zn(3)-Cl(4)	111.6(4)
O(2G)-Zn(3)-Cl(4)	110.4(4)
Cl(5)-Zn(3)-Cl(4)	118.9(3)
O(21G)-Zn(3)-Zn(1G)	42.8(3)
O(2G)-Zn(3)-Zn(1G)	41.4(4)
Cl(5)-Zn(3)-Zn(1G)	124.0(3)
Cl(4)-Zn(3)-Zn(1G)	117.12(18)
O(11)-Zn(4)-Cl(7)	104.3(5)
O(11)-Zn(4)-Cl(6)	99.4(5)
Cl(7)-Zn(4)-Cl(6)	116.4(3)
O(11)-Zn(4)-Cl(8)	103.6(5)
Cl(7)-Zn(4)-Cl(8)	119.3(4)
Cl(6)-Zn(4)-Cl(8)	110.5(4)
C(11)-O(11)-Zn(4)	114.1(10)
O(11)-C(11)-N(11)	121.6(11)
O(11)-C(11)-H(11)	119.2
N(11)-C(11)-H(11)	119.2

C(11)-N(11)-C(112)	118.7(9)
C(11)-N(11)-C(111)	119.7(9)
C(112)-N(11)-C(111)	121.6(10)
N(11)-C(111)-H(11H)	109.5
N(11)-C(111)-H(11I)	109.5
H(11H)-C(111)-H(11I)	109.5
N(11)-C(111)-H(11J)	109.5
H(11H)-C(111)-H(11J)	109.5
H(11I)-C(111)-H(11J)	109.5
N(11)-C(112)-H(11K)	109.5
N(11)-C(112)-H(11L)	109.5
H(11K)-C(112)-H(11L)	109.5
N(11)-C(112)-H(11M)	109.5
H(11K)-C(112)-H(11M)	109.5
H(11L)-C(112)-H(11M)	109.5
O(21)-C(21)-N(21)	122.4(12)
O(21)-C(21)-H(21)	118.8
N(21)-C(21)-H(21)	118.8
C(21)-N(21)-C(211)	120.1(9)
C(21)-N(21)-C(212)	119.5(9)
C(211)-N(21)-C(212)	120.3(11)
N(21)-C(211)-H(21A)	109.5
N(21)-C(211)-H(21B)	109.5
H(21A)-C(211)-H(21B)	109.5
N(21)-C(211)-H(21C)	109.5
H(21A)-C(211)-H(21C)	109.5
H(21B)-C(211)-H(21C)	109.5
N(21)-C(212)-H(21D)	109.5
N(21)-C(212)-H(21E)	109.5
H(21D)-C(212)-H(21E)	109.5

N(21)-C(212)-H(21F)	109.5
H(21D)-C(212)-H(21F)	109.5
H(21E)-C(212)-H(21F)	109.5
O(31)-C(31)-N(31)	122.8(12)
O(31)-C(31)-H(31)	118.6
N(31)-C(31)-H(31)	118.6
C(31)-N(31)-C(312)	120.0(10)
C(31)-N(31)-C(311)	118.6(9)
C(312)-N(31)-C(311)	120.6(11)
N(31)-C(311)-H(31H)	109.5
N(31)-C(311)-H(31I)	109.5
H(31H)-C(311)-H(31I)	109.5
N(31)-C(311)-H(31J)	109.5
H(31H)-C(311)-H(31J)	109.5
H(31I)-C(311)-H(31J)	109.5
N(31)-C(312)-H(31K)	109.5
N(31)-C(312)-H(31L)	109.5
H(31K)-C(312)-H(31L)	109.5
N(31)-C(312)-H(31M)	109.5
H(31K)-C(312)-H(31M)	109.5
H(31L)-C(312)-H(31M)	109.5
O(41)-C(41)-N(41)	121.5(12)
O(41)-C(41)-H(41)	119.3
N(41)-C(41)-H(41)	119.3
C(41)-N(41)-C(412)	119.5(10)
C(41)-N(41)-C(411)	118.5(9)
C(412)-N(41)-C(411)	121.9(11)
N(41)-C(411)-H(41A)	109.5
N(41)-C(411)-H(41B)	109.5
H(41A)-C(411)-H(41B)	109.5

N(41)-C(411)-H(41C)	109.5
H(41A)-C(411)-H(41C)	109.5
H(41B)-C(411)-H(41C)	109.5
N(41)-C(412)-H(41D)	109.5
N(41)-C(412)-H(41E)	109.5
H(41D)-C(412)-H(41E)	109.5
N(41)-C(412)-H(41F)	109.5
H(41D)-C(412)-H(41F)	109.5
H(41E)-C(412)-H(41F)	109.5
O(51)-C(51)-N(51)	121.8(12)
O(51)-C(51)-H(51)	119.1
N(51)-C(51)-H(51)	119.1
C(51)-N(51)-C(511)	119.8(9)
C(51)-N(51)-C(512)	117.8(9)
C(511)-N(51)-C(512)	121.7(11)
N(51)-C(511)-H(51A)	109.5
N(51)-C(511)-H(51B)	109.5
H(51A)-C(511)-H(51B)	109.5
N(51)-C(511)-H(51C)	109.5
H(51A)-C(511)-H(51C)	109.5
H(51B)-C(511)-H(51C)	109.5
N(51)-C(512)-H(51D)	109.5
N(51)-C(512)-H(51E)	109.5
H(51D)-C(512)-H(51E)	109.5
N(51)-C(512)-H(51F)	109.5
H(51D)-C(512)-H(51F)	109.5
H(51E)-C(512)-H(51F)	109.5
O(61)-C(61)-N(61)	123.7(12)
O(61)-C(61)-H(61)	118.2
N(61)-C(61)-H(61)	118.2

C(61)-N(61)-C(611)	120.3(9)
C(61)-N(61)-C(612)	119.8(9)
C(611)-N(61)-C(612)	119.8(11)
N(61)-C(611)-H(61A)	109.5
N(61)-C(611)-H(61B)	109.5
H(61A)-C(611)-H(61B)	109.5
N(61)-C(611)-H(61C)	109.5
H(61A)-C(611)-H(61C)	109.5
H(61B)-C(611)-H(61C)	109.5
N(61)-C(612)-H(61D)	109.5
N(61)-C(612)-H(61E)	109.5
H(61D)-C(612)-H(61E)	109.5
N(61)-C(612)-H(61F)	109.5
H(61D)-C(612)-H(61F)	109.5
H(61E)-C(612)-H(61F)	109.5
O(71)-C(71)-N(71)	119.8(12)
O(71)-C(71)-H(71)	120.1
N(71)-C(71)-H(71)	120.1
C(71)-N(71)-C(711)	119.9(10)
C(71)-N(71)-C(712)	118.6(9)
C(711)-N(71)-C(712)	121.5(11)
N(71)-C(711)-H(71A)	109.5
N(71)-C(711)-H(71B)	109.5
H(71A)-C(711)-H(71B)	109.5
N(71)-C(711)-H(71C)	109.5
H(71A)-C(711)-H(71C)	109.5
H(71B)-C(711)-H(71C)	109.5
N(71)-C(712)-H(71D)	109.5
N(71)-C(712)-H(71E)	109.5
H(71D)-C(712)-H(71E)	109.5

N(71)-C(712)-H(71F)	109.5
H(71D)-C(712)-H(71F)	109.5
H(71E)-C(712)-H(71F)	109.5
O(81)-C(81)-N(81)	119.3(14)
O(81)-C(81)-H(81)	120.3
N(81)-C(81)-H(81)	120.3
C(81)-N(81)-C(812)	117.8(11)
C(81)-N(81)-C(811)	118.1(11)
C(812)-N(81)-C(811)	122.0(13)
N(81)-C(811)-H(81A)	109.5
N(81)-C(811)-H(81B)	109.5
H(81A)-C(811)-H(81B)	109.5
N(81)-C(811)-H(81C)	109.5
H(81A)-C(811)-H(81C)	109.5
H(81B)-C(811)-H(81C)	109.5
N(81)-C(812)-H(81D)	109.5
N(81)-C(812)-H(81E)	109.5
H(81D)-C(812)-H(81E)	109.5
N(81)-C(812)-H(81F)	109.5
H(81D)-C(812)-H(81F)	109.5
H(81E)-C(812)-H(81F)	109.5
O(91)-C(91)-N(91)	124.2(16)
O(91)-C(91)-H(91)	117.9
N(91)-C(91)-H(91)	117.9
C(91)-N(91)-C(912)	119.1(12)
C(91)-N(91)-C(911)	118.5(12)
C(912)-N(91)-C(911)	119.9(13)
N(91)-C(911)-H(91A)	109.5
N(91)-C(911)-H(91B)	109.5
H(91A)-C(911)-H(91B)	109.5

N(91)-C(911)-H(91C)	109.5
H(91A)-C(911)-H(91C)	109.5
H(91B)-C(911)-H(91C)	109.5
N(91)-C(912)-H(91D)	109.5
N(91)-C(912)-H(91E)	109.5
H(91D)-C(912)-H(91E)	109.5
N(91)-C(912)-H(91F)	109.5
H(91D)-C(912)-H(91F)	109.5
H(91E)-C(912)-H(91F)	109.5
O(22)-C(22)-N(22)	123.2(14)
O(22)-C(22)-H(22)	118.4
N(22)-C(22)-H(22)	118.4
C(22)-N(22)-C(221)	119.4(11)
C(22)-N(22)-C(222)	119.4(10)
C(221)-N(22)-C(222)	120.3(12)
N(22)-C(221)-H(22H)	109.5
N(22)-C(221)-H(22I)	109.5
H(22H)-C(221)-H(22I)	109.5
N(22)-C(221)-H(22J)	109.5
H(22H)-C(221)-H(22J)	109.5
H(22I)-C(221)-H(22J)	109.5
N(22)-C(222)-H(22K)	109.5
N(22)-C(222)-H(22L)	109.5
H(22K)-C(222)-H(22L)	109.5
N(22)-C(222)-H(22M)	109.5
H(22K)-C(222)-H(22M)	109.5
H(22L)-C(222)-H(22M)	109.5
O(32)-C(32)-N(32)	121.4(15)
O(32)-C(32)-H(32)	119.3
N(32)-C(32)-H(32)	119.3

C(32)-N(32)-C(322)	119.4(10)
C(32)-N(32)-C(321)	119.3(10)
C(322)-N(32)-C(321)	121.3(12)
N(32)-C(321)-H(32H)	109.5
N(32)-C(321)-H(32I)	109.5
H(32H)-C(321)-H(32I)	109.5
N(32)-C(321)-H(32J)	109.5
H(32H)-C(321)-H(32J)	109.5
H(32I)-C(321)-H(32J)	109.5
N(32)-C(322)-H(32K)	109.5
N(32)-C(322)-H(32L)	109.5
H(32K)-C(322)-H(32L)	109.5
N(32)-C(322)-H(32M)	109.5
H(32K)-C(322)-H(32M)	109.5
H(32L)-C(322)-H(32M)	109.5

Symmetry transformations used to generate equivalent atoms:

[*SP*-4-2]-[{(diphenyl-{benzo-[1,3]- μO^1 : kO^2 -4-ylmethyl}-phosphan- kP)(diphenyl-{benzo-[1,3]- μO^1 -4-ylmethyl}-phosphan- kP -palladium(II)}-[*SAPR*-8-13]- μO^1 : μO^1 : kO^2 -bis-(2,4-pentandionato)-europium(III)] (50)

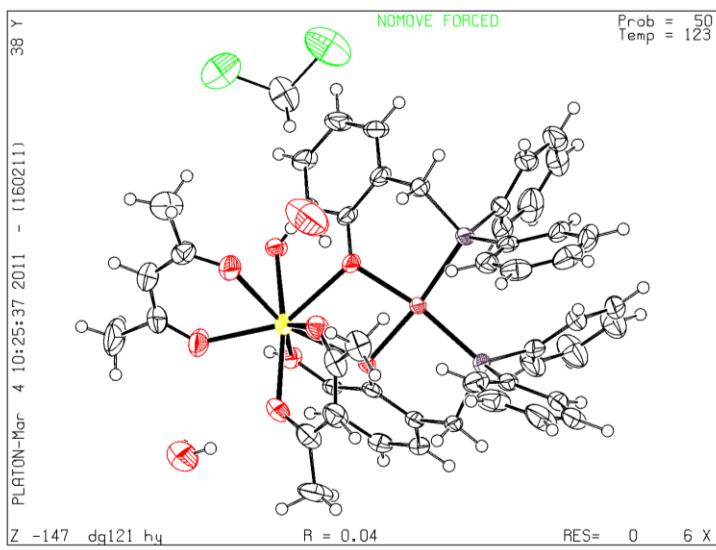


Table 1. Crystal data and structure refinement for dg121_hy.

Identification code	dg121_hy
Empirical formula	C48.50 H50 Cl Eu O10 P2 Pd C48 H45 Eu O8 P2 Pd - 2 H2O, 0.5 CH2Cl2
Formula weight	1148.64
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n (No.14)
Unit cell dimensions	a = 13.205(1) Å alpha = 90 deg. b = 12.857(1) Å beta = 100.60(1) deg. c = 29.164(2) Å gamma = 90 deg.
Volume	4866.9(6) Å^3
Z, Calculated density	4, 1.568 Mg/m^3
Absorption coefficient	1.822 mm^-1
F(000)	2308
Crystal size	0.16 x 0.08 x 0.04 mm
Theta range for data collection	3.14 to 25.00 deg.
Limiting indices	-15<=h<=12, -15<=k<=14, -25<=l<=34
Reflections collected / unique	26211 / 8532 [R(int) = 0.0503]
Completeness to theta = 25.00	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9280 and 0.6176
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8532 / 48 / 605
Goodness-of-fit on F^2	1.040
Final R indices [I>2sigma(I)]	R1 = 0.0443, wR2 = 0.0957
R indices (all data)	R1 = 0.0726, wR2 = 0.1069
Largest diff. peak and hole	1.661 and -0.950 e.Å^-3

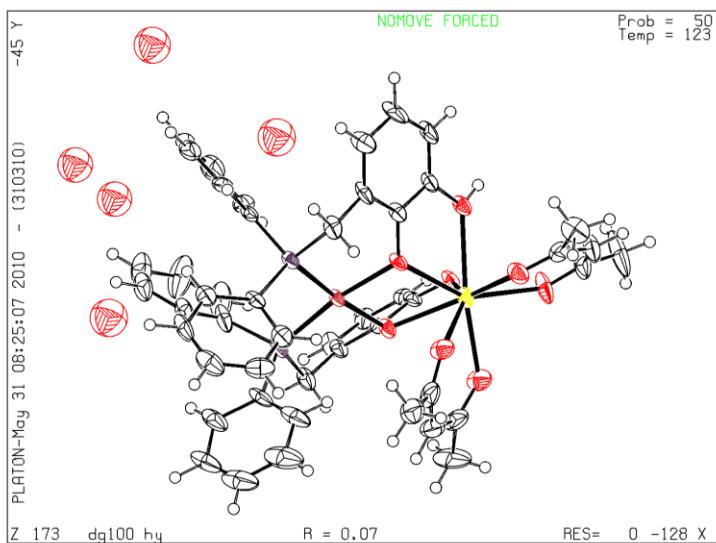


Table 1. Crystal data and structure refinement for dg100_hy.

Identification code	dg100_hy	
Empirical formula	C ₄₈ H ₅₃ Eu O ₁₂ P ₂ Pd C ₄₈ H ₄₅ Eu O ₈ P ₂ Pd - 4 water	
Formula weight	1142.20	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, P2(1)/n (No.14)	
Unit cell dimensions	a = 13.168(1) Å alpha = 90 deg. b = 12.833(1) Å beta = 100.59(1) deg. c = 29.254(2) Å gamma = 90 deg.	
Volume	4859.3(6) Å ³	
Z, Calculated density	4, 1.561 Mg/m ³	
Absorption coefficient	1.774 mm ⁻¹	
F(000)	2304	
Crystal size	0.15 x 0.10 x 0.03 mm	
Theta range for data collection	3.15 to 25.03 deg.	
Limiting indices	-15<=h<=15, -15<=k<=15, -25<=l<=34	
Reflections collected / unique	33443 / 8535 [R(int) = 0.0726]	
Completeness to theta = 25.03	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9562 and 0.6896	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	8535 / 1 / 568	
Goodness-of-fit on F ²	1.106	
Final R indices [I>2sigma(I)]	R1 = 0.0737, wR2 = 0.1611	
R indices (all data)	R1 = 0.1062, wR2 = 0.1745	
Largest diff. peak and hole	2.084 and -1.180 e.Å ⁻³	

[*SP*-4-2]-[{(diphenyl-{benzo-[1,3]- μO^1 : kO^2 -4-ylmethyl}-phosphan-*kP*)(diphenyl-{benzo-[1,3]- μO^1 -4-ylmethyl}-phosphan-*kP*-palladium(II)}-[*SAPR*-8-13]- μO^1 : μO^1 : kO^2 -bis-(6,6,7,7,8,8,8-heptafluoro-2,2-dimethyloctan-3,5-dionato)-europium(III)] (51)

Table 1. Crystal data and structure refinement for gud37.

Identification code	gud37
Empirical formula	C59 H53 Cl2 Eu F14 O8 P2 Pd C58 H51 Eu F14 O8 P2 Pd - CHCl2
Formula weight	1547.21
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1 (no.2)
Unit cell dimensions	a = 14.6078(12) Å alpha = 89.515(4) deg. b = 14.7211(12) Å beta = 71.274(4) deg. c = 16.7575(12) Å gamma = 63.721(4) deg.
Volume	3022.0(4) Å³
Z, Calculated density	2, 1.700 Mg/m³
Absorption coefficient	1.564 mm⁻¹
F(000)	1540
Crystal size	0.18 x 0.12 x 0.06 mm

Theta range for data collection 1.56 to 26.45 deg.

Limiting indices -18<=h<=18, -18<=k<=18, -20<=l<=20

Reflections collected / unique 77691 / 12339 [R(int) = 0.0698]

Completeness to theta = 25.00 99.9 %

Absorption correction Semi-empirical from equivalents

Max. and min. transmission 0.7454 and 0.6367

Refinement method Full-matrix least-squares on F^2

Data / restraints / parameters 12339 / 54 / 777

Goodness-of-fit on F^2 1.037

Final R indices [I>2sigma(I)] R1 = 0.0521, wR2 = 0.1164

R indices (all data) R1 = 0.0969, wR2 = 0.1418

Largest diff. peak and hole 2.455 and -1.937 e.A^-3