Crystal Data

1) Crystal data of 9a

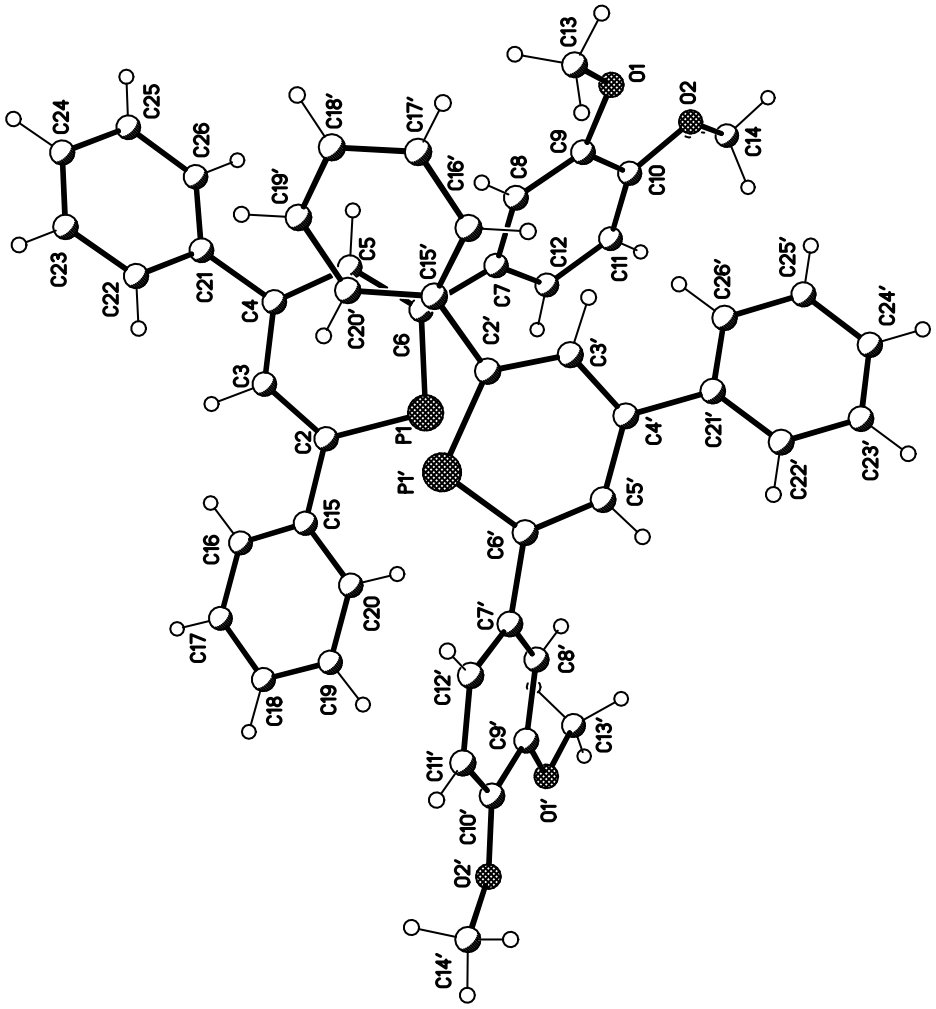

Table 1. Crystal data and structure refinement for dg010_hy.

Identification code	dg010_hy
Empirical formula	C25 H21 O2 P

Formula weight	384.39
Temperature	123(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c (no.14)
Unit cell dimensions	a = 7.609(2) A alpha = 90 deg. b = 25.902(5) A beta = 90.65(3) deg. c = 20.756(4) A gamma = 90 deg.
Volume	4090.5(15) A^3
Z, Calculated density	8, 1.248 Mg/m^3
Absorption coefficient	0.152 mm^-1
F(000)	1616
Crystal size	0.20 x 0.08 x 0.04 mm
Theta range for data collection	2.95 to 25.03 deg.
Limiting indices	-9<=h<=8, -30<=k<=30, -24<=l<=24
Reflections collected / unique	28025 / 7155 [R(int) = 0.1659]
Completeness to theta = 25.03	99.2 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7155 / 0 / 505
Goodness-of-fit on F^2	0.997
Final R indices [I>2sigma(I)]	R1 = 0.0896, wR2 = 0.1805
R indices (all data)	R1 = 0.2396, wR2 = 0.2414
Largest diff. peak and hole	0.804 and -0.424 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for dg010_hy.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
P(1)	1472(2)	2763(1)	2836(1)	24(1)
C(2)	1393(8)	3078(2)	2092(3)	25(2)
C(3)	1123(7)	2823(2)	1504(3)	22(1)
C(4)	852(7)	2293(2)	1434(3)	21(1)
C(5)	821(7)	1963(2)	1966(3)	23(2)
C(6)	1068(7)	2122(2)	2609(3)	20(1)
C(7)	921(7)	1735(2)	3130(3)	21(1)
C(8)	1687(7)	1235(2)	3078(3)	22(2)
C(9)	1413(8)	862(2)	3538(3)	25(2)
C(10)	300(8)	970(2)	4070(3)	24(2)
C(11)	-391(8)	1456(2)	4132(3)	23(2)
C(12)	-59(7)	1840(2)	3677(3)	23(2)
O(1)	2146(5)	377(2)	3547(2)	35(1)
C(13)	3484(10)	268(3)	3098(4)	53(2)
O(2)	18(5)	558(2)	4483(2)	32(1)
C(14)	-1292(8)	635(2)	4960(3)	40(2)
C(15)	1611(8)	3651(2)	2086(3)	24(2)
C(16)	627(8)	3959(2)	1664(3)	28(2)
C(17)	849(9)	4484(2)	1642(3)	35(2)
C(18)	2051(8)	4728(2)	2045(3)	33(2)
C(19)	3007(8)	4426(2)	2481(3)	34(2)
C(20)	2813(8)	3899(2)	2497(3)	26(2)
C(21)	674(8)	2075(2)	770(3)	21(1)
C(22)	1696(8)	2267(2)	269(3)	27(2)
C(23)	1562(8)	2065(2)	-350(3)	29(2)
C(24)	387(9)	1671(2)	-473(3)	33(2)
C(25)	-614(9)	1468(2)	21(3)	36(2)
C(26)	-483(7)	1678(2)	635(3)	25(2)
P(1')	6438(2)	2748(1)	2678(1)	26(1)
C(2')	6017(8)	2102(2)	2851(3)	26(2)
C(3')	5678(7)	1914(2)	3473(3)	24(2)
C(4')	5694(7)	2214(2)	4032(3)	23(2)
C(5')	5990(7)	2745(2)	4010(3)	25(2)
C(6')	6319(7)	3025(2)	3446(3)	24(2)
C(7')	6606(8)	3595(2)	3498(3)	23(2)
C(8')	5519(8)	3895(2)	3896(3)	23(2)
C(9')	5795(8)	4414(2)	3970(3)	24(2)
C(10')	7243(8)	4659(2)	3671(3)	28(2)
C(11')	8300(8)	4362(2)	3269(3)	31(2)
C(12')	7950(8)	3837(2)	3177(3)	29(2)
O(1')	4767(6)	4743(2)	4328(2)	35(1)
C(13')	3214(8)	4525(2)	4606(3)	36(2)
O(2')	7474(6)	5168(2)	3799(2)	41(1)
C(14')	9096(9)	5397(2)	3606(3)	45(2)
C(15')	5965(7)	1726(2)	2306(3)	21(1)
C(16')	6715(8)	1239(2)	2365(3)	23(2)
C(17')	6609(8)	875(2)	1865(3)	26(2)
C(18')	5723(8)	1004(2)	1295(3)	29(2)
C(19')	5021(8)	1493(2)	1221(3)	28(2)
C(20')	5147(7)	1855(2)	1713(3)	27(2)
C(21')	5457(8)	1959(2)	4679(3)	23(2)
C(22')	6433(8)	2119(2)	5212(3)	29(2)
C(23')	6246(9)	1879(3)	5809(3)	37(2)
C(24')	5056(9)	1477(3)	5865(3)	40(2)
C(25')	4059(9)	1309(2)	5343(3)	35(2)
C(26')	4270(8)	1557(2)	4743(3)	25(2)

Table 3. Bond lengths [A] and angles [deg] for dg010_hy.

P(1)-C(2)	1.746(6)
P(1)-C(6)	1.751(6)
P(1)-P(1')	3.797(3)
P(1)-P(1')#1	3.841(3)
C(2)-C(3)	1.401(7)
C(2)-C(15)	1.495(8)
C(3)-C(4)	1.395(7)
C(4)-C(5)	1.396(8)
C(4)-C(21)	1.495(8)
C(5)-C(6)	1.408(7)
C(6)-C(7)	1.480(8)
C(7)-C(12)	1.392(8)
C(7)-C(8)	1.423(8)
C(8)-C(9)	1.376(8)
C(9)-O(1)	1.376(6)
C(9)-C(10)	1.427(8)
C(10)-C(11)	1.370(8)
C(10)-O(2)	1.388(6)
C(11)-C(12)	1.397(8)
O(1)-C(13)	1.417(7)
O(2)-C(14)	1.426(7)
C(15)-C(16)	1.397(8)
C(15)-C(20)	1.398(8)
C(16)-C(17)	1.372(8)
C(17)-C(18)	1.384(8)
C(18)-C(19)	1.395(8)
C(19)-C(20)	1.373(8)
C(21)-C(26)	1.380(8)
C(21)-C(22)	1.397(8)
C(22)-C(23)	1.390(8)
C(23)-C(24)	1.377(8)
C(24)-C(25)	1.388(9)
C(25)-C(26)	1.390(8)
P(1')-C(2')	1.741(6)
P(1')-C(6')	1.752(6)
P(1')-P(1)#2	3.841(3)
C(2')-C(3')	1.406(8)
C(2')-C(15')	1.492(8)
C(3')-C(4')	1.396(8)
C(4')-C(5')	1.394(8)
C(4')-C(21')	1.511(8)
C(5')-C(6')	1.403(8)
C(6')-C(7')	1.496(8)
C(7')-C(12')	1.378(8)
C(7')-C(8')	1.410(8)
C(8')-C(9')	1.369(8)
C(9')-O(1')	1.379(7)
C(9')-C(10')	1.420(8)
C(10')-O(2')	1.356(7)
C(10')-C(11')	1.398(8)
C(11')-C(12')	1.396(8)
O(1')-C(13')	1.436(7)
O(2')-C(14')	1.430(7)
C(15')-C(16')	1.390(8)
C(15')-C(20')	1.414(8)
C(16')-C(17')	1.404(8)
C(17')-C(18')	1.396(8)
C(18')-C(19')	1.383(8)
C(19')-C(20')	1.389(8)
C(21')-C(26')	1.385(8)
C(21')-C(22')	1.389(8)
C(22')-C(23')	1.395(8)
C(23')-C(24')	1.385(9)
C(24')-C(25')	1.387(9)
C(25')-C(26')	1.411(8)

C(2)-P(1)-C(6)	101.6(3)
C(2)-P(1)-P(1')	87.3(2)
C(6)-P(1)-P(1')	97.99(19)
C(2)-P(1)-P(1')#1	84.6(2)
C(6)-P(1)-P(1')#1	78.20(18)
P(1')-P(1)-P(1')#1	170.09(6)
C(3)-C(2)-C(15)	118.4(5)
C(3)-C(2)-P(1)	123.6(5)

C(15)-C(2)-P(1)	118.0(4)
C(4)-C(3)-C(2)	125.0(5)
C(3)-C(4)-C(5)	121.6(5)
C(3)-C(4)-C(21)	118.6(5)
C(5)-C(4)-C(21)	119.8(5)
C(4)-C(5)-C(6)	124.6(5)
C(5)-C(6)-C(7)	119.0(5)
C(5)-C(6)-P(1)	123.6(4)
C(7)-C(6)-P(1)	117.4(4)
C(12)-C(7)-C(8)	117.7(5)
C(12)-C(7)-C(6)	120.5(5)
C(8)-C(7)-C(6)	121.7(5)
C(9)-C(8)-C(7)	121.3(5)
O(1)-C(9)-C(8)	126.0(5)
O(1)-C(9)-C(10)	114.4(5)
C(8)-C(9)-C(10)	119.7(5)
C(11)-C(10)-O(2)	125.9(5)
C(11)-C(10)-C(9)	119.0(5)
O(2)-C(10)-C(9)	115.1(5)
C(10)-C(11)-C(12)	121.2(6)
C(7)-C(12)-C(11)	120.9(6)
C(9)-O(1)-C(13)	117.8(5)
C(10)-O(2)-C(14)	115.8(5)
C(16)-C(15)-C(20)	117.6(5)
C(16)-C(15)-C(2)	120.9(5)
C(20)-C(15)-C(2)	121.5(5)
C(17)-C(16)-C(15)	121.4(6)
C(16)-C(17)-C(18)	120.9(6)
C(17)-C(18)-C(19)	118.1(6)
C(20)-C(19)-C(18)	121.2(6)
C(19)-C(20)-C(15)	120.7(6)
C(26)-C(21)-C(22)	118.3(5)
C(26)-C(21)-C(4)	121.2(5)
C(22)-C(21)-C(4)	120.5(5)
C(23)-C(22)-C(21)	121.2(6)
C(24)-C(23)-C(22)	119.4(6)
C(23)-C(24)-C(25)	120.3(6)
C(24)-C(25)-C(26)	119.6(6)
C(21)-C(26)-C(25)	121.1(6)
C(2')-P(1')-C(6')	101.3(3)
C(2')-P(1')-P(1)	78.8(2)
C(6')-P(1')-P(1)	81.7(2)
C(2')-P(1')-P(1)#2	100.3(2)
C(6')-P(1')-P(1)#2	88.9(2)
P(1)-P(1')-P(1)#2	170.09(6)
C(3')-C(2')-C(15')	117.8(5)
C(3')-C(2')-P(1')	123.9(5)
C(15')-C(2')-P(1')	118.3(4)
C(4')-C(3')-C(2')	124.7(6)
C(5')-C(4')-C(3')	121.5(5)
C(5')-C(4')-C(21')	118.8(5)
C(3')-C(4')-C(21')	119.7(5)
C(4')-C(5')-C(6')	124.7(6)
C(5')-C(6')-C(7')	118.6(5)
C(5')-C(6')-P(1')	123.9(5)
C(7')-C(6')-P(1')	117.5(4)
C(12')-C(7')-C(8')	118.4(5)
C(12')-C(7')-C(6')	121.5(5)
C(8')-C(7')-C(6')	120.0(5)
C(9')-C(8')-C(7')	121.2(5)
C(8')-C(9')-O(1')	125.4(5)
C(8')-C(9')-C(10')	120.5(6)
O(1')-C(9')-C(10')	114.1(5)
O(2')-C(10')-C(11')	125.4(6)
O(2')-C(10')-C(9')	116.6(6)
C(11')-C(10')-C(9')	118.0(5)
C(12')-C(11')-C(10')	120.5(6)
C(7')-C(12')-C(11')	121.2(6)
C(9')-O(1')-C(13')	116.6(4)
C(10')-O(2')-C(14')	117.3(5)
C(16')-C(15')-C(20')	117.9(5)
C(16')-C(15')-C(2')	121.2(5)
C(20')-C(15')-C(2')	120.9(5)
C(15')-C(16')-C(17')	121.6(6)
C(18')-C(17')-C(16')	119.3(6)
C(19')-C(18')-C(17')	119.7(6)
C(18')-C(19')-C(20')	120.9(6)

C(19')-C(20')-C(15')	120.5(6)
C(26')-C(21')-C(22')	119.5(6)
C(26')-C(21')-C(4')	119.9(5)
C(22')-C(21')-C(4')	120.6(6)
C(21')-C(22')-C(23')	120.9(6)
C(24')-C(23')-C(22')	118.9(6)
C(23')-C(24')-C(25')	121.5(6)
C(24')-C(25')-C(26')	118.7(6)
C(21')-C(26')-C(25')	120.5(6)

Symmetry transformations used to generate equivalent atoms:
#1 x-1,y,z #2 x+1,y,z

Table 4. Torsion angles [deg] for dg010_hy.

C(6)-P(1)-C(2)-C(3)	-1.9(6)
P(1')-P(1)-C(2)-C(3)	95.7(5)
P(1')#1-P(1)-C(2)-C(3)	-78.7(5)
C(6)-P(1)-C(2)-C(15)	177.5(5)
P(1')-P(1)-C(2)-C(15)	-84.8(4)
P(1')#1-P(1)-C(2)-C(15)	100.8(4)
C(15)-C(2)-C(3)-C(4)	-178.2(5)
P(1)-C(2)-C(3)-C(4)	1.3(9)
C(2)-C(3)-C(4)-C(5)	0.3(9)
C(2)-C(3)-C(4)-C(21)	-176.9(5)
C(3)-C(4)-C(5)-C(6)	-0.6(9)
C(21)-C(4)-C(5)-C(6)	176.6(5)
C(4)-C(5)-C(6)-C(7)	177.2(5)
C(4)-C(5)-C(6)-P(1)	-0.6(8)
C(2)-P(1)-C(6)-C(5)	1.6(5)
P(1')-P(1)-C(6)-C(5)	-87.2(5)
P(1')#1-P(1)-C(6)-C(5)	83.5(5)
C(2)-P(1)-C(6)-C(7)	-176.2(4)
P(1')-P(1)-C(6)-C(7)	94.9(4)
P(1')#1-P(1)-C(6)-C(7)	-94.4(4)
C(5)-C(6)-C(7)-C(12)	-133.4(6)
P(1)-C(6)-C(7)-C(12)	44.6(7)
C(5)-C(6)-C(7)-C(8)	43.2(8)
P(1)-C(6)-C(7)-C(8)	-138.9(5)
C(12)-C(7)-C(8)-C(9)	2.6(8)
C(6)-C(7)-C(8)-C(9)	-174.1(5)
C(7)-C(8)-C(9)-O(1)	-177.1(5)
C(7)-C(8)-C(9)-C(10)	1.8(9)
O(1)-C(9)-C(10)-C(11)	175.2(5)
C(8)-C(9)-C(10)-C(11)	-3.8(9)
O(1)-C(9)-C(10)-O(2)	-5.0(7)
C(8)-C(9)-C(10)-O(2)	175.9(5)
O(2)-C(10)-C(11)-C(12)	-178.2(5)
C(9)-C(10)-C(11)-C(12)	1.6(9)
C(8)-C(7)-C(12)-C(11)	-4.9(8)
C(6)-C(7)-C(12)-C(11)	171.8(5)
C(10)-C(11)-C(12)-C(7)	2.9(9)
C(8)-C(9)-O(1)-C(13)	9.1(9)
C(10)-C(9)-O(1)-C(13)	-169.9(6)
C(11)-C(10)-O(2)-C(14)	8.8(8)
C(9)-C(10)-O(2)-C(14)	-170.9(5)
C(3)-C(2)-C(15)-C(16)	37.9(8)
P(1)-C(2)-C(15)-C(16)	-141.6(5)
C(3)-C(2)-C(15)-C(20)	-141.4(6)
P(1)-C(2)-C(15)-C(20)	39.0(7)
C(20)-C(15)-C(16)-C(17)	1.2(9)
C(2)-C(15)-C(16)-C(17)	-178.2(5)
C(15)-C(16)-C(17)-C(18)	-0.6(9)
C(16)-C(17)-C(18)-C(19)	-1.1(9)
C(17)-C(18)-C(19)-C(20)	2.3(9)
C(18)-C(19)-C(20)-C(15)	-1.7(9)
C(16)-C(15)-C(20)-C(19)	0.0(9)
C(2)-C(15)-C(20)-C(19)	179.4(5)
C(3)-C(4)-C(21)-C(26)	-142.9(6)
C(5)-C(4)-C(21)-C(26)	39.8(8)
C(3)-C(4)-C(21)-C(22)	37.8(8)
C(5)-C(4)-C(21)-C(22)	-139.5(6)
C(26)-C(21)-C(22)-C(23)	-0.1(9)
C(4)-C(21)-C(22)-C(23)	179.2(5)
C(21)-C(22)-C(23)-C(24)	0.7(9)
C(22)-C(23)-C(24)-C(25)	-2.0(9)
C(23)-C(24)-C(25)-C(26)	2.8(9)
C(22)-C(21)-C(26)-C(25)	1.0(9)
C(4)-C(21)-C(26)-C(25)	-178.4(5)
C(24)-C(25)-C(26)-C(21)	-2.3(9)
C(2)-P(1)-P(1')-C(2')	-129.1(3)
C(6)-P(1)-P(1')-C(2')	-27.7(3)
P(1')#1-P(1)-P(1')-C(2')	-94.4(4)
C(2)-P(1)-P(1')-C(6')	127.6(3)
C(6)-P(1)-P(1')-C(6')	-131.0(3)
P(1')#1-P(1)-P(1')-C(6')	162.3(4)
C(2)-P(1)-P(1')-P(1)#2	145.3(4)
C(6)-P(1)-P(1')-P(1)#2	-113.3(4)
P(1')#1-P(1)-P(1')-P(1)#2	180.0

C(6')-P(1')-C(2')-C(3')	0.4(6)
P(1)-P(1')-C(2')-C(3')	-78.6(5)
P(1)#2-P(1')-C(2')-C(3')	91.3(5)
C(6')-P(1')-C(2')-C(15')	178.8(5)
P(1)-P(1')-C(2')-C(15')	99.8(5)
P(1)#2-P(1')-C(2')-C(15')	-90.3(4)
C(15')-C(2')-C(3')-C(4')	179.3(5)
P(1')-C(2')-C(3')-C(4')	-2.3(8)
C(2')-C(3')-C(4')-C(5')	2.7(9)
C(2')-C(3')-C(4')-C(21')	-174.9(5)
C(3')-C(4')-C(5')-C(6')	-1.0(9)
C(21')-C(4')-C(5')-C(6')	176.6(5)
C(4')-C(5')-C(6')-C(7')	179.8(5)
C(4')-C(5')-C(6')-P(1')	-0.9(8)
C(2')-P(1')-C(6')-C(5')	1.0(6)
P(1)-P(1')-C(6')-C(5')	77.8(5)
P(1)#2-P(1')-C(6')-C(5')	-99.2(5)
C(2')-P(1')-C(6')-C(7')	-179.6(5)
P(1)-P(1')-C(6')-C(7')	-102.9(4)
P(1)#2-P(1')-C(6')-C(7')	80.1(4)
C(5')-C(6')-C(7')-C(12')	135.1(6)
P(1')-C(6')-C(7')-C(12')	-44.3(7)
C(5')-C(6')-C(7')-C(8')	-43.2(8)
P(1')-C(6')-C(7')-C(8')	137.4(5)
C(12')-C(7')-C(8')-C(9')	-0.7(9)
C(6')-C(7')-C(8')-C(9')	177.6(5)
C(7')-C(8')-C(9')-O(1')	177.4(5)
C(7')-C(8')-C(9')-C(10')	-3.2(9)
C(8')-C(9')-C(10')-O(2')	-176.4(5)
O(1')-C(9')-C(10')-O(2')	3.1(8)
C(8')-C(9')-C(10')-C(11')	4.1(9)
O(1')-C(9')-C(10')-C(11')	-176.4(5)
O(2')-C(10')-C(11')-C(12')	179.3(6)
C(9')-C(10')-C(11')-C(12')	-1.3(9)
C(8')-C(7')-C(12')-C(11')	3.6(9)
C(6')-C(7')-C(12')-C(11')	-174.7(5)
C(10')-C(11')-C(12')-C(7')	-2.6(9)
C(8')-C(9')-O(1')-C(13')	-4.7(8)
C(10')-C(9')-O(1')-C(13')	175.8(5)
C(11')-C(10')-O(2')-C(14')	-12.2(9)
C(9')-C(10')-O(2')-C(14')	168.4(5)
C(3')-C(2')-C(15')-C(16')	-42.5(8)
P(1')-C(2')-C(15')-C(16')	139.0(5)
C(3')-C(2')-C(15')-C(20')	137.4(6)
P(1')-C(2')-C(15')-C(20')	-41.1(7)
C(20')-C(15')-C(16')-C(17')	-2.6(8)
C(2')-C(15')-C(16')-C(17')	177.3(5)
C(15')-C(16')-C(17')-C(18')	-0.3(9)
C(16')-C(17')-C(18')-C(19')	2.5(9)
C(17')-C(18')-C(19')-C(20')	-1.6(9)
C(18')-C(19')-C(20')-C(15')	-1.4(9)
C(16')-C(15')-C(20')-C(19')	3.4(8)
C(2')-C(15')-C(20')-C(19')	-176.5(6)
C(5')-C(4')-C(21')-C(26')	143.3(6)
C(3')-C(4')-C(21')-C(26')	-39.0(8)
C(5')-C(4')-C(21')-C(22')	-37.3(8)
C(3')-C(4')-C(21')-C(22')	140.4(6)
C(26')-C(21')-C(22')-C(23')	0.6(9)
C(4')-C(21')-C(22')-C(23')	-178.7(5)
C(21')-C(22')-C(23')-C(24')	-0.5(9)
C(22')-C(23')-C(24')-C(25')	0.3(9)
C(23')-C(24')-C(25')-C(26')	-0.2(9)
C(22')-C(21')-C(26')-C(25')	-0.5(8)
C(4')-C(21')-C(26')-C(25')	178.8(5)
C(24')-C(25')-C(26')-C(21')	0.3(9)

Symmetry transformations used to generate equivalent atoms:
#1 x-1,y,z #2 x+1,y,z

Table 5. Hydrogen bonds for dg010_hy [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(17)-H(17)...O(1)#3	0.95	2.53	3.266(8)	134.8
C(14)-H(14A)...O(2)#4	0.98	2.58	3.435(7)	145.9

Symmetry transformations used to generate equivalent atoms:
#1 x-1,y,z #2 x+1,y,z #3 -x,y+1/2,-z+1/2
#4 -x,-y,-z+1

Crystal data of 9c

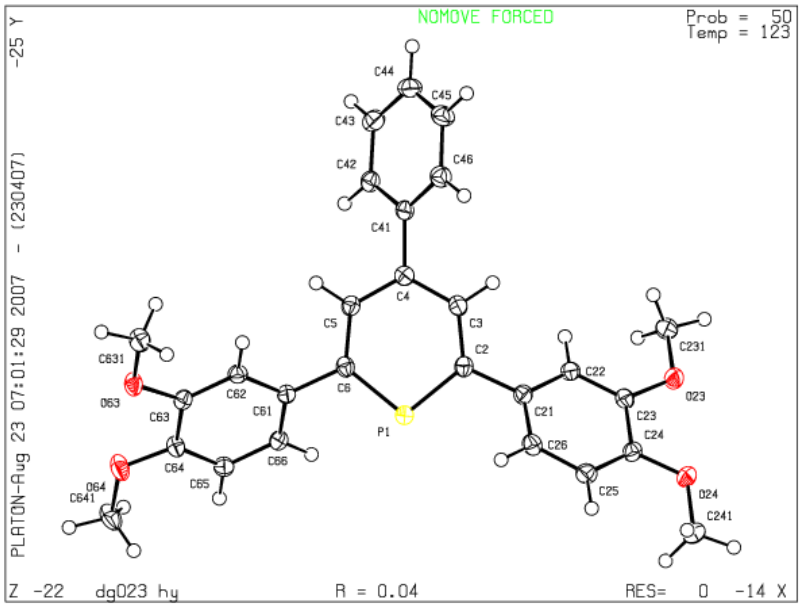

Table 1. Crystal data and structure refinement for dg023_hy.

Identification code	dg023_hy
Empirical formula	C27 H25 O4 P
Formula weight	444.44
Temperature	123(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1 (no.2)
Unit cell dimensions	a = 10.4668(3) A alpha = 106.261(2) deg. b = 11.0141(3) A beta = 106.409(2) deg. c = 11.7927(3) A gamma = 110.307(2) deg.
Volume	1109.83(5) A^3
Z, Calculated density	2, 1.330 Mg/m^3
Absorption coefficient	0.156 mm^-1
F(000)	468
Crystal size	0.30 x 0.20 x 0.10 mm
Theta range for data collection	3.01 to 27.47 deg.

Limiting indices	-13<=h<=13, -14<=k<=14, -15<=l<=15
Reflections collected / unique	17539 / 5036 [R(int) = 0.0265]
Completeness to theta = 25.00	99.0 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5036 / 0 / 293
Goodness-of-fit on F^2	1.043
Final R indices [I>2sigma(I)]	R1 = 0.0355, wR2 = 0.0840
R indices (all data)	R1 = 0.0421, wR2 = 0.0890
Largest diff. peak and hole	0.308 and -0.274 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic

displacement parameters (A^2 x 10^3) for dg023_hy.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
P(1)	8351(1)	2956(1)	2770(1)	21(1)
C(2)	10306(1)	3914(1)	3388(1)	20(1)
C(3)	11032(1)	5104(1)	3186(1)	21(1)
C(4)	10301(1)	5680(1)	2473(1)	20(1)
C(5)	8731(1)	5083(1)	1884(1)	20(1)
C(6)	7758(1)	3882(1)	1936(1)	20(1)
C(21)	11180(1)	3341(1)	4111(1)	20(1)
C(22)	12441(1)	3301(1)	3926(1)	20(1)
C(23)	13217(1)	2706(1)	4547(1)	20(1)
C(24)	12703(1)	2079(1)	5330(1)	20(1)
C(25)	11489(2)	2149(1)	5538(1)	23(1)
C(26)	10741(2)	2788(1)	4937(1)	22(1)
O(23)	14483(1)	2667(1)	4475(1)	25(1)
C(231)	14948(2)	3149(2)	3587(1)	26(1)
O(24)	13493(1)	1449(1)	5834(1)	24(1)
C(241)	12912(2)	680(2)	6514(2)	32(1)
C(41)	11222(1)	6932(1)	2299(1)	20(1)
C(42)	10802(2)	6967(1)	1075(1)	22(1)
C(43)	11714(2)	8088(2)	891(1)	27(1)
C(44)	13024(2)	9203(2)	1924(2)	28(1)
C(45)	13424(2)	9203(1)	3152(2)	28(1)
C(46)	12539(2)	8068(1)	3336(1)	24(1)
C(61)	6102(1)	3296(1)	1222(1)	19(1)
C(62)	5422(1)	4197(1)	1319(1)	19(1)
C(63)	3882(1)	3645(1)	653(1)	19(1)
C(64)	2981(1)	2165(1)	-139(1)	21(1)
C(65)	3651(1)	1277(1)	-227(1)	21(1)
C(66)	5206(1)	1846(1)	452(1)	20(1)
O(63)	3112(1)	4424(1)	701(1)	25(1)
C(631)	3961(2)	5906(1)	1568(1)	26(1)
O(64)	1487(1)	1737(1)	-783(1)	30(1)
C(641)	516(2)	241(2)	-1538(2)	32(1)

Table 3. Bond lengths [A] and angles [deg] for dg023_hy.

P(1)-C(6)	1.7461(13)
P(1)-C(2)	1.7500(13)
C(2)-C(3)	1.3920(18)
C(2)-C(21)	1.4911(17)
C(3)-C(4)	1.4017(17)
C(4)-C(5)	1.4017(17)
C(4)-C(41)	1.4902(17)
C(5)-C(6)	1.3917(18)
C(6)-C(61)	1.4912(17)
C(21)-C(26)	1.3866(18)
C(21)-C(22)	1.4098(18)
C(22)-C(23)	1.3880(17)
C(23)-O(23)	1.3661(15)
C(23)-C(24)	1.4139(18)
C(24)-O(24)	1.3669(15)
C(24)-C(25)	1.3842(18)
C(25)-C(26)	1.3997(18)
O(23)-C(231)	1.4270(16)
O(24)-C(241)	1.4244(16)
C(41)-C(46)	1.3979(18)
C(41)-C(42)	1.4005(18)
C(42)-C(43)	1.3908(19)
C(43)-C(44)	1.386(2)
C(44)-C(45)	1.389(2)
C(45)-C(46)	1.3886(19)
C(61)-C(66)	1.3867(17)
C(61)-C(62)	1.4063(17)
C(62)-C(63)	1.3861(17)
C(63)-O(63)	1.3656(15)
C(63)-C(64)	1.4150(17)
C(64)-O(64)	1.3642(15)
C(64)-C(65)	1.3854(17)
C(65)-C(66)	1.3995(18)
O(63)-C(631)	1.4302(16)
O(64)-C(641)	1.4303(16)

C(6)-P(1)-C(2)	101.88(6)
C(3)-C(2)-C(21)	120.78(11)
C(3)-C(2)-P(1)	123.34(10)
C(21)-C(2)-P(1)	115.83(9)
C(2)-C(3)-C(4)	124.72(12)
C(5)-C(4)-C(3)	121.92(12)
C(5)-C(4)-C(41)	119.12(11)
C(3)-C(4)-C(41)	118.93(11)
C(6)-C(5)-C(4)	124.24(12)
C(5)-C(6)-C(61)	119.78(11)
C(5)-C(6)-P(1)	123.89(10)
C(61)-C(6)-P(1)	116.31(9)
C(26)-C(21)-C(22)	118.65(12)
C(26)-C(21)-C(2)	120.94(12)
C(22)-C(21)-C(2)	120.37(11)
C(23)-C(22)-C(21)	120.72(12)
O(23)-C(23)-C(22)	125.24(12)
O(23)-C(23)-C(24)	114.98(11)
C(22)-C(23)-C(24)	119.78(12)
O(24)-C(24)-C(25)	125.42(12)
O(24)-C(24)-C(23)	115.11(11)
C(25)-C(24)-C(23)	119.47(12)
C(24)-C(25)-C(26)	120.17(12)
C(21)-C(26)-C(25)	121.07(12)
C(23)-O(23)-C(231)	116.75(10)
C(24)-O(24)-C(241)	116.47(11)
C(46)-C(41)-C(42)	118.80(12)
C(46)-C(41)-C(4)	120.98(12)
C(42)-C(41)-C(4)	120.20(12)
C(43)-C(42)-C(41)	120.22(13)
C(44)-C(43)-C(42)	120.41(13)
C(43)-C(44)-C(45)	119.78(13)
C(46)-C(45)-C(44)	120.12(13)
C(45)-C(46)-C(41)	120.61(13)
C(66)-C(61)-C(62)	118.89(11)
C(66)-C(61)-C(6)	120.23(11)
C(62)-C(61)-C(6)	120.88(11)
C(63)-C(62)-C(61)	120.58(11)

O(63)-C(63)-C(62)	125.08(11)
O(63)-C(63)-C(64)	114.92(11)
C(62)-C(63)-C(64)	120.00(11)
O(64)-C(64)-C(65)	125.20(12)
O(64)-C(64)-C(63)	115.40(11)
C(65)-C(64)-C(63)	119.39(11)
C(64)-C(65)-C(66)	120.09(12)
C(61)-C(66)-C(65)	121.04(11)
C(63)-O(63)-C(631)	116.82(10)
C(64)-O(64)-C(641)	117.57(10)

Table 4. Torsion angles [deg] for dg023_hy.

C(6)-P(1)-C(2)-C(3)	0.54(12)
C(6)-P(1)-C(2)-C(21)	-176.81(9)
C(21)-C(2)-C(3)-C(4)	177.23(12)
P(1)-C(2)-C(3)-C(4)	0.00(19)
C(2)-C(3)-C(4)-C(5)	-0.2(2)
C(2)-C(3)-C(4)-C(41)	-178.02(12)
C(3)-C(4)-C(5)-C(6)	-0.4(2)
C(41)-C(4)-C(5)-C(6)	177.40(12)
C(4)-C(5)-C(6)-C(61)	-177.15(12)
C(4)-C(5)-C(6)-P(1)	1.17(19)
C(2)-P(1)-C(6)-C(5)	-1.10(12)
C(2)-P(1)-C(6)-C(61)	177.27(9)
C(3)-C(2)-C(21)-C(26)	143.24(13)
P(1)-C(2)-C(21)-C(26)	-39.34(16)
C(3)-C(2)-C(21)-C(22)	-39.20(18)
P(1)-C(2)-C(21)-C(22)	138.23(11)
C(26)-C(21)-C(22)-C(23)	0.77(19)
C(2)-C(21)-C(22)-C(23)	-176.86(12)
C(21)-C(22)-C(23)-O(23)	-177.21(12)
C(21)-C(22)-C(23)-C(24)	2.68(19)
O(23)-C(23)-C(24)-O(24)	-3.83(16)
C(22)-C(23)-C(24)-O(24)	176.28(11)
O(23)-C(23)-C(24)-C(25)	175.63(12)
C(22)-C(23)-C(24)-C(25)	-4.27(19)
O(24)-C(24)-C(25)-C(26)	-178.18(12)
C(23)-C(24)-C(25)-C(26)	2.42(19)
C(22)-C(21)-C(26)-C(25)	-2.66(19)
C(2)-C(21)-C(26)-C(25)	174.95(12)
C(24)-C(25)-C(26)-C(21)	1.1(2)
C(22)-C(23)-O(23)-C(231)	-6.64(18)
C(24)-C(23)-O(23)-C(231)	173.47(11)
C(25)-C(24)-O(24)-C(241)	6.87(19)
C(23)-C(24)-O(24)-C(241)	-173.71(12)
C(5)-C(4)-C(41)-C(46)	139.26(13)
C(3)-C(4)-C(41)-C(46)	-42.83(17)
C(5)-C(4)-C(41)-C(42)	-42.85(17)
C(3)-C(4)-C(41)-C(42)	135.06(13)
C(46)-C(41)-C(42)-C(43)	2.36(19)
C(4)-C(41)-C(42)-C(43)	-175.57(12)
C(41)-C(42)-C(43)-C(44)	-1.9(2)
C(42)-C(43)-C(44)-C(45)	-0.3(2)
C(43)-C(44)-C(45)-C(46)	1.9(2)
C(44)-C(45)-C(46)-C(41)	-1.5(2)
C(42)-C(41)-C(46)-C(45)	-0.69(19)
C(4)-C(41)-C(46)-C(45)	177.23(12)
C(5)-C(6)-C(61)-C(66)	132.67(13)
P(1)-C(6)-C(61)-C(66)	-45.77(15)
C(5)-C(6)-C(61)-C(62)	-47.55(17)
P(1)-C(6)-C(61)-C(62)	134.01(11)
C(66)-C(61)-C(62)-C(63)	-0.12(19)
C(6)-C(61)-C(62)-C(63)	-179.90(11)
C(61)-C(62)-C(63)-O(63)	178.81(12)
C(61)-C(62)-C(63)-C(64)	-0.47(19)
O(63)-C(63)-C(64)-O(64)	2.60(17)
C(62)-C(63)-C(64)-O(64)	-178.05(12)
O(63)-C(63)-C(64)-C(65)	-178.43(12)
C(62)-C(63)-C(64)-C(65)	0.91(19)
O(64)-C(64)-C(65)-C(66)	178.08(12)
C(63)-C(64)-C(65)-C(66)	-0.8(2)
C(62)-C(61)-C(66)-C(65)	0.26(19)
C(6)-C(61)-C(66)-C(65)	-179.95(12)
C(64)-C(65)-C(66)-C(61)	0.2(2)
C(62)-C(63)-O(63)-C(631)	-3.98(19)
C(64)-C(63)-O(63)-C(631)	175.33(11)
C(65)-C(64)-O(64)-C(641)	4.6(2)
C(63)-C(64)-O(64)-C(641)	-176.49(12)

Table 7. Hydrogen bonds for dg023_hy [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(631)-H(63A)...O(24)#1	0.98	2.61	3.1585(17)	115.8
C(5)-H(5)...O(63)#2	0.95	2.55	3.4124(16)	151.4

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y+1,-z+1 #2 -x+1,-y+1,-z

Crystal data of 11a

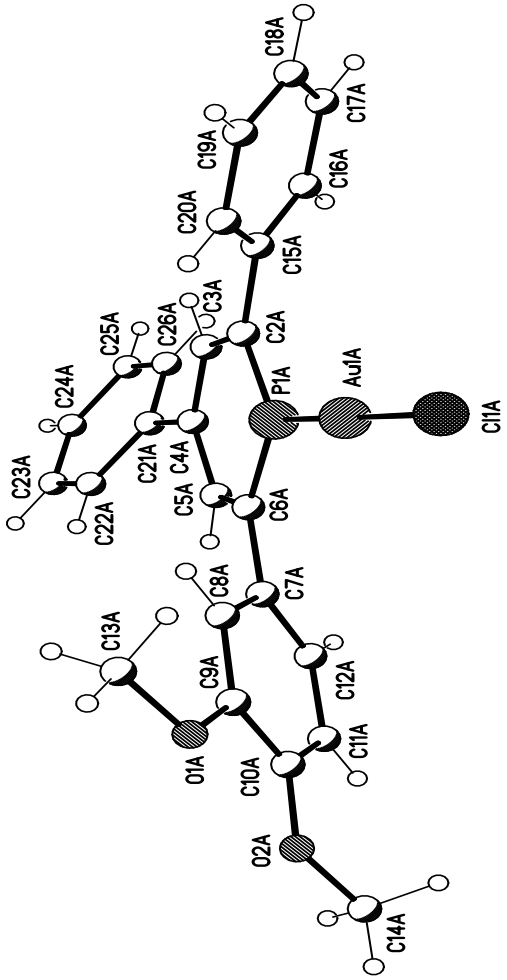

Table 1. Crystal data and structure refinement for dg039_hy.

Identification code	dg039_hy
Empirical formula	C25 H21 Au Cl O2 P
Formula weight	616.80

Temperature	123(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1 (No.2)
Unit cell dimensions	a = 11.376(1) A alpha = 101.68(1) deg. b = 14.232(2) A beta = 98.86(1) deg. c = 21.024(2) A gamma = 92.83(1) deg.
Volume	3282.2(6) A^3
Z, Calculated density	6, 1.872 Mg/m^3
Absorption coefficient	6.938 mm^-1
F(000)	1788
Crystal size	0.30 x 0.20 x 0.15 mm
Theta range for data collection	3.18 to 27.48 deg.
Limiting indices	-14<=h<=14, -18<=k<=18, -27<=l<=27
Reflections collected / unique	63463 / 14992 [R(int) = 0.0352]
Completeness to theta = 25.00	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.4305 and 0.2368
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	14992 / 0 / 817
Goodness-of-fit on F^2	1.069
Final R indices [I>2sigma(I)]	R1 = 0.0229, wR2 = 0.0431
R indices (all data)	R1 = 0.0331, wR2 = 0.0456
Largest diff. peak and hole	0.777 and -1.230 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for dg039_hy.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cl(1A)	2577(1)	5948(1)	3616(1)	24(1)
Au(1A)	2816(1)	4348(1)	3322(1)	14(1)
P(1A)	2922(1)	2777(1)	3057(1)	14(1)
C(2A)	3327(3)	2036(2)	3592(1)	13(1)
C(3A)	3334(3)	1054(2)	3354(2)	15(1)
C(4A)	2995(3)	572(2)	2696(2)	14(1)
C(5A)	2598(3)	1066(2)	2200(1)	14(1)
C(6A)	2566(3)	2061(2)	2283(1)	12(1)
C(7A)	2237(3)	2517(2)	1711(1)	14(1)
C(8A)	2906(3)	3347(2)	1669(1)	15(1)
C(9A)	2629(3)	3781(2)	1136(2)	16(1)
C(10A)	1655(3)	3400(2)	641(2)	17(1)
C(11A)	1003(3)	2573(2)	679(2)	17(1)
C(12A)	1298(3)	2131(2)	1208(2)	16(1)
O(1A)	3260(2)	4571(2)	1045(1)	24(1)
C(13A)	4327(3)	4919(3)	1503(2)	29(1)
O(2A)	1448(2)	3891(2)	152(1)	23(1)
C(14A)	369(3)	3609(3)	-316(2)	27(1)
C(15A)	3690(3)	2475(2)	4305(1)	15(1)
C(16A)	3268(3)	2033(2)	4771(2)	20(1)
C(17A)	3577(3)	2451(3)	5441(2)	26(1)
C(18A)	4307(3)	3295(3)	5642(2)	26(1)
C(19A)	4740(3)	3730(2)	5187(2)	22(1)
C(20A)	4430(3)	3322(2)	4518(2)	18(1)
C(21A)	3123(3)	-476(2)	2508(2)	14(1)
C(22A)	3409(3)	-885(2)	1896(2)	17(1)
C(23A)	3551(3)	-1860(2)	1723(2)	20(1)
C(24A)	3413(3)	-2444(2)	2160(2)	24(1)
C(25A)	3127(3)	-2055(2)	2770(2)	26(1)
C(26A)	2990(3)	-1083(2)	2945(2)	21(1)
Cl(1B)	5648(1)	4299(1)	3009(1)	24(1)
Au(1B)	5830(1)	2687(1)	2772(1)	14(1)
P(1B)	6087(1)	1135(1)	2584(1)	13(1)
C(2B)	6483(3)	491(2)	3180(1)	12(1)
C(3B)	6722(3)	-461(2)	2991(2)	15(1)
C(4B)	6705(3)	-972(2)	2346(2)	14(1)
C(5B)	6426(3)	-552(2)	1802(1)	13(1)
C(6B)	6109(3)	383(2)	1831(1)	13(1)
C(7B)	5759(3)	779(2)	1234(1)	13(1)
C(8B)	6437(3)	652(2)	723(1)	14(1)
C(9B)	6155(3)	1092(2)	196(1)	14(1)
C(10B)	5168(3)	1657(2)	165(1)	14(1)
C(11B)	4482(3)	1750(2)	653(2)	16(1)
C(12B)	4780(3)	1322(2)	1188(2)	16(1)
O(1B)	6803(2)	1067(2)	-302(1)	21(1)
C(13B)	7890(3)	603(3)	-245(2)	28(1)
O(2B)	4991(2)	2089(2)	-360(1)	20(1)
C(14B)	4106(3)	2777(3)	-348(2)	27(1)
C(15B)	6564(3)	938(2)	3891(1)	15(1)
C(16B)	7052(3)	1879(2)	4152(2)	18(1)
C(17B)	7140(3)	2271(2)	4821(2)	22(1)
C(18B)	6772(3)	1723(3)	5236(2)	26(1)
C(19B)	6297(3)	786(3)	4984(2)	25(1)
C(20B)	6178(3)	393(2)	4315(2)	19(1)
C(21B)	6975(3)	-1996(2)	2266(1)	15(1)
C(22B)	7729(3)	-2389(2)	1837(2)	20(1)
C(23B)	7990(3)	-3342(3)	1786(2)	28(1)
C(24B)	7515(3)	-3905(3)	2165(2)	30(1)
C(25B)	6775(3)	-3517(2)	2596(2)	26(1)
C(26B)	6499(3)	-2574(2)	2642(2)	20(1)
Cl(1C)	9262(1)	-720(1)	939(1)	24(1)
Au(1C)	9329(1)	415(1)	1882(1)	15(1)
P(1C)	9530(1)	1506(1)	2813(1)	15(1)
C(2C)	9884(3)	1262(2)	3587(2)	16(1)
C(3C)	10183(3)	2011(2)	4131(2)	16(1)
C(4C)	10283(3)	2987(2)	4123(2)	16(1)

C(5C)	10011(3)	3321(2)	3538(2)	14(1)
C(6C)	9627(3)	2742(2)	2914(2)	13(1)
C(7C)	9262(3)	3157(2)	2325(1)	13(1)
C(8C)	9884(3)	3978(2)	2233(1)	14(1)
C(9C)	9542(3)	4347(2)	1679(2)	13(1)
C(10C)	8545(3)	3915(2)	1211(2)	15(1)
C(11C)	7922(3)	3112(2)	1302(2)	17(1)
C(12C)	8288(3)	2729(2)	1854(2)	17(1)
O(1C)	10100(2)	5125(2)	1534(1)	18(1)
C(13C)	11027(3)	5661(2)	2020(2)	25(1)
O(2C)	8279(2)	4363(2)	697(1)	20(1)
C(14C)	7232(3)	3991(3)	227(2)	34(1)
C(15C)	9783(3)	249(2)	3664(2)	18(1)
C(16C)	10153(3)	-502(2)	3226(2)	27(1)
C(17C)	9956(4)	-1447(3)	3284(2)	35(1)
C(18C)	9399(4)	-1653(3)	3782(2)	41(1)
C(19C)	9059(3)	-915(3)	4236(2)	32(1)
C(20C)	9248(3)	37(2)	4180(2)	22(1)
C(21C)	10691(3)	3673(2)	4766(2)	16(1)
C(22C)	10258(3)	3536(2)	5330(2)	20(1)
C(23C)	10696(3)	4117(2)	5937(2)	23(1)
C(24C)	11590(3)	4839(2)	5998(2)	22(1)
C(25C)	12008(3)	4994(2)	5443(2)	24(1)
C(26C)	11550(3)	4426(2)	4828(2)	21(1)

Table 3. Bond lengths [A] and angles [deg] for dg039_hy.

Cl(1A)-Au(1A)	2.2766(8)
Au(1A)-P(1A)	2.2060(8)
P(1A)-C(6A)	1.715(3)
P(1A)-C(2A)	1.721(3)
C(2A)-C(3A)	1.386(4)
C(2A)-C(15A)	1.487(4)
C(3A)-C(4A)	1.399(4)
C(4A)-C(5A)	1.402(4)
C(4A)-C(21A)	1.484(4)
C(5A)-C(6A)	1.394(4)
C(6A)-C(7A)	1.486(4)
C(7A)-C(12A)	1.385(4)
C(7A)-C(8A)	1.399(4)
C(8A)-C(9A)	1.388(4)
C(9A)-O(1A)	1.367(4)
C(9A)-C(10A)	1.401(4)
C(10A)-O(2A)	1.354(3)
C(10A)-C(11A)	1.383(4)
C(11A)-C(12A)	1.391(4)
O(1A)-C(13A)	1.425(4)
O(2A)-C(14A)	1.434(4)
C(15A)-C(20A)	1.388(5)
C(15A)-C(16A)	1.396(4)
C(16A)-C(17A)	1.396(4)
C(17A)-C(18A)	1.378(5)
C(18A)-C(19A)	1.377(5)
C(19A)-C(20A)	1.392(4)
C(21A)-C(22A)	1.395(4)
C(21A)-C(26A)	1.400(4)
C(22A)-C(23A)	1.386(4)
C(23A)-C(24A)	1.378(5)
C(24A)-C(25A)	1.383(5)
C(25A)-C(26A)	1.381(4)
Cl(1B)-Au(1B)	2.2725(8)
Au(1B)-P(1B)	2.2065(8)
P(1B)-C(2B)	1.716(3)
P(1B)-C(6B)	1.727(3)
C(2B)-C(3B)	1.386(4)
C(2B)-C(15B)	1.488(4)
C(3B)-C(4B)	1.399(4)
C(4B)-C(5B)	1.397(4)
C(4B)-C(21B)	1.485(4)
C(5B)-C(6B)	1.389(4)
C(6B)-C(7B)	1.485(4)
C(7B)-C(12B)	1.389(4)
C(7B)-C(8B)	1.403(4)
C(8B)-C(9B)	1.384(4)
C(9B)-O(1B)	1.365(4)
C(9B)-C(10B)	1.414(4)
C(10B)-O(2B)	1.363(3)
C(10B)-C(11B)	1.370(4)
C(11B)-C(12B)	1.389(4)
O(1B)-C(13B)	1.431(4)
O(2B)-C(14B)	1.438(4)
C(15B)-C(16B)	1.392(4)
C(15B)-C(20B)	1.398(4)
C(16B)-C(17B)	1.390(4)
C(17B)-C(18B)	1.378(5)
C(18B)-C(19B)	1.380(5)
C(19B)-C(20B)	1.388(4)
C(21B)-C(22B)	1.394(4)
C(21B)-C(26B)	1.395(4)
C(22B)-C(23B)	1.389(4)
C(23B)-C(24B)	1.385(5)
C(24B)-C(25B)	1.384(5)
C(25B)-C(26B)	1.382(4)
Cl(1C)-Au(1C)	2.2780(8)
Au(1C)-P(1C)	2.2116(9)
P(1C)-C(2C)	1.724(3)
P(1C)-C(6C)	1.725(3)
C(2C)-C(3C)	1.382(4)
C(2C)-C(15C)	1.484(4)
C(3C)-C(4C)	1.392(4)
C(4C)-C(5C)	1.402(4)

C(4C)-C(21C)	1.492(4)
C(5C)-C(6C)	1.393(4)
C(6C)-C(7C)	1.488(4)
C(7C)-C(12C)	1.389(4)
C(7C)-C(8C)	1.397(4)
C(8C)-C(9C)	1.382(4)
C(9C)-O(1C)	1.361(4)
C(9C)-C(10C)	1.405(4)
C(10C)-O(2C)	1.364(3)
C(10C)-C(11C)	1.377(4)
C(11C)-C(12C)	1.395(4)
O(1C)-C(13C)	1.419(4)
O(2C)-C(14C)	1.428(4)
C(15C)-C(16C)	1.390(5)
C(15C)-C(20C)	1.399(5)
C(16C)-C(17C)	1.385(5)
C(17C)-C(18C)	1.376(6)
C(18C)-C(19C)	1.383(6)
C(19C)-C(20C)	1.392(5)
C(21C)-C(26C)	1.386(5)
C(21C)-C(22C)	1.396(4)
C(22C)-C(23C)	1.377(5)
C(23C)-C(24C)	1.383(5)
C(24C)-C(25C)	1.380(5)
C(25C)-C(26C)	1.387(5)

P(1A)-Au(1A)-Cl(1A)	175.88(3)
C(6A)-P(1A)-C(2A)	107.13(15)
C(6A)-P(1A)-Au(1A)	126.39(10)
C(2A)-P(1A)-Au(1A)	126.45(11)
C(3A)-C(2A)-C(15A)	121.5(3)
C(3A)-C(2A)-P(1A)	120.0(2)
C(15A)-C(2A)-P(1A)	118.5(2)
C(2A)-C(3A)-C(4A)	125.8(3)
C(3A)-C(4A)-C(5A)	121.5(3)
C(3A)-C(4A)-C(21A)	119.6(3)
C(5A)-C(4A)-C(21A)	118.9(3)
C(6A)-C(5A)-C(4A)	125.8(3)
C(5A)-C(6A)-C(7A)	121.3(3)
C(5A)-C(6A)-P(1A)	119.6(2)
C(7A)-C(6A)-P(1A)	119.1(2)
C(12A)-C(7A)-C(8A)	118.8(3)
C(12A)-C(7A)-C(6A)	121.8(3)
C(8A)-C(7A)-C(6A)	119.4(3)
C(9A)-C(8A)-C(7A)	120.6(3)
O(1A)-C(9A)-C(8A)	124.4(3)
O(1A)-C(9A)-C(10A)	115.6(3)
C(8A)-C(9A)-C(10A)	120.0(3)
O(2A)-C(10A)-C(11A)	125.6(3)
O(2A)-C(10A)-C(9A)	115.2(3)
C(11A)-C(10A)-C(9A)	119.3(3)
C(10A)-C(11A)-C(12A)	120.5(3)
C(7A)-C(12A)-C(11A)	120.8(3)
C(9A)-O(1A)-C(13A)	117.2(3)
C(10A)-O(2A)-C(14A)	117.1(3)
C(20A)-C(15A)-C(16A)	119.2(3)
C(20A)-C(15A)-C(2A)	121.4(3)
C(16A)-C(15A)-C(2A)	119.4(3)
C(15A)-C(16A)-C(17A)	120.0(3)
C(18A)-C(17A)-C(16A)	120.0(3)
C(19A)-C(18A)-C(17A)	120.5(3)
C(18A)-C(19A)-C(20A)	119.9(3)
C(15A)-C(20A)-C(19A)	120.4(3)
C(22A)-C(21A)-C(26A)	117.8(3)
C(22A)-C(21A)-C(4A)	120.9(3)
C(26A)-C(21A)-C(4A)	121.3(3)
C(23A)-C(22A)-C(21A)	121.2(3)
C(24A)-C(23A)-C(22A)	120.0(3)
C(23A)-C(24A)-C(25A)	119.8(3)
C(26A)-C(25A)-C(24A)	120.3(3)
C(25A)-C(26A)-C(21A)	120.9(3)
P(1B)-Au(1B)-Cl(1B)	177.01(3)
C(2B)-P(1B)-C(6B)	107.37(14)
C(2B)-P(1B)-Au(1B)	125.20(10)
C(6B)-P(1B)-Au(1B)	127.01(11)
C(3B)-C(2B)-C(15B)	120.0(3)
C(3B)-C(2B)-P(1B)	119.0(2)
C(15B)-C(2B)-P(1B)	121.0(2)

C(2B)-C(3B)-C(4B)	126.5(3)
C(5B)-C(4B)-C(3B)	122.0(3)
C(5B)-C(4B)-C(21B)	121.4(3)
C(3B)-C(4B)-C(21B)	116.6(3)
C(6B)-C(5B)-C(4B)	125.0(3)
C(5B)-C(6B)-C(7B)	122.9(3)
C(5B)-C(6B)-P(1B)	120.0(2)
C(7B)-C(6B)-P(1B)	117.1(2)
C(12B)-C(7B)-C(8B)	118.9(3)
C(12B)-C(7B)-C(6B)	120.0(3)
C(8B)-C(7B)-C(6B)	121.0(3)
C(9B)-C(8B)-C(7B)	120.2(3)
O(1B)-C(9B)-C(8B)	124.7(3)
O(1B)-C(9B)-C(10B)	115.3(3)
C(8B)-C(9B)-C(10B)	119.9(3)
O(2B)-C(10B)-C(11B)	124.8(3)
O(2B)-C(10B)-C(9B)	115.4(3)
C(11B)-C(10B)-C(9B)	119.7(3)
C(10B)-C(11B)-C(12B)	120.3(3)
C(7B)-C(12B)-C(11B)	121.0(3)
C(9B)-O(1B)-C(13B)	116.9(2)
C(10B)-O(2B)-C(14B)	116.1(2)
C(16B)-C(15B)-C(20B)	118.8(3)
C(16B)-C(15B)-C(2B)	121.8(3)
C(20B)-C(15B)-C(2B)	119.4(3)
C(17B)-C(16B)-C(15B)	120.5(3)
C(18B)-C(17B)-C(16B)	120.3(3)
C(17B)-C(18B)-C(19B)	119.8(3)
C(18B)-C(19B)-C(20B)	120.6(3)
C(19B)-C(20B)-C(15B)	120.1(3)
C(22B)-C(21B)-C(26B)	118.8(3)
C(22B)-C(21B)-C(4B)	121.5(3)
C(26B)-C(21B)-C(4B)	119.7(3)
C(23B)-C(22B)-C(21B)	120.1(3)
C(24B)-C(23B)-C(22B)	120.4(3)
C(25B)-C(24B)-C(23B)	119.8(3)
C(26B)-C(25B)-C(24B)	120.0(3)
C(25B)-C(26B)-C(21B)	120.9(3)
P(1C)-Au(1C)-Cl(1C)	175.97(3)
C(2C)-P(1C)-C(6C)	106.84(15)
C(2C)-P(1C)-Au(1C)	124.50(11)
C(6C)-P(1C)-Au(1C)	127.78(11)
C(3C)-C(2C)-C(15C)	120.8(3)
C(3C)-C(2C)-P(1C)	119.8(2)
C(15C)-C(2C)-P(1C)	119.2(2)
C(2C)-C(3C)-C(4C)	126.1(3)
C(3C)-C(4C)-C(5C)	121.9(3)
C(3C)-C(4C)-C(21C)	117.2(3)
C(5C)-C(4C)-C(21C)	120.9(3)
C(6C)-C(5C)-C(4C)	125.4(3)
C(5C)-C(6C)-C(7C)	122.0(3)
C(5C)-C(6C)-P(1C)	119.7(2)
C(7C)-C(6C)-P(1C)	118.2(2)
C(12C)-C(7C)-C(8C)	118.8(3)
C(12C)-C(7C)-C(6C)	120.0(3)
C(8C)-C(7C)-C(6C)	121.2(3)
C(9C)-C(8C)-C(7C)	120.4(3)
O(1C)-C(9C)-C(8C)	125.2(3)
O(1C)-C(9C)-C(10C)	114.4(3)
C(8C)-C(9C)-C(10C)	120.3(3)
O(2C)-C(10C)-C(11C)	125.8(3)
O(2C)-C(10C)-C(9C)	114.7(3)
C(11C)-C(10C)-C(9C)	119.5(3)
C(10C)-C(11C)-C(12C)	119.9(3)
C(7C)-C(12C)-C(11C)	121.0(3)
C(9C)-O(1C)-C(13C)	117.4(2)
C(10C)-O(2C)-C(14C)	117.1(3)
C(16C)-C(15C)-C(20C)	118.8(3)
C(16C)-C(15C)-C(2C)	122.4(3)
C(20C)-C(15C)-C(2C)	118.7(3)
C(17C)-C(16C)-C(15C)	120.7(4)
C(18C)-C(17C)-C(16C)	120.2(4)
C(17C)-C(18C)-C(19C)	120.1(4)
C(18C)-C(19C)-C(20C)	120.1(4)
C(19C)-C(20C)-C(15C)	120.0(3)
C(26C)-C(21C)-C(22C)	118.4(3)
C(26C)-C(21C)-C(4C)	121.2(3)
C(22C)-C(21C)-C(4C)	120.3(3)

C(23C)-C(22C)-C(21C)	121.0(3)
C(22C)-C(23C)-C(24C)	120.2(3)
C(25C)-C(24C)-C(23C)	119.3(3)
C(24C)-C(25C)-C(26C)	120.7(3)
C(21C)-C(26C)-C(25C)	120.3(3)

Table 4. Torsion angles [deg] for dg039_hy.

Cl(1A)-Au(1A)-P(1A)-C(6A)	96.9(4)
Cl(1A)-Au(1A)-P(1A)-C(2A)	-80.7(4)
C(6A)-P(1A)-C(2A)-C(3A)	1.0(3)
Au(1A)-P(1A)-C(2A)-C(3A)	178.93(19)
C(6A)-P(1A)-C(2A)-C(15A)	179.7(2)
Au(1A)-P(1A)-C(2A)-C(15A)	-2.4(3)
C(15A)-C(2A)-C(3A)-C(4A)	179.1(3)
P(1A)-C(2A)-C(3A)-C(4A)	-2.2(4)
C(2A)-C(3A)-C(4A)-C(5A)	-0.3(5)
C(2A)-C(3A)-C(4A)-C(21A)	176.2(3)
C(3A)-C(4A)-C(5A)-C(6A)	4.5(5)
C(21A)-C(4A)-C(5A)-C(6A)	-171.9(3)
C(4A)-C(5A)-C(6A)-C(7A)	174.0(3)
C(4A)-C(5A)-C(6A)-P(1A)	-5.5(4)
C(2A)-P(1A)-C(6A)-C(5A)	2.6(3)
Au(1A)-P(1A)-C(6A)-C(5A)	-175.40(19)
C(2A)-P(1A)-C(6A)-C(7A)	-177.0(2)
Au(1A)-P(1A)-C(6A)-C(7A)	5.1(3)
C(5A)-C(6A)-C(7A)-C(12A)	42.7(4)
P(1A)-C(6A)-C(7A)-C(12A)	-137.8(3)
C(5A)-C(6A)-C(7A)-C(8A)	-136.0(3)
P(1A)-C(6A)-C(7A)-C(8A)	43.5(3)
C(12A)-C(7A)-C(8A)-C(9A)	0.4(4)
C(6A)-C(7A)-C(8A)-C(9A)	179.2(3)
C(7A)-C(8A)-C(9A)-O(1A)	-177.5(3)
C(7A)-C(8A)-C(9A)-C(10A)	1.5(4)
O(1A)-C(9A)-C(10A)-O(2A)	-2.3(4)
C(8A)-C(9A)-C(10A)-O(2A)	178.7(3)
O(1A)-C(9A)-C(10A)-C(11A)	176.9(3)
C(8A)-C(9A)-C(10A)-C(11A)	-2.2(4)
O(2A)-C(10A)-C(11A)-C(12A)	-179.9(3)
C(9A)-C(10A)-C(11A)-C(12A)	1.0(4)
C(8A)-C(7A)-C(12A)-C(11A)	-1.6(4)
C(6A)-C(7A)-C(12A)-C(11A)	179.7(3)
C(10A)-C(11A)-C(12A)-C(7A)	0.9(4)
C(8A)-C(9A)-O(1A)-C(13A)	5.2(4)
C(10A)-C(9A)-O(1A)-C(13A)	-173.8(3)
C(11A)-C(10A)-O(2A)-C(14A)	9.3(4)
C(9A)-C(10A)-O(2A)-C(14A)	-171.6(3)
C(3A)-C(2A)-C(15A)-C(20A)	136.0(3)
P(1A)-C(2A)-C(15A)-C(20A)	-42.7(4)
C(3A)-C(2A)-C(15A)-C(16A)	-44.8(4)
P(1A)-C(2A)-C(15A)-C(16A)	136.5(3)
C(20A)-C(15A)-C(16A)-C(17A)	0.8(5)
C(2A)-C(15A)-C(16A)-C(17A)	-178.4(3)
C(15A)-C(16A)-C(17A)-C(18A)	-0.4(5)
C(16A)-C(17A)-C(18A)-C(19A)	-0.4(5)
C(17A)-C(18A)-C(19A)-C(20A)	0.8(5)
C(16A)-C(15A)-C(20A)-C(19A)	-0.4(4)
C(2A)-C(15A)-C(20A)-C(19A)	178.8(3)
C(18A)-C(19A)-C(20A)-C(15A)	-0.4(5)
C(3A)-C(4A)-C(21A)-C(22A)	-146.2(3)
C(5A)-C(4A)-C(21A)-C(22A)	30.3(4)
C(3A)-C(4A)-C(21A)-C(26A)	32.2(4)
C(5A)-C(4A)-C(21A)-C(26A)	-151.3(3)
C(26A)-C(21A)-C(22A)-C(23A)	0.3(5)
C(4A)-C(21A)-C(22A)-C(23A)	178.8(3)
C(21A)-C(22A)-C(23A)-C(24A)	-0.2(5)
C(22A)-C(23A)-C(24A)-C(25A)	0.3(5)
C(23A)-C(24A)-C(25A)-C(26A)	-0.6(5)
C(24A)-C(25A)-C(26A)-C(21A)	0.8(5)
C(22A)-C(21A)-C(26A)-C(25A)	-0.6(5)
C(4A)-C(21A)-C(26A)-C(25A)	-179.1(3)
Cl(1B)-Au(1B)-P(1B)-C(2B)	38.0(6)
Cl(1B)-Au(1B)-P(1B)-C(6B)	-133.5(6)
C(6B)-P(1B)-C(2B)-C(3B)	-1.1(3)
Au(1B)-P(1B)-C(2B)-C(3B)	-174.03(19)
C(6B)-P(1B)-C(2B)-C(15B)	179.3(2)
Au(1B)-P(1B)-C(2B)-C(15B)	6.3(3)
C(15B)-C(2B)-C(3B)-C(4B)	-178.7(3)
P(1B)-C(2B)-C(3B)-C(4B)	1.7(4)
C(2B)-C(3B)-C(4B)-C(5B)	-0.3(5)
C(2B)-C(3B)-C(4B)-C(21B)	-179.1(3)
C(3B)-C(4B)-C(5B)-C(6B)	-1.9(5)

C(21B)-C(4B)-C(5B)-C(6B)	176.8(3)
C(4B)-C(5B)-C(6B)-C(7B)	-176.8(3)
C(4B)-C(5B)-C(6B)-P(1B)	2.2(4)
C(2B)-P(1B)-C(6B)-C(5B)	-0.7(3)
Au(1B)-P(1B)-C(6B)-C(5B)	172.06(19)
C(2B)-P(1B)-C(6B)-C(7B)	178.3(2)
Au(1B)-P(1B)-C(6B)-C(7B)	-8.9(3)
C(5B)-C(6B)-C(7B)-C(12B)	136.0(3)
P(1B)-C(6B)-C(7B)-C(12B)	-43.0(4)
C(5B)-C(6B)-C(7B)-C(8B)	-46.8(4)
P(1B)-C(6B)-C(7B)-C(8B)	134.1(3)
C(12B)-C(7B)-C(8B)-C(9B)	2.5(5)
C(6B)-C(7B)-C(8B)-C(9B)	-174.7(3)
C(7B)-C(8B)-C(9B)-O(1B)	175.3(3)
C(7B)-C(8B)-C(9B)-C(10B)	-1.2(5)
O(1B)-C(9B)-C(10B)-O(2B)	0.8(4)
C(8B)-C(9B)-C(10B)-O(2B)	177.6(3)
O(1B)-C(9B)-C(10B)-C(11B)	-178.1(3)
C(8B)-C(9B)-C(10B)-C(11B)	-1.2(5)
O(2B)-C(10B)-C(11B)-C(12B)	-176.4(3)
C(9B)-C(10B)-C(11B)-C(12B)	2.4(5)
C(8B)-C(7B)-C(12B)-C(11B)	-1.3(5)
C(6B)-C(7B)-C(12B)-C(11B)	175.9(3)
C(10B)-C(11B)-C(12B)-C(7B)	-1.1(5)
C(8B)-C(9B)-O(1B)-C(13B)	-4.2(5)
C(10B)-C(9B)-O(1B)-C(13B)	172.5(3)
C(11B)-C(10B)-O(2B)-C(14B)	7.7(5)
C(9B)-C(10B)-O(2B)-C(14B)	-171.1(3)
C(3B)-C(2B)-C(15B)-C(16B)	139.8(3)
P(1B)-C(2B)-C(15B)-C(16B)	-40.5(4)
C(3B)-C(2B)-C(15B)-C(20B)	-38.0(4)
P(1B)-C(2B)-C(15B)-C(20B)	141.7(3)
C(20B)-C(15B)-C(16B)-C(17B)	-0.8(4)
C(2B)-C(15B)-C(16B)-C(17B)	-178.6(3)
C(15B)-C(16B)-C(17B)-C(18B)	1.7(5)
C(16B)-C(17B)-C(18B)-C(19B)	-1.0(5)
C(17B)-C(18B)-C(19B)-C(20B)	-0.5(5)
C(18B)-C(19B)-C(20B)-C(15B)	1.4(5)
C(16B)-C(15B)-C(20B)-C(19B)	-0.7(5)
C(2B)-C(15B)-C(20B)-C(19B)	177.2(3)
C(5B)-C(4B)-C(21B)-C(22B)	44.9(4)
C(3B)-C(4B)-C(21B)-C(22B)	-136.4(3)
C(5B)-C(4B)-C(21B)-C(26B)	-137.2(3)
C(3B)-C(4B)-C(21B)-C(26B)	41.5(4)
C(26B)-C(21B)-C(22B)-C(23B)	0.4(5)
C(4B)-C(21B)-C(22B)-C(23B)	178.3(3)
C(21B)-C(22B)-C(23B)-C(24B)	-0.8(5)
C(22B)-C(23B)-C(24B)-C(25B)	0.2(6)
C(23B)-C(24B)-C(25B)-C(26B)	0.8(6)
C(24B)-C(25B)-C(26B)-C(21B)	-1.2(5)
C(22B)-C(21B)-C(26B)-C(25B)	0.6(5)
C(4B)-C(21B)-C(26B)-C(25B)	-177.4(3)
Cl(1C)-Au(1C)-P(1C)-C(2C)	-66.8(5)
Cl(1C)-Au(1C)-P(1C)-C(6C)	101.0(5)
C(6C)-P(1C)-C(2C)-C(3C)	-0.7(3)
Au(1C)-P(1C)-C(2C)-C(3C)	169.2(2)
C(6C)-P(1C)-C(2C)-C(15C)	175.2(2)
Au(1C)-P(1C)-C(2C)-C(15C)	-14.9(3)
C(15C)-C(2C)-C(3C)-C(4C)	-178.7(3)
P(1C)-C(2C)-C(3C)-C(4C)	-2.9(5)
C(2C)-C(3C)-C(4C)-C(5C)	3.9(5)
C(2C)-C(3C)-C(4C)-C(21C)	-176.3(3)
C(3C)-C(4C)-C(5C)-C(6C)	-0.3(5)
C(21C)-C(4C)-C(5C)-C(6C)	179.8(3)
C(4C)-C(5C)-C(6C)-C(7C)	175.0(3)
C(4C)-C(5C)-C(6C)-P(1C)	-3.4(4)
C(2C)-P(1C)-C(6C)-C(5C)	3.6(3)
Au(1C)-P(1C)-C(6C)-C(5C)	-165.92(19)
C(2C)-P(1C)-C(6C)-C(7C)	-174.8(2)
Au(1C)-P(1C)-C(6C)-C(7C)	15.6(3)
C(5C)-C(6C)-C(7C)-C(12C)	-140.4(3)
P(1C)-C(6C)-C(7C)-C(12C)	38.0(4)
C(5C)-C(6C)-C(7C)-C(8C)	39.5(4)
P(1C)-C(6C)-C(7C)-C(8C)	-142.1(2)
C(12C)-C(7C)-C(8C)-C(9C)	-0.9(4)
C(6C)-C(7C)-C(8C)-C(9C)	179.2(3)
C(7C)-C(8C)-C(9C)-O(1C)	-178.3(3)
C(7C)-C(8C)-C(9C)-C(10C)	1.7(4)

O(1C)-C(9C)-C(10C)-O(2C)	-1.8(4)
C(8C)-C(9C)-C(10C)-O(2C)	178.2(3)
O(1C)-C(9C)-C(10C)-C(11C)	179.0(3)
C(8C)-C(9C)-C(10C)-C(11C)	-1.1(4)
O(2C)-C(10C)-C(11C)-C(12C)	-179.6(3)
C(9C)-C(10C)-C(11C)-C(12C)	-0.4(4)
C(8C)-C(7C)-C(12C)-C(11C)	-0.6(4)
C(6C)-C(7C)-C(12C)-C(11C)	179.3(3)
C(10C)-C(11C)-C(12C)-C(7C)	1.3(4)
C(8C)-C(9C)-O(1C)-C(13C)	-7.0(4)
C(10C)-C(9C)-O(1C)-C(13C)	173.0(3)
C(11C)-C(10C)-O(2C)-C(14C)	3.0(4)
C(9C)-C(10C)-O(2C)-C(14C)	-176.2(3)
C(3C)-C(2C)-C(15C)-C(16C)	-142.5(3)
P(1C)-C(2C)-C(15C)-C(16C)	41.7(4)
C(3C)-C(2C)-C(15C)-C(20C)	40.4(4)
P(1C)-C(2C)-C(15C)-C(20C)	-135.5(3)
C(20C)-C(15C)-C(16C)-C(17C)	2.4(5)
C(2C)-C(15C)-C(16C)-C(17C)	-174.7(3)
C(15C)-C(16C)-C(17C)-C(18C)	-0.6(6)
C(16C)-C(17C)-C(18C)-C(19C)	-1.5(6)
C(17C)-C(18C)-C(19C)-C(20C)	1.8(6)
C(18C)-C(19C)-C(20C)-C(15C)	0.0(5)
C(16C)-C(15C)-C(20C)-C(19C)	-2.1(5)
C(2C)-C(15C)-C(20C)-C(19C)	175.2(3)
C(3C)-C(4C)-C(21C)-C(26C)	134.8(3)
C(5C)-C(4C)-C(21C)-C(26C)	-45.4(4)
C(3C)-C(4C)-C(21C)-C(22C)	-41.7(4)
C(5C)-C(4C)-C(21C)-C(22C)	138.1(3)
C(26C)-C(21C)-C(22C)-C(23C)	-1.8(5)
C(4C)-C(21C)-C(22C)-C(23C)	174.8(3)
C(21C)-C(22C)-C(23C)-C(24C)	-1.0(5)
C(22C)-C(23C)-C(24C)-C(25C)	2.3(5)
C(23C)-C(24C)-C(25C)-C(26C)	-0.7(5)
C(22C)-C(21C)-C(26C)-C(25C)	3.4(5)
C(4C)-C(21C)-C(26C)-C(25C)	-173.2(3)
C(24C)-C(25C)-C(26C)-C(21C)	-2.2(5)