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OM0306123: Polyazolyl Chelate Chemistry 13. An Osmaboratrane

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.CIF File	Compound **1b**

Figure S1. The molecular structure of **1b** (50% probability ellipsoids).

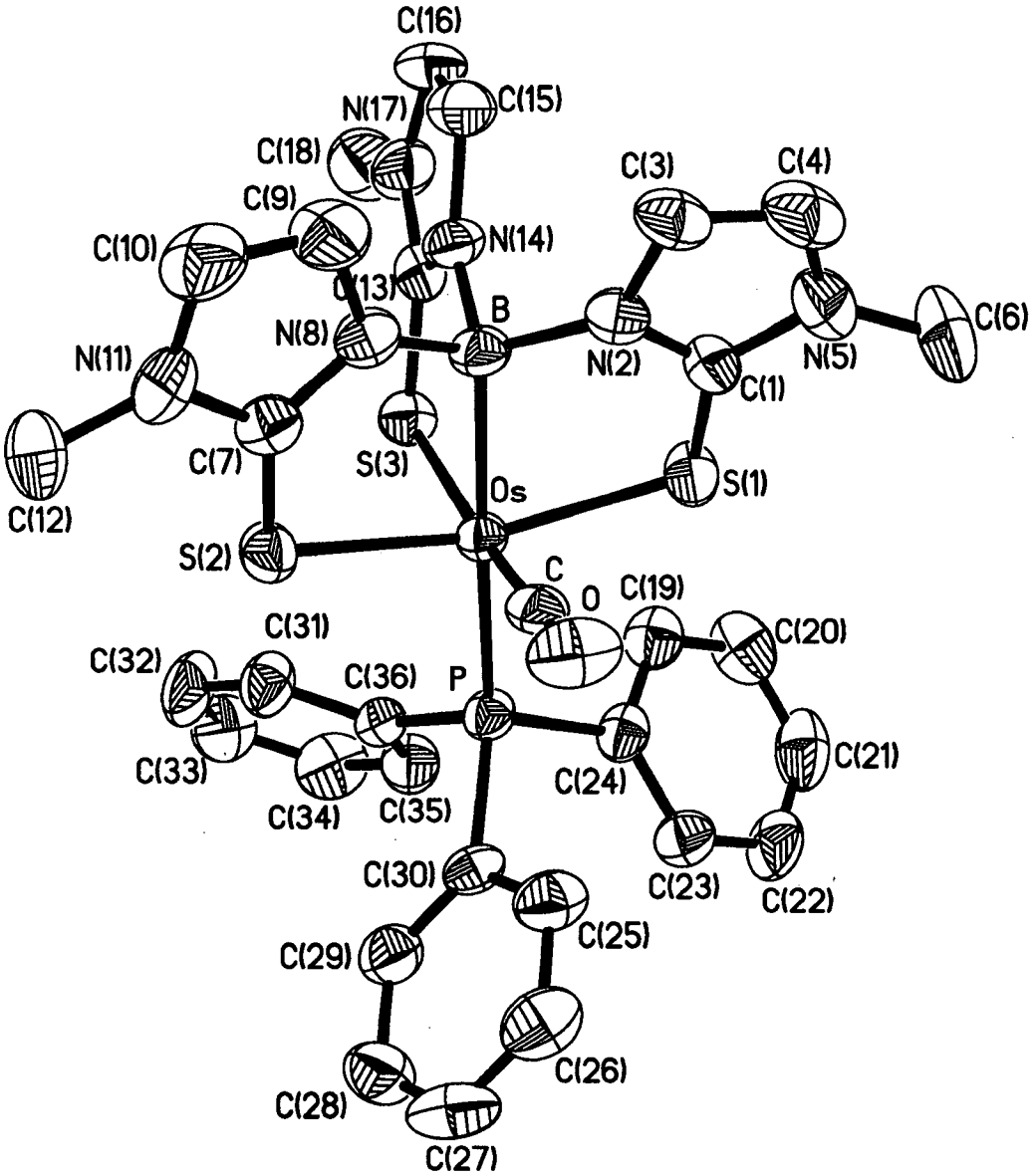

Table S1. Structural and ^{11}B NMR data for complexes with 2c-2e Os–B interactions

Complex	$\delta(^{11}B)$	*d*(Os–B)/Å	ref
6 Co-ordinate Osmium			
Cl(pyO)B OsI(CO)L_2	62.3	2.039(4)	8e
Cl(pyNH)B OsBr(CO)L_2	60.2	2.047(7), 2.053(8)	9b
QuinNHBOsClI(CO)L_2	51.7	2.055(8)	9a
EtO(QuinNH)B OsCl(CO)L_2	-	2.072(3)	9b
EtO(pyNH)B OsCl(CO)L_2	-	2.072(3)	9b
CatBOs(S_2CNEt_2)(CO)L_2	-	2.073(7)	8b
BuNH(pyO)B OsCl(CO)L_2	46.0	2.075(3)	8e
Cl(pyNMe)B OsH(CO)L_2	84.6	2.078(4)	9b
HO(pyNH)B OsCl(CO)L_2	-	2.085(3)	9b
CatBOsI$(CO)_2L_2$-*trans*	36.6	2.090(3)	8c
CatBOs$(NCMe)_2(CO)L_2^+SbF_6^-$	-	2.094(5)	8b
$(\mathbf{CatB})_2$Os(CO)(CNR-4)L_2	45.6	2.104(6), 2.093(6)	8c
Cl(pyNH)B OsH(CO)L_2	73.1	2.104(3)	9b
HO(pyNH)B Os(NCMe)$(CO)L_2^+SbF_6^-$	48.7	2.105(4)	9b
CatBOs(R-2)$(CO)_2L_2$-*trans*	43.3	2.132(7)	8a
CatBOs(NCMe)(CO)(CNR-4)$L_2^+SbF_6^-$	-	2.135(10)	8b
CatBOsI$(CO)_2L_2$-*cis*	44.3	2.145(5)	8c
CatBOs(R-2)$(CO)_2L_2$-*cis*	46.0	2.154(7)	8a,8c
$(\mathbf{mt})_3$**B**Os(CO)L	12.4	2.171(8)	
Cl(pyO)B OsCl(CO)L_2	63.0	-	8e
EtO(pyO)B OsCl(CO)L_2	47.5	-	8e
F(pyO)B OsCl(CO)L_2	48.8	-	8e
CatBOs(R-2)(CO)(CNR-4)L_2	47.2	-	8c
$(\mathbf{CatB})_2$Os$(CO)_2L_2$	43.9	-	8c
CatBOsH$(CO)_2L_2$	45.2	-	8c
CatBOsPh$(CO)_2L_2$	43.3	-	8c
5-Co-odinate Osmium			
$\mathbf{Cl_2B}$OsCl(CO)L_2	52.5	-	9a
CatBOsCl(CO)L_2	-	2.019(3)	8b
$(\mathbf{EtO})_2$**B**OsCl(CO)L_2	-	2.076(3) cited in	8b
CatBOs(R-2)(CO)L_2	26.5	-	8c

L = PPh_3, R = C_6H_4Me, Cat = OC_6H_4O-2, pyO = OC_5H_4N-2, pyNH = HNC_5H_4N-2, pyNMe = $MeNC_5H_4N$-2 Quin = 8-quinonyl.

Table S2. Crystal data and structure refinement for **1b**.

Identification code	Compound **1b**
Empirical formula	C37 H44 N6 O2 B P S3 Cl4 Os
Formula weight	1074.74
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 16.690(2) Å α = 90 deg. b = 11.1483(10)Å β = 107.365(9) deg. c = 24.269(2) Å γ = 90 deg.
Volume	4310.0(7) $Å^3$
Z, Calculated density	4, 1.656 Mg/m^3
Absorption coefficient	3.430 mm^{-1}
F(000)	2144
Crystal size	0.40 x 0.33 x 0.27 mm
Theta range for data collection	1.75 to 25.00 deg.
Limiting indices	0<=h<=19, 0<=k<=13, -28<=l<=27
Reflections collected / unique	7829 / 7548 [R(int) = 0.0346]
Absorption correction	Ellipsoidal
Max. and min. transmission	0.3443 and 0.2816
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6606 / 48 / 460
Goodness-of-fit on F^2	1.021
Final R indices [I>2σ(I)]	R_1 = 0.0438, wR_2 = 0.0859
R indices (all data)	R_1 = 0.0902, wR_2 = 0.1132
Largest diff. peak and hole	1.675 and -0.655 $e.A^{-3}$

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **1b**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Os	2282(1)	2465(1)	638(1)	31(1)
S(1)	2807(1)	462(2)	567(1)	44(1)
S(2)	1460(1)	4161(2)	762(1)	43(1)
S(3)	3131(1)	2619(2)	1673(1)	41(1)
P	3378(1)	3478(2)	367(1)	34(1)
C	1538(5)	2262(6)	-80(3)	39(2)
O	1045(4)	2110(7)	-523(3)	63(2)
B	1419(6)	1460(9)	978(4)	39(2)
C(1)	1903(6)	-300(7)	558(4)	42(2)
N(2)	1243(5)	192(7)	683(3)	41(2)
C(3)	646(6)	-718(8)	637(4)	50(2)
C(4)	967(7)	-1729(9)	482(5)	61(3)
N(5)	1737(5)	-1481(7)	439(4)	52(2)
C(6)	2309(8)	-2297(9)	262(6)	76(3)
C(7)	623(5)	3388(9)	856(4)	41(2)
N(8)	595(5)	2192(7)	926(4)	44(2)
C(9)	-159(7)	1909(11)	1031(5)	62(3)
C(10)	-577(7)	2930(11)	1028(5)	66(3)
N(11)	-99(5)	3876(8)	918(4)	54(2)
C(12)	-330(7)	5130(10)	864(6)	68(3)
C(13)	2526(6)	1686(7)	1950(4)	42(2)
N(14)	1807(4)	1186(6)	1636(3)	41(2)
C(15)	1535(7)	427(9)	2007(4)	53(2)
C(16)	2087(7)	502(9)	2533(4)	58(2)
N(17)	2701(5)	1308(7)	2506(3)	53(2)
C(18)	3400(8)	1687(11)	2979(5)	74(3)
C(19)	4638(3)	1794(6)	737(2)	49(2)
C(20)	5323(4)	1108(5)	715(3)	61(3)
C(21)	5607(3)	1159(6)	232(3)	65(3)
C(22)	5205(4)	1897(6)	-230(2)	64(3)
C(23)	4520(3)	2583(6)	-208(2)	50(2)
C(24)	4237(3)	2532(5)	275(2)	40(1)
C(25)	2558(4)	3729(4)	-808(2)	55(2)
C(26)	2282(4)	4327(6)	-1334(2)	64(3)
C(27)	2506(4)	5517(6)	-1374(2)	65(3)
C(28)	3005(4)	6110(4)	-889(3)	62(3)
C(29)	3281(4)	5512(5)	-363(2)	51(2)
C(30)	3057(3)	4322(5)	-323(2)	37(2)
C(31)	3601(3)	5335(5)	1165(3)	51(2)
C(32)	4047(4)	6194(5)	1551(3)	71(3)
C(33)	4905(4)	6325(6)	1643(3)	63(3)
C(34)	5317(3)	5597(6)	1349(3)	62(3)
C(35)	4871(3)	4737(5)	964(3)	50(2)
C(36)	4013(3)	4606(4)	872(2)	37(2)
C(40)	-788(13)	5529(15)	-2962(8)	127(7)
Cl(1)	-1163(5)	6323(5)	-2487(3)	153(2)

Cl(2)	272(5)	5337(8)	-2672(4)	202(4)
C(50)	357(11)	1702(23)	-2593(7)	145(9)
Cl(3)	1205(4)	2250(7)	-2783(2)	150(2)
Cl(4)	449(3)	1805(5)	-1874(2)	115(1)
O(60)	7769(12)	209(21)	1096(9)	182(7)
C(61)	7932(17)	863(22)	1542(13)	141(8)
C(62)	8199(15)	1246(21)	2027(10)	157(9)
C(63)	7280(28)	-546(44)	1541(22)	293(24)
C(64)	6908(11)	-1090(16)	1676(8)	107(5)

Table S4. Bond lengths [A] and angles [deg] for **1b**.

Os-C	1.826(8)
Os-B	2.171(8)
Os-P	2.403(2)
Os-S(2)	2.406(2)
Os-S(1)	2.424(2)
Os-S(3)	2.493(2)
S(1)-C(1)	1.726(9)
S(2)-C(7)	1.715(9)
S(3)-C(13)	1.720(8)
P-C(24)	1.845(4)
P-C(36)	1.853(4)
P-C(30)	1.854(4)
C-O	1.156(10)
B-N(14)	1.564(12)
B-N(8)	1.572(12)
B-N(2)	1.572(12)
C(1)-N(2)	1.343(11)
C(1)-N(5)	1.359(11)
N(2)-C(3)	1.402(11)
C(3)-C(4)	1.348(15)
C(4)-N(5)	1.349(13)
N(5)-C(6)	1.472(13)
C(7)-N(8)	1.347(13)
C(7)-N(11)	1.370(12)
N(8)-C(9)	1.392(12)
C(9)-C(10)	1.33(2)
C(10)-N(11)	1.395(14)
N(11)-C(12)	1.446(13)
C(13)-N(14)	1.336(11)
C(13)-N(17)	1.359(11)
N(14)-C(15)	1.407(11)
C(15)-C(16)	1.336(15)
C(16)-N(17)	1.380(13)
N(17)-C(18)	1.434(14)
C(19)-C(20)	1.39
C(19)-C(24)	1.39
C(20)-C(21)	1.39
C(21)-C(22)	1.39
C(22)-C(23)	1.39
C(23)-C(24)	1.39
C(25)-C(26)	1.39
C(25)-C(30)	1.39
C(26)-C(27)	1.39
C(27)-C(28)	1.39
C(28)-C(29)	1.39
C(29)-C(30)	1.39
C(31)-C(32)	1.39
C(31)-C(36)	1.39
C(32)-C(33)	1.39
C(33)-C(34)	1.39
C(34)-C(35)	1.39
C(35)-C(36)	1.39

C(40)-Cl(2)	1.71(2)
C(40)-Cl(1)	1.71(2)
C(50)-Cl(4)	1.71(2)
C(50)-Cl(3)	1.72(2)
O(60)-C(61)	1.27(3)
O(60)-C(63)	1.75(4)
C(61)-C(62)	1.21(3)
C(61)-C(63)	1.91(5)
C(63)-C(64)	0.99(5)

C-Os-B	87.7(3)
C-Os-P	98.8(2)
B-Os-P	172.6(3)
C-Os-S(2)	88.0(2)
B-Os-S(2)	83.7(3)
P-Os-S(2)	99.99(7)
C-Os-S(1)	88.6(2)
B-Os-S(1)	81.2(3)
P-Os-S(1)	95.29(7)
S(2)-Os-S(1)	164.67(7)
C-Os-S(3)	171.5(2)
B-Os-S(3)	84.0(3)
P-Os-S(3)	89.61(7)
S(2)-Os-S(3)	89.65(8)
S(1)-Os-S(3)	91.54(8)
C(1)-S(1)-Os	96.9(3)
C(7)-S(2)-Os	98.0(3)
C(13)-S(3)-Os	97.4(3)
C(24)-P-C(36)	99.0(3)
C(24)-P-C(30)	102.0(3)
C(36)-P-C(30)	101.9(3)
C(24)-P-Os	116.5(2)
C(36)-P-Os	118.0(2)
C(30)-P-Os	116.6(2)
O-C-Os	177.1(7)
N(14)-B-N(8)	105.6(7)
N(14)-B-N(2)	104.6(7)
N(8)-B-N(2)	113.0(7)
N(14)-B-Os	111.6(6)
N(8)-B-Os	111.5(6)
N(2)-B-Os	110.3(5)
N(2)-C(1)-N(5)	108.4(8)
N(2)-C(1)-S(1)	124.7(6)
N(5)-C(1)-S(1)	126.9(7)
C(1)-N(2)-C(3)	107.3(7)
C(1)-N(2)-B	114.5(7)
C(3)-N(2)-B	136.0(7)
C(4)-C(3)-N(2)	107.2(8)
N(5)-C(4)-C(3)	108.5(8)
C(4)-N(5)-C(1)	108.6(9)
C(4)-N(5)-C(6)	127.7(9)
C(1)-N(5)-C(6)	123.6(8)
N(8)-C(7)-N(11)	108.3(8)
N(8)-C(7)-S(2)	125.1(7)
N(11)-C(7)-S(2)	126.4(8)
C(7)-N(8)-C(9)	108.3(8)
C(7)-N(8)-B	117.5(7)

C(9)-N(8)-B	133.2(8)
C(10)-C(9)-N(8)	107.8(9)
C(9)-C(10)-N(11)	108.5(8)
C(7)-N(11)-C(10)	107.1(9)
C(7)-N(11)-C(12)	126.4(9)
C(10)-N(11)-C(12)	126.5(9)
N(14)-C(13)-N(17)	109.2(8)
N(14)-C(13)-S(3)	124.1(6)
N(17)-C(13)-S(3)	126.7(7)
C(13)-N(14)-C(15)	107.0(7)
C(13)-N(14)-B	122.0(7)
C(15)-N(14)-B	131.0(8)
C(16)-C(15)-N(14)	108.2(9)
C(15)-C(16)-N(17)	107.8(8)
C(13)-N(17)-C(16)	107.9(8)
C(13)-N(17)-C(18)	125.9(9)
C(16)-N(17)-C(18)	126.3(8)
C(20)-C(19)-C(24)	120.0
C(21)-C(20)-C(19)	120.0
C(20)-C(21)-C(22)	120.0
C(23)-C(22)-C(21)	120.0
C(22)-C(23)-C(24)	120.0
C(23)-C(24)-C(19)	120.0
C(23)-C(24)-P	123.3(3)
C(19)-C(24)-P	116.5(3)
C(26)-C(25)-C(30)	120.0
C(27)-C(26)-C(25)	120.0
C(26)-C(27)-C(28)	120.0
C(29)-C(28)-C(27)	120.0
C(30)-C(29)-C(28)	120.0
C(29)-C(30)-C(25)	120.0
C(29)-C(30)-P	122.5(3)
C(25)-C(30)-P	117.5(3)
C(32)-C(31)-C(36)	120.0
C(31)-C(32)-C(33)	120.0
C(34)-C(33)-C(32)	120.0
C(35)-C(34)-C(33)	120.0
C(34)-C(35)-C(36)	120.0
C(35)-C(36)-C(31)	120.0
C(35)-C(36)-P	122.4(3)
C(31)-C(36)-P	117.6(3)
Cl(2)-C(40)-Cl(1)	109.3(10)
Cl(4)-C(50)-Cl(3)	114.7(10)
C(61)-O(60)-C(63)	76.7(21)
C(62)-C(61)-O(60)	164.1(29)
C(62)-C(61)-C(63)	109.7(29)
O(60)-C(61)-C(63)	63.2(20)
C(64)-C(63)-O(60)	162.0(53)
C(64)-C(63)-C(61)	156.2(51)
O(60)-C(63)-C(61)	40.2(13)

Table S5. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **1b**.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

Atom	U11	U22	U33	U23	U13	U12
Os	30(1)	32(1)	33(1)	0(1)	14(1)	-3(1)
S(1)	38(1)	38(1)	60(1)	-7(1)	20(1)	-3(1)
S(2)	41(1)	37(1)	54(1)	2(1)	20(1)	3(1)
S(3)	41(1)	42(1)	38(1)	1(1)	10(1)	-4(1)
P	32(1)	36(1)	37(1)	-3(1)	16(1)	-4(1)
C	43(4)	37(5)	42(4)	3(3)	20(3)	-9(3)
O	50(4)	90(6)	43(3)	1(3)	3(3)	-25(3)
B	40(5)	41(5)	42(5)	0(4)	21(4)	-9(4)
C(1)	49(4)	33(4)	45(4)	-1(3)	15(4)	-3(3)
N(2)	41(4)	40(4)	46(4)	3(3)	19(3)	-8(3)
C(3)	48(5)	47(5)	51(5)	3(4)	11(4)	-18(4)
C(4)	62(6)	54(6)	63(6)	1(5)	12(5)	-26(5)
N(5)	58(5)	38(4)	56(5)	-1(3)	11(4)	-6(3)
C(6)	78(7)	38(6)	109(9)	-14(5)	25(6)	7(5)
C(7)	35(4)	51(5)	36(4)	4(4)	9(3)	2(4)
N(8)	38(4)	48(5)	54(4)	2(3)	25(3)	-4(3)
C(9)	40(5)	64(6)	91(8)	12(6)	35(6)	1(5)
C(10)	44(5)	85(8)	78(7)	12(6)	31(5)	7(5)
N(11)	46(4)	64(5)	58(5)	-6(4)	25(4)	8(4)
C(12)	63(6)	58(6)	88(8)	7(6)	29(6)	32(5)
C(13)	51(5)	34(4)	43(4)	1(3)	17(4)	3(3)
N(14)	44(4)	46(4)	42(4)	7(3)	23(3)	0(3)
C(15)	68(6)	50(5)	48(5)	4(4)	27(5)	-10(4)
C(16)	81(7)	55(5)	44(5)	17(4)	30(5)	-2(5)
N(17)	68(5)	59(5)	31(3)	5(3)	15(4)	8(4)
C(18)	96(9)	70(7)	48(6)	3(5)	10(6)	-3(6)
C(19)	38(4)	54(5)	57(5)	-5(4)	17(4)	-3(4)
C(20)	40(5)	57(6)	81(7)	4(5)	9(5)	7(4)
C(21)	52(6)	58(6)	90(8)	-21(6)	28(6)	3(5)
C(22)	62(6)	62(6)	85(8)	-15(6)	50(6)	-3(5)
C(23)	51(4)	53(4)	52(4)	0(6)	25(3)	-2(5)
C(24)	34(3)	43(3)	48(4)	-9(5)	19(3)	-8(5)
C(25)	57(6)	62(6)	47(5)	2(4)	20(4)	-13(5)
C(26)	55(6)	85(8)	56(6)	-3(5)	22(5)	-7(5)
C(27)	55(6)	97(8)	43(5)	25(6)	14(5)	-1(6)
C(28)	70(7)	57(6)	63(6)	18(5)	24(5)	14(5)
C(29)	58(5)	53(5)	48(5)	-2(4)	23(4)	-6(4)
C(30)	30(4)	50(4)	38(4)	2(3)	19(3)	-6(3)
C(31)	52(5)	47(5)	59(5)	-17(4)	25(4)	-12(4)
C(32)	96(9)	55(6)	79(7)	-38(6)	49(7)	-24(6)
C(33)	76(7)	56(6)	54(6)	-19(5)	15(5)	-24(5)
C(34)	48(5)	75(7)	57(6)	-11(5)	8(4)	-26(5)
C(35)	46(5)	49(5)	57(5)	-3(4)	21(4)	-5(4)
C(36)	44(4)	37(4)	35(4)	0(3)	17(3)	-2(3)
C(40)	171(19)	84(10)	109(13)	-23(10)	15(13)	-65(12)
Cl(1)	208(7)	88(3)	196(6)	28(3)	111(6)	6(4)
Cl(2)	148(6)	197(8)	247(10)	10(7)	36(6)	36(6)

C(50)	93(11)	236(25)	90(11)	-80(14)	1(9)	14(14)
Cl(3)	147(4)	204(7)	101(3)	-19(4)	40(3)	-7(5)
Cl(4)	105(3)	144(4)	94(3)	-21(3)	25(2)	5(3)
O(60)	169(10)	201(11)	176(10)	16(8)	51(8)	36(8)
C(61)	147(11)	116(10)	156(11)	2(9)	38(9)	14(8
C(62)	161(15)	126(13)	142(14)	34(12)	-19(12)	20(12)
C(63)	286(25)	288(25)	299(25)	6(10)	76(12)	4(10)
C(64)	97(10)	88(9)	120(11)	14(9)	9(9)	27(8)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **1b**.

	x	y	z	U(eq)
H(3A)	126(6)	-639(8)	700(4)	60
H(4A)	703(7)	-2473(9)	417(5)	73
H(6A)	2009(8)	-3004(9)	90(6)	113
H(6B)	2764(8)	-2518(9)	594(6)	113
H(6C)	2528(8)	-1901(9)	-14(6)	113
H(9A)	-338(7)	1145(11)	1093(5)	74
H(10A)	-1100(7)	3000(11)	1088(5)	80
H(12A)	168(7)	5614(10)	964(6)	102
H(12B)	-657(7)	5312(10)	1119(6)	102
H(12C)	-656(7)	5297(10)	473(6)	102
H(15A)	1053(7)	-45(9)	1904(4)	64
H(16A)	2062(7)	85(9)	2860(4)	69
H(18A)	3914(8)	1474(11)	2903(5)	111
H(18B)	3375(8)	1299(11)	3326(5)	111
H(18C)	3378(8)	2541(11)	3024(5)	111
H(19A)	4449(3)	1760(6)	1060(2)	58
H(20A)	5592(5)	614(7)	1024(3)	74
H(21A)	6065(5)	699(8)	217(4)	78
H(22A)	5394(5)	1931(9)	-553(3)	76
H(23A)	4251(5)	3077(8)	-516(2)	60
H(25A)	2408(4)	2933(4)	-781(2)	65
H(26A)	1948(5)	3930(8)	-1658(2)	77
H(27A)	2322(6)	5917(8)	-1725(3)	78
H(28A)	3155(6)	6906(5)	-916(4)	75
H(29A)	3615(5)	5909(7)	-38(3)	61
H(31A)	3026(3)	5247(5)	1104(3)	61
H(32A)	3771(5)	6682(7)	1747(4)	86
H(33A)	5204(5)	6900(8)	1900(4)	76
H(34A)	5891(3)	5684(9)	1411(4)	74
H(35A)	5147(4)	4250(7)	767(4)	60
H(40A)	-1063(13)	4754(15)	-3037(8)	153
H(40B)	-905(13)	5959(15)	-3325(8)	153
H(50A)	-141(11)	2137(23)	-2809(7)	174
H(50B)	276(11)	867(23)	-2708(7)	174
H(61A)	7457(17)	492(22)	1628(13)	169
H(61B)	7706(17)	1621(22)	1366(13)	169
H(62A)	7852(15)	1871(21)	2106(10)	235
H(62B)	8741(15)	1567(21)	2050(10)	235
H(62C)	8259(15)	616(21)	2306(10)	235
H(63A)	7665(28)	-298(44)	1908(22)	352
H(63B)	7540(28)	-1270(44)	1452(22)	352
H(64A)	6739(11)	-1832(16)	1475(8)	160
H(64B)	6420(11)	-634(16)	1674(8)	160
H(64C)	7233(11)	-1253(16)	2067(8)	160

Crystallographic Information File for Complex **1b**.

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R
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 of F^2^ > 2sigma(F^2^) is used only for calculating _R_factor_obs etc.
and is
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C6 C 0.2309(8) -0.2297(9) 0.0262(6) 0.076(3) Uani 1 d . .
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H6B H 0.2764(8) -0.2518(9) 0.0594(6) 0.113 Uiso 1 d R .
H6C H 0.2528(8) -0.1901(9) -0.0014(6) 0.113 Uiso 1 d R .
C7 C 0.0623(5) 0.3388(9) 0.0856(4) 0.041(2) Uani 1 d . .
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H18A H 0.3914(8) 0.1474(11) 0.2903(5) 0.111 Uiso 1 d R .
H18B H 0.3375(8) 0.1299(11) 0.3326(5) 0.111 Uiso 1 d R .
H18C H 0.3378(8) 0.2541(11) 0.3024(5) 0.111 Uiso 1 d R .
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C20 C 0.5323(4) 0.1108(5) 0.0715(3) 0.061(3) Uani 1 d G .
H20A H 0.5592(5) 0.0614(7) 0.1024(3) 0.074 Uiso 1 calc R .
C21 C 0.5607(3) 0.1159(6) 0.0232(3) 0.065(3) Uani 1 d G .
H21A H 0.6065(5) 0.0699(8) 0.0217(4) 0.078 Uiso 1 calc R .
C22 C 0.5205(4) 0.1897(6) -0.0230(2) 0.064(3) Uani 1 d G .
H22A H 0.5394(5) 0.1931(9) -0.0553(3) 0.076 Uiso 1 calc R .
C23 C 0.4520(3) 0.2583(6) -0.0208(2) 0.050(2) Uani 1 d G .
H23A H 0.4251(5) 0.3077(8) -0.0516(2) 0.060 Uiso 1 calc R .
C24 C 0.4237(3) 0.2532(5) 0.0275(2) 0.0401(14) Uani 1 d G .
C25 C 0.2558(4) 0.3729(4) -0.0808(2) 0.055(2) Uani 1 d G .
H25A H 0.2408(4) 0.2933(4) -0.0781(2) 0.065 Uiso 1 calc R .
C26 C 0.2282(4) 0.4327(6) -0.1334(2) 0.064(3) Uani 1 d G .
H26A H 0.1948(5) 0.3930(8) -0.1658(2) 0.077 Uiso 1 calc R .
C27 C 0.2506(4) 0.5517(6) -0.1374(2) 0.065(3) Uani 1 d G .
H27A H 0.2322(6) 0.5917(8) -0.1725(3) 0.078 Uiso 1 calc R .
C28 C 0.3005(4) 0.6110(4) -0.0889(3) 0.062(3) Uani 1 d G .
H28A H 0.3155(6) 0.6906(5) -0.0916(4) 0.075 Uiso 1 calc R .
C29 C 0.3281(4) 0.5512(5) -0.0363(2) 0.051(2) Uani 1 d G .
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C30 C 0.3057(3) 0.4322(5) -0.0323(2) 0.037(2) Uani 1 d G .
C31 C 0.3601(3) 0.5335(5) 0.1165(3) 0.051(2) Uani 1 d G .
H31A H 0.3026(3) 0.5247(5) 0.1104(3) 0.061 Uiso 1 calc R .
C32 C 0.4047(4) 0.6194(5) 0.1551(3) 0.071(3) Uani 1 d G .

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H33A H 0.5204(5) 0.6900(8) 0.1900(4) 0.076 Uiso 1 calc R .
C34 C 0.5317(3) 0.5597(6) 0.1349(3) 0.062(3) Uani 1 d G .
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H61B H 0.7706(17) 0.1621(22) 0.1366(13) 0.169 Uiso 1 d R .
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H63B H 0.7540(28) -0.1270(44) 0.1452(22) 0.352 Uiso 1 d R .
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S3	0.0406(8)	0.0424(11)	0.0382(8)	0.0011(10)	0.0102(7)	-0.0038(10)
P	0.0320(9)	0.0363(9)	0.0366(10)	-0.0029(8)	0.0155(8)	-0.0039(8)
C	0.043(4)	0.037(5)	0.042(4)	0.003(3)	0.020(3)	-0.009(3)
O	0.050(4)	0.090(6)	0.043(3)	0.001(3)	0.003(3)	-0.025(3)
B	0.040(5)	0.041(5)	0.042(5)	0.000(4)	0.021(4)	-0.009(4)
C1	0.049(4)	0.033(4)	0.045(4)	-0.001(3)	0.015(4)	-0.003(3)
N2	0.041(4)	0.040(4)	0.046(4)	0.003(3)	0.019(3)	-0.008(3)
C3	0.048(5)	0.047(5)	0.051(5)	0.003(4)	0.011(4)	-0.018(4)
C4	0.062(6)	0.054(6)	0.063(6)	0.001(5)	0.012(5)	-0.026(5)
N5	0.058(5)	0.038(4)	0.056(5)	-0.001(3)	0.011(4)	-0.006(3)
C6	0.078(7)	0.038(6)	0.109(9)	-0.014(5)	0.025(6)	0.007(5)
C7	0.035(4)	0.051(5)	0.036(4)	0.004(4)	0.009(3)	0.002(4)
N8	0.038(4)	0.048(5)	0.054(4)	0.002(3)	0.025(3)	-0.004(3)
C9	0.040(5)	0.064(6)	0.091(8)	0.012(6)	0.035(6)	0.001(5)
C10	0.044(5)	0.085(8)	0.078(7)	0.012(6)	0.031(5)	0.007(5)
N11	0.046(4)	0.064(5)	0.058(5)	-0.006(4)	0.025(4)	0.008(4)
C12	0.063(6)	0.058(6)	0.088(8)	0.007(6)	0.029(6)	0.032(5)
C13	0.051(5)	0.034(4)	0.043(4)	0.001(3)	0.017(4)	0.003(3)
N14	0.044(4)	0.046(4)	0.042(4)	0.007(3)	0.023(3)	0.000(3)
C15	0.068(6)	0.050(5)	0.048(5)	0.004(4)	0.027(5)	-0.010(4)
C16	0.081(7)	0.055(5)	0.044(5)	0.017(4)	0.030(5)	-0.002(5)
N17	0.068(5)	0.059(5)	0.031(3)	0.005(3)	0.015(4)	0.008(4)
C18	0.096(9)	0.070(7)	0.048(6)	0.003(5)	0.010(6)	-0.003(6)
C19	0.038(4)	0.054(5)	0.057(5)	-0.005(4)	0.017(4)	-0.003(4)
C20	0.040(5)	0.057(6)	0.081(7)	0.004(5)	0.009(5)	0.007(4)
C21	0.052(6)	0.058(6)	0.090(8)	-0.021(6)	0.028(6)	0.003(5)
C22	0.062(6)	0.062(6)	0.085(8)	-0.015(6)	0.050(6)	-0.003(5)
C23	0.051(4)	0.053(4)	0.052(4)	0.000(6)	0.025(3)	-0.002(5)
C24	0.034(3)	0.043(3)	0.048(4)	-0.009(5)	0.019(3)	-0.008(5)
C25	0.057(6)	0.062(6)	0.047(5)	0.002(4)	0.020(4)	-0.013(5)
C26	0.055(6)	0.085(8)	0.056(6)	-0.003(5)	0.022(5)	-0.007(5)

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C27  0.055(6)  0.097(8)  0.043(5)  0.025(6)  0.014(5)  -0.001(6)
C28  0.070(7)  0.057(6)  0.063(6)  0.018(5)  0.024(5)  0.014(5)
C29  0.058(5)  0.053(5)  0.048(5)  -0.002(4)  0.023(4)  -0.006(4)
C30  0.030(4)  0.050(4)  0.038(4)  0.002(3)  0.019(3)  -0.006(3)
C31  0.052(5)  0.047(5)  0.059(5)  -0.017(4)  0.025(4)  -0.012(4)
C32  0.096(9)  0.055(6)  0.079(7)  -0.038(6)  0.049(7)  -0.024(6)
C33  0.076(7)  0.056(6)  0.054(6)  -0.019(5)  0.015(5)  -0.024(5)
C34  0.048(5)  0.075(7)  0.057(6)  -0.011(5)  0.008(4)  -0.026(5)
C35  0.046(5)  0.049(5)  0.057(5)  -0.003(4)  0.021(4)  -0.005(4)
C36  0.044(4)  0.037(4)  0.035(4)  0.000(3)  0.017(3)  -0.002(3)
C40  0.171(19)  0.084(10)  0.109(13)  -0.023(10)  0.015(13)  -.065(12)
Cl1  0.208(7)  0.088(3)  0.196(6)  0.028(3)  0.111(6)  0.006(4)
Cl2  0.148(6)  0.197(8)  0.247(10)  0.010(7)  0.036(6)  0.036(6)
C50  0.093(11)  0.236(25)  0.090(11)  -0.080(14)  0.001(9)  0.014(14)
Cl3  0.147(4)  0.204(7)  0.101(3)  -0.019(4)  0.040(3)  -0.007(5)
Cl4  0.105(3)  0.144(4)  0.094(3)  -0.021(3)  0.025(2)  0.005(3)
O60  0.169(10)  0.201(11)  0.176(10)  0.016(8)  0.051(8)  0.036(8)
C61  0.147(11)  0.116(10)  0.156(11)  0.002(9)  0.038(9)  0.014(8)
C62  0.161(15)  0.126(13)  0.142(14)  0.034(12)  -0.019(12)  0.020(12)
C63  0.286(25)  0.288(25)  0.299(25)  0.006(10)  0.076(12)  0.004(10)
C64  0.097(10)  0.088(9)  0.120(11)  0.014(9)  0.009(9)  0.027(8)

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry.  An approximate
isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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