N(3)-Os(1)-Cl(1)	177.37(14)
N(1)-Os(1)-Cl(1)	92.00(15)
N(5)-Os(1)-Cl(1)	88.06(15)
Cl(1)#2-Os(1)-Cl(1)	91.21(9)

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

Table 11. Anisotropic displacement parameters (A^2 x 10^3) for NH_2Et
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	9(6)	29(6)	34(7)	0	-4(5)	0
C(2)	16(6)	39(7)	30(7)	0	-7(5)	0
C(3)	29(6)	22(6)	14(5)	0	-12(5)	0
C(4)	26(4)	13(4)	32(4)	0(3)	1(3)	-2(3)
C(5)	27(4)	16(4)	55(5)	5(4)	6(4)	-12(3)
C(6)	17(4)	22(4)	45(5)	10(4)	14(3)	1(3)
C(7)	25(6)	36(7)	26(6)	0	0(5)	0
C(8)	24(6)	34(6)	23(6)	0	-6(5)	0
C(9)	14(6)	41(7)	16(5)	0	11(5)	0
C(10)	63(6)	70(7)	66(6)	28(6)	19(5)	32(6)
B(1)	19(6)	35(8)	13(6)	0	4(5)	0
Cl(1)	31(1)	27(1)	29(1)	5(1)	3(1)	-1(1)
N(1)	12(5)	11(4)	21(5)	0	6(4)	0
N(2)	23(5)	12(4)	21(5)	0	12(4)	0
N(3)	16(3)	10(3)	16(3)	0(2)	4(2)	-3(2)
N(4)	12(3)	13(3)	29(3)	5(3)	7(2)	-2(3)
N(5)	13(4)	17(5)	27(5)	0	9(4)	0
Os(1)	11(1)	8(1)	15(1)	0	2(1)	0
O(1)	20(4)	68(6)	37(4)	0	3(4)	0

Table 12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for NH_2Et

	x	y	z	U(eq)
H(1)	9374	2500	7457	26
H(2)	10052	2500	9308	31
H(3)	7126	2500	10172	24
H(4)	2922	-400	6284	26
H(5)	1296	-1398	7705	36
H(6)	1821	135	9181	31
H(7A)	1214	1697	5666	32
H(7B)	1214	3303	5666	32
H(8A)	-623	2500	4382	41
H(8B)	971	1696	3909	41
H(8C)	971	3304	3909	41
H(10A)	5722	-1367	7936	99
H(10B)	7564	-700	7821	99
H(10C)	6701	-746	8873	99
H(1B)	4053	2500	9601	25
H(5A)	3846	3242	4866	21
H(5B)	3846	1758	4866	21

Table 13. Torsion angles [deg] for NH_2Et

N(1)-C(1)-C(2)-C(3)	0.000(4)
C(1)-C(2)-C(3)-N(2)	0.000(4)
N(3)-C(4)-C(5)-C(6)	0.9(8)
C(4)-C(5)-C(6)-N(4)	-0.7(8)
C(2)-C(1)-N(1)-N(2)	0.000(4)
C(2)-C(1)-N(1)-Os(1)	180.000(3)
C(2)-C(3)-N(2)-N(1)	0.000(4)
C(2)-C(3)-N(2)-B(1)	180.000(4)
C(1)-N(1)-N(2)-C(3)	0.000(4)
Os(1)-N(1)-N(2)-C(3)	180.000(3)
C(1)-N(1)-N(2)-B(1)	180.000(3)
Os(1)-N(1)-N(2)-B(1)	0.000(4)
N(4)#2-B(1)-N(2)-C(3)	122.2(5)
N(4)-B(1)-N(2)-C(3)	-122.2(5)
N(4)#2-B(1)-N(2)-N(1)	-57.8(5)
N(4)-B(1)-N(2)-N(1)	57.8(5)
C(5)-C(4)-N(3)-N(4)	-0.6(7)
C(5)-C(4)-N(3)-Os(1)	-176.9(5)
C(5)-C(6)-N(4)-N(3)	0.4(7)
C(5)-C(6)-N(4)-B(1)	178.4(7)
C(4)-N(3)-N(4)-C(6)	0.2(7)
Os(1)-N(3)-N(4)-C(6)	177.0(4)
C(4)-N(3)-N(4)-B(1)	-178.2(6)
Os(1)-N(3)-N(4)-B(1)	-1.3(7)
N(2)-B(1)-N(4)-C(6)	124.8(7)
N(4)#2-B(1)-N(4)-C(6)	-118.4(7)
N(2)-B(1)-N(4)-N(3)	-57.4(7)
N(4)#2-B(1)-N(4)-N(3)	59.4(9)
C(8)-C(7)-N(5)-Os(1)	180.000(1)
C(4)-N(3)-Os(1)-N(3)#2	133.0(5)
N(4)-N(3)-Os(1)-N(3)#2	-42.9(5)
C(4)-N(3)-Os(1)-N(1)	-140.3(6)
N(4)-N(3)-Os(1)-N(1)	43.8(4)
C(4)-N(3)-Os(1)-N(5)	39.7(6)
N(4)-N(3)-Os(1)-N(5)	-136.2(4)
C(4)-N(3)-Os(1)-Cl(1)#2	-48.4(6)
N(4)-N(3)-Os(1)-Cl(1)#2	135.7(4)
C(4)-N(3)-Os(1)-Cl(1)	164(3)
N(4)-N(3)-Os(1)-Cl(1)	-12(3)
C(1)-N(1)-Os(1)-N(3)#2	-136.53(15)
N(2)-N(1)-Os(1)-N(3)#2	43.47(15)
C(1)-N(1)-Os(1)-N(3)	136.53(15)
N(2)-N(1)-Os(1)-N(3)	-43.47(15)
C(1)-N(1)-Os(1)-N(5)	180(16)
N(2)-N(1)-Os(1)-N(5)	0(16)
C(1)-N(1)-Os(1)-Cl(1)#2	45.64(5)
N(2)-N(1)-Os(1)-Cl(1)#2	-134.36(5)
C(1)-N(1)-Os(1)-Cl(1)	-45.64(5)
N(2)-N(1)-Os(1)-Cl(1)	134.36(5)
C(7)-N(5)-Os(1)-N(3)#2	-43.47(15)
C(7)-N(5)-Os(1)-N(3)	43.47(15)
C(7)-N(5)-Os(1)-N(1)	0(16)
C(7)-N(5)-Os(1)-Cl(1)#2	134.36(5)
C(7)-N(5)-Os(1)-Cl(1)	-134.36(5)

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

References:

Instrument:	Nonius KappaCCD
	Nonius (1997). KappaCCD Operations Manual, Delft.
Data Collection Software:	Collect, (1998), Data Collection Software, Nonius.
Data Reduction:	DENZO
	Otinowski, Z., Minor, W., (1996). Processing of X-ray Diffraction Data Collected in Oscillation Mode, Methods in Enzymology, 276, 307-326., C. W. Carter, Jr., R. M. Sweet, Eds., Academic Press.
Cell Refinement:	HKL SCALEPACK
	ibid.
Structure Solution:	SIR92
	Altomare, A., Cascarano, G., Giacovazzo, C., Burla M.C., Polidori, G., Camalli, M.,(1994)., SIR. J. Appl. Cryst. 27, 435-442.
Structure Refinement:	SHELXL-97 (Sheldrick, 1997)
	Sheldrick, G.M. (1997). SHELXL97, Program for the Refinement of Crystal Structures. Univ. of Gottingen, Germany.
Molecular Graphics:	maXus, Zortep
maXus:	MacKay, S., Gilmore, C.J., Edwards, C., Tremayne M., Stewart, N., Shankland, K., (1998), "maXus: a computer program for the solution and refinement of crystal structures from diffraction data" University of Glasgow, Scotland, UK, Nonius BV, Delft, The Netherlands and MacScience Co. Ltd., Yokohama, Japan.
Zortep:	L. Zsolnai, G. Huttner, (1994), University of Heidelberg.

Crystallographic information for $TpOs(NH_2Me)Cl_2$ (**9**) (abbreviated NH_2Me).

A red, plate 0.25 x 0.18 x 0.10 mm was mounted on a glass capillary in epoxy. Data was collected at 25°C with four sets of exposures as follows:

Scan Set	Scan Type	Scan Range (deg.)	θ (deg.)	φ/ω (deg.)	κ (deg.)
1	φ	-46.5 to136.5	4.303	180	0
2	ω	99.8 to 201.4	-1.500	-50.396	-68.957
3	ω	-176.6 to -145.0	-1.500	147.492	-100
4	ω	-176.6 to -72.8	37.224	-189.916	-100

Crystal-to-detector distance was 27 mm and exposure time was 10 seconds for all sets. The scan width was 1°. Data collection was 99.7% complete to 28.28° in θ. A total of 68364 partial and complete reflections were collected covering the indices, h = -13 to 11, k = -20 to 20, l = -23 to 23. 10046 reflections symmetry independent reflections were used and the R_{int} = 0.0668 indicated that the quality of data was good. Indexing and unit cell refinement, based on 727 reflections, indicated a triclinic lattice. The spacegroup was found to be *P* -1 (No. 2). Solution by direct methods (SIR 92) produced a complete heavy atom phasing model inconsistent with the proposed structure submitted. No Mg^{2+} was present instead the Os(IV) complex was present with 2 independent molecules in the asymmetric unit. All hydrogen atoms were placed with idealized geometry except for H1B and H2B (boron H's) which were located. All H atoms were refined with a riding model and U_{iso} values were fixed such that they were 1.1 U_{eq} of their parent atom 1.5 U_{eq} for methyls. All other non-hydrogen atoms were refined anisotropically by full-matrix least-squares. An empirical correction for absorption anisotropy was not applied. Instead, the data were corrected by scaling and averaging using the program SCALEPACK. This program applies a multiplicative correction factor (S) to the observed intensities (I) and has the following form:

$$S = e(2B(\sin\theta/\lambda)^2 / \text{scale}$$

S is calculated from the scale and B factor determined for each frame and is then applied to I to give the corrected intensity (I_{corr}). This method does not, however, calculate minimum and maximum transmission coefficients.

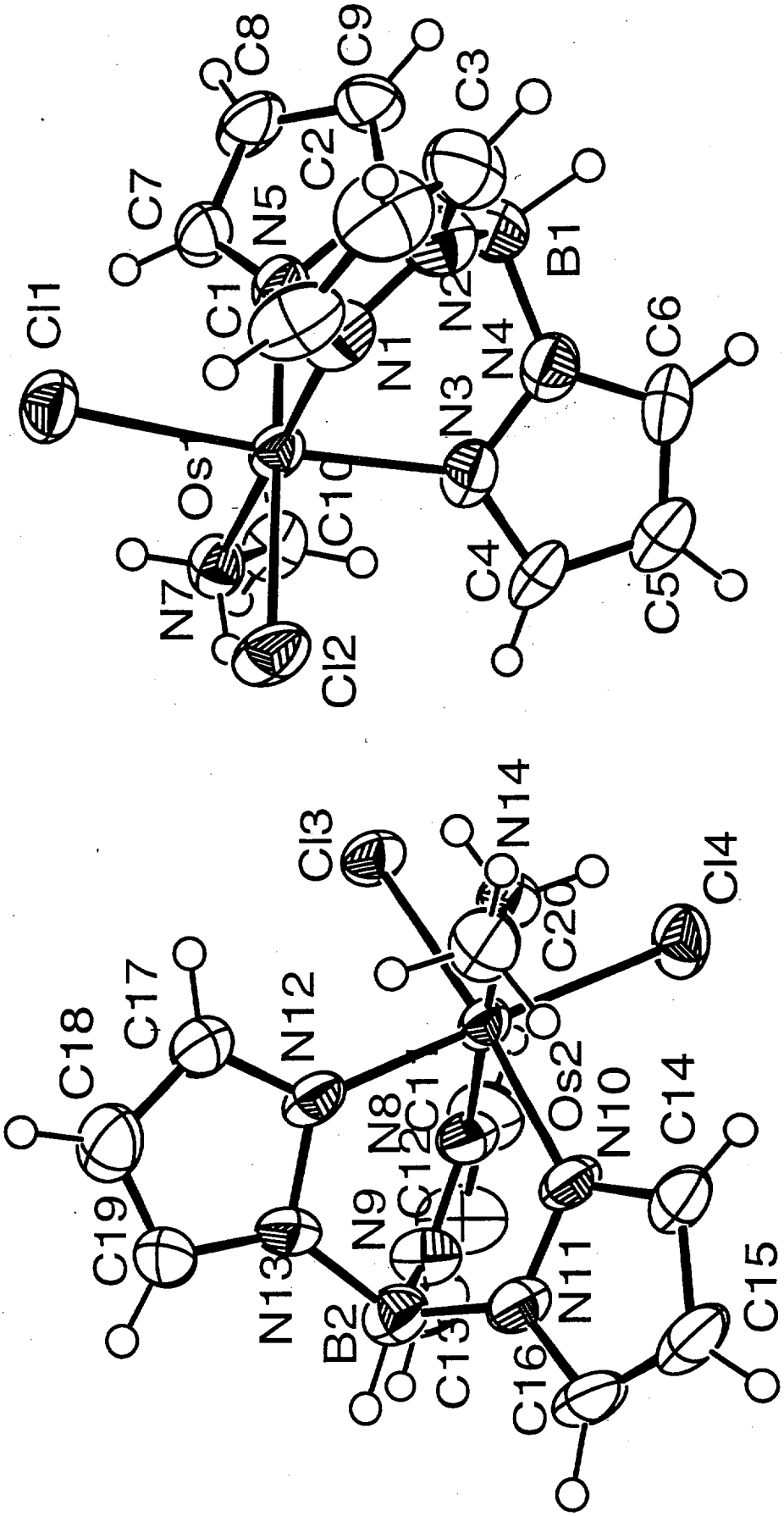


Table 8. Crystal data and structure refinement for NH_2Me

Compound C10H15BCl2N7Os	shelxl
Empirical formula	C10 H15 B Cl2 N7 Os
Formula weight	505.20
Temperature	298(2) K
Wavelength	0.71070 A
Crystal description/color	plate / red
Crystal system, space group	Triclinic, P-1 (No. 2)
Unit cell dimensions	a = 9.4037(2) A alpha = 66.2521(14) deg b = 14.5490(4) A beta = 89.8135(15) de c = 16.3987(3) A gamma = 81.0570(13) de
Volume	2024.27(8) A^3
Z, Calculated density	4, 1.658 Mg/m^3
Absorption coefficient	6.565 mm^-1
F(000)	956
Crystal size	0.25 x 0.18 x 0.10 mm
Reflections for indexing	727
Theta range for data collection	2.44 to 28.28 deg.
Index ranges	-13<=h<=12, -18<=k<=19, -21<=l<=21
Reflections collected / unique	68364 / 10038 [R(int) = 0.0668]
Completeness to theta = 28.28	99.7%
Absorption correction	Scalepack
Max. and min. transmission	0.5597 and 0.2906
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10038 / 0 / 380
Goodness-of-fit on F^2	1.054
Final R indices [I>2sigma(I)]	*R1 = 0.0603, wR2 = 0.1858
R indices (all data) *Report these R factors	R1 = 0.0838, *wR2 = 0.2017
Weighting scheme	calc w=1/[\s^2^(Fo^2^)+(0.1279P)^2^+0.0000P] where P=(F
Extinction coefficient	0.0016(4)

```
Largest diff. peak and hole       3.966 and -3.196 e.A^-3
```

Table 9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for NH_2Me
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	1146(14)	-3693(10)	-1008(8)	61(3)
C(2)	1040(17)	-4681(11)	-962(11)	76(4)
C(3)	750(15)	-4595(10)	-1755(9)	64(3)
C(4)	-2349(9)	-823(8)	-3524(6)	44(2)
C(5)	-3167(11)	-1164(10)	-4013(8)	54(3)
C(6)	-2323(11)	-2024(9)	-4024(8)	52(3)
C(7)	3076(11)	-1410(9)	-3914(7)	46(2)
C(8)	3479(11)	-1841(11)	-4507(8)	58(3)
C(9)	2470(11)	-2550(8)	-4381(6)	46(2)
C(10)	359(12)	651(9)	-4171(7)	48(2)
C(11)	-5740(15)	3636(10)	-3990(7)	61(3)
C(12)	-6306(18)	4657(11)	-4121(9)	74(4)
C(13)	-6497(15)	4546(9)	-3249(9)	69(4)
C(14)	-7736(10)	812(9)	-1459(6)	45(2)
C(15)	-8720(11)	1177(11)	-952(7)	57(3)
C(16)	-8309(11)	2044(10)	-979(7)	51(3)
C(17)	-2634(11)	1425(10)	-1090(8)	52(3)
C(18)	-2497(13)	1882(11)	-528(8)	62(3)
C(19)	-3739(12)	2584(10)	-669(8)	54(3)
C(20)	-4359(13)	-671(10)	-830(7)	50(3)
B(1)	301(13)	-3038(9)	-3364(8)	44(3)
B(2)	-6169(12)	3020(9)	-1631(8)	44(3)
Cl(1)	2930(3)	-1539(2)	-1770(2)	50(1)
Cl(2)	-643(3)	-1143(2)	-1423(2)	53(1)
Cl(3)	-2814(3)	1540(2)	-3231(2)	46(1)
Cl(4)	-6186(3)	1107(2)	-3551(2)	50(1)
N(1)	848(10)	-3011(7)	-1888(5)	45(2)
N(2)	622(10)	-3578(7)	-2352(6)	51(2)
N(3)	-1046(9)	-1460(7)	-3244(5)	42(2)
N(4)	-1060(9)	-2208(7)	-3548(6)	45(2)
N(5)	1931(9)	-1741(7)	-3473(5)	40(2)
N(6)	1579(9)	-2485(6)	-3766(5)	40(2)
N(7)	638(9)	141(6)	-3193(5)	39(2)
N(8)	-5658(9)	2995(7)	-3125(6)	44(2)
N(9)	-6117(10)	3573(7)	-2668(6)	48(2)
N(10)	-6754(8)	1462(7)	-1751(5)	41(2)
N(11)	-7139(9)	2214(7)	-1450(6)	45(2)
N(12)	-3953(8)	1767(6)	-1537(5)	39(2)
N(13)	-4633(9)	2503(7)	-1257(5)	43(2)
N(14)	-4304(9)	-128(6)	-1789(5)	40(2)
Os(1)	744(1)	-1472(1)	-2528(1)	34(1)
Os(2)	-4971(1)	1461(1)	-2463(1)	34(1)

Table 10. Bond lengths [A] and angles [deg] for NH_2Me

C(1)-N(1)	1.381(14)
C(1)-C(2)	1.43(2)
C(1)-H(1)	0.9613
C(2)-C(3)	1.281(19)
C(2)-H(2)	0.9603
C(3)-N(2)	1.393(15)
C(3)-H(3)	0.9606
C(4)-N(3)	1.371(12)
C(4)-C(5)	1.387(15)
C(4)-H(4)	0.9592
C(5)-C(6)	1.380(17)
C(5)-H(5)	0.9605
C(6)-N(4)	1.352(13)
C(6)-H(6)	0.9614
C(7)-N(5)	1.338(13)
C(7)-C(8)	1.378(14)
C(7)-H(7)	0.9602
C(8)-C(9)	1.463(17)
C(8)-H(8)	0.9593
C(9)-N(6)	1.333(12)
C(9)-H(9)	0.9601
C(10)-N(7)	1.476(12)
C(10)-H(10A)	0.9603
C(10)-H(10B)	0.9640
C(10)-H(10C)	0.9570
C(11)-N(8)	1.342(14)
C(11)-C(12)	1.426(19)
C(11)-H(11)	0.9592
C(12)-C(13)	1.387(19)
C(12)-H(12)	0.9603
C(13)-N(9)	1.341(14)
C(13)-H(13)	0.9610
C(14)-N(10)	1.372(13)
C(14)-C(15)	1.424(15)
C(14)-H(14)	0.9600
C(15)-C(16)	1.359(18)
C(15)-H(15)	0.9600
C(16)-N(11)	1.340(13)
C(16)-H(16)	0.9605
C(17)-C(18)	1.352(16)
C(17)-N(12)	1.358(13)
C(17)-H(17)	0.9599
C(18)-C(19)	1.379(18)
C(18)-H(18)	0.9597
C(19)-N(13)	1.334(13)
C(19)-H(19)	0.9595
C(20)-N(14)	1.454(12)
C(20)-H(20A)	0.9593
C(20)-H(20B)	0.9626
C(20)-H(20C)	0.9594
B(1)-N(2)	1.530(15)
B(1)-N(6)	1.548(15)
B(1)-N(4)	1.555(15)
B(1)-H(1B)	1.1802
B(2)-N(13)	1.525(14)
B(2)-N(11)	1.531(15)

B(2)-N(9)	1.567(14)
B(2)-H(2B)	1.0085
Cl(1)-Os(1)	2.374(2)
Cl(2)-Os(1)	2.390(2)
Cl(3)-Os(2)	2.377(2)
Cl(4)-Os(2)	2.386(2)
N(1)-N(2)	1.366(13)
N(1)-Os(1)	2.040(9)
N(3)-N(4)	1.368(12)
N(3)-Os(1)	2.050(8)
N(5)-N(6)	1.429(11)
N(5)-Os(1)	2.034(8)
N(7)-Os(1)	2.139(8)
N(7)-H(7A)	0.9000
N(7)-H(7B)	0.9000
N(8)-N(9)	1.359(12)
N(8)-Os(2)	2.044(9)
N(10)-N(11)	1.373(12)
N(10)-Os(2)	2.040(8)
N(12)-N(13)	1.395(11)
N(12)-Os(2)	2.026(8)
N(14)-Os(2)	2.111(8)
N(14)-H(14A)	0.9000
N(14)-H(14B)	0.9000

N(1)-C(1)-C(2)	107.6(12)
N(1)-C(1)-H(1)	125.7
C(2)-C(1)-H(1)	126.7
C(3)-C(2)-C(1)	108.0(13)
C(3)-C(2)-H(2)	126.2
C(1)-C(2)-H(2)	125.8
C(2)-C(3)-N(2)	109.8(12)
C(2)-C(3)-H(3)	125.2
N(2)-C(3)-H(3)	125.0
N(3)-C(4)-C(5)	109.4(10)
N(3)-C(4)-H(4)	125.4
C(5)-C(4)-H(4)	125.2
C(6)-C(5)-C(4)	105.7(9)
C(6)-C(5)-H(5)	126.7
C(4)-C(5)-H(5)	127.6
N(4)-C(6)-C(5)	109.1(10)
N(4)-C(6)-H(6)	125.5
C(5)-C(6)-H(6)	125.4
N(5)-C(7)-C(8)	113.1(10)
N(5)-C(7)-H(7)	123.4
C(8)-C(7)-H(7)	123.5
C(7)-C(8)-C(9)	103.6(9)
C(7)-C(8)-H(8)	128.2
C(9)-C(8)-H(8)	128.2
N(6)-C(9)-C(8)	108.3(9)
N(6)-C(9)-H(9)	125.5
C(8)-C(9)-H(9)	126.2
N(7)-C(10)-H(10A)	108.9
N(7)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.3
N(7)-C(10)-H(10C)	110.0
H(10A)-C(10)-H(10C)	109.7
H(10B)-C(10)-H(10C)	109.4
N(8)-C(11)-C(12)	111.8(11)
N(8)-C(11)-H(11)	123.6

C(12)-C(11)-H(11)	124.6
C(13)-C(12)-C(11)	101.3(11)
C(13)-C(12)-H(12)	129.4
C(11)-C(12)-H(12)	129.3
N(9)-C(13)-C(12)	111.5(12)
N(9)-C(13)-H(13)	123.7
C(12)-C(13)-H(13)	124.7
N(10)-C(14)-C(15)	107.7(10)
N(10)-C(14)-H(14)	126.5
C(15)-C(14)-H(14)	125.8
C(16)-C(15)-C(14)	106.2(10)
C(16)-C(15)-H(15)	126.1
C(14)-C(15)-H(15)	127.7
N(11)-C(16)-C(15)	109.4(10)
N(11)-C(16)-H(16)	125.4
C(15)-C(16)-H(16)	125.2
C(18)-C(17)-N(12)	110.3(10)
C(18)-C(17)-H(17)	125.3
N(12)-C(17)-H(17)	124.4
C(17)-C(18)-C(19)	106.5(10)
C(17)-C(18)-H(18)	126.6
C(19)-C(18)-H(18)	126.9
N(13)-C(19)-C(18)	108.7(10)
N(13)-C(19)-H(19)	125.3
C(18)-C(19)-H(19)	126.0
N(14)-C(20)-H(20A)	110.2
N(14)-C(20)-H(20B)	109.4
H(20A)-C(20)-H(20B)	109.2
N(14)-C(20)-H(20C)	108.9
H(20A)-C(20)-H(20C)	109.7
H(20B)-C(20)-H(20C)	109.4
N(2)-B(1)-N(6)	107.7(8)
N(2)-B(1)-N(4)	107.8(9)
N(6)-B(1)-N(4)	107.3(9)
N(2)-B(1)-H(1B)	124.3
N(6)-B(1)-H(1B)	109.6
N(4)-B(1)-H(1B)	98.7
N(13)-B(2)-N(11)	109.8(9)
N(13)-B(2)-N(9)	106.9(9)
N(11)-B(2)-N(9)	107.2(9)
N(13)-B(2)-H(2B)	109.3
N(11)-B(2)-H(2B)	110.0
N(9)-B(2)-H(2B)	113.6
N(2)-N(1)-C(1)	105.9(10)
N(2)-N(1)-Os(1)	120.8(6)
C(1)-N(1)-Os(1)	133.3(9)
N(1)-N(2)-C(3)	108.7(9)
N(1)-N(2)-B(1)	118.7(8)
C(3)-N(2)-B(1)	132.6(10)
N(4)-N(3)-C(4)	106.7(8)
N(4)-N(3)-Os(1)	119.6(6)
C(4)-N(3)-Os(1)	133.6(7)
C(6)-N(4)-N(3)	109.0(9)
C(6)-N(4)-B(1)	131.6(10)
N(3)-N(4)-B(1)	119.3(8)
C(7)-N(5)-N(6)	105.6(8)
C(7)-N(5)-Os(1)	136.0(7)
N(6)-N(5)-Os(1)	118.4(6)
C(9)-N(6)-N(5)	109.4(8)
C(9)-N(6)-B(1)	131.8(9)

N(5)-N(6)-B(1)	118.8(8)
C(10)-N(7)-Os(1)	119.8(7)
C(10)-N(7)-H(7A)	107.4
Os(1)-N(7)-H(7A)	107.4
C(10)-N(7)-H(7B)	107.4
Os(1)-N(7)-H(7B)	107.4
H(7A)-N(7)-H(7B)	106.9
C(11)-N(8)-N(9)	106.4(9)
C(11)-N(8)-Os(2)	133.0(8)
N(9)-N(8)-Os(2)	120.6(7)
C(13)-N(9)-N(8)	109.0(9)
C(13)-N(9)-B(2)	133.0(10)
N(8)-N(9)-B(2)	117.9(8)
N(11)-N(10)-C(14)	106.8(8)
N(11)-N(10)-Os(2)	120.2(6)
C(14)-N(10)-Os(2)	132.9(7)
C(16)-N(11)-N(10)	109.9(9)
C(16)-N(11)-B(2)	131.6(10)
N(10)-N(11)-B(2)	118.4(8)
C(17)-N(12)-N(13)	105.6(8)
C(17)-N(12)-Os(2)	134.4(7)
N(13)-N(12)-Os(2)	120.0(6)
C(19)-N(13)-N(12)	108.7(8)
C(19)-N(13)-B(2)	133.0(9)
N(12)-N(13)-B(2)	118.2(8)
C(20)-N(14)-Os(2)	122.8(7)
C(20)-N(14)-H(14A)	106.6
Os(2)-N(14)-H(14A)	106.6
C(20)-N(14)-H(14B)	106.6
Os(2)-N(14)-H(14B)	106.6
H(14A)-N(14)-H(14B)	106.6
N(5)-Os(1)-N(1)	87.3(3)
N(5)-Os(1)-N(3)	87.0(3)
N(1)-Os(1)-N(3)	87.1(3)
N(5)-Os(1)-N(7)	93.0(3)
N(1)-Os(1)-N(7)	179.7(3)
N(3)-Os(1)-N(7)	93.1(3)
N(5)-Os(1)-Cl(1)	88.6(2)
N(1)-Os(1)-Cl(1)	91.8(3)
N(3)-Os(1)-Cl(1)	175.5(2)
N(7)-Os(1)-Cl(1)	88.1(2)
N(5)-Os(1)-Cl(2)	179.5(2)
N(1)-Os(1)-Cl(2)	93.2(3)
N(3)-Os(1)-Cl(2)	93.2(2)
N(7)-Os(1)-Cl(2)	86.6(2)
Cl(1)-Os(1)-Cl(2)	91.26(9)
N(12)-Os(2)-N(10)	86.4(3)
N(12)-Os(2)-N(8)	87.5(3)
N(10)-Os(2)-N(8)	86.0(3)
N(12)-Os(2)-N(14)	93.5(3)
N(10)-Os(2)-N(14)	93.3(3)
N(8)-Os(2)-N(14)	178.7(3)
N(12)-Os(2)-Cl(3)	89.0(2)
N(10)-Os(2)-Cl(3)	175.1(2)
N(8)-Os(2)-Cl(3)	92.2(3)
N(14)-Os(2)-Cl(3)	88.6(2)
N(12)-Os(2)-Cl(4)	179.6(2)
N(10)-Os(2)-Cl(4)	93.2(2)
N(8)-Os(2)-Cl(4)	92.3(3)
N(14)-Os(2)-Cl(4)	86.7(2)

Cl(3)-Os(2)-Cl(4)	91.42(9)

Symmetry transformations used to generate equivalent atoms:

Table 11. Anisotropic displacement parameters (A^2 x 10^3) for NH_2Me . The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	56(7)	69(8)	42(6)	-10(5)	10(5)	6(6)
C(2)	78(10)	57(8)	76(10)	-10(7)	11(8)	-11(7)
C(3)	69(8)	59(8)	75(9)	-33(7)	25(7)	-26(6)
C(4)	20(4)	60(6)	45(5)	-14(5)	4(4)	-6(4)
C(5)	28(5)	72(8)	58(7)	-22(6)	4(4)	-7(5)
C(6)	36(5)	60(7)	62(7)	-22(6)	-3(5)	-21(5)
C(7)	33(5)	68(7)	49(6)	-34(5)	11(4)	-14(5)
C(8)	31(5)	98(10)	55(6)	-45(7)	11(5)	-1(5)
C(9)	50(6)	55(6)	39(5)	-27(5)	8(4)	-2(5)
C(10)	43(6)	56(6)	36(5)	-10(4)	5(4)	-9(5)
C(11)	74(9)	69(8)	36(5)	-20(5)	4(5)	-6(6)
C(12)	92(11)	57(8)	59(8)	-13(6)	17(7)	1(7)
C(13)	68(8)	35(6)	80(9)	-5(6)	12(7)	10(6)
C(14)	28(4)	68(7)	37(5)	-20(5)	0(4)	-5(4)
C(15)	24(5)	96(10)	50(6)	-30(6)	8(4)	-4(5)
C(16)	32(5)	76(8)	44(5)	-29(5)	10(4)	4(5)
C(17)	34(5)	79(8)	57(6)	-43(6)	4(5)	-4(5)
C(18)	48(6)	104(10)	44(6)	-38(7)	2(5)	-16(6)
C(19)	43(6)	77(8)	64(7)	-49(6)	16(5)	-19(6)
C(20)	49(6)	66(7)	35(5)	-20(5)	4(4)	-9(5)
B(1)	43(6)	49(7)	44(6)	-25(5)	4(5)	-7(5)
B(2)	37(6)	48(6)	43(6)	-16(5)	1(5)	1(5)
Cl(1)	36(1)	69(2)	47(1)	-27(1)	-6(1)	-5(1)
Cl(2)	39(1)	80(2)	39(1)	-28(1)	9(1)	3(1)
Cl(3)	36(1)	63(2)	46(1)	-28(1)	15(1)	-9(1)
Cl(4)	46(1)	74(2)	38(1)	-26(1)	1(1)	-20(1)
N(1)	44(5)	56(5)	26(4)	-10(4)	3(3)	-2(4)
N(2)	53(6)	37(5)	57(5)	-13(4)	12(4)	-10(4)
N(3)	33(4)	57(5)	36(4)	-18(4)	2(3)	-9(4)
N(4)	37(4)	57(5)	44(5)	-22(4)	4(4)	-12(4)
N(5)	34(4)	53(5)	34(4)	-19(4)	2(3)	-8(4)
N(6)	41(4)	46(5)	37(4)	-22(4)	7(3)	-9(4)
N(7)	38(4)	49(5)	30(4)	-16(3)	0(3)	-9(4)
N(8)	36(4)	46(5)	49(5)	-23(4)	4(4)	2(4)
N(9)	50(5)	45(5)	46(5)	-18(4)	7(4)	-1(4)
N(10)	24(4)	55(5)	45(4)	-23(4)	7(3)	-1(3)
N(11)	31(4)	57(5)	50(5)	-27(4)	7(4)	-2(4)
N(12)	26(4)	53(5)	34(4)	-16(4)	7(3)	-1(3)
N(13)	40(4)	55(5)	44(5)	-32(4)	9(4)	-2(4)
N(14)	40(4)	47(5)	36(4)	-20(3)	6(3)	-6(4)
Os(1)	26(1)	48(1)	30(1)	-19(1)	4(1)	-4(1)
Os(2)	26(1)	47(1)	30(1)	-18(1)	4(1)	-4(1)

Table 12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for NH_2Me

	x	y	z	U(eq)
H(1)	1393	-3527	-521	68
H(2)	1176	-5301	-430	83
H(3)	614	-5145	-1913	71
H(4)	-2652	-235	-3399	48
H(5)	-4123	-869	-4288	60
H(6)	-2592	-2430	-4319	57
H(7)	3574	-929	-3820	50
H(8)	4239	-1706	-4909	64
H(9)	2441	-2984	-4691	50
H(10A)	351	1368	-4358	72
H(10B)	-566	545	-4335	72
H(10C)	1095	379	-4456	72
H(11)	-5464	3425	-4460	67
H(12)	-6471	5263	-4665	82
H(13)	-6888	5089	-3079	76
H(14)	-7761	217	-1573	50
H(15)	-9519	881	-650	63
H(16)	-8779	2464	-698	56
H(17)	-1913	922	-1160	58
H(18)	-1686	1751	-120	68
H(19)	-3934	3056	-393	59
H(20A)	-4017	-1385	-652	75
H(20B)	-5339	-575	-669	75
H(20C)	-3766	-403	-534	75
H(1B)	-54	-3432	-3816	48
H(2B)	-6541	3494	-1339	49
H(7A)	-56	432	-2951	47
H(7B)	1479	286	-3058	47
H(14A)	-4828	-420	-2046	48
H(14B)	-3383	-262	-1916	48

Table 13. Torsion angles [deg] for NH_2Me.

N(1)-C(1)-C(2)-C(3)	2.0(17)
C(1)-C(2)-C(3)-N(2)	-1.2(17)
N(3)-C(4)-C(5)-C(6)	-0.1(12)
C(4)-C(5)-C(6)-N(4)	1.1(13)
N(5)-C(7)-C(8)-C(9)	-2.2(13)
C(7)-C(8)-C(9)-N(6)	0.7(12)
N(8)-C(11)-C(12)-C(13)	1.7(17)
C(11)-C(12)-C(13)-N(9)	-1.0(17)
N(10)-C(14)-C(15)-C(16)	1.5(12)
C(14)-C(15)-C(16)-N(11)	-1.1(12)
N(12)-C(17)-C(18)-C(19)	-3.9(15)
C(17)-C(18)-C(19)-N(13)	3.8(15)
C(2)-C(1)-N(1)-N(2)	-1.9(13)
C(2)-C(1)-N(1)-Os(1)	179.3(9)
C(1)-N(1)-N(2)-C(3)	1.3(12)
Os(1)-N(1)-N(2)-C(3)	-179.8(8)
C(1)-N(1)-N(2)-B(1)	-178.4(10)
Os(1)-N(1)-N(2)-B(1)	0.5(12)
C(2)-C(3)-N(2)-N(1)	-0.1(15)
C(2)-C(3)-N(2)-B(1)	179.6(13)
N(6)-B(1)-N(2)-N(1)	57.9(12)
N(4)-B(1)-N(2)-N(1)	-57.7(12)
N(6)-B(1)-N(2)-C(3)	-121.7(13)
N(4)-B(1)-N(2)-C(3)	122.7(13)
C(5)-C(4)-N(3)-N(4)	-0.9(11)
C(5)-C(4)-N(3)-Os(1)	178.6(7)
C(5)-C(6)-N(4)-N(3)	-1.7(12)
C(5)-C(6)-N(4)-B(1)	-177.6(10)
C(4)-N(3)-N(4)-C(6)	1.6(11)
Os(1)-N(3)-N(4)-C(6)	-178.0(7)
C(4)-N(3)-N(4)-B(1)	178.1(9)
Os(1)-N(3)-N(4)-B(1)	-1.5(11)
N(2)-B(1)-N(4)-C(6)	-126.0(11)
N(6)-B(1)-N(4)-C(6)	118.2(12)
N(2)-B(1)-N(4)-N(3)	58.5(12)
N(6)-B(1)-N(4)-N(3)	-57.4(11)
C(8)-C(7)-N(5)-N(6)	2.7(12)
C(8)-C(7)-N(5)-Os(1)	-179.9(8)
C(8)-C(9)-N(6)-N(5)	0.8(11)
C(8)-C(9)-N(6)-B(1)	179.7(10)
C(7)-N(5)-N(6)-C(9)	-2.1(11)
Os(1)-N(5)-N(6)-C(9)	180.0(7)
C(7)-N(5)-N(6)-B(1)	178.9(9)
Os(1)-N(5)-N(6)-B(1)	0.9(11)
N(2)-B(1)-N(6)-C(9)	122.6(11)
N(4)-B(1)-N(6)-C(9)	-121.5(11)
N(2)-B(1)-N(6)-N(5)	-58.6(11)
N(4)-B(1)-N(6)-N(5)	57.3(11)
C(12)-C(11)-N(8)-N(9)	-1.8(15)
C(12)-C(11)-N(8)-Os(2)	180.0(10)
C(12)-C(13)-N(9)-N(8)	0.0(16)
C(12)-C(13)-N(9)-B(2)	-177.2(13)
C(11)-N(8)-N(9)-C(13)	1.1(13)
Os(2)-N(8)-N(9)-C(13)	179.6(8)
C(11)-N(8)-N(9)-B(2)	178.8(10)
Os(2)-N(8)-N(9)-B(2)	-2.8(12)

N(13)-B(2)-N(9)-C(13)	-122.4(13)
N(11)-B(2)-N(9)-C(13)	119.9(14)
N(13)-B(2)-N(9)-N(8)	60.7(12)
N(11)-B(2)-N(9)-N(8)	-57.0(11)
C(15)-C(14)-N(10)-N(11)	-1.2(10)
C(15)-C(14)-N(10)-Os(2)	177.2(7)
C(15)-C(16)-N(11)-N(10)	0.4(12)
C(15)-C(16)-N(11)-B(2)	-174.7(10)
C(14)-N(10)-N(11)-C(16)	0.5(11)
Os(2)-N(10)-N(11)-C(16)	-178.1(6)
C(14)-N(10)-N(11)-B(2)	176.4(8)
Os(2)-N(10)-N(11)-B(2)	-2.3(11)
N(13)-B(2)-N(11)-C(16)	118.8(11)
N(9)-B(2)-N(11)-C(16)	-125.4(11)
N(13)-B(2)-N(11)-N(10)	-55.9(12)
N(9)-B(2)-N(11)-N(10)	59.9(11)
C(18)-C(17)-N(12)-N(13)	2.5(13)
C(18)-C(17)-N(12)-Os(2)	-179.5(8)
C(18)-C(19)-N(13)-N(12)	-2.3(13)
C(18)-C(19)-N(13)-B(2)	175.9(11)
C(17)-N(12)-N(13)-C(19)	0.0(12)
Os(2)-N(12)-N(13)-C(19)	-178.4(7)
C(17)-N(12)-N(13)-B(2)	-178.6(9)
Os(2)-N(12)-N(13)-B(2)	3.1(12)
N(11)-B(2)-N(13)-C(19)	-122.7(13)
N(9)-B(2)-N(13)-C(19)	121.3(12)
N(11)-B(2)-N(13)-N(12)	55.4(12)
N(9)-B(2)-N(13)-N(12)	-60.6(12)
C(7)-N(5)-Os(1)-N(1)	-134.7(10)
N(6)-N(5)-Os(1)-N(1)	42.4(6)
C(7)-N(5)-Os(1)-N(3)	138.0(10)
N(6)-N(5)-Os(1)-N(3)	-44.9(6)
C(7)-N(5)-Os(1)-N(7)	45.1(10)
N(6)-N(5)-Os(1)-N(7)	-137.8(6)
C(7)-N(5)-Os(1)-Cl(1)	-42.9(10)
N(6)-N(5)-Os(1)-Cl(1)	134.2(6)
C(7)-N(5)-Os(1)-Cl(2)	26(25)
N(6)-N(5)-Os(1)-Cl(2)	-157(24)
N(2)-N(1)-Os(1)-N(5)	-44.6(8)
C(1)-N(1)-Os(1)-N(5)	134.0(11)
N(2)-N(1)-Os(1)-N(3)	42.6(8)
C(1)-N(1)-Os(1)-N(3)	-138.9(11)
N(2)-N(1)-Os(1)-N(7)	174(100)
C(1)-N(1)-Os(1)-N(7)	-8(56)
N(2)-N(1)-Os(1)-Cl(1)	-133.1(8)
C(1)-N(1)-Os(1)-Cl(1)	45.5(11)
N(2)-N(1)-Os(1)-Cl(2)	135.6(8)
C(1)-N(1)-Os(1)-Cl(2)	-45.9(11)
N(4)-N(3)-Os(1)-N(5)	46.0(7)
C(4)-N(3)-Os(1)-N(5)	-133.4(9)
N(4)-N(3)-Os(1)-N(1)	-41.4(7)
C(4)-N(3)-Os(1)-N(1)	139.2(9)
N(4)-N(3)-Os(1)-N(7)	138.8(7)
C(4)-N(3)-Os(1)-N(7)	-40.6(9)
N(4)-N(3)-Os(1)-Cl(1)	34(4)
C(4)-N(3)-Os(1)-Cl(1)	-145(3)
N(4)-N(3)-Os(1)-Cl(2)	-134.4(7)
C(4)-N(3)-Os(1)-Cl(2)	46.1(9)
C(10)-N(7)-Os(1)-N(5)	42.7(8)
C(10)-N(7)-Os(1)-N(1)	-176(100)

C(10)-N(7)-Os(1)-N(3)	-44.4(8)
C(10)-N(7)-Os(1)-Cl(1)	131.2(7)
C(10)-N(7)-Os(1)-Cl(2)	-137.4(7)
C(17)-N(12)-Os(2)-N(10)	137.2(11)
N(13)-N(12)-Os(2)-N(10)	-45.1(7)
C(17)-N(12)-Os(2)-N(8)	-136.6(11)
N(13)-N(12)-Os(2)-N(8)	41.1(7)
C(17)-N(12)-Os(2)-N(14)	44.1(11)
N(13)-N(12)-Os(2)-N(14)	-138.2(7)
C(17)-N(12)-Os(2)-Cl(3)	-44.4(10)
N(13)-N(12)-Os(2)-Cl(3)	133.3(7)
C(17)-N(12)-Os(2)-Cl(4)	162(29)
N(13)-N(12)-Os(2)-Cl(4)	-21(30)
N(11)-N(10)-Os(2)-N(12)	44.9(7)
C(14)-N(10)-Os(2)-N(12)	-133.3(9)
N(11)-N(10)-Os(2)-N(8)	-42.9(7)
C(14)-N(10)-Os(2)-N(8)	138.9(9)
N(11)-N(10)-Os(2)-N(14)	138.2(7)
C(14)-N(10)-Os(2)-N(14)	-40.0(9)
N(11)-N(10)-Os(2)-Cl(3)	25(3)
C(14)-N(10)-Os(2)-Cl(3)	-153(2)
N(11)-N(10)-Os(2)-Cl(4)	-134.9(7)
C(14)-N(10)-Os(2)-Cl(4)	46.9(9)
C(11)-N(8)-Os(2)-N(12)	136.8(11)
N(9)-N(8)-Os(2)-N(12)	-41.2(8)
C(11)-N(8)-Os(2)-N(10)	-136.7(11)
N(9)-N(8)-Os(2)-N(10)	45.4(8)
C(11)-N(8)-Os(2)-N(14)	-77(14)
N(9)-N(8)-Os(2)-N(14)	105(14)
C(11)-N(8)-Os(2)-Cl(3)	47.9(11)
N(9)-N(8)-Os(2)-Cl(3)	-130.1(7)
C(11)-N(8)-Os(2)-Cl(4)	-43.6(11)
N(9)-N(8)-Os(2)-Cl(4)	138.4(7)
C(20)-N(14)-Os(2)-N(12)	44.3(8)
C(20)-N(14)-Os(2)-N(10)	-42.3(8)
C(20)-N(14)-Os(2)-N(8)	-102(14)
C(20)-N(14)-Os(2)-Cl(3)	133.2(8)
C(20)-N(14)-Os(2)-Cl(4)	-135.3(8)

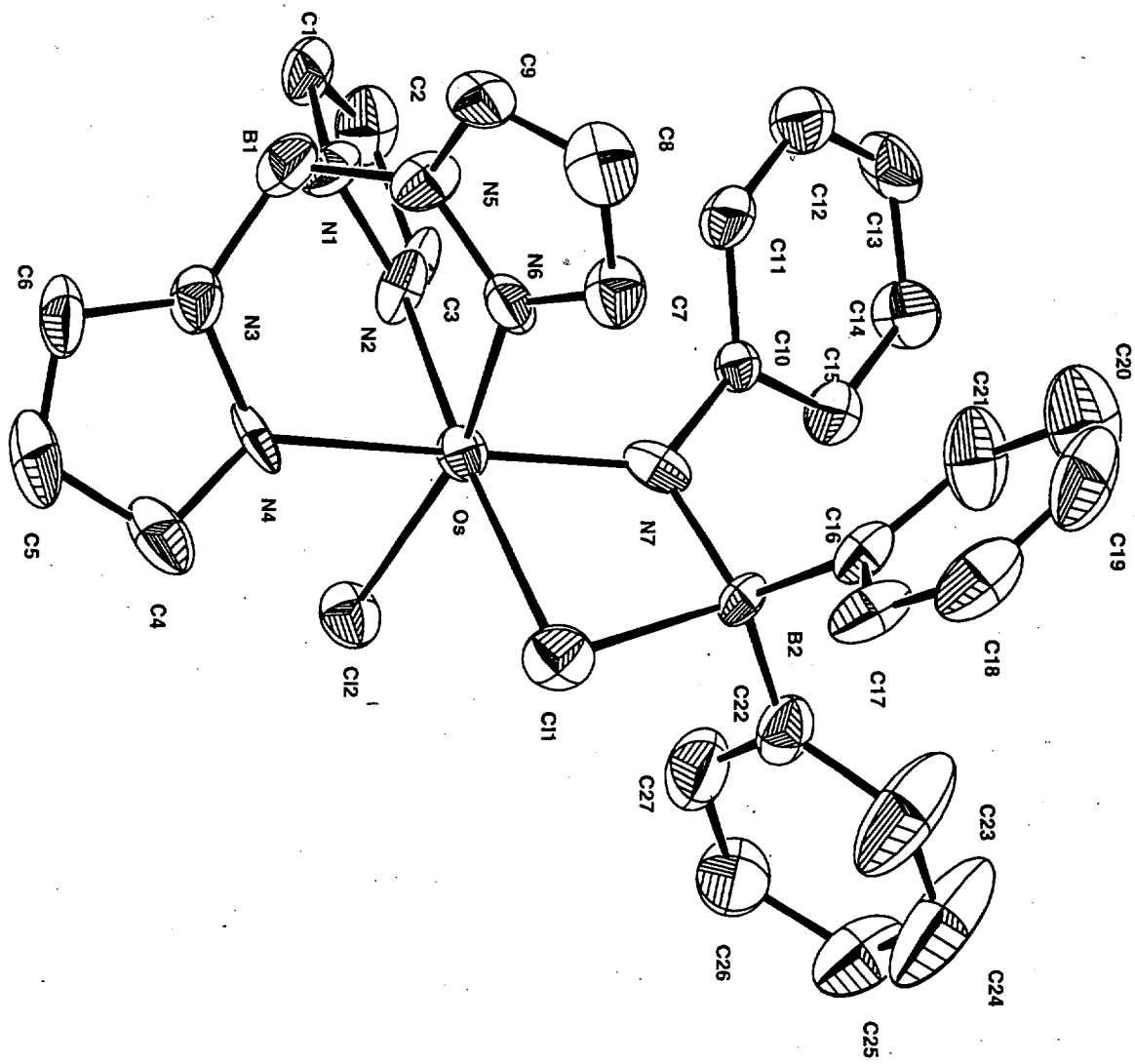
Symmetry transformations used to generate equivalent atoms:

References:

Instrument:	Nonius KappaCCD
	Nonius (1997). KappaCCD Operations Manual, Delft.
Data Collection Software:	Collect, (1998), Data Collection Software, Nonius.
Data Reduction:	DENZO
	Otinowski, Z., Minor, W., (1996). Processing of X-ray Diffraction Data Collected in Oscillation Mode, Methods in Enzymology, 276, 307-326., C. W. Carter, Jr., R. M. Sweet, Eds., Academic Press.
Cell Refinement:	HKL SCALEPACK
	ibid.
Structure Solution:	SIR92
	Altomare, A., Cascarano, G., Giacovazzo, C., Burla M.C., Polidori, G., Camalli, M.,(1994)., SIR. J. Appl. Cryst. 27, 435-442.
Structure Refinement:	SHELXL-97 (Sheldrick, 1997)
	Sheldrick, G.M. (1997). SHELXL97, Program for the Refinement of Crystal Structures. Univ. of Gottingen, Germany.
Molecular Graphics:	maXus, Zortep
maXus:	MacKay, S., Gilmore, C.J., Edwards, C., Tremayne M., Stewart, N., Shankland, K., (1998), "maXus: a computer program for the solution and refinement of crystal structures from diffraction data" University of Glasgow, Scotland, UK, Nonius BV, Delft, The Netherlands and MacScience Co. Ltd., Yokohama, Japan.
Zortep:	L. Zsolnai, G. Huttner, (1994), University of Heidelberg.

Crystal Data and Structural Refinement for $TpOs([N(Ph)(BPh_2)]Cl_2$ (**11**)

Identification code	tc972
Empirical formula	$C_{27}H_{25}B_2Cl_2N_7Os$
Formula weight	730.26
Temperature	183 K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C12/c1
Unit cell dimensions	a = 21.268(4) Å α = 90° b = 9.739(2) Å β = 108.88(2)° c = 28.269(5) Å γ = 90°
Volume	5540(1) $Å^3$
Z	8
Density (calculated)	1.751 Mg/m^3
Absorption coefficient	4.828 mm^{-1}
F(000)	2848
Crystal size	.28 x .24 x .10 mm
θ range for data collection	1.52 to 22.48°
Index ranges	$0 \le h \le 22$, $-1 \le k \le 10$, $-30 \le \ell \le 28$
Reflections collected	4258
Independent reflections	3629 (R_{int} = 0.0519)
Absorption correction	Semi-empirical from ψ-scans
Max. and min. transmission	1.000 and 0.722
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3601 / 0 / 352
Goodness-of-fit on F^2	1.051
Final R indices [I>2σ(I)]	R1 = 0.0387, wR2 = 0.0914
R indices (all data)	R1 = 0.0932, wR2 = 0.1436
Largest diff. peak and hole	2.580 and -1.395 $eÅ^{-3}$



Bond lengths (Å) and Angles (°) for $TpOs([N(Ph)(BPh_2)]Cl_2$ (11)

Os-N(7)	1.884(10)	Os-N(2)	2.029(9)
Os-N(6)	2.068(10)	Os-N(4)	2.100(9)
Os-Cl(2)	2.354(3)	Os-Cl(1)	2.404(3)
Cl(1)-B(2)	2.078(14)	B(1)-N(1)	1.53(2)
B(1)-N(5)	1.53(2)	B(1)-N(3)	1.53(2)
B(2)-C(22)	1.60(2)	B(2)-N(7)	1.60(2)
B(2)-C(16)	1.61(2)	N(1)-C(1)	1.34(2)
N(1)-N(2)	1.376(13)	N(2)-C(3)	1.319(14)
N(3)-C(6)	1.33(2)	N(3)-N(4)	1.392(13)
N(4)-C(4)	1.33(2)	N(5)-C(9)	1.34(2)
N(5)-N(6)	1.376(13)	N(6)-C(7)	1.33(2)
N(7)-C(10)	1.401(14)	C(1)-C(2)	1.39(2)
C(2)-C(3)	1.40(2)	C(4)-C(5)	1.41(2)
C(5)-C(6)	1.35(2)	C(7)-C(8)	1.38(2)
C(8)-C(9)	1.34(2)	C(10)-C(11)	1.39(2)
C(10)-C(15)	1.42(2)	C(11)-C(12)	1.36(2)
C(12)-C(13)	1.35(2)	C(13)-C(14)	1.40(2)
C(14)-C(15)	1.37(2)	C(16)-C(17)	1.36(2)
C(16)-C(21)	1.38(2)	C(17)-C(18)	1.37(2)
C(18)-C(19)	1.37(2)	C(19)-C(20)	1.36(2)
C(20)-C(21)	1.39(2)	C(22)-C(23)	1.33(2)
C(22)-C(27)	1.38(2)	C(23)-C(24)	1.37(2)
C(24)-C(25)	1.33(2)	C(25)-C(26)	1.37(2)
C(26)-C(27)	1.38(2)		

N(7)-Os-N(2)	97.5(4)	N(7)-Os-N(6)	93.8(4)
N(2)-Os-N(6)	89.2(4)	N(7)-Os-N(4)	172.7(3)
N(2)-Os-N(4)	87.5(4)	N(6)-Os-N(4)	80.8(4)
N(7)-Os-Cl(2)	100.3(3)	N(2)-Os-Cl(2)	88.5(3)
N(6)-Os-Cl(2)	165.9(3)	N(4)-Os-Cl(2)	85.2(3)
N(7)-Os-Cl(1)	75.8(3)	N(2)-Os-Cl(1)	172.5(3)
N(6)-Os-Cl(1)	94.7(3)	N(4)-Os-Cl(1)	99.5(3)
Cl(2)-Os-Cl(1)	89.24(11)	B(2)-Cl(1)-Os	80.0(4)
N(1)-B(1)-N(5)	107.6(10)	N(1)-B(1)-N(3)	107.3(11)
N(5)-B(1)-N(3)	106.6(11)	C(22)-B(2)-N(7)	115.5(10)

C(1)-N(1)-B(1)	130.5(11)	N(2)-N(1)-B(1)	120.5(9)
C(3)-N(2)-N(1)	107.4(9)	C(3)-N(2)-Os	132.5(8)
N(1)-N(2)-Os	120.1(6)	C(6)-N(3)-N(4)	107.8(10)
C(6)-N(3)-B(1)	131.6(12)	N(4)-N(3)-B(1)	120.3(9)
C(4)-N(4)-N(3)	108.6(10)	C(4)-N(4)-Os	133.4(9)
N(3)-N(4)-Os	117.9(7)	C(9)-N(5)-N(6)	108.4(10)
C(9)-N(5)-B(1)	131.7(11)	N(6)-N(5)-B(1)	119.6(10)
C(7)-N(6)-N(5)	105.9(10)	C(7)-N(6)-Os	134.2(9)
N(5)-N(6)-Os	119.8(7)	C(10)-N(7)-B(2)	119.3(10)
C(10)-N(7)-Os	127.8(7)	B(2)-N(7)-Os	112.1(7)
N(1)-C(1)-C(2)	108.6(11)	C(1)-C(2)-C(3)	104.7(11)
N(2)-C(3)-C(2)	110.2(11)	N(4)-C(4)-C(5)	107.0(13)
C(6)-C(5)-C(4)	107.5(12)	N(3)-C(6)-C(5)	109.2(12)
N(6)-C(7)-C(8)	110.6(12)	C(9)-C(8)-C(7)	105.4(12)
N(5)-C(9)-C(8)	109.6(11)	C(11)-C(10)-N(7)	121.9(10)
C(11)-C(10)-C(15)	117.1(10)	N(7)-C(10)-C(15)	121.0(10)
C(12)-C(11)-C(10)	122.0(11)	C(13)-C(12)-C(11)	120.2(13)
C(12)-C(13)-C(14)	120.8(12)	C(15)-C(14)-C(13)	119.3(12)
C(14)-C(15)-C(10)	120.6(12)	C(17)-C(16)-C(21)	116.3(12)
C(17)-C(16)-B(2)	122.9(12)	C(21)-C(16)-B(2)	120.6(11)
C(16)-C(17)-C(18)	123(2)	C(19)-C(18)-C(17)	120.6(14)
C(20)-C(19)-C(18)	118(2)	C(19)-C(20)-C(21)	121(2)
C(16)-C(21)-C(20)	121.3(13)	C(23)-C(22)-C(27)	114.9(14)
C(23)-C(22)-B(2)	123.9(13)	C(27)-C(22)-B(2)	121.1(11)
C(22)-C(23)-C(24)	123(2)	C(25)-C(24)-C(23)	122(2)
C(24)-C(25)-C(26)	117(2)	C(25)-C(26)-C(27)	119.6(14)
C(22)-C(27)-C(26)	122.7(14)		

C(22)-B(2)-C(16)	116.5(10)	N(7)-B(2)-C(16)	114.9(10)
C(22)-B(2)-Cl(1)	108.8(8)	N(7)-B(2)-Cl(1)	92.0(7)
C(16)-B(2)-Cl(1)	105.4(8)	C(1)-N(1)-N(2)	108.9(9)

Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for $TpOs([N(Ph)(BPh_2)])Cl_2$ (**11**)

	U11	U22	U33	U23	U13	U12
Os	24(1)	27(1)	20(1)	-1(1)	5(1)	2(1)
Cl(1)	44(2)	45(2)	32(2)	3(2)	20(2)	-2(2)
Cl(2)	36(2)	31(2)	33(2)	-4(1)	8(2)	6(1)
B(1)	33(9)	35(9)	44(10)	-5(8)	3(8)	-11(7)
B(2)	14(7)	31(9)	40(9)	2(7)	11(6)	-6(6)
N(1)	26(6)	20(6)	46(7)	-7(5)	14(5)	-4(5)
N(2)	15(5)	43(7)	25(5)	-15(5)	12(4)	-3(5)
N(3)	28(6)	32(7)	36(7)	-10(5)	2(5)	0(5)
N(4)	35(6)	30(7)	20(5)	0(5)	-2(4)	24(5)
N(5)	38(6)	23(6)	38(6)	-15(5)	18(5)	-5(5)
N(6)	26(6)	32(6)	31(6)	10(5)	7(5)	9(5)
N(7)	40(6)	14(6)	27(6)	1(4)	16(5)	14(5)
C(1)	15(6)	49(9)	52(9)	7(7)	12(6)	0(6)
C(2)	28(7)	61(10)	37(8)	2(7)	17(6)	5(7)
C(3)	13(6)	45(8)	40(7)	-13(7)	5(5)	-6(6)
C(4)	48(9)	35(9)	39(8)	0(6)	1(7)	21(7)
C(5)	44(9)	64(12)	26(7)	-13(7)	-12(6)	15(8)
C(6)	28(8)	45(10)	42(8)	-17(7)	-14(7)	6(7)
C(7)	36(8)	40(9)	34(8)	-6(6)	6(6)	3(7)
C(8)	53(10)	48(10)	39(8)	-12(7)	9(7)	8(8)
C(9)	48(9)	17(7)	35(7)	-8(6)	8(6)	0(6)
C(10)	21(6)	23(9)	18(6)	-1(5)	3(5)	-1(5)
C(11)	28(7)	30(8)	33(7)	-8(6)	5(6)	-5(6)
C(12)	40(8)	42(8)	31(8)	1(7)	7(6)	-4(7)
C(13)	43(8)	53(11)	26(8)	16(7)	6(6)	6(7)
C(14)	59(9)	49(9)	13(6)	-1(6)	0(6)	-12(8)
C(15)	31(7)	36(8)	33(8)	-3(6)	2(6)	-6(6)
C(16)	23(6)	38(7)	45(8)	-4(7)	15(6)	-11(7)
C(17)	49(9)	33(7)	61(9)	-15(7)	31(7)	-17(8)
C(18)	45(9)	53(9)	78(11)	-26(9)	43(9)	-15(8)
C(19)	27(8)	81(13)	84(13)	-25(11)	18(9)	-2(8)
C(20)	48(10)	101(14)	60(11)	-1(10)	25(9)	22(10)
C(21)	29(8)	92(12)	49(9)	-7(9)	14(7)	18(9)
C(22)	28(7)	54(9)	27(7)	1(6)	11(6)	-9(7)
C(23)	44(10)	97(15)	156(19)	-78(14)	53(12)	-25(10)
C(24)	46(11)	101(15)	195(25)	-92(17)	58(14)	-30(11)
C(25)	58(11)	58(11)	78(11)	-20(9)	38(9)	-17(9)
C(26)	47(9)	38(11)	65(10)	-12(7)	12(7)	4(7)
C(27)	37(9)	45(10)	80(12)	-12(8)	0(8)	-4(7)

Hydrogen Coordinates (10^4) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for $TpOs([N(Ph)(BPh_2)]Cl_2$ (**11**)

	x	y	z	U(eq)
H(1B)	5727(7)	1785(16)	382(6)	50
H(1A)	5507(6)	2051(14)	1321(5)	50
H(2A)	5791(6)	3744(14)	2042(5)	50
H(3A)	6487(5)	5590(14)	1823(4)	50
H(4A)	6137(7)	6519(14)	-311(5)	50
H(5A)	5127(7)	5193(16)	-856(5)	50
H(6A)	5063(6)	3025(15)	-410(5)	50
H(7A)	8258(7)	3291(14)	726(5)	50
H(8A)	8102(7)	765(15)	553(5)	50
H(9A)	6924(7)	254(12)	462(4)	50
H(11A)	7595(6)	3014(13)	1659(5)	50
H(12A)	7814(6)	2077(14)	2440(4)	50
H(13A)	8297(6)	3382(15)	3145(5)	50
H(14A)	8570(7)	5701(15)	3075(4)	50
H(15A)	8374(6)	6666(13)	2290(4)	50
H(17A)	9021(7)	5878(14)	583(5)	50
H(18A)	9962(7)	4631(16)	613(6)	50
H(19A)	10480(7)	3238(18)	1294(7)	50
H(20A)	10109(8)	3302(19)	1985(6)	50
H(21A)	9194(6)	4671(17)	1970(5)	50
H(23A)	9494(8)	7844(20)	1557(8)	50
H(24A)	9729(9)	10013(21)	1886(9)	50
H(25A)	8940(7)	11332(17)	2060(6)	50
H(26A)	7844(7)	10500(14)	1821(5)	50
H(27A)	7604(7)	8330(15)	1448(6)	50

Atomic Coordinates (10^4) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for $TpOs([N(Ph)(BPh_2)]Cl_2$ (**11**)

	x	y	z	U(eq)
Os	7022(1)	5297(1)	848(1)	24(1)
Cl(1)	7781(2)	6464(3)	513(1)	38(1)
Cl(2)	6483(2)	7401(3)	860(1)	34(1)
B(1)	6110(7)	2614(16)	547(6)	40(4)
B(2)	8368(6)	6312(14)	1259(5)	28(3)
N(1)	6103(5)	3245(10)	1040(4)	30(2)
N(2)	6446(4)	4437(10)	1216(3)	26(2)
N(3)	5879(5)	3720(10)	146(4)	34(3)
N(4)	6242(5)	4927(10)	181(3)	31(3)
N(5)	6834(5)	2299(10)	598(4)	32(2)
N(6)	7289(5)	3352(10)	689(4)	30(2)
N(7)	7795(5)	5534(9)	1404(3)	26(2)
C(1)	5787(6)	2844(14)	1359(5)	38(3)
C(2)	5931(6)	3770(14)	1751(5)	41(3)
C(3)	6325(5)	4777(14)	1630(4)	34(3)
C(4)	5973(7)	5660(14)	-233(5)	44(4)
C(5)	5424(7)	4909(16)	-536(5)	50(4)
C(6)	5388(6)	3736(15)	-291(5)	44(4)
C(7)	7852(7)	2791(14)	672(5)	38(3)
C(8)	7772(7)	1400(15)	582(5)	48(4)
C(9)	7134(7)	1137(12)	533(4)	35(3)
C(10)	7939(5)	4949(11)	1880(4)	21(3)
C(11)	7793(6)	3583(13)	1946(5)	31(3)
C(12)	7922(6)	3021(14)	2407(4)	39(3)
C(13)	8208(6)	3785(15)	2820(5)	42(4)
C(14)	8370(7)	5163(15)	2780(4)	43(4)
C(15)	8250(6)	5729(13)	2317(4)	35(3)
C(16)	8989(6)	5365(14)	1260(5)	35(3)
C(17)	9239(7)	5338(14)	874(5)	45(3)
C(18)	9796(7)	4602(16)	890(6)	53(4)
C(19)	10108(7)	3798(18)	1293(7)	64(5)
C(20)	9885(8)	3834(19)	1693(6)	68(5)
C(21)	9337(6)	4629(17)	1681(5)	56(4)
C(22)	8539(6)	7821(14)	1483(4)	36(3)
C(23)	9144(8)	8379(20)	1609(8)	94(7)
C(24)	9288(9)	9658(21)	1818(9)	110(9)
C(25)	8823(7)	10459(17)	1897(6)	61(4)
C(26)	8188(7)	9950(14)	1766(5)	51(4)
C(27)	8053(7)	8661(15)	1552(6)	59(4)

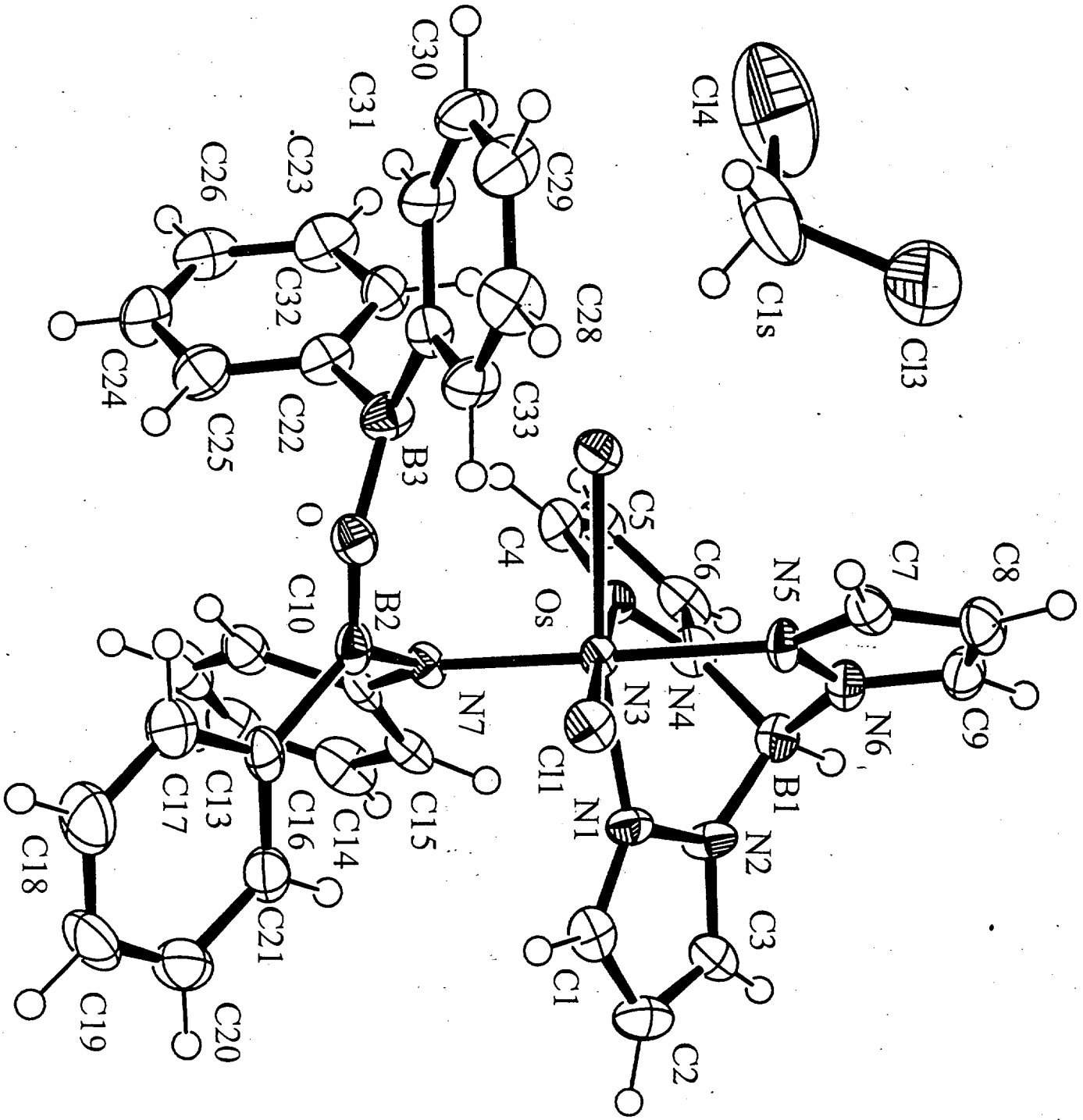


Figure 1. ORTEP of $TpOs[N(Ph)(BPhOBPh_2)]Cl_2$ (12).

Table 1. Crystal data and structural refinement for **$TpOs[N(Ph)(BPhOBPh_2)]Cl_2$ (12)**.

Compound C34H32B3Cl4N7OOs	shelxl
Empirical formula	C34 H32 B3 Cl4 N7 O Os
Formula weight	919.10
Temperature	183(2) K
Wavelength	0.71073 A
Crystal description/color	prism / red
Crystal system, space group	Triclinic, P -1 (No. 2)
Unit cell dimensions	a = 11.578(3) A alpha = 91.31(2) deg. b = 12.343(5) A beta = 110.59(2) deg. c = 15.482(5) A gamma = 115.35(2) deg.
Volume	1832.0(11) A^3
Z, Calculated density	2, 1.666 Mg/m^3
Absorption coefficient	3.811 mm^-1
F(000)	904
Crystal size	0.38 x 0.34 x 0.30 mm
Reflections for indexing	24
Theta range for data collection	1.44 to 24.97 deg.
Index ranges	-13<=h<=13, -14<=k<=13, -14<=l<=17
Reflections collected / unique	6391 / 5974 [R(int) = 0.0298]
Completeness to theta = 24.97	92.8%
Absorption correction	Psi scan
Max. and min. transmission	0.3943 and 0.3253
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5974 / 0 / 451
Goodness-of-fit on F^2	1.099
Final R indices [I>2sigma(I)]	*R1 = 0.0592, wR2 = 0.1459
R indices (all data) *Report these R factors	R1 = 0.0748, *wR2 = 0.1564
Weighting scheme	calc w=1/[\s^2^(Fo^2^)+(0.1228P)^2^+0.3476P] where P=
Largest diff. peak and hole	4.345 and -5.910 e.A^-3

Table 2. Atomic coordinates (10^4) and equivalent isotropic displacement parameters ($A^2 \cdot 10^3$) for **TpOs[N(Ph)(BPhOBPh$_2$)]Cl$_2$ (12)**. U (eq) is defined as one third of the trace orthogonalized Uij tensor.

	x	y	z	U(eq)
Os	341(1)	686(1)	2669(1)	19(1)
Cl(1)	1608(2)	1611(2)	4287(2)	28(1)
Cl(2)	1633(2)	2523(2)	2256(2)	28(1)
B(1)	-116(11)	-1833(10)	1711(9)	31(2)
B(2)	-585(10)	2266(10)	3350(7)	25(2)
B(3)	859(11)	3974(9)	2679(8)	30(2)
N(1)	-521(7)	-977(6)	3011(5)	25(2)
N(2)	-676(8)	-1993(6)	2476(5)	26(2)
N(3)	-664(7)	-140(6)	1278(5)	23(2)
N(4)	-821(8)	-1267(7)	997(6)	30(2)
N(5)	1864(7)	214(7)	2681(5)	26(2)
N(6)	1449(8)	-922(7)	2208(5)	28(2)
N(7)	-1078(7)	1144(6)	2640(5)	22(2)
C(1)	-945(9)	-1341(8)	3695(7)	29(2)
C(2)	-1435(10)	-2597(9)	3618(7)	37(2)
C(3)	-1252(10)	-2959(9)	2869(7)	32(2)
C(4)	-1313(9)	181(9)	492(6)	30(2)
C(5)	-1846(9)	-691(9)	-275(7)	31(2)
C(6)	-1516(9)	-1594(9)	53(7)	33(2)
C(7)	3247(9)	751(9)	3095(7)	28(2)
C(8)	3755(10)	15(9)	2896(7)	36(2)
C(9)	2603(10)	-1040(9)	2335(7)	35(2)
C(10)	-2502(9)	524(9)	2067(7)	26(2)
C(11)	-3274(10)	1170(9)	1875(7)	33(2)
C(12)	-4654(11)	596(12)	1307(8)	46(3)
C(13)	-5340(10)	-638(11)	911(8)	44(3)
C(14)	-4593(10)	-1290(10)	1098(7)	41(3)
C(15)	-3189(9)	-732(8)	1684(7)	29(2)
C(16)	-1240(9)	2151(9)	4099(7)	28(2)
C(17)	-1030(12)	3216(10)	4605(8)	40(2)
C(18)	-1566(15)	3194(13)	5258(9)	56(3)
C(19)	-2376(13)	2090(12)	5441(9)	49(3)
C(20)	-2603(11)	1023(11)	4960(8)	44(3)
C(21)	-2050(10)	1041(9)	4289(7)	34(2)
C(22)	-247(10)	3896(8)	1696(7)	31(2)
C(23)	-1171(12)	3687(10)	4(8)	45(3)
C(24)	-2239(11)	4233(10)	859(9)	45(3)
C(25)	-1289(11)	4177(9)	1706(8)	40(2)
C(26)	-2167(10)	4007(9)	39(8)	41(3)
C(27)	-223(10)	3654(9)	828(7)	34(2)
C(28)	2377(9)	5097(8)	3124(6)	26(2)
C(29)	3295(10)	5269(9)	4041(7)	33(2)
C(30)	4615(10)	6251(9)	4412(7)	38(2)
C(31)	5036(10)	7092(9)	3885(8)	42(3)
C(32)	4168(10)	6951(9)	2970(8)	39(2)
C(33)	2847(10)	5973(9)	2606(7)	33(2)
O	327(6)	3382(5)	3323(4)	28(1)
Cl(3)	6164(5)	3947(4)	3036(5)	116(2)
Cl(4)	4784(6)	4693(7)	1374(4)	132(2)
C(1S)	5124(15)	4656(14)	2560(13)	83(5)

Table 3. Bond Lengths (Å) and angles (deg) for **TpOs[N(Ph)(BPhOBPh$_2$)]Cl$_2$ (12)**.

Os-N(7)	1.940(7)
Os-N(3)	2.038(7)
Os-N(1)	2.038(7)
Os-N(5)	2.075(7)
Os-Cl(1)	2.363(2)
Os-Cl(2)	2.371(2)
B(1)-N(4)	1.505(13)
B(1)-N(2)	1.516(15)
B(1)-N(6)	1.541(13)
B(1)-H(1B1)	1.0228
B(2)-O	1.343(13)
B(2)-N(7)	1.506(12)
B(2)-C(16)	1.572(14)
B(3)-O	1.409(13)
B(3)-C(22)	1.575(13)
B(3)-C(28)	1.582(13)
N(1)-C(1)	1.329(13)
N(1)-N(2)	1.395(10)
N(2)-C(3)	1.370(12)
N(3)-C(4)	1.355(11)
N(3)-N(4)	1.363(10)
N(4)-C(6)	1.348(12)
N(5)-C(7)	1.328(12)
N(5)-N(6)	1.365(10)
N(6)-C(9)	1.353(12)
N(7)-C(10)	1.397(11)
C(1)-C(2)	1.390(13)
C(1)-H(1A)	0.9600
C(2)-C(3)	1.349(15)
C(2)-H(2A)	0.9602
C(3)-H(3A)	0.9599
C(4)-C(5)	1.344(13)
C(4)-H(4A)	0.9600
C(5)-C(6)	1.377(14)
C(5)-H(5A)	0.9600
C(6)-H(6A)	0.9600
C(7)-C(8)	1.356(13)
C(7)-H(7A)	0.9600
C(8)-C(9)	1.370(14)
C(8)-H(8A)	0.9600
C(9)-H(9A)	0.9599
C(10)-C(11)	1.399(13)
C(10)-C(15)	1.400(13)
C(11)-C(12)	1.357(14)
C(11)-H(11A)	0.9601
C(12)-C(13)	1.381(16)
C(12)-H(12A)	0.9598
C(13)-C(14)	1.382(16)
C(13)-H(13A)	0.9602
C(14)-C(15)	1.384(13)
C(14)-H(14A)	0.9601
C(15)-H(15A)	0.9599
C(16)-C(17)	1.394(14)
C(16)-C(21)	1.399(14)
C(17)-C(18)	1.355(17)
C(17)-H(17A)	0.9602

C(18)-C(19)	1.388(17)
C(18)-H(18A)	0.9600
C(19)-C(20)	1.370(16)
C(19)-H(19A)	0.9601
C(20)-C(21)	1.395(15)
C(20)-H(20A)	0.9602
C(21)-H(21A)	0.9600
C(22)-C(27)	1.383(15)
C(22)-C(25)	1.395(15)
C(23)-C(27)	1.376(14)
C(23)-C(26)	1.386(16)
C(23)-H(23A)	0.9600
C(24)-C(26)	1.330(17)
C(24)-C(25)	1.411(14)
C(24)-H(24A)	0.9599
C(25)-H(25A)	0.9601
C(26)-H(26A)	0.9600
C(27)-H(27A)	0.9600
C(28)-C(29)	1.386(13)
C(28)-C(33)	1.397(13)
C(29)-C(30)	1.379(13)
C(29)-H(29A)	0.9601
C(30)-C(31)	1.367(15)
C(30)-H(30A)	0.9601
C(31)-C(32)	1.372(14)
C(31)-H(31A)	0.9602
C(32)-C(33)	1.377(14)
C(32)-H(32A)	0.9600
C(33)-H(33A)	0.9600
Cl(3)-C(1S)	1.751(17)
Cl(4)-C(1S)	1.743(19)
C(1S)-H(1SA)	0.9600
C(1S)-H(1SB)	0.9602

N(7)-Os-N(3)	93.5(3)
N(7)-Os-N(1)	96.8(3)
N(3)-Os-N(1)	89.6(3)
N(7)-Os-N(5)	178.9(3)
N(3)-Os-N(5)	86.0(3)
N(1)-Os-N(5)	84.1(3)
N(7)-Os-Cl(1)	89.9(2)
N(3)-Os-Cl(1)	176.7(2)
N(1)-Os-Cl(1)	89.9(2)
N(5)-Os-Cl(1)	90.7(2)
N(7)-Os-Cl(2)	93.1(2)
N(3)-Os-Cl(2)	89.1(2)
N(1)-Os-Cl(2)	170.1(2)
N(5)-Os-Cl(2)	86.0(2)
Cl(1)-Os-Cl(2)	90.78(8)
N(4)-B(1)-N(2)	108.6(8)
N(4)-B(1)-N(6)	108.9(8)
N(2)-B(1)-N(6)	105.6(8)
N(4)-B(1)-H(1B1)	109.4
N(2)-B(1)-H(1B1)	111.5
N(6)-B(1)-H(1B1)	112.8
O-B(2)-N(7)	121.8(9)
O-B(2)-C(16)	118.7(8)
N(7)-B(2)-C(16)	119.3(8)
O-B(3)-C(22)	116.4(8)
O-B(3)-C(28)	116.1(8)

C(22)-B(3)-C(28)	121.4(8)
C(1)-N(1)-N(2)	108.2(7)
C(1)-N(1)-Os	133.6(6)
N(2)-N(1)-Os	118.1(6)
C(3)-N(2)-N(1)	105.2(7)
C(3)-N(2)-B(1)	134.4(8)
N(1)-N(2)-B(1)	120.2(7)
C(4)-N(3)-N(4)	106.7(7)
C(4)-N(3)-Os	133.0(6)
N(4)-N(3)-Os	120.2(6)
C(6)-N(4)-N(3)	107.9(8)
C(6)-N(4)-B(1)	132.6(9)
N(3)-N(4)-B(1)	119.1(8)
C(7)-N(5)-N(6)	106.6(7)
C(7)-N(5)-Os	135.0(6)
N(6)-N(5)-Os	118.3(5)
C(9)-N(6)-N(5)	108.1(7)
C(9)-N(6)-B(1)	131.8(8)
N(5)-N(6)-B(1)	120.0(7)
C(10)-N(7)-B(2)	116.8(7)
C(10)-N(7)-Os	127.5(6)
B(2)-N(7)-Os	115.6(5)
N(1)-C(1)-C(2)	110.3(9)
N(1)-C(1)-H(1A)	124.7
C(2)-C(1)-H(1A)	124.9
C(3)-C(2)-C(1)	104.8(9)
C(3)-C(2)-H(2A)	127.9
C(1)-C(2)-H(2A)	127.4
C(2)-C(3)-N(2)	111.5(9)
C(2)-C(3)-H(3A)	125.5
N(2)-C(3)-H(3A)	123.0
C(5)-C(4)-N(3)	110.7(9)
C(5)-C(4)-H(4A)	124.5
N(3)-C(4)-H(4A)	124.8
C(4)-C(5)-C(6)	105.5(8)
C(4)-C(5)-H(5A)	128.6
C(6)-C(5)-H(5A)	125.8
N(4)-C(6)-C(5)	109.2(9)
N(4)-C(6)-H(6A)	125.0
C(5)-C(6)-H(6A)	125.8
N(5)-C(7)-C(8)	111.4(9)
N(5)-C(7)-H(7A)	123.4
C(8)-C(7)-H(7A)	125.1
C(7)-C(8)-C(9)	105.1(9)
C(7)-C(8)-H(8A)	127.5
C(9)-C(8)-H(8A)	127.4
N(6)-C(9)-C(8)	108.8(9)
N(6)-C(9)-H(9A)	125.7
C(8)-C(9)-H(9A)	125.5
N(7)-C(10)-C(11)	119.4(8)
N(7)-C(10)-C(15)	121.9(8)
C(11)-C(10)-C(15)	118.7(8)
C(12)-C(11)-C(10)	120.6(10)
C(12)-C(11)-H(11A)	120.5
C(10)-C(11)-H(11A)	118.8
C(11)-C(12)-C(13)	121.3(10)
C(11)-C(12)-H(12A)	119.3
C(13)-C(12)-H(12A)	119.4
C(12)-C(13)-C(14)	118.8(9)
C(12)-C(13)-H(13A)	121.2

C(14)-C(13)-H(13A)	120.0
C(13)-C(14)-C(15)	121.2(10)
C(13)-C(14)-H(14A)	119.6
C(15)-C(14)-H(14A)	119.2
C(14)-C(15)-C(10)	119.4(9)
C(14)-C(15)-H(15A)	120.3
C(10)-C(15)-H(15A)	120.3
C(17)-C(16)-C(21)	116.8(9)
C(17)-C(16)-B(2)	118.8(9)
C(21)-C(16)-B(2)	124.4(9)
C(18)-C(17)-C(16)	122.4(11)
C(18)-C(17)-H(17A)	119.1
C(16)-C(17)-H(17A)	118.5
C(17)-C(18)-C(19)	120.6(11)
C(17)-C(18)-H(18A)	120.6
C(19)-C(18)-H(18A)	118.8
C(20)-C(19)-C(18)	118.7(10)
C(20)-C(19)-H(19A)	120.4
C(18)-C(19)-H(19A)	120.9
C(19)-C(20)-C(21)	120.8(10)
C(19)-C(20)-H(20A)	119.9
C(21)-C(20)-H(20A)	119.3
C(20)-C(21)-C(16)	120.6(9)
C(20)-C(21)-H(21A)	120.6
C(16)-C(21)-H(21A)	118.7
C(27)-C(22)-C(25)	117.0(9)
C(27)-C(22)-B(3)	125.7(9)
C(25)-C(22)-B(3)	117.2(9)
C(27)-C(23)-C(26)	119.3(11)
C(27)-C(23)-H(23A)	120.6
C(26)-C(23)-H(23A)	120.1
C(26)-C(24)-C(25)	120.8(11)
C(26)-C(24)-H(24A)	120.0
C(25)-C(24)-H(24A)	119.2
C(22)-C(25)-C(24)	120.2(11)
C(22)-C(25)-H(25A)	120.0
C(24)-C(25)-H(25A)	119.8
C(24)-C(26)-C(23)	120.3(10)
C(24)-C(26)-H(26A)	119.7
C(23)-C(26)-H(26A)	120.0
C(23)-C(27)-C(22)	122.4(10)
C(23)-C(27)-H(27A)	118.7
C(22)-C(27)-H(27A)	118.9
C(29)-C(28)-C(33)	116.9(8)
C(29)-C(28)-B(3)	122.1(8)
C(33)-C(28)-B(3)	121.0(8)
C(30)-C(29)-C(28)	121.0(9)
C(30)-C(29)-H(29A)	120.1
C(28)-C(29)-H(29A)	118.9
C(31)-C(30)-C(29)	120.4(9)
C(31)-C(30)-H(30A)	120.1
C(29)-C(30)-H(30A)	119.5
C(30)-C(31)-C(32)	120.5(9)
C(30)-C(31)-H(31A)	119.6
C(32)-C(31)-H(31A)	119.9
C(31)-C(32)-C(33)	118.8(9)
C(31)-C(32)-H(32A)	120.5
C(33)-C(32)-H(32A)	120.7
C(32)-C(33)-C(28)	122.3(9)
C(32)-C(33)-H(33A)	119.0

C(28)-C(33)-H(33A)	118.8
B(2)-O-B(3)	138.5(8)
Cl(4)-C(1S)-Cl(3)	113.1(8)
Cl(4)-C(1S)-H(1SA)	109.9
Cl(3)-C(1S)-H(1SA)	109.3
Cl(4)-C(1S)-H(1SB)	108.2
Cl(3)-C(1S)-H(1SB)	108.5
H(1SA)-C(1S)-H(1SB)	107.8

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($A^2 \cdot 10^3$) for **TpOs[N(Ph)(BPhOBPh$_2$)]Cl$_2$ (12)**. The anisotropic displacement exponent takes the form: $-2\pi^2(h^2 \cdot a^2 \cdot U_{11} + ... + 2h \cdot k \cdot a \cdot b U_{12})$.

	U11	U22	U33	U23	U13	U12
Os	15(1)	27(1)	13(1)	3(1)	2(1)	10(1)
Cl(1)	22(1)	38(1)	15(1)	1(1)	1(1)	12(1)
Cl(2)	24(1)	31(1)	26(1)	8(1)	11(1)	11(1)
B(1)	29(6)	35(6)	34(7)	10(5)	13(5)	19(5)
B(2)	24(5)	39(5)	19(5)	5(4)	5(4)	23(4)
B(3)	28(5)	31(5)	26(6)	8(4)	5(5)	14(4)
N(1)	25(4)	26(4)	22(4)	10(3)	8(3)	10(3)
N(2)	41(4)	13(3)	17(4)	0(3)	11(3)	9(3)
N(3)	24(4)	28(4)	17(4)	4(3)	8(3)	14(3)
N(4)	29(4)	33(4)	21(4)	-1(3)	5(3)	12(3)
N(5)	18(4)	35(4)	25(4)	3(3)	4(3)	17(3)
N(6)	28(4)	37(4)	24(4)	5(3)	9(3)	21(3)
N(7)	12(3)	31(4)	19(4)	3(3)	3(3)	9(3)
C(1)	22(4)	37(5)	19(5)	-2(4)	1(4)	12(4)
C(2)	34(5)	39(5)	28(6)	13(4)	10(4)	10(4)
C(3)	29(5)	36(5)	33(6)	8(4)	17(4)	13(4)
C(4)	18(4)	48(5)	17(5)	5(4)	-2(4)	17(4)
C(5)	21(4)	52(6)	17(5)	7(4)	4(4)	16(4)
C(6)	21(5)	41(5)	21(5)	-4(4)	7(4)	4(4)
C(7)	25(5)	38(5)	22(5)	6(4)	9(4)	15(4)
C(8)	24(5)	53(6)	31(6)	10(5)	9(4)	21(5)
C(9)	36(5)	48(6)	33(6)	14(4)	14(4)	29(5)
C(10)	19(4)	43(5)	23(5)	9(4)	13(4)	16(4)
C(11)	27(5)	48(6)	26(6)	11(4)	11(4)	20(4)
C(12)	27(5)	85(9)	34(6)	20(6)	11(5)	32(6)
C(13)	18(5)	73(8)	28(6)	10(5)	1(4)	16(5)
C(14)	19(5)	53(6)	25(6)	-5(5)	0(4)	3(4)
C(15)	22(5)	39(5)	24(5)	5(4)	13(4)	10(4)
C(16)	24(5)	45(5)	22(5)	6(4)	7(4)	23(4)
C(17)	48(6)	41(6)	41(7)	6(5)	23(5)	25(5)
C(18)	76(9)	73(8)	48(8)	14(6)	36(7)	51(7)
C(19)	56(7)	80(8)	38(7)	23(6)	34(6)	42(7)
C(20)	40(6)	57(7)	44(7)	25(5)	21(5)	25(5)
C(21)	34(5)	43(5)	32(6)	9(4)	14(4)	24(4)
C(22)	28(5)	29(5)	27(6)	4(4)	5(4)	11(4)
C(23)	50(7)	48(6)	26(6)	6(5)	7(5)	21(5)
C(24)	26(5)	54(6)	55(8)	20(5)	8(5)	25(5)
C(25)	42(6)	42(6)	35(6)	10(5)	12(5)	21(5)
C(26)	26(5)	39(6)	33(7)	10(4)	-4(4)	7(4)
C(27)	29(5)	47(6)	29(6)	12(4)	9(4)	23(4)
C(28)	26(5)	33(5)	19(5)	4(4)	7(4)	15(4)
C(29)	31(5)	38(5)	26(5)	13(4)	5(4)	18(4)
C(30)	27(5)	48(6)	20(5)	0(4)	-4(4)	12(4)
C(31)	19(5)	33(5)	53(7)	9(5)	1(4)	6(4)
C(32)	31(5)	40(5)	43(7)	22(5)	9(5)	17(4)
C(33)	25(5)	41(5)	28(6)	13(4)	2(4)	17(4)
O	22(3)	32(3)	27(4)	4(3)	9(3)	12(3)
Cl(3)	92(3)	78(3)	217(7)	62(3)	92(4)	49(3)
Cl(4)	81(3)	205(7)	98(4)	-16(4)	17(3)	75(4)
C(1S)	40(7)	74(9)	124(15)	-16(9)	40(8)	13(7)

Table 5. Hydrogen coordinates (10^4) and isotropic displacement parameters ($A^2 \cdot 10^3$) for **TpOs[N(Ph)(BPhOBPh$_2$)]Cl$_2$ (12).**

	x	y	z	U(eq)
H(1B1)	-296	-2653	1383	35
H(1A)	-890	-806	4185	32
H(2A)	-1836	-3096	4006	41
H(3A)	-1500	-3785	2625	35
H(4A)	-1357	940	480	33
H(5A)	-2338	-699	-922	34
H(6A)	-1767	-2350	-325	36
H(7A)	3804	1571	3464	31
H(8A)	4715	199	3097	39
H(9A)	2614	-1756	2091	39
H(11A)	-2812	2025	2156	36
H(12A)	-5165	1056	1186	51
H(13A)	-6312	-1040	499	49
H(14A)	-5058	-2149	828	45
H(15A)	-2689	-1202	1824	32
H(17A)	-469	3991	4493	44
H(18A)	-1402	3942	5597	61
H(19A)	-2769	2071	5896	54
H(20A)	-3161	251	5077	49
H(21A)	-2213	292	3952	37
H(23A)	-1136	3508	-590	49
H(24A)	-2947	4431	877	49
H(25A)	-1368	4323	2290	44
H(26A)	-2821	4050	-530	45
H(27A)	483	3459	799	37
H(29A)	2992	4696	4422	36
H(30A)	5240	6340	5044	42
H(31A)	5950	7783	4156	46
H(32A)	4475	7530	2594	43
H(33A)	2226	5889	1974	37
H(1SA)	5568	5473	2921	91
H(1SB)	4249	4210	2616	91

Table 6. Torsion angles (deg) for **TpOs[N(Ph)(BPhOBPh$_2$)]Cl$_2$ (12)**.

N(7)-Os-N(1)-C(1)	-53.3(9)
N(3)-Os-N(1)-C(1)	-146.7(8)
N(5)-Os-N(1)-C(1)	127.3(9)
Cl(1)-Os-N(1)-C(1)	36.6(8)
Cl(2)-Os-N(1)-C(1)	130.7(11)
N(7)-Os-N(1)-N(2)	130.4(6)
N(3)-Os-N(1)-N(2)	37.0(6)
N(5)-Os-N(1)-N(2)	-49.0(6)
Cl(1)-Os-N(1)-N(2)	-139.7(6)
Cl(2)-Os-N(1)-N(2)	-45.5(16)
C(1)-N(1)-N(2)-C(3)	2.0(9)
Os-N(1)-N(2)-C(3)	179.2(6)
C(1)-N(1)-N(2)-B(1)	-172.8(8)
Os-N(1)-N(2)-B(1)	4.4(10)
N(4)-B(1)-N(2)-C(3)	127.1(11)
N(6)-B(1)-N(2)-C(3)	-116.2(11)
N(4)-B(1)-N(2)-N(1)	-59.9(11)
N(6)-B(1)-N(2)-N(1)	56.7(10)
N(7)-Os-N(3)-C(4)	43.8(8)
N(1)-Os-N(3)-C(4)	140.6(8)
N(5)-Os-N(3)-C(4)	-135.3(9)
Cl(1)-Os-N(3)-C(4)	-137(3)
Cl(2)-Os-N(3)-C(4)	-49.3(8)
N(7)-Os-N(3)-N(4)	-133.6(6)
N(1)-Os-N(3)-N(4)	-36.8(6)
N(5)-Os-N(3)-N(4)	47.3(6)
Cl(1)-Os-N(3)-N(4)	45(4)
Cl(2)-Os-N(3)-N(4)	133.4(6)
C(4)-N(3)-N(4)-C(6)	1.9(10)
Os-N(3)-N(4)-C(6)	179.9(6)
C(4)-N(3)-N(4)-B(1)	175.6(8)
Os-N(3)-N(4)-B(1)	-6.4(11)
N(2)-B(1)-N(4)-C(6)	-127.2(10)
N(6)-B(1)-N(4)-C(6)	118.3(11)
N(2)-B(1)-N(4)-N(3)	60.9(11)
N(6)-B(1)-N(4)-N(3)	-53.6(11)
N(7)-Os-N(5)-C(7)	83(14)
N(3)-Os-N(5)-C(7)	141.8(9)
N(1)-Os-N(5)-C(7)	-128.1(9)
Cl(1)-Os-N(5)-C(7)	-38.3(9)
Cl(2)-Os-N(5)-C(7)	52.5(9)
N(7)-Os-N(5)-N(6)	-101(14)
N(3)-Os-N(5)-N(6)	-42.0(6)
N(1)-Os-N(5)-N(6)	48.1(6)
Cl(1)-Os-N(5)-N(6)	137.9(6)
Cl(2)-Os-N(5)-N(6)	-131.3(6)
C(7)-N(5)-N(6)-C(9)	-1.0(10)
Os-N(5)-N(6)-C(9)	-178.2(6)
C(7)-N(5)-N(6)-B(1)	175.1(8)
Os-N(5)-N(6)-B(1)	-2.1(11)
N(4)-B(1)-N(6)-C(9)	-126.4(11)
N(2)-B(1)-N(6)-C(9)	117.1(11)
N(4)-B(1)-N(6)-N(5)	58.6(11)
N(2)-B(1)-N(6)-N(5)	-57.9(10)
O-B(2)-N(7)-C(10)	-117.7(9)
C(16)-B(2)-N(7)-C(10)	57.5(11)