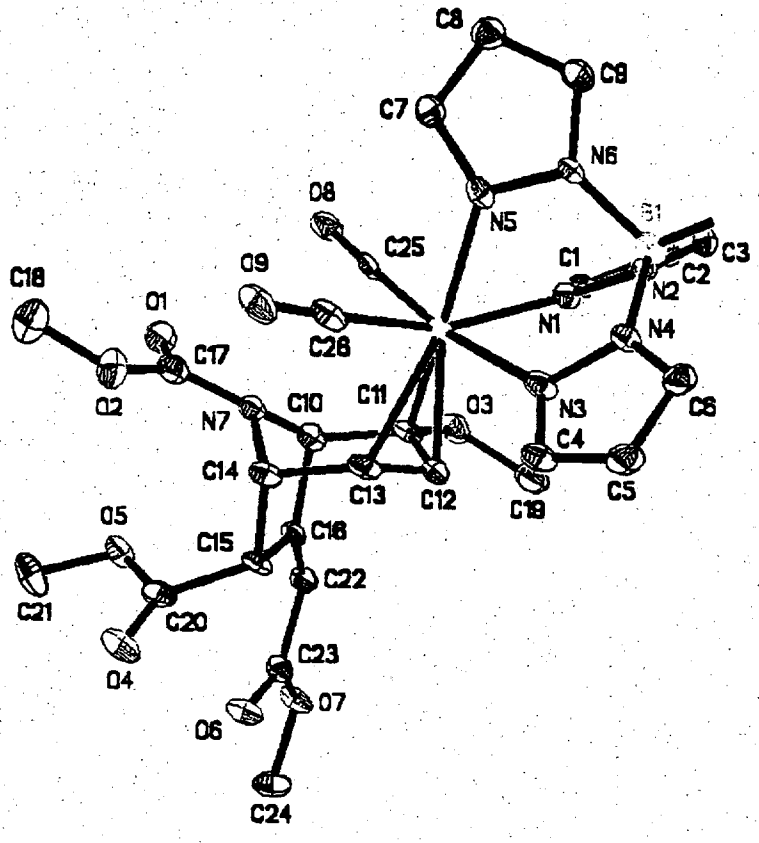
C(14)-N(7)-C(17)-O(1)	155.2(6)
C(16)-C(15)-C(20)-O(4)	1(2)
C(14)-C(15)-C(20)-O(4)	-117.3(15)
C(10)-C(16)-C(21)-C(22)	66.4(10)
C(15)-C(16)-C(21)-C(22)	-172.5(7)
C(24)-Mo(1)-C(23)-O(5)	24(12)
N(1)-Mo(1)-C(23)-O(5)	-72(12)
N(5)-Mo(1)-C(23)-O(5)	-45(13)
C(12)-Mo(1)-C(23)-O(5)	127(12)
C(13)-Mo(1)-C(23)-O(5)	129(12)
N(3)-Mo(1)-C(23)-O(5)	-151(12)
C(23)-Mo(1)-C(24)-O(6)	-71(13)
N(1)-Mo(1)-C(24)-O(6)	11(13)
N(5)-Mo(1)-C(24)-O(6)	90(13)
C(12)-Mo(1)-C(24)-O(6)	-174(13)
C(13)-Mo(1)-C(24)-O(6)	-136(13)
N(3)-Mo(1)-C(24)-O(6)	63(14)

Symmetry transformations used to generate equivalent atoms:

Ortep Drawing of Compound (±)-12



$C_{26}H_{28}N_7O_9MoB \cdot CH_2Cl_2$

(d53b)

Crystal Structure Analysis

A suitable crystal of **D53b2** was coated with Paratone N oil, suspended in a small fiber loop and placed in a cooled nitrogen gas stream at 100 K on a Bruker D8 SMART APEX CCD sealed tube diffractometer with graphite monochromated MoK_α (0.071073Å) radiation. A hemisphere of data were measured using a series of combinations of phi and omega scans with 10 second frame exposures and 0.3° frame widths. Data collection, indexing and initial cell refinements were all handled using SMART[1] software. Frame integration and final cell refinements were carried out using SAINT[2] software. The final cell parameters were determined from least-squares refinement on 8192 reflections. The SADABS[3] program was used to carry out absorption corrections.

The structure was solved using Direct methods and difference Fourier techniques (SHELXTL, V5.10).[4] Hydrogen atoms were placed their expected chemical positions using the HFIX command and were included in the final cycles of least squares with isotropic U_{ij} 's related to the atom's ridden upon. The C-H distances were fixed at 0.93 Å, 0.98 Å (methine), 0.97 Å (methylene), or 0.96 Å (methyl). All non-hydrogen atoms were refined anisotropically. Scattering factors and anomalous dispersion corrections are taken from the *International Tables for X-ray Crystallography*[5]. Structure solution, refinement, graphics and generation of publication materials were performed by using SHELXTL, V5.10 software. Additional details of data collection and structure refinement are given in Table 1.

References

1. SMART Version 5.55, **2000**, Bruker AXS, Inc., Analytical X-ray Systems, 5465 East Cheryl Parkway, Madison WI 53711-5373.
2. SAINT Version 6.02, **1999**, Bruker AXS, Inc., Analytical X-ray Systems, 5465 East Cheryl Parkway, Madison WI 53711-5373.
3. SADABS, **1996**, George Sheldrick, University of Göttingen,
4. SHELXTL V5.10, **1997**, Bruker AXS, Inc., Analytical X-ray Systems, 5465 East Cheryl Parkway, Madison WI 53711-5373.
5. A. J. C. Wilson (ed), *International Tables for X-ray Crystallography, Volume C.* Kynoch, Academic Publishers, Dordrecht, **1992**, Tables 6.1.1.4 (pp. 500-502) and 4.2.6.8 (pp. 219-222).

Data for Compound (±)-12

Table 1. Crystal data and structure refinement for $C_{26}H_{28}N_7O_9MoB \cdot CH_2Cl_2$.

Identification code	d53b2m	
Empirical formula	C27 H30 B Cl2 Mo N7 O9	
Formula weight	772.21	
Temperature	100(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 8.7904(8) Å	α= 90°.
	b = 33.831(3) Å	β= 108.339(2)°.
	c = 11.1697(10) Å	γ = 90°.
Volume	3153.0(5) Å^3	
Z	4	
Density (calculated)	1.627 Mg/m^3	
Absorption coefficient	0.650 mm^{-1}	
F(000)	1568	
Crystal size	0.13 x 0.10 x 0.02 mm^3	
Theta range for data collection	2.01 to 30.57°.	
Index ranges	$-12 \le h \le 11$, $-48 \le k \le$ v47, $-10 \le l \le 15$	
Reflections collected	27580	
Independent reflections	9605 [R(int) = 0.0783]	
Completeness to theta = 30.57°	99.5 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9605 / 0 / 428	
Goodness-of-fit on F^2	1.121	
Final R indices [I>2sigma(I)]	R1 = 0.0829, wR2 = 0.1538	
R indices (all data)	R1 = 0.1209, wR2 = 0.1681	
Largest diff. peak and hole	0.901 and -2.100 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $C_{26}H_{28}N_7O_9MoB{\cdot}CH_2Cl_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	-1679(1)	-3475(1)	-6186(1)	13(1)
O(1)	-1867(5)	-4208(1)	-10133(3)	28(1)
O(2)	-3657(4)	-4503(1)	-9353(4)	30(1)
O(3)	2016(4)	-3632(1)	-6511(3)	22(1)
O(4)	-1319(4)	-5391(1)	-7016(4)	27(1)
O(5)	-665(4)	-5080(1)	-8566(3)	24(1)
O(6)	2376(4)	-5260(1)	-6226(3)	25(1)
O(7)	4621(4)	-5056(1)	-6574(3)	24(1)
O(8)	-1910(5)	-3362(1)	-9006(3)	25(1)
O(9)	-4797(4)	-3959(1)	-7356(4)	31(1)
N(1)	-21(5)	-2951(1)	-5592(4)	17(1)
N(2)	-238(4)	-2685(1)	-4742(3)	14(1)
N(3)	-1765(5)	-3454(1)	-4161(4)	18(1)
N(4)	-1735(5)	-3096(1)	-3596(4)	16(1)
N(5)	-3386(5)	-2985(1)	-6379(4)	17(1)
N(6)	-3187(4)	-2697(1)	-5484(4)	15(1)
N(7)	-1481(5)	-4219(1)	-8018(4)	16(1)
B(1)	-1716(6)	-2705(2)	-4285(5)	16(1)
C(1)	1111(5)	-2798(1)	-6020(4)	17(1)
C(2)	1634(6)	-2435(1)	-5458(5)	21(1)
C(3)	745(6)	-2373(1)	-4664(4)	18(1)
C(4)	-1964(6)	-3722(1)	-3346(5)	21(1)
C(5)	-2064(6)	-3543(1)	-2255(5)	22(1)
C(6)	-1932(6)	-3145(1)	-2464(5)	20(1)
C(7)	-4702(6)	-2885(1)	-7336(5)	20(1)
C(8)	-5326(6)	-2531(1)	-7070(5)	24(1)
C(9)	-4330(6)	-2423(1)	-5897(5)	19(1)
C(10)	205(6)	-4114(1)	-7654(4)	18(1)
C(11)	648(6)	-3825(1)	-6535(5)	17(1)
C(12)	195(6)	-3926(1)	-5465(5)	21(1)
C(13)	-1282(6)	-4140(1)	-5808(4)	18(1)

C(14)	-1624(6)	-4428(1)	-6922(5)	18(1)
C(15)	-215(6)	-4730(1)	-6664(5)	17(1)
C(16)	1011(6)	-4503(1)	-7100(4)	17(1)
C(17)	-2299(6)	-4308(1)	-9256(5)	24(1)
C(18)	-4580(8)	-4578(2)	-10663(6)	45(2)
C(19)	3210(6)	-3576(2)	-5300(5)	29(1)
C(20)	-767(6)	-5111(1)	-7404(5)	20(1)
C(21)	-1127(7)	-5422(2)	-9373(6)	36(1)
C(22)	2488(6)	-4613(1)	-7061(5)	19(1)
C(23)	3113(6)	-5005(1)	-6573(5)	20(1)
C(24)	5299(6)	-5443(2)	-6165(5)	29(1)
C(25)	-1785(6)	-3409(1)	-7942(4)	17(1)
C(26)	-3619(6)	-3785(1)	-6900(5)	21(1)
C(1S)	-2085(7)	-6395(2)	-8433(5)	34(1)
Cl(1)	-2486(2)	-6380(1)	-10084(1)	41(1)
Cl(2)	-3865(2)	-6480(1)	-8050(2)	46(1)

Table 3. Bond lengths [Å] and angles [°] for $C_{26}H_{28}N_7O_9MoB{\cdot}CH_2Cl_2$.

Mo(1)-C(26)	1.947(5)	N(7)-C(10)	1.452(6)
Mo(1)-C(25)	1.947(5)	N(7)-C(14)	1.453(6)
Mo(1)-N(5)	2.200(4)	C(1)-C(2)	1.391(6)
Mo(1)-C(12)	2.202(5)	C(2)-C(3)	1.370(7)
Mo(1)-N(1)	2.259(4)	C(4)-C(5)	1.388(7)
Mo(1)-N(3)	2.288(4)	C(5)-C(6)	1.378(7)
Mo(1)-C(13)	2.295(4)	C(7)-C(8)	1.388(7)
Mo(1)-C(11)	2.498(5)	C(8)-C(9)	1.377(7)
O(1)-C(17)	1.206(6)	C(10)-C(16)	1.530(6)
O(2)-C(17)	1.337(6)	C(10)-C(11)	1.537(6)
O(2)-C(18)	1.454(7)	C(11)-C(12)	1.415(7)
O(3)-C(11)	1.363(6)	C(12)-C(13)	1.431(7)
O(3)-C(19)	1.440(6)	C(13)-C(14)	1.533(7)
O(4)-C(20)	1.205(6)	C(14)-C(15)	1.562(6)
O(5)-C(20)	1.333(6)	C(15)-C(16)	1.523(7)
O(5)-C(21)	1.444(6)	C(15)-C(20)	1.524(6)
O(6)-C(23)	1.214(6)	C(16)-C(22)	1.339(7)
O(7)-C(23)	1.337(6)	C(22)-C(23)	1.472(6)
O(7)-C(24)	1.453(6)	C(1S)-Cl(1)	1.766(6)
O(8)-C(25)	1.169(6)	C(1S)-Cl(2)	1.770(6)
O(9)-C(26)	1.160(6)		
N(1)-C(1)	1.336(6)	C(26)-Mo(1)-C(25)	83.7(2)
N(1)-N(2)	1.363(5)	C(26)-Mo(1)-N(5)	83.31(17)
N(2)-C(3)	1.351(6)	C(25)-Mo(1)-N(5)	89.99(17)
N(2)-B(1)	1.539(7)	C(26)-Mo(1)-C(12)	103.59(19)
N(3)-C(4)	1.334(6)	C(25)-Mo(1)-C(12)	103.95(19)
N(3)-N(4)	1.364(5)	N(5)-Mo(1)-C(12)	164.94(17)
N(4)-C(6)	1.339(6)	C(26)-Mo(1)-N(1)	160.85(17)
N(4)-B(1)	1.532(6)	C(25)-Mo(1)-N(1)	91.60(16)
N(5)-C(7)	1.349(6)	N(5)-Mo(1)-N(1)	78.12(14)
N(5)-N(6)	1.368(5)	C(12)-Mo(1)-N(1)	95.56(16)
N(6)-C(9)	1.338(6)	C(26)-Mo(1)-N(3)	97.17(18)
N(6)-B(1)	1.542(7)	C(25)-Mo(1)-N(3)	170.54(16)
N(7)-C(17)	1.375(6)	N(5)-Mo(1)-N(3)	80.78(14)

C(12)-Mo(1)-N(3)	85.04(17)	N(5)-N(6)-B(1)	120.1(4)
N(1)-Mo(1)-N(3)	84.50(14)	C(17)-N(7)-C(10)	120.0(4)
C(26)-Mo(1)-C(13)	67.04(19)	C(17)-N(7)-C(14)	125.8(4)
C(25)-Mo(1)-C(13)	104.72(17)	C(10)-N(7)-C(14)	103.5(4)
N(5)-Mo(1)-C(13)	144.66(16)	N(4)-B(1)-N(2)	110.4(4)
C(12)-Mo(1)-C(13)	37.03(17)	N(4)-B(1)-N(6)	108.3(4)
N(1)-Mo(1)-C(13)	132.00(16)	N(2)-B(1)-N(6)	106.0(4)
N(3)-Mo(1)-C(13)	84.20(15)	N(1)-C(1)-C(2)	110.9(4)
C(26)-Mo(1)-C(11)	109.58(18)	C(3)-C(2)-C(1)	104.6(4)
C(25)-Mo(1)-C(11)	71.30(18)	N(2)-C(3)-C(2)	108.8(4)
N(5)-Mo(1)-C(11)	155.30(15)	N(3)-C(4)-C(5)	111.3(4)
C(12)-Mo(1)-C(11)	34.30(17)	C(6)-C(5)-C(4)	104.1(4)
N(1)-Mo(1)-C(11)	86.22(14)	N(4)-C(6)-C(5)	109.0(4)
N(3)-Mo(1)-C(11)	116.89(15)	N(5)-C(7)-C(8)	110.3(4)
C(13)-Mo(1)-C(11)	58.64(16)	C(9)-C(8)-C(7)	104.9(4)
C(17)-O(2)-C(18)	111.7(5)	N(6)-C(9)-C(8)	109.1(4)
C(11)-O(3)-C(19)	117.4(4)	N(7)-C(10)-C(16)	101.8(4)
C(20)-O(5)-C(21)	117.0(4)	N(7)-C(10)-C(11)	111.0(4)
C(23)-O(7)-C(24)	115.2(4)	C(16)-C(10)-C(11)	104.5(4)
C(1)-N(1)-N(2)	106.1(4)	O(3)-C(11)-C(12)	125.5(4)
C(1)-N(1)-Mo(1)	133.1(3)	O(3)-C(11)-C(10)	108.5(4)
N(2)-N(1)-Mo(1)	120.2(3)	C(12)-C(11)-C(10)	117.9(4)
C(3)-N(2)-N(1)	109.5(4)	O(3)-C(11)-Mo(1)	122.0(3)
C(3)-N(2)-B(1)	127.0(4)	C(12)-C(11)-Mo(1)	61.3(3)
N(1)-N(2)-B(1)	121.3(4)	C(10)-C(11)-Mo(1)	114.7(3)
C(4)-N(3)-N(4)	105.9(4)	C(11)-C(12)-C(13)	111.6(4)
C(4)-N(3)-Mo(1)	134.9(3)	C(11)-C(12)-Mo(1)	84.4(3)
N(4)-N(3)-Mo(1)	118.9(3)	C(13)-C(12)-Mo(1)	75.0(3)
C(6)-N(4)-N(3)	109.7(4)	C(12)-C(13)-C(14)	117.9(4)
C(6)-N(4)-B(1)	127.4(4)	C(12)-C(13)-Mo(1)	67.9(3)
N(3)-N(4)-B(1)	122.4(4)	C(14)-C(13)-Mo(1)	119.5(3)
C(7)-N(5)-N(6)	106.2(4)	N(7)-C(14)-C(13)	109.3(4)
C(7)-N(5)-Mo(1)	131.0(3)	N(7)-C(14)-C(15)	101.5(4)
N(6)-N(5)-Mo(1)	122.6(3)	C(13)-C(14)-C(15)	109.0(4)
C(9)-N(6)-N(5)	109.5(4)	C(16)-C(15)-C(20)	112.9(4)
C(9)-N(6)-B(1)	130.2(4)	C(16)-C(15)-C(14)	102.1(3)

C(20)-C(15)-C(14)	110.8(4)	O(5)-C(20)-C(15)	110.7(4)
C(22)-C(16)-C(15)	128.7(4)	C(16)-C(22)-C(23)	120.5(5)
C(22)-C(16)-C(10)	125.0(4)	O(6)-C(23)-O(7)	122.5(4)
C(15)-C(16)-C(10)	106.2(4)	O(6)-C(23)-C(22)	125.7(5)
O(1)-C(17)-O(2)	125.0(5)	O(7)-C(23)-C(22)	111.8(4)
O(1)-C(17)-N(7)	123.8(5)	O(8)-C(25)-Mo(1)	177.2(4)
O(2)-C(17)-N(7)	111.1(5)	O(9)-C(26)-Mo(1)	177.5(4)
O(4)-C(20)-O(5)	124.7(5)	Cl(1)-C(1S)-Cl(2)	110.8(3)
O(4)-C(20)-C(15)	124.4(5)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $C_{26}H_{28}N_7O_9MoB{\cdot}CH_2Cl_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	18(1)	9(1)	15(1)	1(1)	8(1)	1(1)
O(1)	43(2)	24(2)	16(2)	0(2)	8(2)	3(2)
O(2)	25(2)	32(2)	29(2)	-7(2)	5(2)	-6(2)
O(3)	19(2)	16(2)	30(2)	-1(2)	7(2)	-3(1)
O(4)	31(2)	15(2)	41(2)	4(2)	19(2)	-1(1)
O(5)	33(2)	14(2)	27(2)	-3(2)	14(2)	-5(1)
O(6)	28(2)	16(2)	33(2)	7(2)	14(2)	4(1)
O(7)	26(2)	13(2)	37(2)	2(2)	15(2)	3(1)
O(8)	44(2)	15(2)	19(2)	3(1)	13(2)	2(2)
O(9)	28(2)	16(2)	50(3)	-4(2)	16(2)	-5(2)
N(1)	21(2)	17(2)	16(2)	0(2)	8(2)	4(2)
N(2)	15(2)	14(2)	12(2)	2(1)	4(2)	2(1)
N(3)	24(2)	15(2)	20(2)	1(2)	12(2)	3(2)
N(4)	18(2)	13(2)	18(2)	1(2)	8(2)	3(1)
N(5)	25(2)	12(2)	17(2)	-1(2)	11(2)	-3(2)
N(6)	19(2)	9(2)	18(2)	0(2)	7(2)	1(1)
N(7)	21(2)	12(2)	16(2)	1(2)	7(2)	0(2)
B(1)	21(3)	12(2)	17(3)	0(2)	8(2)	2(2)
C(1)	18(2)	15(2)	18(2)	2(2)	6(2)	5(2)
C(2)	16(2)	17(2)	29(3)	4(2)	7(2)	2(2)
C(3)	20(2)	15(2)	17(2)	-1(2)	1(2)	-2(2)
C(4)	25(3)	14(2)	25(3)	4(2)	12(2)	0(2)
C(5)	27(3)	22(2)	18(2)	5(2)	9(2)	1(2)
C(6)	23(2)	22(2)	14(2)	2(2)	7(2)	4(2)
C(7)	21(2)	16(2)	21(2)	0(2)	3(2)	-3(2)
C(8)	18(2)	20(2)	30(3)	1(2)	3(2)	1(2)
C(9)	19(2)	18(2)	24(3)	0(2)	10(2)	2(2)
C(10)	22(2)	16(2)	18(2)	1(2)	12(2)	2(2)
C(11)	19(2)	10(2)	22(2)	3(2)	7(2)	3(2)
C(12)	30(3)	12(2)	19(2)	0(2)	4(2)	1(2)
C(13)	29(3)	13(2)	17(2)	4(2)	14(2)	4(2)
C(14)	20(2)	14(2)	22(2)	5(2)	10(2)	2(2)

C(15)	25(2)	8(2)	20(2)	2(2)	12(2)	4(2)
C(16)	25(2)	9(2)	16(2)	1(2)	5(2)	-1(2)
C(17)	25(3)	17(2)	29(3)	-1(2)	8(2)	4(2)
C(18)	41(4)	45(4)	38(4)	-7(3)	-2(3)	-1(3)
C(19)	27(3)	18(2)	40(3)	1(2)	6(2)	4(2)
C(20)	20(2)	15(2)	28(3)	2(2)	9(2)	6(2)
C(21)	47(4)	21(3)	44(4)	-15(3)	22(3)	-5(2)
C(22)	22(2)	14(2)	20(2)	1(2)	6(2)	1(2)
C(23)	24(3)	14(2)	21(2)	-2(2)	7(2)	2(2)
C(24)	25(3)	25(3)	35(3)	7(2)	9(2)	11(2)
C(25)	25(2)	7(2)	19(2)	-2(2)	10(2)	-1(2)
C(26)	27(3)	14(2)	26(3)	2(2)	15(2)	1(2)
C(1S)	32(3)	33(3)	32(3)	-4(3)	2(3)	-3(2)
Cl(1)	62(1)	28(1)	31(1)	-4(1)	12(1)	-12(1)
Cl(2)	52(1)	34(1)	55(1)	-6(1)	24(1)	-14(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $C_{26}H_{28}N_7O_9MoB•CH_2Cl_2$.

	x	y	z	U(eq)
H(1A)	1507	-2921	-6627	20
H(2A)	2431	-2267	-5594	25
H(3A)	810	-2147	-4144	22
H(4A)	-2029	-3998	-3494	25
H(5A)	-2194	-3667	-1530	27
H(6A)	-1973	-2939	-1897	24
H(7A)	-5139	-3034	-8085	24
H(8A)	-6240	-2393	-7585	28
H(9A)	-4437	-2191	-5451	23
H(10A)	543	-4018	-8379	21
H(12A)	960	-3921	-4587	25
H(13A)	-1599	-4240	-5077	22
H(14A)	-2687	-4561	-7097	22
H(15A)	224	-4788	-5741	20
H(18A)	-5564	-4720	-10700	67
H(18B)	-3941	-4738	-11059	67
H(18C)	-4855	-4326	-11113	67
H(19A)	4131	-3435	-5409	44
H(19B)	3560	-3834	-4912	44
H(19C)	2753	-3421	-4754	44
H(21A)	-995	-5364	-10195	53
H(21B)	-2251	-5486	-9488	53
H(21C)	-449	-5647	-8985	53
H(22A)	3138	-4437	-7350	23
H(24A)	6398	-5454	-6202	43
H(24B)	4649	-5646	-6720	43
H(24C)	5309	-5490	-5297	43
H(1SA)	-1601	-6142	-8059	41
H(1SB)	-1306	-6609	-8071	41
H(1)	-1780(50)	-2461(12)	-3690(40)	3(11)

Table 6. Torsion angles [°] for $C_{26}H_{28}N_7O_9MoB{\cdot}CH_2Cl_2$.

C(26)-Mo(1)-N(1)-C(1)	-107.4(6)
C(25)-Mo(1)-N(1)-C(1)	-32.1(4)
N(5)-Mo(1)-N(1)-C(1)	-121.8(4)
C(12)-Mo(1)-N(1)-C(1)	72.1(4)
N(3)-Mo(1)-N(1)-C(1)	156.5(4)
C(13)-Mo(1)-N(1)-C(1)	79.4(5)
C(11)-Mo(1)-N(1)-C(1)	39.0(4)
C(26)-Mo(1)-N(1)-N(2)	62.4(7)
C(25)-Mo(1)-N(1)-N(2)	137.7(3)
N(5)-Mo(1)-N(1)-N(2)	48.1(3)
C(12)-Mo(1)-N(1)-N(2)	-118.1(3)
N(3)-Mo(1)-N(1)-N(2)	-33.6(3)
C(13)-Mo(1)-N(1)-N(2)	-110.7(3)
C(11)-Mo(1)-N(1)-N(2)	-151.1(3)
C(1)-N(1)-N(2)-C(3)	0.5(5)
Mo(1)-N(1)-N(2)-C(3)	-171.8(3)
C(1)-N(1)-N(2)-B(1)	164.9(4)
Mo(1)-N(1)-N(2)-B(1)	-7.4(5)
C(26)-Mo(1)-N(3)-C(4)	49.1(5)
C(25)-Mo(1)-N(3)-C(4)	143.9(10)
N(5)-Mo(1)-N(3)-C(4)	131.0(5)
C(12)-Mo(1)-N(3)-C(4)	-54.1(5)
N(1)-Mo(1)-N(3)-C(4)	-150.1(5)
C(13)-Mo(1)-N(3)-C(4)	-16.9(5)
C(11)-Mo(1)-N(3)-C(4)	-67.2(5)
C(26)-Mo(1)-N(3)-N(4)	-124.8(3)
C(25)-Mo(1)-N(3)-N(4)	-29.9(12)
N(5)-Mo(1)-N(3)-N(4)	-42.8(3)
C(12)-Mo(1)-N(3)-N(4)	132.1(3)
N(1)-Mo(1)-N(3)-N(4)	36.0(3)
C(13)-Mo(1)-N(3)-N(4)	169.3(3)
C(11)-Mo(1)-N(3)-N(4)	119.0(3)
C(4)-N(3)-N(4)-C(6)	-0.7(5)
Mo(1)-N(3)-N(4)-C(6)	174.8(3)
C(4)-N(3)-N(4)-B(1)	-172.9(4)

Mo(1)-N(3)-N(4)-B(1)	2.6(5)
C(26)-Mo(1)-N(5)-C(7)	-44.5(4)
C(25)-Mo(1)-N(5)-C(7)	39.2(4)
C(12)-Mo(1)-N(5)-C(7)	-162.8(6)
N(1)-Mo(1)-N(5)-C(7)	130.8(4)
N(3)-Mo(1)-N(5)-C(7)	-142.9(4)
C(13)-Mo(1)-N(5)-C(7)	-76.9(5)
C(11)-Mo(1)-N(5)-C(7)	79.0(6)
C(26)-Mo(1)-N(5)-N(6)	140.0(4)
C(25)-Mo(1)-N(5)-N(6)	-136.3(3)
C(12)-Mo(1)-N(5)-N(6)	21.7(8)
N(1)-Mo(1)-N(5)-N(6)	-44.6(3)
N(3)-Mo(1)-N(5)-N(6)	41.6(3)
C(13)-Mo(1)-N(5)-N(6)	107.7(4)
C(11)-Mo(1)-N(5)-N(6)	-96.4(4)
C(7)-N(5)-N(6)-C(9)	-1.3(5)
Mo(1)-N(5)-N(6)-C(9)	175.1(3)
C(7)-N(5)-N(6)-B(1)	-176.1(4)
Mo(1)-N(5)-N(6)-B(1)	0.3(5)
C(6)-N(4)-B(1)-N(2)	130.1(5)
N(3)-N(4)-B(1)-N(2)	-59.1(5)
C(6)-N(4)-B(1)-N(6)	-114.3(5)
N(3)-N(4)-B(1)-N(6)	56.5(5)
C(3)-N(2)-B(1)-N(4)	-136.3(4)
N(1)-N(2)-B(1)-N(4)	62.2(5)
C(3)-N(2)-B(1)-N(6)	106.7(5)
N(1)-N(2)-B(1)-N(6)	-54.8(5)
C(9)-N(6)-B(1)-N(4)	127.6(5)
N(5)-N(6)-B(1)-N(4)	-58.9(5)
C(9)-N(6)-B(1)-N(2)	-114.0(5)
N(5)-N(6)-B(1)-N(2)	59.5(5)
N(2)-N(1)-C(1)-C(2)	-0.1(5)
Mo(1)-N(1)-C(1)-C(2)	170.8(3)
N(1)-C(1)-C(2)-C(3)	-0.4(5)
N(1)-N(2)-C(3)-C(2)	-0.8(5)
B(1)-N(2)-C(3)-C(2)	-164.1(4)
C(1)-C(2)-C(3)-N(2)	0.7(5)

N(4)-N(3)-C(4)-C(5)	-0.1(5)
Mo(1)-N(3)-C(4)-C(5)	-174.4(3)
N(3)-C(4)-C(5)-C(6)	0.7(6)
N(3)-N(4)-C(6)-C(5)	1.2(5)
B(1)-N(4)-C(6)-C(5)	172.9(4)
C(4)-C(5)-C(6)-N(4)	-1.1(6)
N(6)-N(5)-C(7)-C(8)	1.1(5)
Mo(1)-N(5)-C(7)-C(8)	-174.9(3)
N(5)-C(7)-C(8)-C(9)	-0.5(6)
N(5)-N(6)-C(9)-C(8)	1.1(5)
B(1)-N(6)-C(9)-C(8)	175.1(5)
C(7)-C(8)-C(9)-N(6)	-0.3(6)
C(17)-N(7)-C(10)-C(16)	-99.9(5)
C(14)-N(7)-C(10)-C(16)	46.5(4)
C(17)-N(7)-C(10)-C(11)	149.3(4)
C(14)-N(7)-C(10)-C(11)	-64.2(4)
C(19)-O(3)-C(11)-C(12)	9.9(6)
C(19)-O(3)-C(11)-C(10)	-137.8(4)
C(19)-O(3)-C(11)-Mo(1)	85.4(4)
N(7)-C(10)-C(11)-O(3)	-158.9(4)
C(16)-C(10)-C(11)-O(3)	92.1(4)
N(7)-C(10)-C(11)-C(12)	50.6(5)
C(16)-C(10)-C(11)-C(12)	-58.4(5)
N(7)-C(10)-C(11)-Mo(1)	-18.7(4)
C(16)-C(10)-C(11)-Mo(1)	-127.7(3)
C(26)-Mo(1)-C(11)-O(3)	158.6(4)
C(25)-Mo(1)-C(11)-O(3)	82.6(4)
N(5)-Mo(1)-C(11)-O(3)	40.0(6)
C(12)-Mo(1)-C(11)-O(3)	-116.0(5)
N(1)-Mo(1)-C(11)-O(3)	-10.3(4)
N(3)-Mo(1)-C(11)-O(3)	-92.2(4)
C(13)-Mo(1)-C(11)-O(3)	-156.0(4)
C(26)-Mo(1)-C(11)-C(12)	-85.5(3)
C(25)-Mo(1)-C(11)-C(12)	-161.4(3)
N(5)-Mo(1)-C(11)-C(12)	156.0(3)
N(1)-Mo(1)-C(11)-C(12)	105.6(3)
N(3)-Mo(1)-C(11)-C(12)	23.7(3)

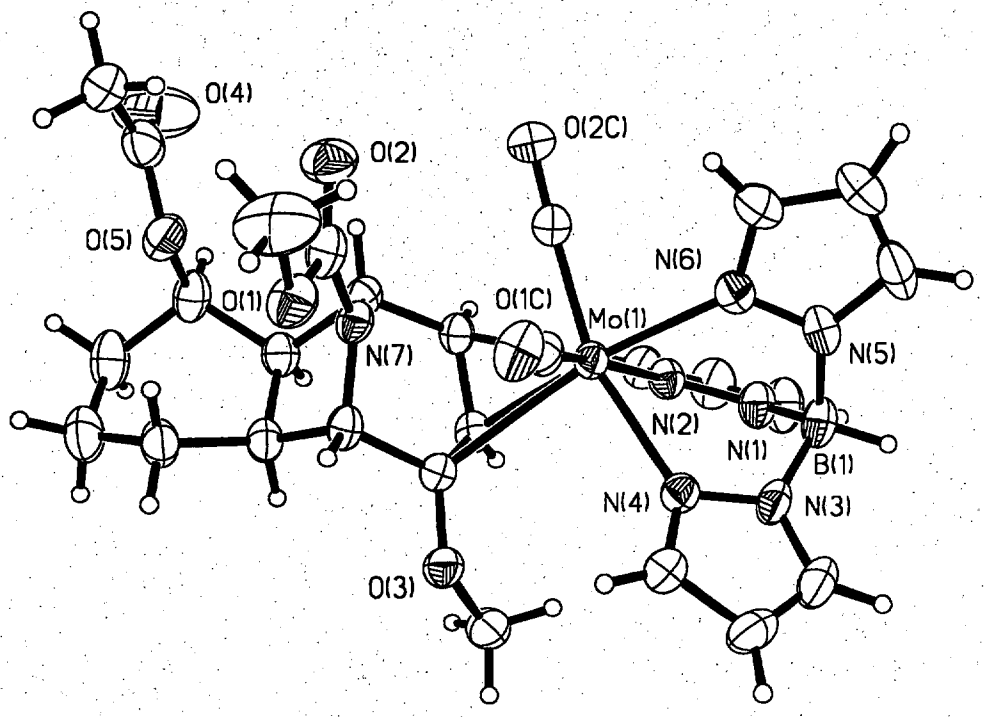
C(13)-Mo(1)-C(11)-C(12)	-40.0(3)
C(26)-Mo(1)-C(11)-C(10)	24.2(4)
C(25)-Mo(1)-C(11)-C(10)	-51.8(3)
N(5)-Mo(1)-C(11)-C(10)	-94.4(4)
C(12)-Mo(1)-C(11)-C(10)	109.6(4)
N(1)-Mo(1)-C(11)-C(10)	-144.8(3)
N(3)-Mo(1)-C(11)-C(10)	133.4(3)
C(13)-Mo(1)-C(11)-C(10)	69.6(3)
O(3)-C(11)-C(12)-C(13)	-178.0(4)
C(10)-C(11)-C(12)-C(13)	-33.0(6)
Mo(1)-C(11)-C(12)-C(13)	71.5(3)
O(3)-C(11)-C(12)-Mo(1)	110.6(4)
C(10)-C(11)-C(12)-Mo(1)	-104.4(4)
C(26)-Mo(1)-C(12)-C(11)	104.9(3)
C(25)-Mo(1)-C(12)-C(11)	18.1(3)
N(5)-Mo(1)-C(12)-C(11)	-139.2(6)
N(1)-Mo(1)-C(12)-C(11)	-74.9(3)
N(3)-Mo(1)-C(12)-C(11)	-158.9(3)
C(13)-Mo(1)-C(12)-C(11)	114.2(4)
C(26)-Mo(1)-C(12)-C(13)	-9.3(3)
C(25)-Mo(1)-C(12)-C(13)	-96.1(3)
N(5)-Mo(1)-C(12)-C(13)	106.6(6)
N(1)-Mo(1)-C(12)-C(13)	170.9(3)
N(3)-Mo(1)-C(12)-C(13)	86.9(3)
C(11)-Mo(1)-C(12)-C(13)	-114.2(4)
C(11)-C(12)-C(13)-C(14)	35.2(6)
Mo(1)-C(12)-C(13)-C(14)	112.8(4)
C(11)-C(12)-C(13)-Mo(1)	-77.6(3)
C(26)-Mo(1)-C(13)-C(12)	170.2(3)
C(25)-Mo(1)-C(13)-C(12)	93.8(3)
N(5)-Mo(1)-C(13)-C(12)	-154.5(3)
N(1)-Mo(1)-C(13)-C(12)	-12.2(4)
N(3)-Mo(1)-C(13)-C(12)	-89.4(3)
C(11)-Mo(1)-C(13)-C(12)	37.0(3)
C(26)-Mo(1)-C(13)-C(14)	59.6(4)
C(25)-Mo(1)-C(13)-C(14)	-16.8(4)
N(5)-Mo(1)-C(13)-C(14)	94.9(4)

C(12)-Mo(1)-C(13)-C(14)	-110.6(5)
N(1)-Mo(1)-C(13)-C(14)	-122.8(3)
N(3)-Mo(1)-C(13)-C(14)	160.0(4)
C(11)-Mo(1)-C(13)-C(14)	-73.6(4)
C(17)-N(7)-C(14)-C(13)	-150.7(4)
C(10)-N(7)-C(14)-C(13)	65.4(4)
C(17)-N(7)-C(14)-C(15)	94.3(5)
C(10)-N(7)-C(14)-C(15)	-49.6(4)
C(12)-C(13)-C(14)-N(7)	-54.2(5)
Mo(1)-C(13)-C(14)-N(7)	24.9(5)
C(12)-C(13)-C(14)-C(15)	55.9(5)
Mo(1)-C(13)-C(14)-C(15)	135.0(3)
N(7)-C(14)-C(15)-C(16)	31.8(4)
C(13)-C(14)-C(15)-C(16)	-83.4(4)
N(7)-C(14)-C(15)-C(20)	-88.7(4)
C(13)-C(14)-C(15)-C(20)	156.1(4)
C(20)-C(15)-C(16)-C(22)	-63.4(6)
C(14)-C(15)-C(16)-C(22)	177.6(5)
C(20)-C(15)-C(16)-C(10)	114.8(4)
C(14)-C(15)-C(16)-C(10)	-4.3(5)
N(7)-C(10)-C(16)-C(22)	153.5(5)
C(11)-C(10)-C(16)-C(22)	-90.9(5)
N(7)-C(10)-C(16)-C(15)	-24.7(5)
C(11)-C(10)-C(16)-C(15)	90.9(4)
C(18)-O(2)-C(17)-O(1)	-0.6(7)
C(18)-O(2)-C(17)-N(7)	176.6(4)
C(10)-N(7)-C(17)-O(1)	-20.5(7)
C(14)-N(7)-C(17)-O(1)	-159.0(5)
C(10)-N(7)-C(17)-O(2)	162.2(4)
C(14)-N(7)-C(17)-O(2)	23.7(6)
C(21)-O(5)-C(20)-O(4)	-5.5(7)
C(21)-O(5)-C(20)-C(15)	179.1(4)
C(16)-C(15)-C(20)-O(4)	156.5(5)
C(14)-C(15)-C(20)-O(4)	-89.7(6)
C(16)-C(15)-C(20)-O(5)	-28.1(5)
C(14)-C(15)-C(20)-O(5)	85.8(5)
C(15)-C(16)-C(22)-C(23)	1.5(8)

C(10)-C(16)-C(22)-C(23)	-176.4(4)
C(24)-O(7)-C(23)-O(6)	1.7(7)
C(24)-O(7)-C(23)-C(22)	-177.0(4)
C(16)-C(22)-C(23)-O(6)	3.2(8)
C(16)-C(22)-C(23)-O(7)	-178.2(4)
C(26)-Mo(1)-C(25)-O(8)	61(8)
N(5)-Mo(1)-C(25)-O(8)	-22(8)
C(12)-Mo(1)-C(25)-O(8)	163(8)
N(1)-Mo(1)-C(25)-O(8)	-101(8)
N(3)-Mo(1)-C(25)-O(8)	-35(9)
C(13)-Mo(1)-C(25)-O(8)	125(8)
C(11)-Mo(1)-C(25)-O(8)	174(100)
C(25)-Mo(1)-C(26)-O(9)	-48(11)
N(5)-Mo(1)-C(26)-O(9)	43(11)
C(12)-Mo(1)-C(26)-O(9)	-151(11)
N(1)-Mo(1)-C(26)-O(9)	29(11)
N(3)-Mo(1)-C(26)-O(9)	122(11)
C(13)-Mo(1)-C(26)-O(9)	-157(11)
C(11)-Mo(1)-C(26)-O(9)	-116(11)

Symmetry transformations used to generate equivalent atoms:

Ortep Drawing for Compound (±)-15



30% probability ellipsoids

Crystal Structure Analysis for Compound (±)-15

A suitable crystal of **HMB 99b** (Compound **(±)-15)** was mounted on a glass fiber using epoxy cement. Diffraction intensity data were measured at room temperature (omega scans) using graphite monochromated CuK_α radiation (1.54178 Å) on a Siemens P4/RA diffractometer. Three representative reflections were monitored after every 97 reflections as a check on instrument and crystal stability; no appreciable decay was observed. Lorentz, polarization, and an absorption correction, based on a series of psi scans, were applied to the data (XSCANS).[1]

The structure was solved using Direct methods and difference Fourier techniques (SHELXTL, V5.10).[2] Hydrogen atoms were placed their expected chemical positions using the HFIX command and were included in the final cycles of least squares with isotropic U_{ij} 's related to the atom's ridden upon. The C-H distances were fixed at 0.93 Å, 0.98 Å (methine), 0.97 Å (methylene), or 0.96 Å (methyl). All non-hydrogen atoms were refined anisotropically. The weighting scheme used during refinement was $1/\sigma^2$, based on counting statistics. Scattering factors and anomalous dispersion corrections are taken from the *International Tables for X-ray Crystallography.*[3] Structure solution, refinement, graphics and generation of publication materials were performed by using SHELXTL, V5.10 software. Additional details of data collection and structure refinement are given in Table 1.

References

1. XSCANS V2.31, **1997**, Bruker AXS, Inc., Analytical X-ray Systems, 5465 East Cheryl Parkway, Madison WI 53711-5373.
2. SHELXTL V5.10, **1997**, Bruker AXS, Inc., Analytical X-ray Systems, 5465 East Cheryl Parkway, Madison WI 53711-5373.
3. A. J. C. Wilson (ed), *International Tables for X-ray Crystallography, Volume C.* Kynoch, Academic Publishers, Dordrecht, **1992**, Tables 6.1.1.4 (pp. 500-502) and 4.2.6.8 (pp. 219-222).

Data for Compound (±)-15

Table 1. Crystal data and structure refinement for hmb99ab.

Identification code	hmb99ab	
Empirical formula	$C_{27}H_{32}BMoN_7O_7$	
Formula weight	673.35	
Temperature	299(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 14.2329(6) Å	α= 90°.
	b = 15.8683(6) Å	β= 112.107(4)°.
	c = 14.3681(5) Å	γ = 90°.
Volume	3006.5(2) Å^3	
Z	4	
Density (calculated)	1.488 Mg/m^3	
Absorption coefficient	4.048 mm^{-1}	
F(000)	1384	
Crystal size	0.10 x 0.28 x 0.22 mm^3	
Theta range for data collection	3.35 to 56.76°.	
Index ranges	-1<=h<=15, -17<=k<=1, -14<=l<=13	
Reflections collected	4859	
Independent reflections	3937 [R(int) = 0.0387]	
Completeness to theta = 56.76°	97.7 %	
Absorption correction	Integration	
Max. and min. transmission	0.6781 and 0.4292	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3937 / 0 / 401	
Goodness-of-fit on F^2	1.066	
Final R indices [I>2sigma(I)]	R1 = 0.0395, wR2 = 0.0948	
R indices (all data)	R1 = 0.0472, wR2 = 0.1009	
Extinction coefficient	0.00028(3)	
Largest diff. peak and hole	0.551 and -0.687 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for hmb99ab. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	8213(1)	2379(1)	7599(1)	43(1)
N(1)	6151(3)	3187(3)	6095(3)	63(1)
N(2)	7128(3)	3059(2)	6196(3)	55(1)
N(3)	6360(3)	3272(3)	7905(3)	58(1)
N(4)	7381(3)	3149(2)	8357(3)	51(1)
N(5)	5888(3)	1926(3)	6991(3)	64(1)
N(6)	6844(3)	1598(3)	7303(3)	60(1)
N(7)	10703(3)	2036(2)	8524(3)	49(1)
O(1)	11443(3)	1317(2)	9930(3)	72(1)
O(1C)	9290(3)	1498(2)	9638(3)	72(1)
O(2)	11034(3)	629(2)	8455(3)	82(1)
O(2C)	8842(3)	799(2)	6693(3)	82(1)
O(3)	9748(2)	3933(2)	9203(2)	57(1)
O(4)	12712(6)	1147(4)	6724(5)	157(3)
O(5)	12616(3)	1796(2)	8041(3)	70(1)
C(1C)	8917(3)	1831(3)	8861(4)	51(1)
C(1)	9780(3)	3333(3)	8546(3)	45(1)
C(2)	9307(3)	3365(3)	7530(4)	47(1)
C(2C)	8622(4)	1410(3)	7021(4)	58(1)
C(3)	9474(3)	2641(3)	7013(4)	48(1)
C(4)	10519(3)	2237(3)	7492(4)	53(1)
C(5)	11357(3)	2922(3)	7618(4)	56(1)
C(6)	11557(3)	3310(3)	8666(4)	54(1)
C(7)	10787(3)	2844(3)	9009(3)	50(1)
C(9)	12651(3)	3177(4)	9390(4)	66(1)
C(10)	13422(4)	3469(4)	8965(5)	85(2)
C(11)	13165(4)	3200(4)	7884(5)	85(2)
C(12)	12301(4)	2574(4)	7480(4)	65(1)
C(14)	12849(4)	1139(4)	7591(5)	79(2)
C(15)	13253(5)	416(4)	8259(6)	103(2)
C(16)	11057(4)	1257(4)	8917(4)	63(1)

C(17)	11647(7)	475(4)	10387(6)	132(3)
C(13)	9186(4)	4699(3)	8770(4)	68(1)
C(18)	5639(4)	3547(4)	5193(5)	84(2)
C(19)	6278(5)	3684(4)	4719(4)	81(2)
C(20)	7198(4)	3364(3)	5369(4)	62(1)
C(21)	6032(4)	3633(3)	8568(5)	71(2)
C(22)	6824(5)	3770(4)	9444(5)	78(2)
C(23)	7654(4)	3453(3)	9283(4)	59(1)
C(24)	5221(4)	1297(5)	6822(5)	84(2)
C(25)	5729(5)	550(4)	7028(6)	99(2)
C(26)	6737(5)	760(3)	7325(5)	77(2)
B(1)	5741(4)	2878(4)	6882(5)	65(2)

Table 3. Bond lengths [Å] and angles [°] for hmb99ab.

Mo(1)-C(1C)	1.919(5)	C(1)-C(7)	1.543(6)
Mo(1)-C(2C)	1.938(5)	C(2)-C(3)	1.436(7)
Mo(1)-N(6)	2.211(4)	C(3)-C(4)	1.524(6)
Mo(1)-C(2)	2.235(5)	C(4)-C(5)	1.573(7)
Mo(1)-N(4)	2.247(4)	C(5)-C(12)	1.533(7)
Mo(1)-C(3)	2.289(5)	C(5)-C(6)	1.551(7)
Mo(1)-N(2)	2.294(4)	C(6)-C(9)	1.528(6)
Mo(1)-C(1)	2.614(4)	C(6)-C(7)	1.548(6)
N(1)-C(18)	1.351(7)	C(9)-C(10)	1.515(7)
N(1)-N(2)	1.359(5)	C(10)-C(11)	1.517(8)
N(1)-B(1)	1.536(8)	C(11)-C(12)	1.516(8)
N(2)-C(20)	1.321(6)	C(14)-C(15)	1.467(9)
N(3)-C(21)	1.336(6)	C(18)-C(19)	1.343(8)
N(3)-N(4)	1.365(5)	C(19)-C(20)	1.387(7)
N(3)-B(1)	1.534(8)	C(21)-C(22)	1.354(8)
N(4)-C(23)	1.329(6)	C(22)-C(23)	1.382(7)
N(5)-C(24)	1.337(7)	C(24)-C(25)	1.361(9)
N(5)-N(6)	1.365(5)	C(25)-C(26)	1.375(8)
N(5)-B(1)	1.525(8)		
N(6)-C(26)	1.341(7)	C(1C)-Mo(1)-C(2C)	84.9(2)
N(7)-C(16)	1.374(6)	C(1C)-Mo(1)-N(6)	92.06(17)
N(7)-C(4)	1.442(6)	C(2C)-Mo(1)-N(6)	81.83(18)
N(7)-C(7)	1.443(6)	C(1C)-Mo(1)-C(2)	103.55(18)
O(1)-C(16)	1.351(6)	C(2C)-Mo(1)-C(2)	102.1(2)
O(1)-C(17)	1.468(7)	N(6)-Mo(1)-C(2)	164.14(16)
O(1C)-C(1C)	1.166(5)	C(1C)-Mo(1)-N(4)	88.32(17)
O(2)-C(16)	1.191(6)	C(2C)-Mo(1)-N(4)	159.51(18)
O(2C)-C(2C)	1.171(6)	N(6)-Mo(1)-N(4)	79.12(14)
O(3)-C(1)	1.352(5)	C(2)-Mo(1)-N(4)	98.29(16)
O(3)-C(13)	1.460(6)	C(1C)-Mo(1)-C(3)	103.11(18)
O(4)-C(14)	1.186(7)	C(2C)-Mo(1)-C(3)	65.32(19)
O(5)-C(14)	1.332(7)	N(6)-Mo(1)-C(3)	141.90(16)
O(5)-C(12)	1.450(6)	C(2)-Mo(1)-C(3)	36.99(17)
C(1)-C(2)	1.360(6)	N(4)-Mo(1)-C(3)	135.15(15)

C(1C)-Mo(1)-N(2)	169.27(16)	C(14)-O(5)-C(12)	118.5(5)
C(2C)-Mo(1)-N(2)	102.02(18)	O(1C)-C(1C)-Mo(1)	175.9(4)
N(6)-Mo(1)-N(2)	80.94(14)	O(3)-C(1)-C(2)	126.2(4)
C(2)-Mo(1)-N(2)	83.21(15)	O(3)-C(1)-C(7)	108.8(4)
N(4)-Mo(1)-N(2)	82.40(14)	C(2)-C(1)-C(7)	119.1(4)
C(3)-Mo(1)-N(2)	87.32(16)	O(3)-C(1)-Mo(1)	121.6(3)
C(1C)-Mo(1)-C(1)	74.36(17)	C(2)-C(1)-Mo(1)	58.7(3)
C(2C)-Mo(1)-C(1)	110.30(17)	C(7)-C(1)-Mo(1)	114.0(3)
N(6)-Mo(1)-C(1)	160.38(15)	C(1)-C(2)-C(3)	114.5(4)
C(2)-Mo(1)-C(1)	31.34(15)	C(1)-C(2)-Mo(1)	89.9(3)
N(4)-Mo(1)-C(1)	86.26(13)	C(3)-C(2)-Mo(1)	73.6(3)
C(3)-Mo(1)-C(1)	56.85(16)	O(2C)-C(2C)-Mo(1)	176.6(5)
N(2)-Mo(1)-C(1)	110.21(14)	C(2)-C(3)-C(4)	115.2(4)
C(18)-N(1)-N(2)	109.1(4)	C(2)-C(3)-Mo(1)	69.4(3)
C(18)-N(1)-B(1)	128.6(5)	C(4)-C(3)-Mo(1)	121.6(3)
N(2)-N(1)-B(1)	122.1(4)	N(7)-C(4)-C(3)	109.0(4)
C(20)-N(2)-N(1)	105.6(4)	N(7)-C(4)-C(5)	101.5(4)
C(20)-N(2)-Mo(1)	135.1(3)	C(3)-C(4)-C(5)	109.3(4)
N(1)-N(2)-Mo(1)	119.2(3)	C(12)-C(5)-C(6)	114.8(4)
C(21)-N(3)-N(4)	108.5(4)	C(12)-C(5)-C(4)	113.6(4)
C(21)-N(3)-B(1)	129.0(4)	C(6)-C(5)-C(4)	103.9(4)
N(4)-N(3)-B(1)	121.5(4)	C(9)-C(6)-C(7)	112.3(4)
C(23)-N(4)-N(3)	106.3(4)	C(9)-C(6)-C(5)	112.0(4)
C(23)-N(4)-Mo(1)	132.4(3)	C(7)-C(6)-C(5)	103.1(4)
N(3)-N(4)-Mo(1)	120.6(3)	N(7)-C(7)-C(1)	110.1(4)
C(24)-N(5)-N(6)	109.1(5)	N(7)-C(7)-C(6)	102.2(4)
C(24)-N(5)-B(1)	131.3(5)	C(1)-C(7)-C(6)	106.1(4)
N(6)-N(5)-B(1)	119.6(4)	C(10)-C(9)-C(6)	113.0(5)
C(26)-N(6)-N(5)	106.1(4)	C(9)-C(10)-C(11)	113.3(5)
C(26)-N(6)-Mo(1)	130.7(4)	C(12)-C(11)-C(10)	115.1(5)
N(5)-N(6)-Mo(1)	123.1(3)	O(5)-C(12)-C(11)	108.0(4)
C(16)-N(7)-C(4)	121.3(4)	O(5)-C(12)-C(5)	109.7(4)
C(16)-N(7)-C(7)	130.6(4)	C(11)-C(12)-C(5)	109.8(5)
C(4)-N(7)-C(7)	104.4(4)	O(4)-C(14)-O(5)	121.9(7)
C(16)-O(1)-C(17)	110.4(5)	O(4)-C(14)-C(15)	124.4(7)
C(1)-O(3)-C(13)	116.5(4)	O(5)-C(14)-C(15)	113.7(6)

O(2)-C(16)-O(1)	125.1(5)	N(4)-C(23)-C(22)	110.7(5)
O(2)-C(16)-N(7)	126.5(5)	N(5)-C(24)-C(25)	109.1(5)
O(1)-C(16)-N(7)	108.5(5)	C(24)-C(25)-C(26)	105.3(5)
C(19)-C(18)-N(1)	109.3(5)	N(6)-C(26)-C(25)	110.3(6)
C(18)-C(19)-C(20)	104.4(5)	N(5)-B(1)-N(3)	107.4(4)
N(2)-C(20)-C(19)	111.6(5)	N(5)-B(1)-N(1)	108.4(5)
N(3)-C(21)-C(22)	109.9(5)	N(3)-B(1)-N(1)	109.6(5)
C(21)-C(22)-C(23)	104.5(5)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for hmb99ab. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	38(1)	42(1)	48(1)	2(1)	15(1)	1(1)
N(1)	47(2)	74(3)	64(3)	12(2)	16(2)	4(2)
N(2)	45(2)	59(2)	55(3)	4(2)	14(2)	1(2)
N(3)	41(2)	59(2)	78(3)	11(2)	27(2)	11(2)
N(4)	46(2)	50(2)	56(3)	2(2)	17(2)	4(2)
N(5)	47(2)	74(3)	68(3)	2(2)	17(2)	-14(2)
N(6)	53(3)	54(3)	73(3)	-3(2)	22(2)	-4(2)
N(7)	43(2)	51(2)	52(2)	14(2)	17(2)	9(2)
O(1)	72(2)	66(2)	77(3)	22(2)	25(2)	16(2)
O(1C)	67(2)	86(3)	68(2)	32(2)	32(2)	19(2)
O(2)	96(3)	56(2)	85(3)	3(2)	24(2)	13(2)
O(2C)	75(3)	65(2)	108(3)	-23(2)	35(2)	3(2)
O(3)	50(2)	61(2)	54(2)	-3(2)	11(2)	10(2)
O(4)	268(9)	116(4)	128(5)	-30(4)	120(6)	-16(5)
O(5)	60(2)	82(3)	70(2)	-2(2)	25(2)	15(2)
C(1C)	46(3)	48(3)	64(3)	9(2)	25(2)	3(2)
C(1)	44(2)	49(3)	44(3)	4(2)	18(2)	2(2)
C(2)	43(3)	44(3)	48(3)	17(2)	10(2)	6(2)
C(2C)	49(3)	58(3)	66(3)	-3(3)	20(3)	-1(2)
C(3)	42(2)	58(3)	41(3)	5(2)	13(2)	1(2)
C(4)	52(3)	50(3)	64(3)	6(2)	31(2)	0(2)
C(5)	50(3)	62(3)	54(3)	7(2)	19(2)	-1(2)
C(6)	43(3)	55(3)	62(3)	7(2)	16(2)	0(2)
C(7)	40(2)	62(3)	46(3)	8(2)	14(2)	5(2)
C(9)	44(3)	81(4)	66(3)	-3(3)	13(2)	-1(3)
C(10)	52(3)	97(5)	104(5)	4(4)	26(3)	-11(3)
C(11)	53(3)	115(5)	92(5)	24(4)	34(3)	-6(3)
C(12)	50(3)	94(4)	56(3)	11(3)	26(2)	3(3)
C(14)	60(3)	93(5)	92(5)	-24(4)	38(3)	-19(3)
C(15)	64(4)	79(4)	144(6)	-18(4)	14(4)	12(3)
C(16)	49(3)	82(4)	57(4)	16(3)	19(3)	11(3)

C(17)	197(9)	81(5)	100(6)	38(4)	36(6)	43(5)
C(13)	62(3)	55(3)	76(4)	0(3)	14(3)	9(3)
C(18)	53(3)	105(5)	76(4)	29(4)	5(3)	17(3)
C(19)	75(4)	101(5)	54(3)	23(3)	9(3)	16(3)
C(20)	59(3)	74(3)	49(3)	5(3)	16(3)	5(3)
C(21)	55(3)	71(4)	96(5)	12(3)	40(3)	17(3)
C(22)	85(4)	80(4)	87(4)	-10(3)	51(4)	13(3)
C(23)	58(3)	61(3)	61(3)	4(3)	25(3)	7(2)
C(24)	57(3)	108(5)	82(4)	-13(4)	22(3)	-36(4)
C(25)	90(5)	74(4)	137(6)	-20(4)	45(4)	-37(4)
C(26)	76(4)	55(3)	97(5)	-8(3)	30(3)	-13(3)
B(1)	39(3)	81(4)	72(4)	11(3)	17(3)	11(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for hmb99ab.

	x	y	z	U(eq)
H(2)	9000(30)	3760(30)	7220(30)	28(11)
H(3)	9260(30)	2660(20)	6350(40)	40(12)
H(4A)	10595	1745	7115	63
H(5A)	11062	3360	7111	67
H(6A)	11400	3914	8597	65
H(7A)	11020	2798	9742	60
H(9A)	12760	3482	10008	79
H(9B)	12758	2583	9555	79
H(10A)	14082	3244	9375	102
H(10B)	13467	4079	9003	102
H(11A)	12993	3698	7462	102
H(11B)	13766	2954	7829	102
H(12A)	12150	2469	6766	78
H(15A)	13414	-30	7893	154
H(15B)	12755	223	8511	154
H(15C)	13855	583	8811	154
H(17A)	11929	528	11105	198
H(17B)	12120	186	10168	198
H(17C)	11026	161	10186	198
H(13A)	9209	5077	9299	102
H(13B)	8493	4558	8377	102
H(13C)	9485	4965	8349	102
H(18A)	4952	3680	4939	101
H(19A)	6136	3936	4097	98
H(20A)	7791	3364	5238	74
H(21A)	5361	3770	8446	85
H(22A)	6811	4021	10025	94
H(23A)	8314	3452	9758	71
H(24A)	4521	1359	6600	101
H(25A)	5453	13	6978	119
H(26A)	7269	375	7514	93
H(1)	4980(40)	3050(30)	6670(30)	65(14)

Table 6. Torsion angles [°] for hmb99ab.

C(18)-N(1)-N(2)-C(20)	1.7(6)	N(2)-Mo(1)-N(4)-N(3)	39.2(3)
B(1)-N(1)-N(2)-C(20)	176.8(5)	C(1)-Mo(1)-N(4)-N(3)	150.2(3)
C(18)-N(1)-N(2)-Mo(1)	-176.2(4)	C(24)-N(5)-N(6)-C(26)	-0.3(6)
B(1)-N(1)-N(2)-Mo(1)	-1.0(6)	B(1)-N(5)-N(6)-C(26)	-179.9(5)
C(1C)-Mo(1)-N(2)-C(20)	174.0(8)	C(24)-N(5)-N(6)-Mo(1)	176.5(4)
C(2C)-Mo(1)-N(2)-C(20)	-56.7(5)	B(1)-N(5)-N(6)-Mo(1)	-3.1(6)
N(6)-Mo(1)-N(2)-C(20)	-136.3(5)	C(1C)-Mo(1)-N(6)-C(26)	-51.5(5)
C(2)-Mo(1)-N(2)-C(20)	44.3(5)	C(2C)-Mo(1)-N(6)-C(26)	33.0(5)
N(4)-Mo(1)-N(2)-C(20)	143.6(5)	C(2)-Mo(1)-N(6)-C(26)	138.6(6)
C(3)-Mo(1)-N(2)-C(20)	7.4(5)	N(4)-Mo(1)-N(6)-C(26)	-139.4(5)
C(1)-Mo(1)-N(2)-C(20)	60.5(5)	C(3)-Mo(1)-N(6)-C(26)	62.9(6)
C(1C)-Mo(1)-N(2)-N(1)	-8.9(11)	N(2)-Mo(1)-N(6)-C(26)	136.6(5)
C(2C)-Mo(1)-N(2)-N(1)	120.4(4)	C(1)-Mo(1)-N(6)-C(26)	-96.9(6)
N(6)-Mo(1)-N(2)-N(1)	40.8(3)	C(1C)-Mo(1)-N(6)-N(5)	132.5(4)
C(2)-Mo(1)-N(2)-N(1)	-138.6(4)	C(2C)-Mo(1)-N(6)-N(5)	-143.0(4)
N(4)-Mo(1)-N(2)-N(1)	-39.3(3)	C(2)-Mo(1)-N(6)-N(5)	-37.4(8)
C(3)-Mo(1)-N(2)-N(1)	-175.6(4)	N(4)-Mo(1)-N(6)-N(5)	44.6(4)
C(1)-Mo(1)-N(2)-N(1)	-122.5(3)	C(3)-Mo(1)-N(6)-N(5)	-113.1(4)
C(21)-N(3)-N(4)-C(23)	-1.0(5)	N(2)-Mo(1)-N(6)-N(5)	-39.4(4)
B(1)-N(3)-N(4)-C(23)	-170.3(5)	C(1)-Mo(1)-N(6)-N(5)	87.1(6)
C(21)-N(3)-N(4)-Mo(1)	170.6(3)	C(2C)-Mo(1)-C(1C)-O(1C)	-121(6)
B(1)-N(3)-N(4)-Mo(1)	1.3(6)	N(6)-Mo(1)-C(1C)-O(1C)	-40(6)
C(1C)-Mo(1)-N(4)-C(23)	33.7(4)	C(2)-Mo(1)-C(1C)-O(1C)	138(6)
C(2C)-Mo(1)-N(4)-C(23)	104.2(6)	N(4)-Mo(1)-C(1C)-O(1C)	39(6)
N(6)-Mo(1)-N(4)-C(23)	126.1(4)	C(3)-Mo(1)-C(1C)-O(1C)	176(6)
C(2)-Mo(1)-N(4)-C(23)	-69.8(4)	N(2)-Mo(1)-C(1C)-O(1C)	9(7)
C(3)-Mo(1)-N(4)-C(23)	-73.3(5)	C(1)-Mo(1)-C(1C)-O(1C)	126(6)
N(2)-Mo(1)-N(4)-C(23)	-151.7(4)	C(13)-O(3)-C(1)-C(2)	-2.8(7)
C(1)-Mo(1)-N(4)-C(23)	-40.8(4)	C(13)-O(3)-C(1)-C(7)	149.5(4)
C(1C)-Mo(1)-N(4)-N(3)	-135.4(3)	C(13)-O(3)-C(1)-Mo(1)	-75.0(4)
C(2C)-Mo(1)-N(4)-N(3)	-64.9(6)	C(1C)-Mo(1)-C(1)-O(3)	-86.1(3)
N(6)-Mo(1)-N(4)-N(3)	-43.0(3)	C(2C)-Mo(1)-C(1)-O(3)	-164.4(3)
C(2)-Mo(1)-N(4)-N(3)	121.2(3)	N(6)-Mo(1)-C(1)-O(3)	-38.5(6)
C(3)-Mo(1)-N(4)-N(3)	117.6(3)	C(2)-Mo(1)-C(1)-O(3)	115.9(5)

N(4)-Mo(1)-C(1)-O(3)	3.2(3)
C(3)-Mo(1)-C(1)-O(3)	156.3(4)
N(2)-Mo(1)-C(1)-O(3)	83.7(3)
C(1C)-Mo(1)-C(1)-C(2)	158.0(3)
C(2C)-Mo(1)-C(1)-C(2)	79.7(3)
N(6)-Mo(1)-C(1)-C(2)	-154.3(4)
N(4)-Mo(1)-C(1)-C(2)	-112.6(3)
C(3)-Mo(1)-C(1)-C(2)	40.4(3)
N(2)-Mo(1)-C(1)-C(2)	-32.2(3)
C(1C)-Mo(1)-C(1)-C(7)	47.4(3)
C(2C)-Mo(1)-C(1)-C(7)	-30.9(4)
N(6)-Mo(1)-C(1)-C(7)	95.0(5)
C(2)-Mo(1)-C(1)-C(7)	-110.6(4)
N(4)-Mo(1)-C(1)-C(7)	136.7(3)
C(3)-Mo(1)-C(1)-C(7)	-70.2(3)
N(2)-Mo(1)-C(1)-C(7)	-142.8(3)
O(3)-C(1)-C(2)-C(3)	179.7(4)
C(7)-C(1)-C(2)-C(3)	30.0(6)
Mo(1)-C(1)-C(2)-C(3)	-71.9(4)
O(3)-C(1)-C(2)-Mo(1)	-108.4(4)
C(7)-C(1)-C(2)-Mo(1)	101.9(4)
C(1C)-Mo(1)-C(2)-C(1)	-21.7(3)
C(2C)-Mo(1)-C(2)-C(1)	-109.3(3)
N(6)-Mo(1)-C(2)-C(1)	147.9(5)
N(4)-Mo(1)-C(2)-C(1)	68.5(3)
C(3)-Mo(1)-C(2)-C(1)	-115.6(4)
N(2)-Mo(1)-C(2)-C(1)	149.8(3)
C(1C)-Mo(1)-C(2)-C(3)	93.9(3)
C(2C)-Mo(1)-C(2)-C(3)	6.3(3)
N(6)-Mo(1)-C(2)-C(3)	-96.5(6)
N(4)-Mo(1)-C(2)-C(3)	-175.8(3)
N(2)-Mo(1)-C(2)-C(3)	-94.6(3)
C(1)-Mo(1)-C(2)-C(3)	115.6(4)
C(1C)-Mo(1)-C(2C)-O(2C)	60(8)
N(6)-Mo(1)-C(2C)-O(2C)	-32(8)
C(2)-Mo(1)-C(2C)-O(2C)	163(8)
N(4)-Mo(1)-C(2C)-O(2C)	-11(8)
C(3)-Mo(1)-C(2C)-O(2C)	167(8)
N(2)-Mo(1)-C(2C)-O(2C)	-111(8)
C(1)-Mo(1)-C(2C)-O(2C)	132(8)
C(1)-C(2)-C(3)-C(4)	-34.1(6)
Mo(1)-C(2)-C(3)-C(4)	-116.3(4)
C(1)-C(2)-C(3)-Mo(1)	82.2(4)
C(1C)-Mo(1)-C(3)-C(2)	-95.2(3)
C(2C)-Mo(1)-C(3)-C(2)	-173.2(3)
N(6)-Mo(1)-C(3)-C(2)	153.9(3)
N(4)-Mo(1)-C(3)-C(2)	5.8(4)
N(2)-Mo(1)-C(3)-C(2)	82.3(3)
C(1)-Mo(1)-C(3)-C(2)	-34.1(3)
C(1C)-Mo(1)-C(3)-C(4)	12.4(4)
C(2C)-Mo(1)-C(3)-C(4)	-65.6(4)
N(6)-Mo(1)-C(3)-C(4)	-98.5(4)
C(2)-Mo(1)-C(3)-C(4)	107.6(5)
N(4)-Mo(1)-C(3)-C(4)	113.5(4)
N(2)-Mo(1)-C(3)-C(4)	-170.1(4)
C(1)-Mo(1)-C(3)-C(4)	73.6(4)
C(16)-N(7)-C(4)-C(3)	131.8(4)
C(7)-N(7)-C(4)-C(3)	-67.8(4)
C(16)-N(7)-C(4)-C(5)	-112.9(5)
C(7)-N(7)-C(4)-C(5)	47.5(4)
C(2)-C(3)-C(4)-N(7)	54.9(5)
Mo(1)-C(3)-C(4)-N(7)	-25.6(5)
C(2)-C(3)-C(4)-C(5)	-55.3(5)
Mo(1)-C(3)-C(4)-C(5)	-135.7(3)
N(7)-C(4)-C(5)-C(12)	99.3(4)
C(3)-C(4)-C(5)-C(12)	-145.7(4)
N(7)-C(4)-C(5)-C(6)	-26.1(4)
C(3)-C(4)-C(5)-C(6)	89.0(5)
C(12)-C(5)-C(6)-C(9)	-6.2(6)
C(4)-C(5)-C(6)-C(9)	118.4(4)
C(12)-C(5)-C(6)-C(7)	-127.1(4)
C(4)-C(5)-C(6)-C(7)	-2.5(4)

C(16)-N(7)-C(7)-C(1)	-139.7(5)	C(4)-N(7)-C(16)-O(1)	161.9(4)
C(4)-N(7)-C(7)-C(1)	62.5(4)	C(7)-N(7)-C(16)-O(1)	7.2(7)
C(16)-N(7)-C(7)-C(6)	107.9(5)	N(2)-N(1)-C(18)-C(19)	-2.2(7)
C(4)-N(7)-C(7)-C(6)	-49.9(4)	B(1)-N(1)-C(18)-C(19)	-177.0(6)
O(3)-C(1)-C(7)-N(7)	159.5(4)	N(1)-C(18)-C(19)-C(20)	1.8(7)
C(2)-C(1)-C(7)-N(7)	-46.0(5)	N(1)-N(2)-C(20)-C(19)	-0.6(6)
Mo(1)-C(1)-C(7)-N(7)	20.2(4)	Mo(1)-N(2)-C(20)-C(19)	176.8(4)
O(3)-C(1)-C(7)-C(6)	-90.7(4)	C(18)-C(19)-C(20)-N(2)	-0.7(7)
C(2)-C(1)-C(7)-C(6)	63.8(5)	N(4)-N(3)-C(21)-C(22)	1.5(6)
Mo(1)-C(1)-C(7)-C(6)	130.1(3)	B(1)-N(3)-C(21)-C(22)	169.6(5)
C(9)-C(6)-C(7)-N(7)	-90.3(5)	N(3)-C(21)-C(22)-C(23)	-1.3(7)
C(5)-C(6)-C(7)-N(7)	30.4(4)	N(3)-N(4)-C(23)-C(22)	0.2(6)
C(9)-C(6)-C(7)-C(1)	154.4(4)	Mo(1)-N(4)-C(23)-C(22)	-170.0(4)
C(5)-C(6)-C(7)-C(1)	-84.9(4)	C(21)-C(22)-C(23)-N(4)	0.6(6)
C(7)-C(6)-C(9)-C(10)	167.9(5)	N(6)-N(5)-C(24)-C(25)	0.4(7)
C(5)-C(6)-C(9)-C(10)	52.5(6)	B(1)-N(5)-C(24)-C(25)	179.8(6)
C(6)-C(9)-C(10)-C(11)	-44.4(7)	N(5)-C(24)-C(25)-C(26)	-0.2(8)
C(9)-C(10)-C(11)-C(12)	-9.9(8)	N(5)-N(6)-C(26)-C(25)	0.2(7)
C(14)-O(5)-C(12)-C(11)	-106.4(5)	Mo(1)-N(6)-C(26)-C(25)	-176.3(4)
C(14)-O(5)-C(12)-C(5)	133.9(5)	C(24)-C(25)-C(26)-N(6)	0.0(8)
C(10)-C(11)-C(12)-O(5)	-64.9(6)	C(24)-N(5)-B(1)-N(3)	123.3(6)
C(10)-C(11)-C(12)-C(5)	54.7(7)	N(6)-N(5)-B(1)-N(3)	-57.3(6)
C(6)-C(5)-C(12)-O(5)	73.1(5)	C(24)-N(5)-B(1)-N(1)	-118.4(6)
C(4)-C(5)-C(12)-O(5)	-46.2(6)	N(6)-N(5)-B(1)-N(1)	61.1(6)
C(6)-C(5)-C(12)-C(11)	-45.4(6)	C(21)-N(3)-B(1)-N(5)	-108.5(6)
C(4)-C(5)-C(12)-C(11)	-164.8(4)	N(4)-N(3)-B(1)-N(5)	58.3(6)
C(12)-O(5)-C(14)-O(4)	-7.5(9)	C(21)-N(3)-B(1)-N(1)	133.9(5)
C(12)-O(5)-C(14)-C(15)	174.2(5)	N(4)-N(3)-B(1)-N(1)	-59.2(6)
C(17)-O(1)-C(16)-O(2)	-11.1(8)	C(18)-N(1)-B(1)-N(5)	115.9(6)
C(17)-O(1)-C(16)-N(7)	168.9(5)	N(2)-N(1)-B(1)-N(5)	-58.3(6)
C(4)-N(7)-C(16)-O(2)	-18.1(8)	C(18)-N(1)-B(1)-N(3)	-127.2(6)
C(7)-N(7)-C(16)-O(2)	-172.8(5)	N(2)-N(1)-B(1)-N(3)	58.6(6)

Symmetry transformations used to generate equivalent atoms: