Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $C_{24}H_{28}BMoN_7O_7$. 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)	37(1)	32(1)	41(1)	0(1)	2(1)	-1(1)
B(1)	39(3)	40(3)	49(3)	-2(2)	2(2)	7(2)
N(1)	40(2)	44(2)	45(2)	0(2)	-2(2)	2(2)
N(2)	42(2)	41(2)	48(2)	2(2)	1(2)	-2(2)
N(3)	44(2)	36(2)	46(2)	-2(2)	7(2)	-2(2)
N(4)	40(2)	40(2)	49(2)	2(2)	7(2)	1(2)
N(5)	43(2)	38(2)	46(2)	4(2)	6(2)	1(2)
N(6)	38(2)	37(2)	49(2)	1(2)	2(2)	-1(2)
N(7)	39(2)	33(2)	48(2)	1(2)	3(2)	2(2)
O(1)	56(2)	49(2)	53(2)	2(2)	12(2)	9(2)
O(2)	52(2)	34(2)	70(2)	1(2)	7(1)	6(1)
O(3)	53(2)	29(2)	61(2)	3(1)	10(1)	0(1)
O(4)	50(2)	96(3)	97(3)	24(2)	18(2)	12(2)
O(5)	66(2)	74(3)	72(2)	19(2)	11(2)	24(2)
O(6)	60(2)	93(3)	48(2)	-3(2)	10(2)	7(2)
O(7)	61(2)	40(2)	96(3)	-2(2)	-6(2)	6(2)
C(1)	52(3)	44(3)	54(2)	-9(2)	-1(2)	-2(2)
C(2)	57(3)	47(3)	66(3)	-5(2)	-8(2)	-14(2)
C(3)	43(2)	49(3)	62(3)	-3(2)	-6(2)	-12(2)
C(4)	55(3)	47(3)	43(2)	-4(2)	-1(2)	1(2)
C(5)	63(3)	65(4)	40(2)	-5(2)	10(2)	2(3)
C(6)	52(3)	50(3)	53(3)	-3(2)	15(2)	2(2)
C(7)	54(3)	50(3)	57(3)	4(2)	8(2)	-3(2)
C(8)	67(3)	48(3)	59(3)	14(2)	3(2)	4(3)
C(9)	52(3)	43(3)	57(3)	1(2)	0(2)	10(2)
C(10)	42(2)	39(3)	47(2)	3(2)	0(2)	-2(2)
C(11)	41(2)	39(2)	45(2)	-2(2)	3(2)	-3(2)
C(12)	41(2)	44(3)	44(2)	-7(2)	2(2)	-4(2)
C(13)	40(2)	34(2)	52(3)	-4(2)	-1(2)	-2(2)
C(14)	41(2)	32(2)	49(2)	4(2)	6(2)	-5(2)
C(15)	43(2)	39(3)	61(3)	-1(2)	1(2)	-6(2)

C(16)	38(2)	47(3)	52(3)	-4(2)	-3(2)	-3(2)
C(17)	35(2)	44(3)	48(2)	-3(2)	-3(2)	1(2)
C(18)	59(3)	47(3)	86(3)	-5(3)	9(3)	13(2)
C(19)	73(3)	31(3)	78(3)	-8(2)	6(3)	5(2)
C(20)	42(3)	56(3)	52(3)	-2(2)	-2(2)	-2(2)
C(21)	92(4)	96(5)	89(4)	22(4)	10(3)	46(4)
C(22)	49(3)	67(3)	52(3)	-8(3)	0(2)	1(3)
C(23)	43(3)	39(3)	53(3)	4(2)	-2(2)	4(2)
C(24)	40(2)	42(3)	56(2)	-1(2)	0(2)	-5(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $C_{24}H_{28}BMoN_7O_7$.

	x	y	z	U(eq)
H(1)	-3200(30)	2840(30)	1910(20)	32(10)
H(1A)	-836	82	599	60
H(2A)	-2800	-247	335	69
H(3A)	-3725	1143	1002	62
H(4A)	123	2122	4001	58
H(5A)	-1556	2512	4705	67
H(6A)	-2983	2774	3553	62
H(7A)	186	4258	592	64
H(8A)	-1468	5265	286	70
H(9A)	-2914	4428	999	61
H(10A)	2775	678	2776	51
H(11A)	1392	1635	3340	50
H(12A)	1264	3344	3003	51
H(14A)	3263	2818	1136	49
H(15A)	4573	2827	2253	58
H(15B)	3699	3476	2670	58
H(18A)	4477	-1205	1487	95
H(18B)	5173	-267	1316	95
H(18C)	4275	-622	640	95
H(19A)	1624	5452	1693	91
H(19B)	2049	4901	2518	91
H(19C)	857	4735	2144	91
H(21A)	5438	-458	4315	138
H(21B)	6192	380	4010	138
H(21C)	5633	-362	3358	138
H(22A)	4072	2736	4183	84
H(22B)	3347	1804	4304	84
H(22C)	2830	2776	3917	84

Table 6. Torsion angles [°] for $C_{24}H_{28}BMoN_7O_7$.

C(23)-Mo(1)-N(1)-C(1)	47.8(4)
C(24)-Mo(1)-N(1)-C(1)	-34.5(4)
C(12)-Mo(1)-N(1)-C(1)	-145.1(5)
N(5)-Mo(1)-N(1)-C(1)	138.6(4)
C(11)-Mo(1)-N(1)-C(1)	-70.9(5)
N(3)-Mo(1)-N(1)-C(1)	-138.6(4)
C(13)-Mo(1)-N(1)-C(1)	87.0(6)
C(23)-Mo(1)-N(1)-N(2)	-134.8(3)
C(24)-Mo(1)-N(1)-N(2)	142.9(3)
C(12)-Mo(1)-N(1)-N(2)	32.3(7)
N(5)-Mo(1)-N(1)-N(2)	-44.0(3)
C(11)-Mo(1)-N(1)-N(2)	106.5(3)
N(3)-Mo(1)-N(1)-N(2)	38.8(3)
C(13)-Mo(1)-N(1)-N(2)	-95.6(5)
C(1)-N(1)-N(2)-C(3)	0.3(5)
Mo(1)-N(1)-N(2)-C(3)	-177.7(3)
C(1)-N(1)-N(2)-B(1)	-179.9(4)
Mo(1)-N(1)-N(2)-B(1)	2.2(5)
N(4)-B(1)-N(2)-C(3)	120.0(5)
N(6)-B(1)-N(2)-C(3)	-122.2(5)
N(4)-B(1)-N(2)-N(1)	-59.8(5)
N(6)-B(1)-N(2)-N(1)	58.1(5)
C(23)-Mo(1)-N(3)-C(4)	-160.5(11)
C(24)-Mo(1)-N(3)-C(4)	65.8(5)
C(12)-Mo(1)-N(3)-C(4)	-36.6(5)
N(1)-Mo(1)-N(3)-C(4)	145.3(5)
N(5)-Mo(1)-N(3)-C(4)	-134.7(5)
C(11)-Mo(1)-N(3)-C(4)	1.1(5)
C(13)-Mo(1)-N(3)-C(4)	-49.9(5)
C(23)-Mo(1)-N(3)-N(4)	14.7(13)
C(24)-Mo(1)-N(3)-N(4)	-119.0(3)
C(12)-Mo(1)-N(3)-N(4)	138.6(3)
N(1)-Mo(1)-N(3)-N(4)	-39.5(3)
N(5)-Mo(1)-N(3)-N(4)	40.5(3)

C(11)-Mo(1)-N(3)-N(4)	176.3(3)
C(13)-Mo(1)-N(3)-N(4)	125.3(3)
C(4)-N(3)-N(4)-C(6)	-1.0(5)
Mo(1)-N(3)-N(4)-C(6)	-177.5(3)
C(4)-N(3)-N(4)-B(1)	176.1(4)
Mo(1)-N(3)-N(4)-B(1)	-0.4(5)
N(2)-B(1)-N(4)-C(6)	-125.6(5)
N(6)-B(1)-N(4)-C(6)	118.4(5)
N(2)-B(1)-N(4)-N(3)	57.9(5)
N(6)-B(1)-N(4)-N(3)	-58.1(5)
C(23)-Mo(1)-N(5)-C(7)	-35.1(4)
C(24)-Mo(1)-N(5)-C(7)	-108.9(6)
C(12)-Mo(1)-N(5)-C(7)	67.6(4)
N(1)-Mo(1)-N(5)-C(7)	-128.8(4)
C(11)-Mo(1)-N(5)-C(7)	76.3(5)
N(3)-Mo(1)-N(5)-C(7)	148.3(4)
C(13)-Mo(1)-N(5)-C(7)	35.7(4)
C(23)-Mo(1)-N(5)-N(6)	136.9(3)
C(24)-Mo(1)-N(5)-N(6)	63.1(5)
C(12)-Mo(1)-N(5)-N(6)	-120.3(3)
N(1)-Mo(1)-N(5)-N(6)	43.3(3)
C(11)-Mo(1)-N(5)-N(6)	-111.6(3)
N(3)-Mo(1)-N(5)-N(6)	-39.7(3)
C(13)-Mo(1)-N(5)-N(6)	-152.2(3)
C(7)-N(5)-N(6)-C(9)	-0.2(5)
Mo(1)-N(5)-N(6)-C(9)	-174.2(3)
C(7)-N(5)-N(6)-B(1)	172.8(4)
Mo(1)-N(5)-N(6)-B(1)	-1.2(5)
N(4)-B(1)-N(6)-C(9)	-128.8(4)
N(2)-B(1)-N(6)-C(9)	113.6(5)
N(4)-B(1)-N(6)-N(5)	59.5(5)
N(2)-B(1)-N(6)-N(5)	-58.1(5)
N(2)-N(1)-C(1)-C(2)	-0.8(5)
Mo(1)-N(1)-C(1)-C(2)	176.9(3)
N(1)-C(1)-C(2)-C(3)	0.9(6)
N(1)-N(2)-C(3)-C(2)	0.3(5)

B(1)-N(2)-C(3)-C(2)	-179.5(4)
C(1)-C(2)-C(3)-N(2)	-0.7(5)
N(4)-N(3)-C(4)-C(5)	1.1(6)
Mo(1)-N(3)-C(4)-C(5)	176.8(3)
N(3)-C(4)-C(5)-C(6)	-0.8(6)
N(3)-N(4)-C(6)-C(5)	0.5(6)
B(1)-N(4)-C(6)-C(5)	-176.3(5)
C(4)-C(5)-C(6)-N(4)	0.2(6)
N(6)-N(5)-C(7)-C(8)	0.7(5)
Mo(1)-N(5)-C(7)-C(8)	173.6(3)
N(5)-C(7)-C(8)-C(9)	-1.0(6)
N(5)-N(6)-C(9)-C(8)	-0.4(5)
B(1)-N(6)-C(9)-C(8)	-172.8(4)
C(7)-C(8)-C(9)-N(6)	0.8(5)
C(17)-N(7)-C(10)-C(11)	-158.5(4)
C(14)-N(7)-C(10)-C(11)	65.7(4)
C(17)-N(7)-C(10)-C(16)	85.1(5)
C(14)-N(7)-C(10)-C(16)	-50.7(4)
N(7)-C(10)-C(11)-C(12)	-55.8(5)
C(16)-C(10)-C(11)-C(12)	54.7(5)
N(7)-C(10)-C(11)-Mo(1)	25.1(5)
C(16)-C(10)-C(11)-Mo(1)	135.6(3)
C(23)-Mo(1)-C(11)-C(12)	91.8(3)
C(24)-Mo(1)-C(11)-C(12)	167.6(3)
N(1)-Mo(1)-C(11)-C(12)	-152.8(3)
N(5)-Mo(1)-C(11)-C(12)	-14.3(3)
N(3)-Mo(1)-C(11)-C(12)	-85.6(3)
C(13)-Mo(1)-C(11)-C(12)	36.0(3)
C(23)-Mo(1)-C(11)-C(10)	-17.7(4)
C(24)-Mo(1)-C(11)-C(10)	58.1(4)
C(12)-Mo(1)-C(11)-C(10)	-109.6(4)
N(1)-Mo(1)-C(11)-C(10)	97.7(4)
N(5)-Mo(1)-C(11)-C(10)	-123.9(3)
N(3)-Mo(1)-C(11)-C(10)	164.8(4)
C(13)-Mo(1)-C(11)-C(10)	-73.6(3)
C(10)-C(11)-C(12)-C(13)	37.1(5)

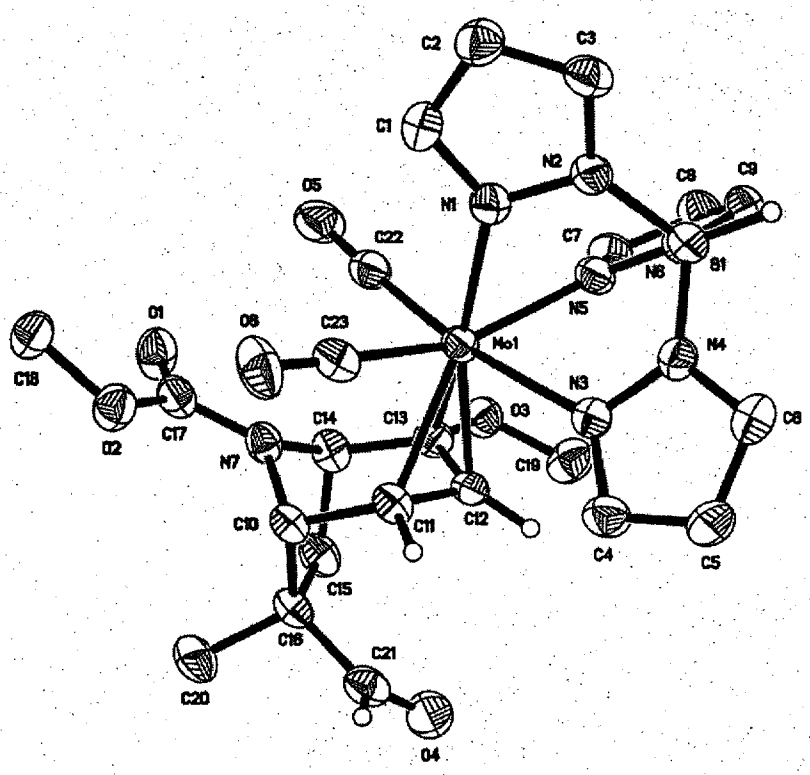
Mo(1)-C(11)-C(12)-C(13)	-79.4(3)
C(10)-C(11)-C(12)-Mo(1)	116.5(4)
C(23)-Mo(1)-C(12)-C(13)	16.5(3)
C(24)-Mo(1)-C(12)-C(13)	102.2(3)
N(1)-Mo(1)-C(12)-C(13)	-150.3(5)
N(5)-Mo(1)-C(12)-C(13)	-76.6(3)
C(11)-Mo(1)-C(12)-C(13)	113.9(4)
N(3)-Mo(1)-C(12)-C(13)	-156.8(3)
C(23)-Mo(1)-C(12)-C(11)	-97.4(3)
C(24)-Mo(1)-C(12)-C(11)	-11.7(3)
N(1)-Mo(1)-C(12)-C(11)	95.8(6)
N(5)-Mo(1)-C(12)-C(11)	169.5(2)
N(3)-Mo(1)-C(12)-C(11)	89.3(3)
C(13)-Mo(1)-C(12)-C(11)	-113.9(4)
C(19)-O(3)-C(13)-C(12)	11.6(6)
C(19)-O(3)-C(13)-C(14)	-136.4(4)
C(19)-O(3)-C(13)-Mo(1)	86.4(4)
C(11)-C(12)-C(13)-O(3)	-179.0(4)
Mo(1)-C(12)-C(13)-O(3)	109.8(4)
C(11)-C(12)-C(13)-C(14)	-33.9(5)
Mo(1)-C(12)-C(13)-C(14)	-105.1(4)
C(11)-C(12)-C(13)-Mo(1)	71.2(3)
C(23)-Mo(1)-C(13)-O(3)	80.6(3)
C(24)-Mo(1)-C(13)-O(3)	156.2(3)
C(12)-Mo(1)-C(13)-O(3)	-116.4(5)
N(1)-Mo(1)-C(13)-O(3)	38.8(6)
N(5)-Mo(1)-C(13)-O(3)	-11.5(3)
C(11)-Mo(1)-C(13)-O(3)	-157.4(4)
N(3)-Mo(1)-C(13)-O(3)	-91.6(3)
C(23)-Mo(1)-C(13)-C(12)	-162.9(3)
C(24)-Mo(1)-C(13)-C(12)	-87.4(3)
N(1)-Mo(1)-C(13)-C(12)	155.2(4)
N(5)-Mo(1)-C(13)-C(12)	104.9(3)
C(11)-Mo(1)-C(13)-C(12)	-41.0(3)
N(3)-Mo(1)-C(13)-C(12)	24.9(3)
C(23)-Mo(1)-C(13)-C(14)	-53.5(3)

C(24)-Mo(1)-C(13)-C(14)	22.0(4)
C(12)-Mo(1)-C(13)-C(14)	109.4(4)
N(1)-Mo(1)-C(13)-C(14)	-95.3(5)
N(5)-Mo(1)-C(13)-C(14)	-145.7(3)
C(11)-Mo(1)-C(13)-C(14)	68.4(3)
N(3)-Mo(1)-C(13)-C(14)	134.3(3)
C(17)-N(7)-C(14)-C(13)	157.0(4)
C(10)-N(7)-C(14)-C(13)	-63.5(4)
C(17)-N(7)-C(14)-C(15)	-89.8(4)
C(10)-N(7)-C(14)-C(15)	49.6(4)
O(3)-C(13)-C(14)-N(7)	-158.2(3)
C(12)-C(13)-C(14)-N(7)	50.9(5)
Mo(1)-C(13)-C(14)-N(7)	-18.0(4)
O(3)-C(13)-C(14)-C(15)	91.8(4)
C(12)-C(13)-C(14)-C(15)	-59.1(5)
Mo(1)-C(13)-C(14)-C(15)	-128.0(3)
N(7)-C(14)-C(15)-C(16)	-28.6(4)
C(13)-C(14)-C(15)-C(16)	88.1(4)
C(14)-C(15)-C(16)-C(22)	-125.7(4)
C(14)-C(15)-C(16)-C(20)	112.1(4)
C(14)-C(15)-C(16)-C(10)	-1.4(4)
N(7)-C(10)-C(16)-C(22)	155.2(4)
C(11)-C(10)-C(16)-C(22)	39.9(5)
N(7)-C(10)-C(16)-C(20)	-84.5(4)
C(11)-C(10)-C(16)-C(20)	160.2(4)
N(7)-C(10)-C(16)-C(15)	30.6(4)
C(11)-C(10)-C(16)-C(15)	-84.7(4)
C(18)-O(2)-C(17)-O(1)	5.1(6)
C(18)-O(2)-C(17)-N(7)	-175.7(4)
C(14)-N(7)-C(17)-O(1)	-21.0(6)
C(10)-N(7)-C(17)-O(1)	-151.1(4)
C(14)-N(7)-C(17)-O(2)	159.8(3)
C(10)-N(7)-C(17)-O(2)	29.8(5)
C(21)-O(5)-C(20)-O(4)	2.8(8)
C(21)-O(5)-C(20)-C(16)	-179.4(5)
C(22)-C(16)-C(20)-O(4)	-133.9(6)

C(15)-C(16)-C(20)-O(4)	-8.0(7)
C(10)-C(16)-C(20)-O(4)	102.3(6)
C(22)-C(16)-C(20)-O(5)	48.4(5)
C(15)-C(16)-C(20)-O(5)	174.3(4)
C(10)-C(16)-C(20)-O(5)	-75.4(5)
C(24)-Mo(1)-C(23)-O(6)	84(13)
C(12)-Mo(1)-C(23)-O(6)	-173(100)
N(1)-Mo(1)-C(23)-O(6)	3(13)
N(5)-Mo(1)-C(23)-O(6)	-76(13)
C(11)-Mo(1)-C(23)-O(6)	148(13)
N(3)-Mo(1)-C(23)-O(6)	-51(13)
C(13)-Mo(1)-C(23)-O(6)	-164(13)
C(23)-Mo(1)-C(24)-O(7)	-38(6)
C(12)-Mo(1)-C(24)-O(7)	-139(6)
N(1)-Mo(1)-C(24)-O(7)	57(6)
N(5)-Mo(1)-C(24)-O(7)	37(7)
C(11)-Mo(1)-C(24)-O(7)	-147(6)
N(3)-Mo(1)-C(24)-O(7)	136(6)
C(13)-Mo(1)-C(24)-O(7)	-105(6)

Symmetry transformations used to generate equivalent atoms:

Ortep Drawing of Compound (±)-**9b**



Crystal Structure Analysis

A suitable crystal of **HMB219a** 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 (±)-9b

Table 1. Crystal data and structure refinement for $C_{23}H_{26}N_7BMoO_6$.

Identification code	hmb219a	
Empirical formula	$C_{23}H_{26}N_7BMoO_6$	
Formula weight	603.26	
Temperature	295(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 14.6934(13) Å	α= 90°.
	b = 7.8476(5) Å	β= 102.939(5)°.
	c = 22.7805(15) Å	γ = 90°.
Volume	2560.1(3) Å^3	
Z	4	
Density (calculated)	1.565 Mg/m^3	
Absorption coefficient	4.650 mm^{-1}	
F(000)	1232	
Crystal size	0.32 x 0.30 x 0.06 mm^3	
Theta range for data collection	3.28 to 56.74°.	
Index ranges	$-14 \le h \le 15$, $-8 \le k \le 8$, $-24 \le l \le 24$	
Reflections collected	6885	
Independent reflections	3384 [R(int) = 0.0409]	
Completeness to theta = 56.74°	98.8 %	
Absorption correction	Empirical	
Max. and min. transmission	0.2026 and 0.0582	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3384 / 0 / 347	
Goodness-of-fit on F^2	2.584	
Final R indices [I>2sigma(I)]	R1 = 0.0542, wR2 = 0.1197	
R indices (all data)	R1 = 0.0601, wR2 = 0.1210	
Largest diff. peak and hole	1.111 and -1.248 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $C_{23}H_{26}N_7BMoO_6$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	8458(1)	3510(1)	1236(1)	41(1)
B(1)	6889(5)	3826(10)	-87(3)	51(2)
N(1)	7016(3)	2532(6)	937(2)	49(1)
N(2)	6477(3)	2838(6)	382(2)	48(1)
N(3)	7802(3)	5842(6)	672(2)	48(1)
N(4)	7169(3)	5611(6)	160(2)	46(1)
N(5)	8467(3)	2480(6)	307(2)	48(1)
N(6)	7757(4)	2864(6)	-170(2)	48(1)
N(7)	10124(3)	3225(6)	2500(2)	47(1)
O(1)	10491(4)	765(7)	3029(2)	73(1)
O(2)	9545(3)	2735(6)	3313(2)	64(1)
O(3)	10744(3)	2714(6)	1070(2)	57(1)
O(4)	11433(4)	7863(8)	1906(3)	84(2)
O(5)	9072(4)	37(6)	1838(2)	81(2)
O(6)	7785(3)	4175(8)	2419(2)	78(2)
C(1)	6504(5)	1551(8)	1225(3)	57(2)
C(2)	5636(4)	1242(9)	852(3)	59(2)
C(3)	5649(4)	2058(8)	328(3)	54(2)
C(4)	7882(5)	7537(8)	756(3)	56(2)
C(5)	7307(5)	8389(8)	270(3)	60(2)
C(6)	6869(5)	7121(9)	-95(3)	56(2)
C(7)	9039(5)	1431(8)	97(3)	58(2)
C(8)	8716(5)	1172(9)	-513(3)	65(2)
C(9)	7906(5)	2079(8)	-665(3)	56(2)
C(10)	9934(4)	5049(7)	2467(3)	46(2)
C(11)	9365(4)	5463(8)	1843(3)	45(1)
C(12)	9782(4)	5003(7)	1344(3)	47(2)
C(13)	10275(5)	3464(8)	1452(3)	51(2)
C(14)	10750(4)	2972(9)	2099(3)	52(2)
C(15)	11496(4)	4376(9)	2328(3)	61(2)
C(16)	10947(4)	5793(9)	2572(3)	51(2)

C(17)	10095(5)	2116(9)	2957(3)	58(2)
C(18)	9236(6)	1464(10)	3678(3)	77(2)
C(19)	10917(6)	3711(10)	584(4)	74(2)
C(20)	11349(5)	6159(10)	3237(3)	69(2)
C(21)	10959(5)	7482(9)	2247(3)	61(2)
C(22)	8868(5)	1376(9)	1621(3)	58(2)
C(23)	8034(4)	3954(8)	1983(3)	56(2)

Table 3. Bond lengths [Å] and angles [°] for $C_{23}H_{26}N_7BMoO_6$.

Mo(1)-C(22)	1.923(7)	C(5)-C(6)	1.363(10)
Mo(1)-C(23)	1.970(8)	C(7)-C(8)	1.380(10)
Mo(1)-N(1)	2.213(5)	C(8)-C(9)	1.363(10)
Mo(1)-C(12)	2.236(6)	C(10)-C(11)	1.513(8)
Mo(1)-N(5)	2.269(5)	C(10)-C(16)	1.567(8)
Mo(1)-C(11)	2.283(6)	C(11)-C(12)	1.454(8)
Mo(1)-N(3)	2.318(5)	C(12)-C(13)	1.402(8)
Mo(1)-C(13)	2.604(7)	C(13)-C(14)	1.531(9)
B(1)-N(4)	1.531(9)	C(14)-C(15)	1.560(9)
B(1)-N(6)	1.530(9)	C(15)-C(16)	1.548(9)
B(1)-N(2)	1.547(9)	C(16)-C(21)	1.519(10)
N(1)-C(1)	1.345(8)	C(16)-C(20)	1.525(9)
N(1)-N(2)	1.355(7)		
N(2)-C(3)	1.343(8)	C(22)-Mo(1)-C(23)	83.5(3)
N(3)-N(4)	1.331(7)	C(22)-Mo(1)-N(1)	91.0(2)
N(3)-C(4)	1.345(8)	C(23)-Mo(1)-N(1)	82.0(2)
N(4)-C(6)	1.351(8)	C(22)-Mo(1)-C(12)	103.4(3)
N(5)-C(7)	1.339(8)	C(23)-Mo(1)-C(12)	104.4(2)
N(5)-N(6)	1.360(7)	N(1)-Mo(1)-C(12)	164.7(2)
N(6)-C(9)	1.346(8)	C(22)-Mo(1)-N(5)	92.8(2)
N(7)-C(17)	1.365(8)	C(23)-Mo(1)-N(5)	159.7(2)
N(7)-C(14)	1.449(8)	N(1)-Mo(1)-N(5)	78.12(17)
N(7)-C(10)	1.457(7)	C(12)-Mo(1)-N(5)	95.9(2)
O(1)-C(17)	1.202(8)	C(22)-Mo(1)-C(11)	103.2(3)
O(2)-C(17)	1.357(8)	C(23)-Mo(1)-C(11)	67.2(2)
O(2)-C(18)	1.435(8)	N(1)-Mo(1)-C(11)	143.91(19)
O(3)-C(13)	1.358(7)	C(12)-Mo(1)-C(11)	37.5(2)
O(3)-C(19)	1.425(8)	N(5)-Mo(1)-C(11)	132.86(19)
O(4)-C(21)	1.193(9)	C(22)-Mo(1)-N(3)	171.4(2)
O(5)-C(22)	1.171(8)	C(23)-Mo(1)-N(3)	99.6(2)
O(6)-C(23)	1.146(8)	N(1)-Mo(1)-N(3)	81.50(18)
C(1)-C(2)	1.387(9)	C(12)-Mo(1)-N(3)	83.73(19)
C(2)-C(3)	1.358(10)	N(5)-Mo(1)-N(3)	81.53(18)
C(4)-C(5)	1.403(9)	C(11)-Mo(1)-N(3)	85.4(2)

C(22)-Mo(1)-C(13)	72.5(2)	N(3)-C(4)-C(5)	110.0(6)
C(23)-Mo(1)-C(13)	110.4(2)	C(6)-C(5)-C(4)	104.6(6)
N(1)-Mo(1)-C(13)	157.47(19)	N(4)-C(6)-C(5)	108.3(6)
C(12)-Mo(1)-C(13)	32.6(2)	N(5)-C(7)-C(8)	110.4(6)
N(5)-Mo(1)-C(13)	87.21(18)	C(9)-C(8)-C(7)	105.2(6)
C(11)-Mo(1)-C(13)	57.35(19)	N(6)-C(9)-C(8)	108.8(6)
N(3)-Mo(1)-C(13)	113.41(19)	N(7)-C(10)-C(11)	108.6(5)
N(4)-B(1)-N(6)	109.5(5)	N(7)-C(10)-C(16)	101.1(5)
N(4)-B(1)-N(2)	108.7(6)	C(11)-C(10)-C(16)	111.7(5)
N(6)-B(1)-N(2)	107.7(5)	C(12)-C(11)-C(10)	116.2(5)
C(1)-N(1)-N(2)	106.4(5)	C(12)-C(11)-Mo(1)	69.5(3)
C(1)-N(1)-Mo(1)	130.5(4)	C(10)-C(11)-Mo(1)	123.3(4)
N(2)-N(1)-Mo(1)	123.0(4)	C(13)-C(12)-C(11)	111.6(6)
C(3)-N(2)-N(1)	109.4(5)	C(13)-C(12)-Mo(1)	88.3(4)
C(3)-N(2)-B(1)	130.7(5)	C(11)-C(12)-Mo(1)	73.0(3)
N(1)-N(2)-B(1)	119.7(5)	O(3)-C(13)-C(12)	125.2(6)
N(4)-N(3)-C(4)	106.3(5)	O(3)-C(13)-C(14)	108.7(5)
N(4)-N(3)-Mo(1)	120.0(4)	C(12)-C(13)-C(14)	119.5(5)
C(4)-N(3)-Mo(1)	133.6(4)	O(3)-C(13)-Mo(1)	122.0(4)
N(3)-N(4)-C(6)	110.8(5)	C(12)-C(13)-Mo(1)	59.1(3)
N(3)-N(4)-B(1)	121.6(5)	C(14)-C(13)-Mo(1)	114.3(4)
C(6)-N(4)-B(1)	127.6(5)	N(7)-C(14)-C(13)	110.9(5)
C(7)-N(5)-N(6)	106.4(5)	N(7)-C(14)-C(15)	100.9(5)
C(7)-N(5)-Mo(1)	133.4(4)	C(13)-C(14)-C(15)	106.2(6)
N(6)-N(5)-Mo(1)	120.2(4)	C(16)-C(15)-C(14)	104.1(5)
C(9)-N(6)-N(5)	109.2(5)	C(21)-C(16)-C(20)	106.0(5)
C(9)-N(6)-B(1)	128.7(5)	C(21)-C(16)-C(15)	112.8(6)
N(5)-N(6)-B(1)	121.5(5)	C(20)-C(16)-C(15)	112.0(6)
C(17)-N(7)-C(14)	121.8(5)	C(21)-C(16)-C(10)	111.4(5)
C(17)-N(7)-C(10)	128.9(5)	C(20)-C(16)-C(10)	111.4(5)
C(14)-N(7)-C(10)	104.1(5)	C(15)-C(16)-C(10)	103.4(5)
C(17)-O(2)-C(18)	113.9(6)	O(1)-C(17)-O(2)	124.6(7)
C(13)-O(3)-C(19)	117.7(5)	O(1)-C(17)-N(7)	124.8(7)
N(1)-C(1)-C(2)	109.8(6)	O(2)-C(17)-N(7)	110.6(6)
C(3)-C(2)-C(1)	105.3(6)	O(4)-C(21)-C(16)	127.5(7)
N(2)-C(3)-C(2)	109.0(6)	O(5)-C(22)-Mo(1)	176.3(6)

O(6)-C(23)-Mo(1)	178.5(6)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for $C_{23}H_{26}N_7BMoO_6$. 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)	44(1)	39(1)	38(1)	-3(1)	5(1)	1(1)
B(1)	51(4)	52(5)	45(4)	0(3)	2(3)	-7(3)
N(1)	49(3)	52(3)	46(3)	-2(3)	11(2)	-7(2)
N(2)	45(3)	49(3)	46(3)	2(2)	3(2)	-1(2)
N(3)	53(3)	44(3)	44(3)	3(2)	6(2)	-1(2)
N(4)	47(3)	45(3)	44(3)	6(2)	7(2)	1(2)
N(5)	50(3)	46(3)	47(3)	-6(2)	7(2)	-4(2)
N(6)	60(3)	46(3)	37(3)	-2(2)	7(2)	-7(2)
N(7)	53(3)	47(3)	41(3)	-4(2)	8(2)	8(2)
O(1)	102(4)	60(3)	58(3)	9(2)	19(3)	25(3)
O(2)	73(3)	65(3)	60(3)	3(2)	26(3)	2(2)
O(3)	68(3)	57(3)	49(3)	-6(2)	23(2)	3(2)
O(4)	82(4)	98(4)	74(4)	-1(3)	20(3)	-27(3)
O(5)	100(4)	44(3)	83(4)	1(3)	-16(3)	0(3)
O(6)	68(3)	122(5)	48(3)	-15(3)	18(3)	1(3)
C(1)	64(4)	58(4)	48(4)	10(3)	13(3)	1(3)
C(2)	47(4)	68(5)	64(5)	7(4)	14(3)	-6(3)
C(3)	44(3)	56(4)	59(4)	-5(3)	2(3)	-7(3)
C(4)	63(4)	41(4)	59(4)	-7(3)	7(3)	0(3)
C(5)	74(4)	34(4)	67(5)	8(3)	7(4)	7(3)
C(6)	59(4)	54(4)	55(4)	14(3)	16(3)	7(3)
C(7)	65(4)	51(4)	61(4)	-9(3)	17(3)	4(3)
C(8)	78(5)	66(5)	54(4)	-17(4)	23(4)	1(4)
C(9)	71(4)	56(4)	42(4)	-8(3)	16(3)	-10(3)
C(10)	46(3)	49(4)	41(3)	-9(3)	6(3)	1(3)
C(11)	38(3)	51(4)	45(3)	-7(3)	4(3)	7(3)
C(12)	51(3)	41(4)	44(4)	-4(3)	2(3)	-5(3)
C(13)	67(4)	38(3)	51(4)	-10(3)	20(3)	1(3)
C(14)	49(3)	54(4)	52(4)	-4(3)	9(3)	15(3)
C(15)	48(4)	73(5)	56(4)	-7(4)	0(3)	5(3)
C(16)	47(3)	59(4)	42(3)	-11(3)	0(3)	-3(3)

C(17)	65(4)	59(4)	45(4)	-5(3)	4(3)	4(4)
C(18)	81(5)	89(6)	62(5)	14(4)	17(4)	-21(4)
C(19)	80(5)	72(5)	80(5)	3(4)	41(4)	-1(4)
C(20)	59(4)	88(6)	52(4)	-8(4)	-7(3)	-5(4)
C(21)	53(4)	62(5)	62(5)	-10(4)	0(4)	-5(3)
C(22)	69(4)	46(4)	52(4)	-3(3)	1(3)	-6(3)
C(23)	51(4)	55(4)	57(4)	-10(3)	3(3)	-1(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $C_{23}H_{26}N_7BMoO_6$.

	x	y	z	U(eq)
H(1)	6410(40)	3970(80)	-530(30)	63(19)
H(1A)	6703	1141	1616	68
H(2A)	5148	612	941	71
H(3A)	5163	2073	-13	65
H(4A)	8263	8066	1087	67
H(5A)	7240	9559	210	72
H(6A)	6436	7271	-458	67
H(7A)	9578	945	330	70
H(8A)	8992	520	-767	78
H(9A)	7519	2144	-1048	67
H(10A)	9617	5418	2781	55
H(11A)	9097	6611	1810	54
H(12A)	9886	5833	1044	56
H(14A)	11017	1824	2127	63
H(15A)	11996	3938	2644	73
H(15B)	11759	4801	2002	73
H(18A)	8860	1991	3921	116
H(18B)	9769	933	3933	116
H(18C)	8874	620	3423	116
H(19A)	11256	3042	352	111
H(19B)	11278	4696	741	111
H(19C)	10334	4066	332	111
H(20A)	11968	6614	3287	104
H(20B)	11372	5122	3463	104
H(20C)	10960	6971	3379	104
H(21A)	10550	8313	2324	73

Table 6. Torsion angles [°] for $C_{23}H_{26}N_7BMoO_6$.

C(22)-Mo(1)-N(1)-C(1)	40.2(6)
C(23)-Mo(1)-N(1)-C(1)	-43.2(6)
C(12)-Mo(1)-N(1)-C(1)	-159.1(7)
N(5)-Mo(1)-N(1)-C(1)	132.8(6)
C(11)-Mo(1)-N(1)-C(1)	-74.2(7)
N(3)-Mo(1)-N(1)-C(1)	-144.2(6)
C(13)-Mo(1)-N(1)-C(1)	82.3(7)
C(22)-Mo(1)-N(1)-N(2)	-138.4(5)
C(23)-Mo(1)-N(1)-N(2)	138.2(5)
C(12)-Mo(1)-N(1)-N(2)	22.3(10)
N(5)-Mo(1)-N(1)-N(2)	-45.8(4)
C(11)-Mo(1)-N(1)-N(2)	107.2(5)
N(3)-Mo(1)-N(1)-N(2)	37.2(4)
C(13)-Mo(1)-N(1)-N(2)	-96.3(6)
C(1)-N(1)-N(2)-C(3)	-0.1(7)
Mo(1)-N(1)-N(2)-C(3)	178.8(4)
C(1)-N(1)-N(2)-B(1)	-175.3(6)
Mo(1)-N(1)-N(2)-B(1)	3.6(7)
N(4)-B(1)-N(2)-C(3)	124.4(7)
N(6)-B(1)-N(2)-C(3)	-117.1(7)
N(4)-B(1)-N(2)-N(1)	-61.5(7)
N(6)-B(1)-N(2)-N(1)	56.9(7)
C(22)-Mo(1)-N(3)-N(4)	-7.7(18)
C(23)-Mo(1)-N(3)-N(4)	-118.2(4)
N(1)-Mo(1)-N(3)-N(4)	-37.9(4)
C(12)-Mo(1)-N(3)-N(4)	138.2(4)
N(5)-Mo(1)-N(3)-N(4)	41.3(4)
C(11)-Mo(1)-N(3)-N(4)	175.8(4)
C(13)-Mo(1)-N(3)-N(4)	124.5(4)
C(22)-Mo(1)-N(3)-C(4)	168.7(15)
C(23)-Mo(1)-N(3)-C(4)	58.1(6)
N(1)-Mo(1)-N(3)-C(4)	138.4(6)
C(12)-Mo(1)-N(3)-C(4)	-45.5(6)
N(5)-Mo(1)-N(3)-C(4)	-142.4(6)

C(11)-Mo(1)-N(3)-C(4)	-7.8(6)
C(13)-Mo(1)-N(3)-C(4)	-59.2(6)
C(4)-N(3)-N(4)-C(6)	2.2(7)
Mo(1)-N(3)-N(4)-C(6)	179.4(4)
C(4)-N(3)-N(4)-B(1)	180.0(6)
Mo(1)-N(3)-N(4)-B(1)	-2.8(7)
N(6)-B(1)-N(4)-N(3)	-57.0(7)
N(2)-B(1)-N(4)-N(3)	60.3(7)
N(6)-B(1)-N(4)-C(6)	120.4(6)
N(2)-B(1)-N(4)-C(6)	-122.3(6)
C(22)-Mo(1)-N(5)-C(7)	-39.1(6)
C(23)-Mo(1)-N(5)-C(7)	-117.9(8)
N(1)-Mo(1)-N(5)-C(7)	-129.6(6)
C(12)-Mo(1)-N(5)-C(7)	64.7(6)
C(11)-Mo(1)-N(5)-C(7)	71.8(6)
N(3)-Mo(1)-N(5)-C(7)	147.4(6)
C(13)-Mo(1)-N(5)-C(7)	33.2(6)
C(22)-Mo(1)-N(5)-N(6)	137.6(4)
C(23)-Mo(1)-N(5)-N(6)	58.8(8)
N(1)-Mo(1)-N(5)-N(6)	47.1(4)
C(12)-Mo(1)-N(5)-N(6)	-118.6(4)
C(11)-Mo(1)-N(5)-N(6)	-111.5(4)
N(3)-Mo(1)-N(5)-N(6)	-35.9(4)
C(13)-Mo(1)-N(5)-N(6)	-150.1(4)
C(7)-N(5)-N(6)-C(9)	-1.0(7)
Mo(1)-N(5)-N(6)-C(9)	-178.5(4)
C(7)-N(5)-N(6)-B(1)	170.8(5)
Mo(1)-N(5)-N(6)-B(1)	-6.7(7)
N(4)-B(1)-N(6)-C(9)	-126.5(6)
N(2)-B(1)-N(6)-C(9)	115.5(7)
N(4)-B(1)-N(6)-N(5)	63.4(7)
N(2)-B(1)-N(6)-N(5)	-54.5(7)
N(2)-N(1)-C(1)-C(2)	-0.4(7)
Mo(1)-N(1)-C(1)-C(2)	-179.1(4)
N(1)-C(1)-C(2)-C(3)	0.6(8)
N(1)-N(2)-C(3)-C(2)	0.5(7)

B(1)-N(2)-C(3)-C(2)	175.1(6)
C(1)-C(2)-C(3)-N(2)	-0.7(8)
N(4)-N(3)-C(4)-C(5)	-2.2(7)
Mo(1)-N(3)-C(4)-C(5)	-178.9(4)
N(3)-C(4)-C(5)-C(6)	1.4(8)
N(3)-N(4)-C(6)-C(5)	-1.3(7)
B(1)-N(4)-C(6)-C(5)	-178.9(6)
C(4)-C(5)-C(6)-N(4)	-0.1(8)
N(6)-N(5)-C(7)-C(8)	1.6(7)
Mo(1)-N(5)-C(7)-C(8)	178.6(4)
N(5)-C(7)-C(8)-C(9)	-1.5(8)
N(5)-N(6)-C(9)-C(8)	0.1(7)
B(1)-N(6)-C(9)-C(8)	-170.9(6)
C(7)-C(8)-C(9)-N(6)	0.8(8)
C(17)-N(7)-C(10)-C(11)	-137.9(6)
C(14)-N(7)-C(10)-C(11)	67.9(5)
C(17)-N(7)-C(10)-C(16)	104.5(7)
C(14)-N(7)-C(10)-C(16)	-49.7(6)
N(7)-C(10)-C(11)-C(12)	-57.8(7)
C(16)-C(10)-C(11)-C(12)	52.9(7)
N(7)-C(10)-C(11)-Mo(1)	24.0(6)
C(16)-C(10)-C(11)-Mo(1)	134.6(4)
C(22)-Mo(1)-C(11)-C(12)	94.9(4)
C(23)-Mo(1)-C(11)-C(12)	171.9(4)
N(1)-Mo(1)-C(11)-C(12)	-154.5(3)
N(5)-Mo(1)-C(11)-C(12)	-11.7(5)
N(3)-Mo(1)-C(11)-C(12)	-85.7(3)
C(13)-Mo(1)-C(11)-C(12)	36.0(3)
C(22)-Mo(1)-C(11)-C(10)	-13.7(5)
C(23)-Mo(1)-C(11)-C(10)	63.4(5)
N(1)-Mo(1)-C(11)-C(10)	97.0(5)
C(12)-Mo(1)-C(11)-C(10)	-108.6(6)
N(5)-Mo(1)-C(11)-C(10)	-120.3(4)
N(3)-Mo(1)-C(11)-C(10)	165.8(5)
C(13)-Mo(1)-C(11)-C(10)	-72.6(5)
C(10)-C(11)-C(12)-C(13)	36.9(7)

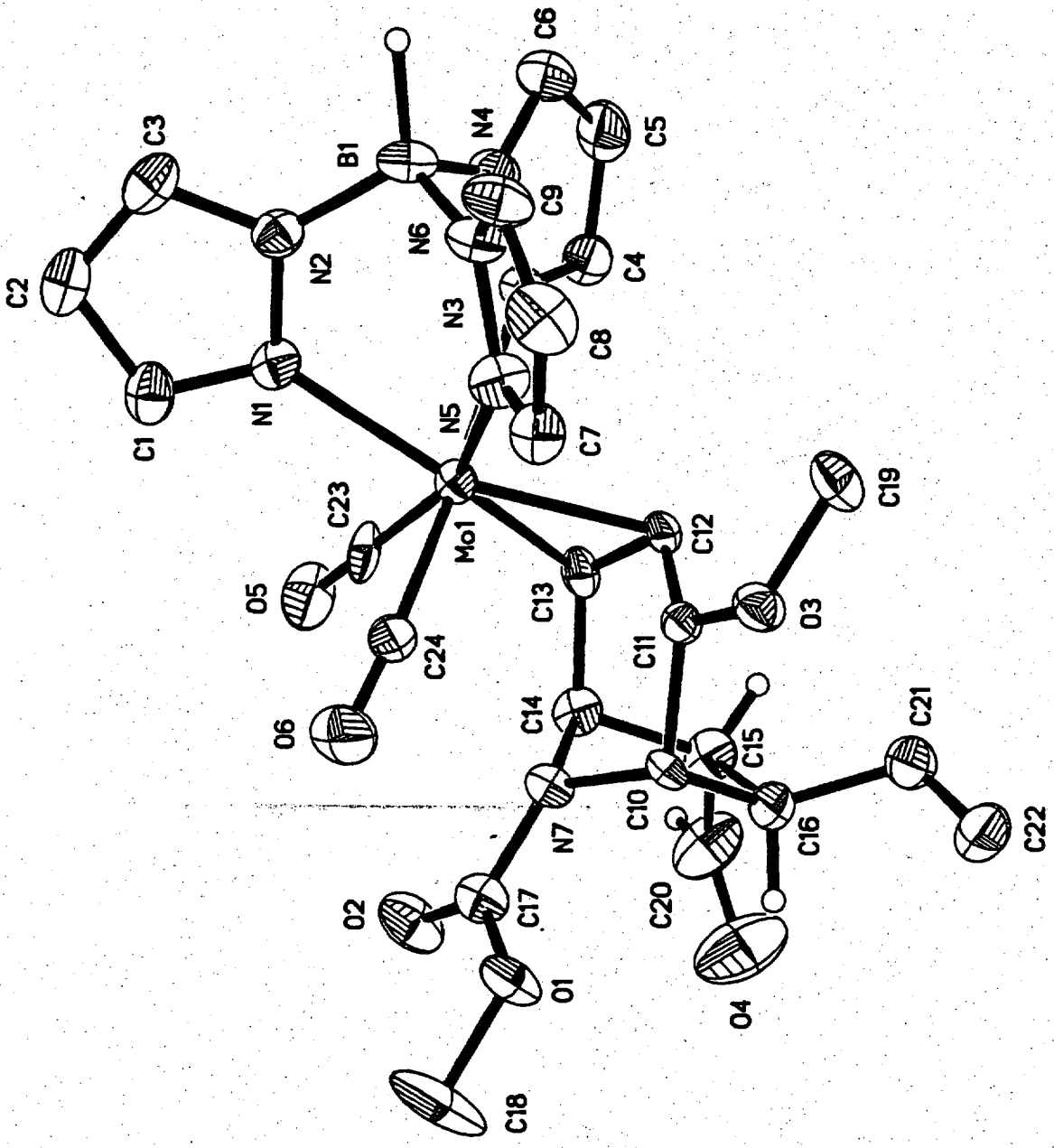
Mo(1)-C(11)-C(12)-C(13)	-81.1(4)
C(10)-C(11)-C(12)-Mo(1)	118.0(5)
C(22)-Mo(1)-C(12)-C(13)	18.9(4)
C(23)-Mo(1)-C(12)-C(13)	105.5(4)
N(1)-Mo(1)-C(12)-C(13)	-141.3(7)
N(5)-Mo(1)-C(12)-C(13)	-75.4(4)
C(11)-Mo(1)-C(12)-C(13)	113.2(5)
N(3)-Mo(1)-C(12)-C(13)	-156.2(4)
C(22)-Mo(1)-C(12)-C(11)	-94.3(4)
C(23)-Mo(1)-C(12)-C(11)	-7.7(4)
N(1)-Mo(1)-C(12)-C(11)	105.5(8)
N(5)-Mo(1)-C(12)-C(11)	171.4(3)
N(3)-Mo(1)-C(12)-C(11)	90.6(4)
C(13)-Mo(1)-C(12)-C(11)	-113.2(5)
C(19)-O(3)-C(13)-C(12)	13.9(9)
C(19)-O(3)-C(13)-C(14)	-137.2(6)
C(19)-O(3)-C(13)-Mo(1)	86.5(6)
C(11)-C(12)-C(13)-O(3)	-179.5(6)
Mo(1)-C(12)-C(13)-O(3)	109.5(6)
C(11)-C(12)-C(13)-C(14)	-31.3(8)
Mo(1)-C(12)-C(13)-C(14)	-102.3(5)
C(11)-C(12)-C(13)-Mo(1)	71.0(4)
C(22)-Mo(1)-C(13)-O(3)	84.5(5)
C(23)-Mo(1)-C(13)-O(3)	160.4(5)
N(1)-Mo(1)-C(13)-O(3)	39.8(8)
C(12)-Mo(1)-C(13)-O(3)	-114.8(7)
N(5)-Mo(1)-C(13)-O(3)	-9.3(5)
C(11)-Mo(1)-C(13)-O(3)	-156.4(6)
N(3)-Mo(1)-C(13)-O(3)	-88.8(5)
C(22)-Mo(1)-C(13)-C(12)	-160.7(5)
C(23)-Mo(1)-C(13)-C(12)	-84.8(4)
N(1)-Mo(1)-C(13)-C(12)	154.5(5)
N(5)-Mo(1)-C(13)-C(12)	105.5(4)
C(11)-Mo(1)-C(13)-C(12)	-41.7(4)
N(3)-Mo(1)-C(13)-C(12)	25.9(4)
C(22)-Mo(1)-C(13)-C(14)	-49.7(4)

C(23)-Mo(1)-C(13)-C(14)	26.2(5)
N(1)-Mo(1)-C(13)-C(14)	-94.4(6)
C(12)-Mo(1)-C(13)-C(14)	111.1(6)
N(5)-Mo(1)-C(13)-C(14)	-143.5(4)
C(11)-Mo(1)-C(13)-C(14)	69.4(4)
N(3)-Mo(1)-C(13)-C(14)	137.0(4)
C(17)-N(7)-C(14)-C(13)	141.5(6)
C(10)-N(7)-C(14)-C(13)	-62.0(6)
C(17)-N(7)-C(14)-C(15)	-106.3(7)
C(10)-N(7)-C(14)-C(15)	50.2(6)
O(3)-C(13)-C(14)-N(7)	-160.4(5)
C(12)-C(13)-C(14)-N(7)	46.6(8)
Mo(1)-C(13)-C(14)-N(7)	-20.4(6)
O(3)-C(13)-C(14)-C(15)	90.8(6)
C(12)-C(13)-C(14)-C(15)	-62.2(7)
Mo(1)-C(13)-C(14)-C(15)	-129.2(4)
N(7)-C(14)-C(15)-C(16)	-29.8(6)
C(13)-C(14)-C(15)-C(16)	86.0(6)
C(14)-C(15)-C(16)-C(21)	-119.6(6)
C(14)-C(15)-C(16)-C(20)	120.9(6)
C(14)-C(15)-C(16)-C(10)	0.8(7)
N(7)-C(10)-C(16)-C(21)	149.7(5)
C(11)-C(10)-C(16)-C(21)	34.3(7)
N(7)-C(10)-C(16)-C(20)	-92.2(6)
C(11)-C(10)-C(16)-C(20)	152.4(6)
N(7)-C(10)-C(16)-C(15)	28.2(6)
C(11)-C(10)-C(16)-C(15)	-87.1(6)
C(18)-O(2)-C(17)-O(1)	-17.7(9)
C(18)-O(2)-C(17)-N(7)	161.2(6)
C(14)-N(7)-C(17)-O(1)	-8.7(10)
C(10)-N(7)-C(17)-O(1)	-158.9(6)
C(14)-N(7)-C(17)-O(2)	172.4(5)
C(10)-N(7)-C(17)-O(2)	22.2(9)
C(20)-C(16)-C(21)-O(4)	111.6(8)
C(15)-C(16)-C(21)-O(4)	-11.3(9)
C(10)-C(16)-C(21)-O(4)	-127.1(7)

C(23)-Mo(1)-C(22)-O(5)	98(11)
N(1)-Mo(1)-C(22)-O(5)	16(11)
C(12)-Mo(1)-C(22)-O(5)	-159(11)
N(5)-Mo(1)-C(22)-O(5)	-62(11)
C(11)-Mo(1)-C(22)-O(5)	162(11)
N(3)-Mo(1)-C(22)-O(5)	-14(12)
C(13)-Mo(1)-C(22)-O(5)	-149(11)
C(22)-Mo(1)-C(23)-O(6)	-26(22)
N(1)-Mo(1)-C(23)-O(6)	66(22)
C(12)-Mo(1)-C(23)-O(6)	-128(22)
N(5)-Mo(1)-C(23)-O(6)	55(22)
C(11)-Mo(1)-C(23)-O(6)	-133(22)
N(3)-Mo(1)-C(23)-O(6)	146(22)
C(13)-Mo(1)-C(23)-O(6)	-94(22)

Symmetry transformations used to generate equivalent atoms:

Ortep Drawing of Compound (±)-10a



Crystal Structure Analysis

A suitable crystal of **HMB133b** 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 (±)-10a

Table 1. Crystal data and structure refinement for $C_{24}H_{28}N_7BMoO_6$.

Identification code	mhb133b	
Empirical formula	$C_{24}H_{28}BMoN_7O_6$	
Formula weight	617.28	
Temperature	293(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 10.7530(5) Å	α= 90°.
	b = 12.0967(4) Å	β= 90°.
	c = 20.9602(7) Å	γ = 90°.
Volume	2726.42(18) Å^3	
Z	4	
Density (calculated)	1.504 Mg/m^3	
Absorption coefficient	4.380 mm^{-1}	
F(000)	1264	
Crystal size	0.36 x 0.20 x 0.06 mm^3	
Theta range for data collection	4.22 to 56.73°.	
Index ranges	$-11 \le h \le 11$, $-12 \le k \le 13$, $-22 \le l \le 22$	
Reflections collected	4661	
Independent reflections	3463 [R(int) = 0.0481]	
Completeness to theta = 56.73°	98.1 %	
Absorption correction	Empirical	
Max. and min. transmission	0.2504 and 0.1040	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3463 / 0 / 357	
Goodness-of-fit on F^2	2.326	
Final R indices [I>2sigma(I)]	R1 = 0.0494, wR2 = 0.1112	
R indices (all data)	R1 = 0.0532, wR2 = 0.1155	
Absolute structure parameter	-0.011(19)	
Extinction coefficient	0.00241(10)	
Largest diff. peak and hole	0.831 and -0.622 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $C_{24}H_{28}N_7BMoO_6$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	3213(1)	6314(1)	1902(1)	34(1)
B(1)	5566(10)	5845(9)	879(4)	51(3)
N(1)	3735(6)	7122(5)	994(3)	40(2)
N(2)	4727(6)	6777(6)	649(3)	43(2)
N(3)	3733(6)	4764(6)	1313(3)	41(2)
N(4)	4783(7)	4800(6)	955(3)	48(2)
N(5)	5270(6)	6482(6)	2016(3)	47(2)
N(6)	6073(6)	6194(6)	1536(3)	47(2)
N(7)	1325(5)	6693(5)	3152(3)	36(1)
O(1)	1163(5)	8123(5)	3811(3)	55(2)
O(2)	-342(5)	7830(5)	3079(3)	69(2)
O(3)	4391(5)	5667(5)	3467(2)	44(1)
O(4)	-1091(7)	5169(10)	4121(4)	123(4)
O(5)	544(6)	6850(6)	1451(3)	71(2)
O(6)	2861(7)	8541(5)	2604(3)	73(2)
C(1)	3220(9)	7948(7)	671(3)	50(2)
C(2)	3905(9)	8158(8)	115(4)	55(2)
C(3)	4834(9)	7404(8)	123(4)	56(2)
C(4)	3235(9)	3749(6)	1248(3)	50(2)
C(5)	3981(11)	3125(8)	848(4)	69(3)
C(6)	4934(9)	3789(8)	671(4)	65(3)
C(7)	5953(8)	6954(7)	2473(4)	45(2)
C(8)	7209(8)	6954(9)	2296(5)	59(3)
C(9)	7225(7)	6503(8)	1712(4)	54(3)
C(10)	2291(6)	6229(6)	3563(3)	35(2)
C(11)	3289(7)	5686(5)	3148(3)	34(2)
C(12)	2952(8)	5004(6)	2652(3)	39(2)
C(13)	1752(8)	5222(6)	2381(3)	39(2)
C(14)	801(7)	5715(6)	2835(4)	40(2)
C(15)	617(9)	4917(7)	3403(4)	50(2)
C(16)	1546(8)	5317(7)	3919(3)	45(2)

C(17)	616(8)	7577(7)	3325(4)	45(2)
C(18)	541(11)	9105(9)	4008(7)	114(5)
C(19)	5253(9)	4800(8)	3314(4)	64(3)
C(20)	-691(11)	4903(11)	3620(5)	84(4)
C(21)	2301(9)	4413(7)	4248(4)	59(3)
C(22)	3075(11)	4836(10)	4809(4)	84(4)
C(23)	1543(8)	6615(7)	1617(4)	49(2)
C(24)	2992(8)	7677(7)	2358(4)	49(2)

Table 3. Bond lengths [Å] and angles [°] for $C_{24}H_{28}N_7BMoO_6$.

Mo(1)-C(24)	1.920(9)	C(7)-C(8)	1.401(12)
Mo(1)-C(23)	1.928(9)	C(8)-C(9)	1.339(12)
Mo(1)-N(1)	2.213(6)	C(10)-C(11)	1.529(9)
Mo(1)-N(5)	2.233(6)	C(10)-C(16)	1.555(11)
Mo(1)-C(12)	2.250(7)	C(11)-C(12)	1.375(10)
Mo(1)-C(13)	2.285(8)	C(12)-C(13)	1.434(11)
Mo(1)-N(3)	2.313(6)	C(13)-C(14)	1.518(11)
B(1)-N(4)	1.527(13)	C(14)-C(15)	1.546(11)
B(1)-N(2)	1.523(12)	C(15)-C(20)	1.479(14)
B(1)-N(6)	1.539(11)	C(15)-C(16)	1.550(11)
N(1)-C(1)	1.326(10)	C(16)-C(21)	1.526(11)
N(1)-N(2)	1.355(8)	C(21)-C(22)	1.528(12)
N(2)-C(3)	1.343(10)		
N(3)-C(4)	1.347(10)	C(24)-Mo(1)-C(23)	83.0(4)
N(3)-N(4)	1.358(9)	C(24)-Mo(1)-N(1)	94.6(3)
N(4)-C(6)	1.369(11)	C(23)-Mo(1)-N(1)	83.4(3)
N(5)-C(7)	1.336(9)	C(24)-Mo(1)-N(5)	89.5(3)
N(5)-N(6)	1.372(8)	C(23)-Mo(1)-N(5)	159.8(3)
N(6)-C(9)	1.346(10)	N(1)-Mo(1)-N(5)	78.5(2)
N(7)-C(17)	1.363(10)	C(24)-Mo(1)-C(12)	104.0(3)
N(7)-C(10)	1.462(9)	C(23)-Mo(1)-C(12)	103.5(3)
N(7)-C(14)	1.469(9)	N(1)-Mo(1)-C(12)	160.8(2)
O(1)-C(17)	1.349(10)	N(5)-Mo(1)-C(12)	96.5(3)
O(1)-C(18)	1.424(10)	C(24)-Mo(1)-C(13)	101.1(3)
O(2)-C(17)	1.192(10)	C(23)-Mo(1)-C(13)	66.7(3)
O(3)-C(11)	1.361(9)	N(1)-Mo(1)-C(13)	143.9(2)
O(3)-C(19)	1.436(10)	N(5)-Mo(1)-C(13)	133.4(3)
O(4)-C(20)	1.179(12)	C(12)-Mo(1)-C(13)	36.9(3)
O(5)-C(23)	1.165(10)	C(24)-Mo(1)-N(3)	172.4(3)
O(6)-C(24)	1.174(10)	C(23)-Mo(1)-N(3)	102.3(3)
C(1)-C(2)	1.402(11)	N(1)-Mo(1)-N(3)	80.7(2)
C(2)-C(3)	1.353(12)	N(5)-Mo(1)-N(3)	83.8(2)
C(4)-C(5)	1.384(12)	C(12)-Mo(1)-N(3)	80.3(2)
C(5)-C(6)	1.354(13)	C(13)-Mo(1)-N(3)	86.1(2)

N(4)-B(1)-N(2)	108.6(7)	N(5)-C(7)-C(8)	109.9(8)
N(4)-B(1)-N(6)	109.2(7)	C(9)-C(8)-C(7)	104.8(8)
N(2)-B(1)-N(6)	106.9(7)	N(6)-C(9)-C(8)	110.6(8)
C(1)-N(1)-N(2)	106.8(7)	N(7)-C(10)-C(11)	109.1(5)
C(1)-N(1)-Mo(1)	131.7(6)	N(7)-C(10)-C(16)	100.9(6)
N(2)-N(1)-Mo(1)	121.5(5)	C(11)-C(10)-C(16)	109.2(6)
C(3)-N(2)-N(1)	109.4(7)	O(3)-C(11)-C(12)	126.2(7)
C(3)-N(2)-B(1)	128.8(8)	O(3)-C(11)-C(10)	109.8(5)
N(1)-N(2)-B(1)	121.7(6)	C(12)-C(11)-C(10)	120.2(7)
C(4)-N(3)-N(4)	107.7(7)	C(11)-C(12)-C(13)	115.2(7)
C(4)-N(3)-Mo(1)	134.2(5)	C(11)-C(12)-Mo(1)	94.2(5)
N(4)-N(3)-Mo(1)	118.1(5)	C(13)-C(12)-Mo(1)	72.9(4)
N(3)-N(4)-C(6)	108.1(7)	C(12)-C(13)-C(14)	115.5(6)
N(3)-N(4)-B(1)	122.9(7)	C(12)-C(13)-Mo(1)	70.3(4)
C(6)-N(4)-B(1)	129.0(7)	C(14)-C(13)-Mo(1)	120.7(5)
C(7)-N(5)-N(6)	106.8(6)	N(7)-C(14)-C(13)	109.9(6)
C(7)-N(5)-Mo(1)	131.3(6)	N(7)-C(14)-C(15)	101.8(6)
N(6)-N(5)-Mo(1)	121.5(4)	C(13)-C(14)-C(15)	108.9(7)
C(9)-N(6)-N(5)	107.9(6)	C(20)-C(15)-C(16)	113.7(8)
C(9)-N(6)-B(1)	130.4(7)	C(20)-C(15)-C(14)	111.5(9)
N(5)-N(6)-B(1)	120.2(6)	C(16)-C(15)-C(14)	105.1(6)
C(17)-N(7)-C(10)	122.8(6)	C(21)-C(16)-C(10)	116.8(7)
C(17)-N(7)-C(14)	122.5(6)	C(21)-C(16)-C(15)	115.8(7)
C(10)-N(7)-C(14)	103.3(6)	C(10)-C(16)-C(15)	102.6(6)
C(17)-O(1)-C(18)	115.0(8)	O(2)-C(17)-O(1)	125.3(8)
C(11)-O(3)-C(19)	117.6(6)	O(2)-C(17)-N(7)	124.7(8)
N(1)-C(1)-C(2)	109.9(8)	O(1)-C(17)-N(7)	110.0(7)
C(3)-C(2)-C(1)	104.8(8)	O(4)-C(20)-C(15)	128.2(11)
N(2)-C(3)-C(2)	109.1(8)	C(16)-C(21)-C(22)	113.5(8)
N(3)-C(4)-C(5)	109.2(8)	O(5)-C(23)-Mo(1)	176.7(8)
C(6)-C(5)-C(4)	106.3(8)	O(6)-C(24)-Mo(1)	176.1(7)
C(5)-C(6)-N(4)	108.8(8)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $C_{24}H_{28}N_7BMoO_6$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	33(1)	31(1)	37(1)	0(1)	0(1)	-2(1)
B(1)	44(6)	58(7)	51(5)	-11(5)	12(5)	7(6)
N(1)	38(4)	35(4)	47(3)	0(3)	6(3)	-17(3)
N(2)	33(3)	49(4)	45(3)	1(3)	4(3)	-3(4)
N(3)	43(4)	43(4)	37(3)	1(3)	2(3)	7(4)
N(4)	46(4)	52(5)	45(4)	-3(3)	0(3)	11(4)
N(5)	38(3)	57(5)	47(4)	-6(4)	-2(3)	-7(4)
N(6)	36(4)	51(5)	55(4)	-8(4)	7(3)	7(4)
N(7)	27(3)	34(3)	45(3)	-5(3)	-2(3)	-2(3)
O(1)	51(4)	42(3)	71(4)	-16(3)	-7(3)	16(3)
O(2)	43(3)	67(4)	96(4)	-16(4)	-21(4)	15(3)
O(3)	37(3)	48(4)	45(3)	-4(3)	-3(3)	12(3)
O(4)	75(5)	210(11)	85(5)	-18(7)	23(5)	-33(7)
O(5)	51(4)	89(5)	74(4)	24(4)	-4(4)	-4(4)
O(6)	92(5)	37(3)	90(4)	-7(4)	33(4)	-15(4)
C(1)	58(5)	43(5)	49(4)	5(4)	-11(5)	-10(6)
C(2)	65(6)	53(6)	46(4)	12(4)	-13(5)	-18(6)
C(3)	60(6)	62(6)	46(5)	8(5)	6(4)	-18(6)
C(4)	70(5)	38(4)	43(4)	-7(4)	-2(4)	-6(7)
C(5)	110(9)	41(5)	58(5)	-8(5)	-7(6)	5(7)
C(6)	81(7)	53(6)	59(5)	-10(5)	9(5)	16(7)
C(7)	50(5)	38(5)	48(4)	-2(4)	-9(4)	-10(5)
C(8)	41(5)	60(7)	77(6)	-7(6)	-17(5)	-6(5)
C(9)	27(4)	66(7)	70(6)	-11(5)	2(4)	8(5)
C(10)	34(4)	31(4)	41(3)	0(4)	2(3)	14(4)
C(11)	33(4)	30(4)	38(3)	7(3)	10(5)	3(4)
C(12)	52(5)	22(4)	43(4)	7(3)	13(4)	8(4)
C(13)	47(4)	24(4)	47(4)	4(3)	-9(4)	-3(5)
C(14)	35(4)	36(5)	48(4)	-1(4)	2(4)	-17(4)
C(15)	57(6)	38(5)	55(5)	0(4)	4(4)	-18(5)
C(16)	47(5)	44(5)	43(4)	6(4)	7(4)	3(5)

C(17)	35(5)	43(5)	56(5)	-4(4)	3(4)	-4(5)
C(18)	94(9)	77(8)	172(13)	-73(9)	-32(9)	45(8)
C(19)	55(5)	62(6)	75(6)	12(5)	1(5)	29(6)
C(20)	77(8)	110(10)	65(6)	0(7)	6(6)	-39(8)
C(21)	71(6)	46(5)	59(5)	14(4)	21(5)	5(5)
C(22)	92(8)	115(9)	45(4)	13(6)	6(6)	43(9)
C(23)	51(5)	50(6)	47(4)	29(4)	0(4)	-10(5)
C(24)	50(5)	45(5)	50(4)	9(4)	17(4)	8(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $C_{24}H_{28}N_7BMoO_6$.

	x	y	z	U(eq)
H(1A)	2510	8331	796	60
H(2A)	3754	8697	-191	65
H(3A)	5448	7331	-187	67
H(4A)	2505	3506	1440	60
H(5A)	3854	2395	726	83
H(6A)	5583	3592	401	78
H(7A)	5642	7239	2853	54
H(8A)	7883	7210	2531	71
H(9A)	7935	6415	1463	65
H(10A)	2640	6780	3856	42
H(12A)	3340	4276	2603	47
H(13A)	1430	4627	2110	47
H(14A)	15	5882	2619	48
H(15A)	852	4169	3269	60
H(16A)	1057	5687	4251	53
H(18A)	979	9429	4360	172
H(18B)	-292	8927	4136	172
H(18C)	517	9619	3659	172
H(19A)	5984	4875	3573	96
H(19B)	5479	4851	2871	96
H(19C)	4872	4096	3394	96
H(20A)	-1271	4652	3325	101
H(21A)	2853	4076	3938	71
H(21B)	1738	3845	4400	71
H(22A)	3513	4229	5001	126
H(22B)	2536	5169	5120	126
H(22C)	3662	5374	4660	126
H(1)	6430(60)	5630(50)	530(30)	33(19)

Table 6. Torsion angles [°] for $C_{24}H_{28}N_7BMoO_6$.

C(24)-Mo(1)-N(1)-C(1)	-48.0(7)
C(23)-Mo(1)-N(1)-C(1)	34.3(7)
N(5)-Mo(1)-N(1)-C(1)	-136.5(7)
C(12)-Mo(1)-N(1)-C(1)	146.9(9)
C(13)-Mo(1)-N(1)-C(1)	68.0(8)
N(3)-Mo(1)-N(1)-C(1)	138.0(7)
C(24)-Mo(1)-N(1)-N(2)	133.5(6)
C(23)-Mo(1)-N(1)-N(2)	-144.1(6)
N(5)-Mo(1)-N(1)-N(2)	45.0(5)
C(12)-Mo(1)-N(1)-N(2)	-31.6(11)
C(13)-Mo(1)-N(1)-N(2)	-110.5(6)
N(3)-Mo(1)-N(1)-N(2)	-40.5(5)
C(1)-N(1)-N(2)-C(3)	1.1(8)
Mo(1)-N(1)-N(2)-C(3)	179.9(5)
C(1)-N(1)-N(2)-B(1)	178.8(7)
Mo(1)-N(1)-N(2)-B(1)	-2.3(9)
N(4)-B(1)-N(2)-C(3)	-122.7(9)
N(6)-B(1)-N(2)-C(3)	119.5(9)
N(4)-B(1)-N(2)-N(1)	60.0(9)
N(6)-B(1)-N(2)-N(1)	-57.7(9)
C(24)-Mo(1)-N(3)-C(4)	170(2)
C(23)-Mo(1)-N(3)-C(4)	-57.3(7)
N(1)-Mo(1)-N(3)-C(4)	-138.4(7)
N(5)-Mo(1)-N(3)-C(4)	142.3(7)
C(12)-Mo(1)-N(3)-C(4)	44.6(7)
C(13)-Mo(1)-N(3)-C(4)	7.9(7)
C(24)-Mo(1)-N(3)-N(4)	-8(2)
C(23)-Mo(1)-N(3)-N(4)	125.2(5)
N(1)-Mo(1)-N(3)-N(4)	44.1(5)
N(5)-Mo(1)-N(3)-N(4)	-35.2(5)
C(12)-Mo(1)-N(3)-N(4)	-132.9(5)
C(13)-Mo(1)-N(3)-N(4)	-169.6(5)
C(4)-N(3)-N(4)-C(6)	-0.6(8)
Mo(1)-N(3)-N(4)-C(6)	177.6(5)

C(4)-N(3)-N(4)-B(1)	176.4(7)
Mo(1)-N(3)-N(4)-B(1)	-5.4(9)
N(2)-B(1)-N(4)-N(3)	-54.1(9)
N(6)-B(1)-N(4)-N(3)	62.1(10)
N(2)-B(1)-N(4)-C(6)	122.3(9)
N(6)-B(1)-N(4)-C(6)	-121.5(9)
C(24)-Mo(1)-N(5)-C(7)	30.1(8)
C(23)-Mo(1)-N(5)-C(7)	97.8(11)
N(1)-Mo(1)-N(5)-C(7)	124.9(8)
C(12)-Mo(1)-N(5)-C(7)	-73.9(8)
C(13)-Mo(1)-N(5)-C(7)	-74.8(8)
N(3)-Mo(1)-N(5)-C(7)	-153.4(8)
C(24)-Mo(1)-N(5)-N(6)	-141.4(6)
C(23)-Mo(1)-N(5)-N(6)	-73.6(12)
N(1)-Mo(1)-N(5)-N(6)	-46.6(6)
C(12)-Mo(1)-N(5)-N(6)	114.6(6)
C(13)-Mo(1)-N(5)-N(6)	113.8(6)
N(3)-Mo(1)-N(5)-N(6)	35.1(6)
C(7)-N(5)-N(6)-C(9)	-0.3(10)
Mo(1)-N(5)-N(6)-C(9)	173.0(6)
C(7)-N(5)-N(6)-B(1)	-167.6(8)
Mo(1)-N(5)-N(6)-B(1)	5.7(11)
N(4)-B(1)-N(6)-C(9)	133.6(10)
N(2)-B(1)-N(6)-C(9)	-109.1(11)
N(4)-B(1)-N(6)-N(5)	-62.4(10)
N(2)-B(1)-N(6)-N(5)	54.9(10)
N(2)-N(1)-C(1)-C(2)	-1.3(8)
Mo(1)-N(1)-C(1)-C(2)	-179.9(5)
N(1)-C(1)-C(2)-C(3)	0.9(9)
N(1)-N(2)-C(3)-C(2)	-0.6(9)
B(1)-N(2)-C(3)-C(2)	-178.1(8)
C(1)-C(2)-C(3)-N(2)	-0.2(10)
N(4)-N(3)-C(4)-C(5)	0.7(9)
Mo(1)-N(3)-C(4)-C(5)	-177.0(5)
N(3)-C(4)-C(5)-C(6)	-0.5(10)
C(4)-C(5)-C(6)-N(4)	0.1(10)

N(3)-N(4)-C(6)-C(5)	0.3(10)
B(1)-N(4)-C(6)-C(5)	-176.5(8)
N(6)-N(5)-C(7)-C(8)	-1.1(10)
Mo(1)-N(5)-C(7)-C(8)	-173.5(6)
N(5)-C(7)-C(8)-C(9)	2.1(12)
N(5)-N(6)-C(9)-C(8)	1.7(11)
B(1)-N(6)-C(9)-C(8)	167.3(9)
C(7)-C(8)-C(9)-N(6)	-2.3(12)
C(17)-N(7)-C(10)-C(11)	-152.4(7)
C(14)-N(7)-C(10)-C(11)	63.5(7)
C(17)-N(7)-C(10)-C(16)	92.7(8)
C(14)-N(7)-C(10)-C(16)	-51.4(7)
C(19)-O(3)-C(11)-C(12)	-5.6(10)
C(19)-O(3)-C(11)-C(10)	152.1(6)
N(7)-C(10)-C(11)-O(3)	154.7(6)
C(16)-C(10)-C(11)-O(3)	-95.8(7)
N(7)-C(10)-C(11)-C(12)	-46.0(9)
C(16)-C(10)-C(11)-C(12)	63.5(8)
O(3)-C(11)-C(12)-C(13)	-177.7(6)
C(10)-C(11)-C(12)-C(13)	26.7(9)
O(3)-C(11)-C(12)-Mo(1)	-104.6(6)
C(10)-C(11)-C(12)-Mo(1)	99.7(6)
C(24)-Mo(1)-C(12)-C(11)	-25.2(6)
C(23)-Mo(1)-C(12)-C(11)	-111.1(5)
N(1)-Mo(1)-C(12)-C(11)	139.5(7)
N(5)-Mo(1)-C(12)-C(11)	65.9(5)
C(13)-Mo(1)-C(12)-C(11)	-115.1(7)
N(3)-Mo(1)-C(12)-C(11)	148.5(5)
C(24)-Mo(1)-C(12)-C(13)	90.0(5)
C(23)-Mo(1)-C(12)-C(13)	4.0(5)
N(1)-Mo(1)-C(12)-C(13)	-105.3(9)
N(5)-Mo(1)-C(12)-C(13)	-178.9(4)
N(3)-Mo(1)-C(12)-C(13)	-96.4(4)
C(11)-C(12)-C(13)-C(14)	-29.0(9)
Mo(1)-C(12)-C(13)-C(14)	-115.5(6)
C(11)-C(12)-C(13)-Mo(1)	86.5(6)

C(24)-Mo(1)-C(13)-C(12)	-98.5(5)
C(23)-Mo(1)-C(13)-C(12)	-175.8(5)
N(1)-Mo(1)-C(13)-C(12)	147.4(4)
N(5)-Mo(1)-C(13)-C(12)	1.4(6)
N(3)-Mo(1)-C(13)-C(12)	79.1(4)
C(24)-Mo(1)-C(13)-C(14)	10.0(7)
C(23)-Mo(1)-C(13)-C(14)	-67.2(6)
N(1)-Mo(1)-C(13)-C(14)	-104.1(6)
N(5)-Mo(1)-C(13)-C(14)	110.0(6)
C(12)-Mo(1)-C(13)-C(14)	108.5(7)
N(3)-Mo(1)-C(13)-C(14)	-172.4(6)
C(17)-N(7)-C(14)-C(13)	147.5(7)
C(10)-N(7)-C(14)-C(13)	-68.3(7)
C(17)-N(7)-C(14)-C(15)	-97.2(8)
C(10)-N(7)-C(14)-C(15)	47.0(7)
C(12)-C(13)-C(14)-N(7)	52.0(9)
Mo(1)-C(13)-C(14)-N(7)	-29.3(8)
C(12)-C(13)-C(14)-C(15)	-58.7(9)
Mo(1)-C(13)-C(14)-C(15)	-139.9(5)
N(7)-C(14)-C(15)-C(20)	100.1(8)
C(13)-C(14)-C(15)-C(20)	-143.8(8)
N(7)-C(14)-C(15)-C(16)	-23.5(8)
C(13)-C(14)-C(15)-C(16)	92.6(7)
N(7)-C(10)-C(16)-C(21)	162.1(6)
C(11)-C(10)-C(16)-C(21)	47.2(8)
N(7)-C(10)-C(16)-C(15)	34.3(8)
C(11)-C(10)-C(16)-C(15)	-80.6(8)
C(20)-C(15)-C(16)-C(21)	102.9(11)
C(14)-C(15)-C(16)-C(21)	-134.9(7)
C(20)-C(15)-C(16)-C(10)	-128.7(9)
C(14)-C(15)-C(16)-C(10)	-6.5(9)
C(18)-O(1)-C(17)-O(2)	-3.3(14)
C(18)-O(1)-C(17)-N(7)	176.4(8)
C(10)-N(7)-C(17)-O(2)	-162.5(8)
C(14)-N(7)-C(17)-O(2)	-25.2(13)
C(10)-N(7)-C(17)-O(1)	17.8(10)