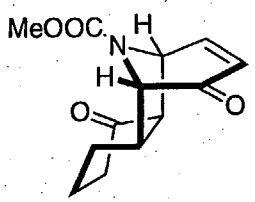
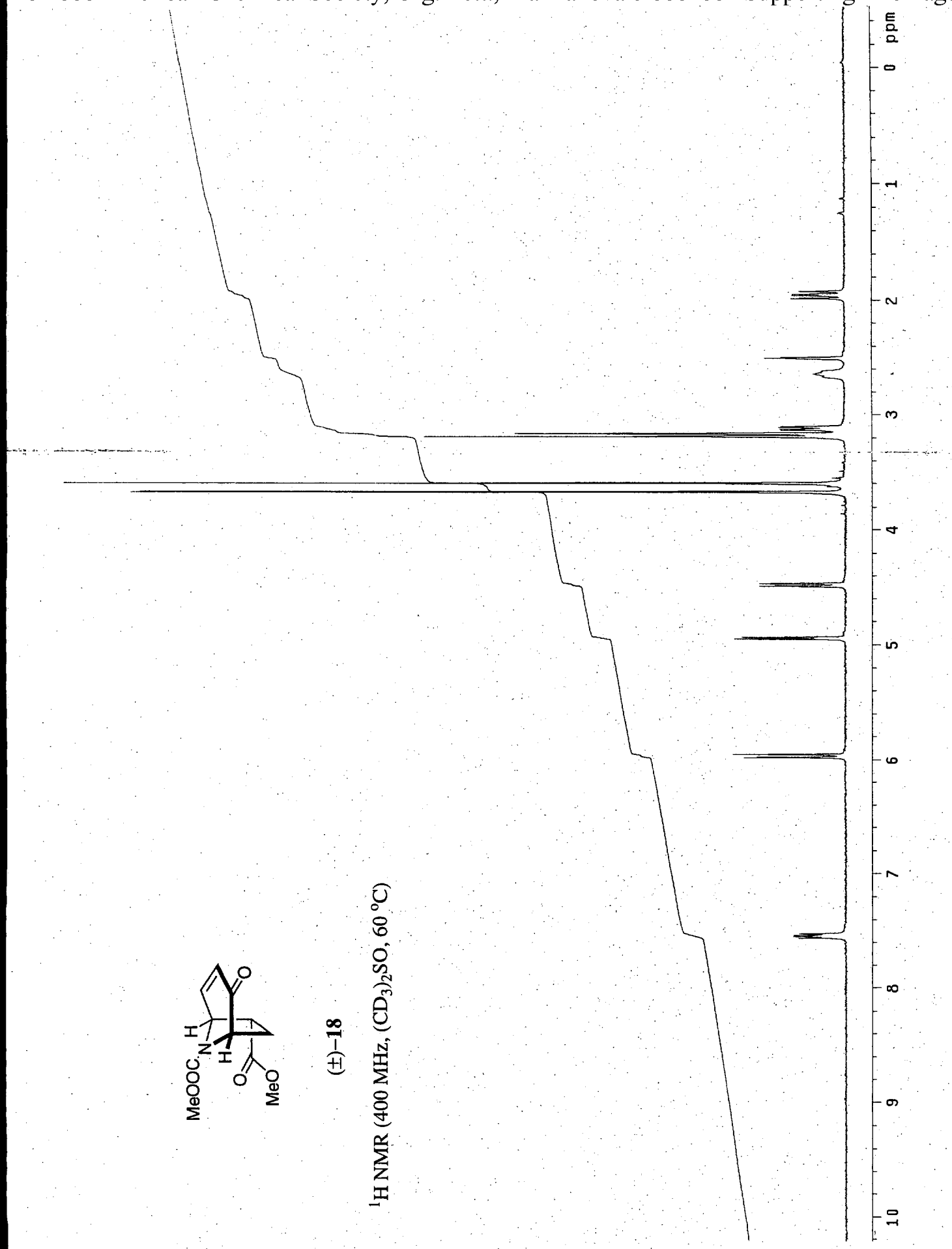


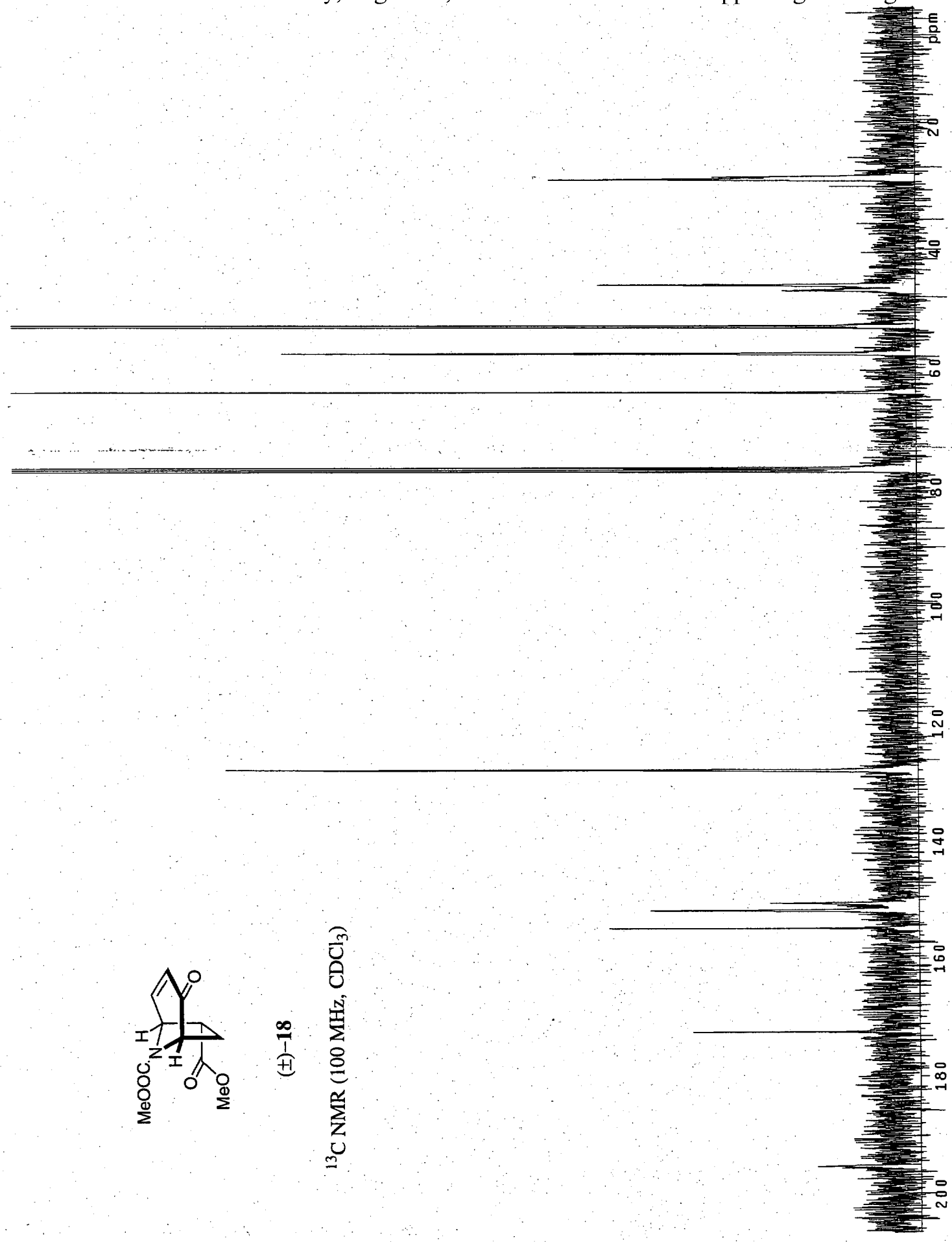
(±)–**17**

^{13}C NMR (100 MHz, $CDCl_3$)



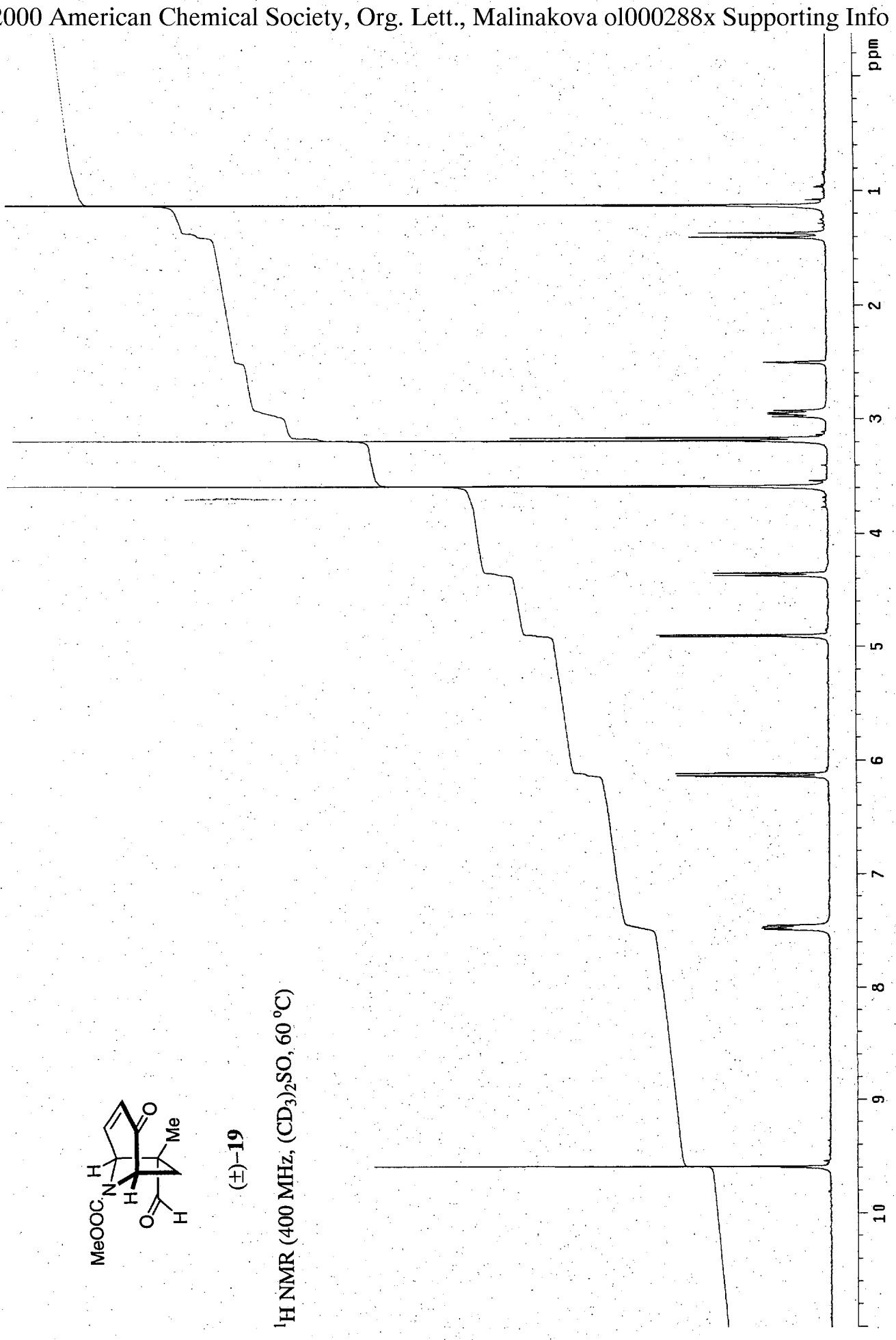
(±)–**18**

^{1}H NMR (400 MHz, $(CD_3)_2SO$, 60 °C)



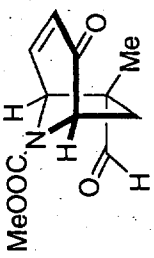
(±)-**18**

^{13}C NMR (100 MHz, $CDCl_3$)



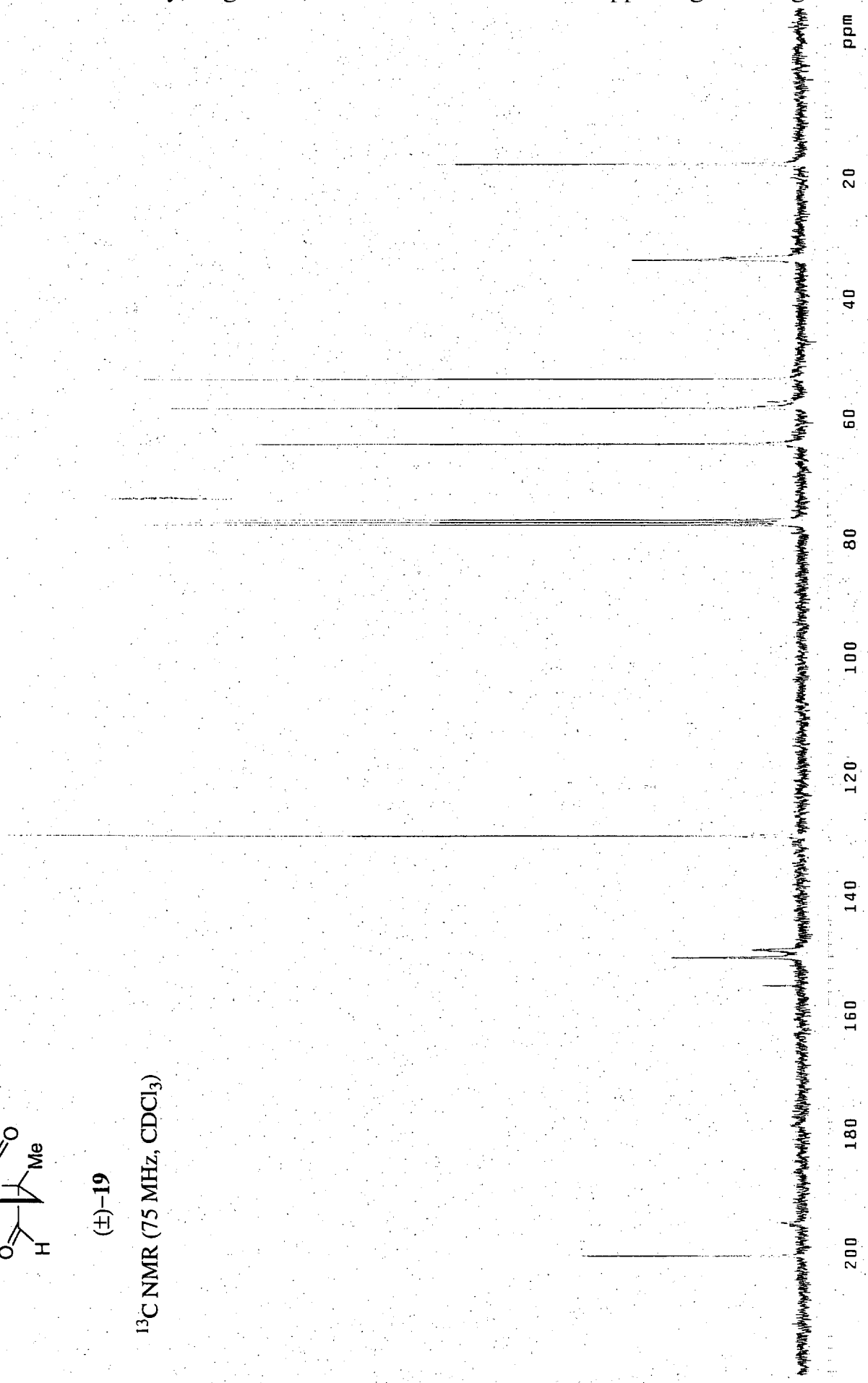
(±)–**19**

^{1}H NMR (400 MHz, $(CD_3)_2SO$, 60 °C)

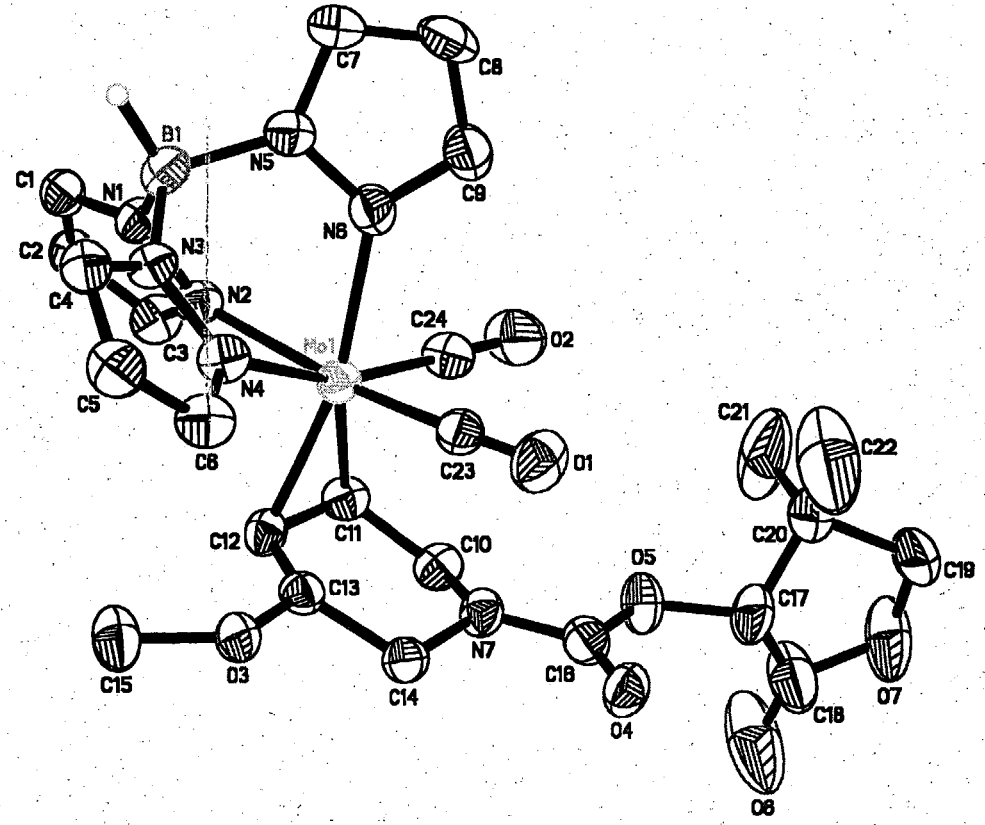


(±)-**19**

^{13}C NMR (75 MHz, $CDCl_3$)



Ortep Drawing of Compound **(-)-2b**



$C_{24}H_2N_7BMoO_7$

Crystallographic Studies for Compound (-)-2b

Crystals of AM7067 were obtained as described in the experimental section. A fragment with dimensions 0.36 x 0.18 x 0.14 mm cut from a single crystal was mounted on a quartz fiber with superglue. The diffraction intensities, including Friedel pairs, were collected using Cu Kα graphite monochromated radiation (1.54178 Å) on a Siemens P4/RA single-crystal x-ray diffractometer. Three representative reflections were monitored after every 97 reflections and no decay was observed. The structure was solved using direct methods (SHELXTL Ver 5.0) and refined by full-matrix least squares methods (SHELX-97). An empirical absorption correction was applied to the reflection data using psi-scan data. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included at calculated positions with the C-H bond distance fixed at 0.93, 0.96, 0.97, or 0.98 Å. These values are the default effective C-H distances for T=27°C and were chosen to give the best fit to the x-ray data and so avoid the introduction of systematic error. The true internuclear distances are longer and do not vary with temperature. The apparent variation with temperature is caused by libration. The B-H hydrogen was located in the difference map and was refined. The absolute configuration was based on the enantiomer with a Flack parameter of –0.017 (17).

Data for Compound (-)-2b

Table 1. Crystal data and structure refinement for $C_{24}H_{28}N_7BMoO_7$.

Identification code	am7067b
Empirical formula	$C_{24}H_{28}N_7BMoO_7$
Formula weight	633.28
Temperature	300(2) K
Wavelength	1.54178 è
Crystal system, space group	Orthorhombic, P2(1)2(1)2
Unit cell dimensions	a = 32.187(3) è α = 90°. b = 7.4807(7) è β = 90°. c = 12.9722(14) è γ = 90°.
Volume	3123.4(5) è^3
Z, Calculated density	4, 1.347 Mg/m^3
Absorption coefficient	3.862 mm^{-1}
F(000)	1296
Crystal size	0.36 x 0.18 x 0.14 mm
Theta range for data collection	2.75° to 56.75°.
Limiting indices	-32 ≤ h ≤ 32, -8 ≤ k ≤ 8, -14 ≤ l ≤ 14
Reflections collected / unique	4686 / 4045 [R(int) = 0.0340]
Completeness to theta = 56.75	98.2 %
Absorption correction	Empirical
Max. and min. transmission	0.1913 and 0.0982
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4045 / 0 / 366
Goodness-of-fit on F^2	1.077
Final R indices [I>2sigma(I)]	R1 = 0.0507, wR2 = 0.1518

R indices (all data)	R1 = 0.0528, wR2 = 0.1558
Absolute structure parameter	-0.017(17)
Extinction coefficient	0.0026(3)
Largest diff. peak and hole	0.769 and -0.351 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $C_{24}H_{28}N_7BMoO_7$.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Mo(1)	3721(1)	8884(1)	4419(1)	49(1)
B(1)	4297(3)	10591(12)	2464(7)	59(2)
N(1)	4304(2)	8552(8)	2413(4)	57(1)
N(2)	4104(2)	7532(8)	3140(5)	57(2)
N(3)	3839(2)	11232(8)	2380(4)	54(1)
N(4)	3558(2)	10817(7)	3124(4)	57(1)
N(5)	4462(2)	11177(9)	3541(4)	59(1)
N(6)	4260(2)	10685(8)	4424(5)	64(2)
N(7)	3003(2)	7188(8)	6172(4)	58(2)
O(1)	3288(2)	11250(8)	6033(5)	86(2)
O(2)	4161(2)	7429(11)	6365(6)	101(2)
O(3)	2676(1)	8729(8)	3654(3)	62(1)
O(4)	2642(2)	8832(9)	7356(4)	70(1)
O(5)	3147(2)	6888(8)	7858(4)	75(2)
O(6)	2768(5)	4899(15)	9489(7)	226(8)
O(7)	3154(3)	6556(11)	10563(5)	127(3)
C(1)	4493(2)	7463(11)	1735(6)	62(2)
C(2)	4423(2)	5744(10)	1990(6)	64(2)
C(3)	4177(3)	5826(10)	2872(7)	67(2)
C(4)	3674(2)	12405(9)	1727(5)	59(2)
C(5)	3275(3)	12780(10)	2044(6)	64(2)
C(6)	3223(3)	11751(10)	2920(7)	67(2)
C(7)	4792(2)	12259(11)	3786(7)	65(2)
C(8)	4797(3)	12454(14)	4824(8)	80(2)
C(9)	4467(3)	11480(12)	5196(6)	78(2)
C(10)	3287(3)	5725(10)	5932(6)	62(2)
C(11)	3497(2)	6059(10)	4896(5)	56(2)
C(12)	3257(2)	6719(9)	4046(5)	54(2)
C(13)	2938(2)	7900(9)	4314(5)	55(2)
C(14)	2728(2)	7883(10)	5346(5)	55(2)
C(15)	2662(3)	8120(13)	2601(6)	82(3)
C(16)	2898(3)	7769(11)	7141(6)	65(2)
C(17)	3104(3)	7568(14)	8875(6)	81(3)
C(18)	2973(5)	6126(18)	9620(8)	126(5)
C(19)	3387(4)	8150(20)	10475(7)	122(4)
C(20)	3486(4)	8350(30)	9314(8)	140(6)
C(21)	3837(5)	7100(50)	9095(12)	340(30)
C(22)	3543(10)	10260(30)	9055(11)	320(20)
C(23)	3444(2)	10351(10)	5411(6)	57(2)
C(24)	3995(2)	7895(11)	5618(7)	67(2)

Table 3. Bond lengths [è] and angles [deg] for $C_{24}H_{28}N_7BMoO_7$.

Mo(1)-C(23)	1.912(8)
Mo(1)-C(24)	1.934(9)
Mo(1)-N(6)	2.195(6)
Mo(1)-C(12)	2.256(7)
Mo(1)-N(4)	2.278(6)
Mo(1)-N(2)	2.301(6)
Mo(1)-C(11)	2.317(7)
B(1)-N(1)	1.527(11)
B(1)-N(3)	1.554(11)
B(1)-N(5)	1.557(11)
N(1)-C(1)	1.344(9)
N(1)-N(2)	1.373(8)
N(2)-C(3)	1.343(10)
N(3)-C(4)	1.331(9)
N(3)-N(4)	1.358(8)
N(4)-C(6)	1.313(10)
N(5)-N(6)	1.367(8)
N(5)-C(7)	1.373(10)
N(6)-C(9)	1.342(10)
N(7)-C(16)	1.373(10)
N(7)-C(10)	1.459(10)
N(7)-C(14)	1.483(9)
O(1)-C(23)	1.165(9)
O(2)-C(24)	1.161(10)
O(3)-C(13)	1.352(8)
O(3)-C(15)	1.441(9)
O(4)-C(16)	1.179(10)
O(5)-C(16)	1.393(10)
O(5)-C(17)	1.421(10)
O(6)-C(18)	1.145(14)
O(7)-C(18)	1.392(13)
O(7)-C(19)	1.413(14)
C(1)-C(2)	1.347(11)
C(2)-C(3)	1.392(11)
C(4)-C(5)	1.376(11)
C(5)-C(6)	1.382(11)
C(7)-C(8)	1.354(12)
C(8)-C(9)	1.375(12)
C(10)-C(11)	1.525(10)
C(11)-C(12)	1.433(10)
C(12)-C(13)	1.399(10)
C(13)-C(14)	1.500(9)
C(17)-C(20)	1.476(15)
C(17)-C(18)	1.507(14)
C(19)-C(20)	1.547(14)
C(20)-C(22)	1.48(3)
C(20)-C(21)	1.49(3)
C(23)-Mo(1)-C(24)	83.7(4)

C(23)-Mo(1)-N(6)	90.8(3)
C(24)-Mo(1)-N(6)	82.7(3)
C(23)-Mo(1)-C(12)	104.3(3)
C(24)-Mo(1)-C(12)	101.5(3)
N(6)-Mo(1)-C(12)	164.6(2)
C(23)-Mo(1)-N(4)	91.4(3)
C(24)-Mo(1)-N(4)	160.2(3)
N(6)-Mo(1)-N(4)	78.1(2)
C(12)-Mo(1)-N(4)	98.4(2)
C(23)-Mo(1)-N(2)	170.9(3)
C(24)-Mo(1)-N(2)	99.7(3)
N(6)-Mo(1)-N(2)	81.3(2)
C(12)-Mo(1)-N(2)	83.3(2)
N(4)-Mo(1)-N(2)	82.5(2)
C(23)-Mo(1)-C(11)	101.4(3)
C(24)-Mo(1)-C(11)	65.0(3)
N(6)-Mo(1)-C(11)	143.6(2)
C(12)-Mo(1)-C(11)	36.5(3)
N(4)-Mo(1)-C(11)	134.8(2)
N(2)-Mo(1)-C(11)	87.6(2)
N(1)-B(1)-N(3)	108.6(6)
N(1)-B(1)-N(5)	108.4(6)
N(3)-B(1)-N(5)	107.4(6)
C(1)-N(1)-N(2)	109.0(6)
C(1)-N(1)-B(1)	129.8(7)
N(2)-N(1)-B(1)	121.2(6)
C(3)-N(2)-N(1)	105.6(6)
C(3)-N(2)-Mo(1)	134.2(5)
N(1)-N(2)-Mo(1)	120.2(4)
C(4)-N(3)-N(4)	109.7(6)
C(4)-N(3)-B(1)	128.9(6)
N(4)-N(3)-B(1)	120.8(5)
C(6)-N(4)-N(3)	106.4(6)
C(6)-N(4)-Mo(1)	132.5(5)
N(3)-N(4)-Mo(1)	121.0(4)
N(6)-N(5)-C(7)	109.5(6)
N(6)-N(5)-B(1)	120.9(6)
C(7)-N(5)-B(1)	129.5(7)
C(9)-N(6)-N(5)	105.6(6)
C(9)-N(6)-Mo(1)	131.8(6)
N(5)-N(6)-Mo(1)	122.6(4)
C(16)-N(7)-C(10)	125.9(6)
C(16)-N(7)-C(14)	113.8(6)
C(10)-N(7)-C(14)	118.9(6)
C(13)-O(3)-C(15)	118.4(6)
C(16)-O(5)-C(17)	113.2(7)
C(18)-O(7)-C(19)	110.2(8)
N(1)-C(1)-C(2)	110.0(7)
C(1)-C(2)-C(3)	104.8(6)
N(2)-C(3)-C(2)	110.7(7)
N(3)-C(4)-C(5)	108.5(6)
C(4)-C(5)-C(6)	104.2(7)
N(4)-C(6)-C(5)	111.3(8)
C(8)-C(7)-N(5)	107.6(7)

C(7)-C(8)-C(9)	106.4(8)
N(6)-C(9)-C(8)	110.9(7)
N(7)-C(10)-C(11)	110.0(6)
C(12)-C(11)-C(10)	119.7(6)
C(12)-C(11)-Mo(1)	69.4(4)
C(10)-C(11)-Mo(1)	121.5(5)
C(13)-C(12)-C(11)	115.0(6)
C(13)-C(12)-Mo(1)	88.8(4)
C(11)-C(12)-Mo(1)	74.1(4)
O(3)-C(13)-C(12)	126.2(6)
O(3)-C(13)-C(14)	106.8(6)
C(12)-C(13)-C(14)	123.2(6)
N(7)-C(14)-C(13)	112.2(6)
O(4)-C(16)-N(7)	127.0(7)
O(4)-C(16)-O(5)	124.3(7)
N(7)-C(16)-O(5)	108.7(7)
O(5)-C(17)-C(20)	114.7(9)
O(5)-C(17)-C(18)	111.5(8)
C(20)-C(17)-C(18)	105.6(9)
O(6)-C(18)-O(7)	123.9(12)
O(6)-C(18)-C(17)	129.8(11)
O(7)-C(18)-C(17)	106.3(9)
O(7)-C(19)-C(20)	105.6(9)
C(17)-C(20)-C(22)	113.5(18)
C(17)-C(20)-C(21)	107.9(15)
C(22)-C(20)-C(21)	118.0(19)
C(17)-C(20)-C(19)	99.5(9)
C(22)-C(20)-C(19)	109.8(13)
C(21)-C(20)-C(19)	106.3(16)
O(1)-C(23)-Mo(1)	177.7(7)
O(2)-C(24)-Mo(1)	174.9(8)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (è^2 x 10^3) for $C_{24}H_{28}N_7BMoO_7$. 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
Mo(1)	49(1)	48(1)	50(1)	0(1)	2(1)	-1(1)
B(1)	56(5)	67(5)	54(5)	6(4)	10(4)	4(4)
N(1)	57(3)	59(3)	54(3)	-1(3)	6(3)	1(3)
N(2)	51(3)	54(3)	65(4)	-3(3)	5(3)	0(3)
N(3)	49(3)	55(3)	56(3)	4(3)	6(3)	1(3)
N(4)	54(3)	52(3)	66(3)	5(3)	2(3)	4(3)
N(5)	51(3)	60(3)	66(3)	-1(3)	1(3)	-3(3)
N(6)	71(4)	63(4)	58(3)	-5(3)	-2(3)	-7(3)
N(7)	69(4)	57(4)	48(3)	6(3)	1(3)	-4(3)
O(1)	104(5)	65(3)	89(4)	-16(3)	25(4)	-3(4)
O(2)	89(5)	130(6)	85(4)	39(4)	-24(4)	-8(4)
O(3)	56(3)	84(4)	46(2)	7(3)	-6(2)	1(3)
O(4)	69(3)	82(4)	59(3)	-10(3)	7(2)	14(3)
O(5)	103(4)	78(4)	43(3)	6(3)	-13(3)	10(3)
O(6)	420(20)	158(9)	97(6)	6(7)	-29(10)	-169(13)
O(7)	229(10)	103(5)	50(3)	3(4)	-15(5)	-2(6)
C(1)	54(4)	74(5)	59(4)	-16(4)	6(4)	4(4)
C(2)	64(5)	56(5)	70(5)	-19(3)	5(4)	8(3)
C(3)	74(5)	52(4)	76(5)	-3(4)	7(4)	4(4)
C(4)	65(5)	54(4)	57(4)	1(3)	-2(4)	-1(3)
C(5)	74(5)	54(4)	65(4)	15(3)	-10(4)	-3(4)
C(6)	65(5)	56(4)	80(5)	1(4)	2(4)	1(4)
C(7)	51(4)	60(5)	82(5)	2(4)	1(4)	-11(4)
C(8)	58(5)	82(6)	100(6)	-13(5)	-13(4)	-23(4)
C(9)	91(6)	83(6)	61(4)	-4(4)	-9(4)	-15(5)
C(10)	68(5)	53(4)	64(4)	8(3)	2(4)	-2(4)
C(11)	59(4)	44(3)	65(4)	-2(3)	4(3)	-1(3)
C(12)	63(4)	51(4)	48(3)	-5(3)	5(3)	1(3)
C(13)	56(4)	57(4)	52(4)	7(3)	-4(3)	-14(3)
C(14)	53(4)	60(4)	53(4)	5(3)	-2(3)	0(3)
C(15)	105(7)	88(6)	52(4)	0(4)	-13(4)	-4(5)
C(16)	74(5)	69(5)	52(4)	5(4)	-3(4)	-20(4)
C(17)	106(7)	95(6)	42(4)	5(4)	5(4)	-1(6)
C(18)	189(13)	121(9)	68(6)	-1(6)	-16(7)	-61(10)
C(19)	116(9)	189(13)	60(5)	-20(7)	-15(6)	-52(9)
C(20)	124(10)	234(16)	64(6)	-42(9)	19(6)	-81(11)
C(21)	95(9)	820(80)	92(9)	-140(20)	-31(8)	80(20)
C(22)	560(50)	290(30)	97(10)	-29(14)	72(18)	-330(30)
C(23)	61(4)	53(4)	58(4)	-2(4)	5(4)	-11(3)
C(24)	61(5)	66(5)	75(5)	5(4)	-4(4)	-4(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $C_{24}H_{28}N_7BMoO_7$.

	x	y	z	U(eq)
H(1A)	4649	7841	1172	74
H(2A)	4518	4727	1653	76
H(3A)	4076	4836	3227	81
H(4A)	3806	12890	1154	70
H(5A)	3084	13549	1738	77
H(6A)	2982	11725	3313	80
H(7A)	4978	12767	3323	77
H(8A)	4986	13116	5209	96
H(9A)	4397	11385	5889	94
H(10A)	3134	4608	5907	74
H(10B)	3496	5631	6468	74
H(11A)	3691	5109	4700	67
H(12A)	3259	6112	3377	65
H(14A)	2642	9089	5520	66
H(14B)	2480	7146	5307	66
H(15A)	2466	8828	2221	123
H(15B)	2578	6888	2585	123
H(15C)	2932	8237	2296	123
H(17A)	2889	8493	8869	97
H(19A)	3641	8071	10875	146
H(19B)	3227	9163	10719	146
H(21A)	3908	7160	8377	504
H(21B)	3755	5899	9264	504
H(21C)	4074	7427	9503	504
H(22A)	3596	10384	8331	476
H(22B)	3774	10736	9438	476
H(22C)	3296	10914	9231	476
H(1)	4487(16)	11320(70)	1920(40)	26(13)

Table 6. Torsion angles [deg] for $C_{24}H_{28}N_7BMoO_7$.

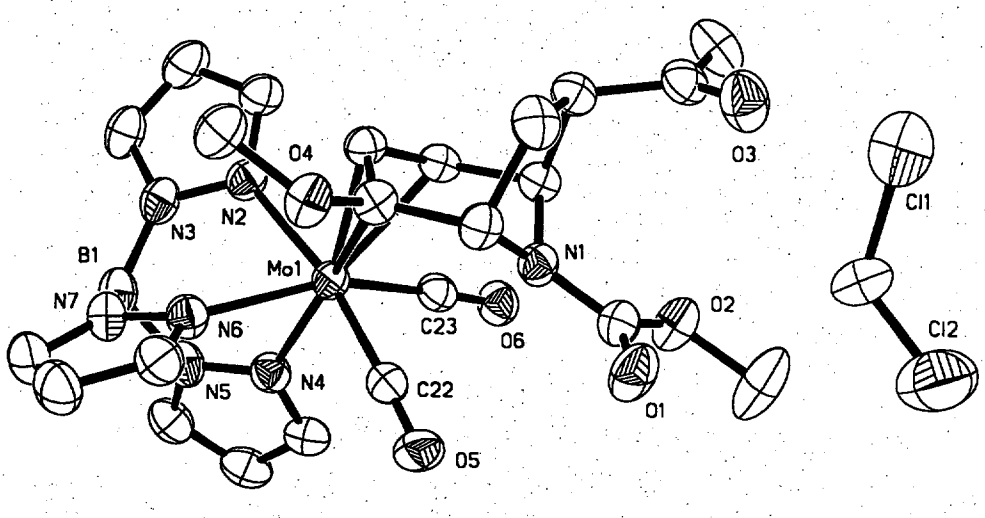
N(3)-B(1)-N(1)-C(1)	120.2(8)
N(5)-B(1)-N(1)-C(1)	-123.5(8)
N(3)-B(1)-N(1)-N(2)	-61.1(9)
N(5)-B(1)-N(1)-N(2)	55.2(9)
C(1)-N(1)-N(2)-C(3)	-0.3(8)
B(1)-N(1)-N(2)-C(3)	-179.3(7)
C(1)-N(1)-N(2)-Mo(1)	-178.0(5)
B(1)-N(1)-N(2)-Mo(1)	3.1(9)
C(23)-Mo(1)-N(2)-C(3)	171.6(16)
C(24)-Mo(1)-N(2)-C(3)	60.0(8)
N(6)-Mo(1)-N(2)-C(3)	141.1(8)
C(12)-Mo(1)-N(2)-C(3)	-40.5(8)
N(4)-Mo(1)-N(2)-C(3)	-139.9(8)
C(11)-Mo(1)-N(2)-C(3)	-4.1(8)
C(23)-Mo(1)-N(2)-N(1)	-12(2)
C(24)-Mo(1)-N(2)-N(1)	-123.1(5)
N(6)-Mo(1)-N(2)-N(1)	-42.1(5)
C(12)-Mo(1)-N(2)-N(1)	136.3(5)
N(4)-Mo(1)-N(2)-N(1)	36.9(5)
C(11)-Mo(1)-N(2)-N(1)	172.7(5)
N(1)-B(1)-N(3)-C(4)	-126.3(7)
N(5)-B(1)-N(3)-C(4)	116.7(7)
N(1)-B(1)-N(3)-N(4)	64.5(8)
N(5)-B(1)-N(3)-N(4)	-52.5(8)
C(4)-N(3)-N(4)-C(6)	-0.2(8)
B(1)-N(3)-N(4)-C(6)	170.8(6)
C(4)-N(3)-N(4)-Mo(1)	-178.9(4)
B(1)-N(3)-N(4)-Mo(1)	-7.8(8)
C(23)-Mo(1)-N(4)-C(6)	-39.3(7)
C(24)-Mo(1)-N(4)-C(6)	-114.6(10)
N(6)-Mo(1)-N(4)-C(6)	-129.9(7)
C(12)-Mo(1)-N(4)-C(6)	65.4(7)
N(2)-Mo(1)-N(4)-C(6)	147.5(7)
C(11)-Mo(1)-N(4)-C(6)	68.3(8)
C(23)-Mo(1)-N(4)-N(3)	138.9(5)
C(24)-Mo(1)-N(4)-N(3)	63.6(10)
N(6)-Mo(1)-N(4)-N(3)	48.3(5)
C(12)-Mo(1)-N(4)-N(3)	-116.4(5)
N(2)-Mo(1)-N(4)-N(3)	-34.3(5)
C(11)-Mo(1)-N(4)-N(3)	-113.5(5)
N(1)-B(1)-N(5)-N(6)	-61.5(8)
N(3)-B(1)-N(5)-N(6)	55.6(9)
N(1)-B(1)-N(5)-C(7)	122.0(8)
N(3)-B(1)-N(5)-C(7)	-120.9(8)
C(7)-N(5)-N(6)-C(9)	0.4(8)
B(1)-N(5)-N(6)-C(9)	-176.8(7)
C(7)-N(5)-N(6)-Mo(1)	-178.1(5)
B(1)-N(5)-N(6)-Mo(1)	4.7(9)
C(23)-Mo(1)-N(6)-C(9)	44.2(8)

C(24)-Mo(1)-N(6)-C(9)	-39.3(8)
C(12)-Mo(1)-N(6)-C(9)	-146.3(9)
N(4)-Mo(1)-N(6)-C(9)	135.5(8)
N(2)-Mo(1)-N(6)-C(9)	-140.4(8)
C(11)-Mo(1)-N(6)-C(9)	-66.5(9)
C(23)-Mo(1)-N(6)-N(5)	-137.7(6)
C(24)-Mo(1)-N(6)-N(5)	138.7(6)
C(12)-Mo(1)-N(6)-N(5)	31.8(12)
N(4)-Mo(1)-N(6)-N(5)	-46.4(5)
N(2)-Mo(1)-N(6)-N(5)	37.7(5)
C(11)-Mo(1)-N(6)-N(5)	111.6(6)
N(2)-N(1)-C(1)-C(2)	0.1(8)
B(1)-N(1)-C(1)-C(2)	178.9(8)
N(1)-C(1)-C(2)-C(3)	0.1(9)
N(1)-N(2)-C(3)-C(2)	0.4(9)
Mo(1)-N(2)-C(3)-C(2)	177.6(5)
C(1)-C(2)-C(3)-N(2)	-0.3(10)
N(4)-N(3)-C(4)-C(5)	0.1(8)
B(1)-N(3)-C(4)-C(5)	-170.1(7)
N(3)-C(4)-C(5)-C(6)	0.1(8)
N(3)-N(4)-C(6)-C(5)	0.3(8)
Mo(1)-N(4)-C(6)-C(5)	178.7(5)
C(4)-C(5)-C(6)-N(4)	-0.3(9)
N(6)-N(5)-C(7)-C(8)	-0.2(10)
B(1)-N(5)-C(7)-C(8)	176.6(8)
N(5)-C(7)-C(8)-C(9)	0.0(12)
N(5)-N(6)-C(9)-C(8)	-0.4(10)
Mo(1)-N(6)-C(9)-C(8)	177.9(6)
C(7)-C(8)-C(9)-N(6)	0.3(12)
C(16)-N(7)-C(10)-C(11)	-150.7(7)
C(14)-N(7)-C(10)-C(11)	43.7(9)
N(7)-C(10)-C(11)-C(12)	-42.5(9)
N(7)-C(10)-C(11)-Mo(1)	40.3(8)
C(23)-Mo(1)-C(11)-C(12)	98.7(5)
C(24)-Mo(1)-C(11)-C(12)	176.1(5)
N(6)-Mo(1)-C(11)-C(12)	-153.9(4)
N(4)-Mo(1)-C(11)-C(12)	-5.0(5)
N(2)-Mo(1)-C(11)-C(12)	-82.0(4)
C(23)-Mo(1)-C(11)-C(10)	-14.3(6)
C(24)-Mo(1)-C(11)-C(10)	63.2(6)
N(6)-Mo(1)-C(11)-C(10)	93.1(7)
C(12)-Mo(1)-C(11)-C(10)	-113.0(7)
N(4)-Mo(1)-C(11)-C(10)	-117.9(6)
N(2)-Mo(1)-C(11)-C(10)	165.0(6)
C(10)-C(11)-C(12)-C(13)	34.4(10)
Mo(1)-C(11)-C(12)-C(13)	-81.0(6)
C(10)-C(11)-C(12)-Mo(1)	115.4(6)
C(23)-Mo(1)-C(12)-C(13)	26.5(5)
C(24)-Mo(1)-C(12)-C(13)	112.8(5)
N(6)-Mo(1)-C(12)-C(13)	-142.7(8)
N(4)-Mo(1)-C(12)-C(13)	-67.2(4)
N(2)-Mo(1)-C(12)-C(13)	-148.6(4)
C(11)-Mo(1)-C(12)-C(13)	116.4(6)
C(23)-Mo(1)-C(12)-C(11)	-89.9(5)

C(24)-Mo(1)-C(12)-C(11)	-3.6(5)
N(6)-Mo(1)-C(12)-C(11)	100.9(9)
N(4)-Mo(1)-C(12)-C(11)	176.4(4)
N(2)-Mo(1)-C(12)-C(11)	95.0(4)
C(15)-O(3)-C(13)-C(12)	12.9(10)
C(15)-O(3)-C(13)-C(14)	-145.2(6)
C(11)-C(12)-C(13)-O(3)	178.5(6)
Mo(1)-C(12)-C(13)-O(3)	106.7(7)
C(11)-C(12)-C(13)-C(14)	-26.7(10)
Mo(1)-C(12)-C(13)-C(14)	-98.6(6)
C(16)-N(7)-C(14)-C(13)	155.9(6)
C(10)-N(7)-C(14)-C(13)	-36.8(8)
O(3)-C(13)-C(14)-N(7)	-173.6(6)
C(12)-C(13)-C(14)-N(7)	27.4(9)
C(10)-N(7)-C(16)-O(4)	-172.5(8)
C(14)-N(7)-C(16)-O(4)	-6.3(11)
C(10)-N(7)-C(16)-O(5)	7.5(10)
C(14)-N(7)-C(16)-O(5)	173.8(6)
C(17)-O(5)-C(16)-O(4)	-8.1(11)
C(17)-O(5)-C(16)-N(7)	171.9(7)
C(16)-O(5)-C(17)-C(20)	-117.4(12)
C(16)-O(5)-C(17)-C(18)	122.6(9)
C(19)-O(7)-C(18)-O(6)	-179.6(18)
C(19)-O(7)-C(18)-C(17)	0.2(16)
O(5)-C(17)-C(18)-O(6)	-33(2)
C(20)-C(17)-C(18)-O(6)	-158(2)
O(5)-C(17)-C(18)-O(7)	147.7(10)
C(20)-C(17)-C(18)-O(7)	22.5(15)
C(18)-O(7)-C(19)-C(20)	-21.7(17)
O(5)-C(17)-C(20)-C(22)	87.0(16)
C(18)-C(17)-C(20)-C(22)	-149.8(13)
O(5)-C(17)-C(20)-C(21)	-45.7(17)
C(18)-C(17)-C(20)-C(21)	77.5(15)
O(5)-C(17)-C(20)-C(19)	-156.4(11)
C(18)-C(17)-C(20)-C(19)	-33.2(15)
O(7)-C(19)-C(20)-C(17)	33.8(16)
O(7)-C(19)-C(20)-C(22)	153.1(18)
O(7)-C(19)-C(20)-C(21)	-78.2(17)
C(24)-Mo(1)-C(23)-O(1)	41(16)
N(6)-Mo(1)-C(23)-O(1)	-41(16)
C(12)-Mo(1)-C(23)-O(1)	141(16)
N(4)-Mo(1)-C(23)-O(1)	-120(16)
N(2)-Mo(1)-C(23)-O(1)	-72(17)
C(11)-Mo(1)-C(23)-O(1)	104(16)
C(23)-Mo(1)-C(24)-O(2)	-42(9)
N(6)-Mo(1)-C(24)-O(2)	49(9)
C(12)-Mo(1)-C(24)-O(2)	-146(9)
N(4)-Mo(1)-C(24)-O(2)	34(9)
N(2)-Mo(1)-C(24)-O(2)	129(9)
C(11)-Mo(1)-C(24)-O(2)	-148(9)

Symmetry transformations used to generate equivalent atoms:

Ortep Drawing of Compound (±)-**5a**



Crystal Structure Analysis for Compound (±)-5a

A suitable crystal of HMA103b (Compound **(±)-5a)** 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 (±)-5a

Table 1. Crystal data and structure refinement for $Mo(CO)_2(Tp)(C_{12}H_{16}NO_4)(CH_2Cl_2)1/2$. +

Identification code	hma103b	
Empirical formula	$C_{23.5}0\ H_{27}\ B\ Cl\ Mo\ N_7\ O_6$	
Formula weight	645.72	
Temperature	299(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 10.7760(10) Å	α= 90°.
	b = 22.6470(10) Å	β= 103.830(10)°.
	c = 11.7810(10) Å	γ = 90°.
Volume	2791.7(4) $Å^3$	
Z	4	
Density (calculated)	1.536 Mg/m^3	
Absorption coefficient	5.165 mm^{-1}	
F(000)	1316	
Crystal size	.144 x .42 x .50 mm^3	
Theta range for data collection	3.90 to 56.72°.	
Index ranges	-1<=h<=11, -24<=k<=1, -12<=l<=12	
Reflections collected	4550	
Independent reflections	3649 [R(int) = 0.0400]	
Completeness to theta = 56.72°	97.6 %	
Absorption correction	Empirical	
Max. and min. transmission	0.1372 and 0.0268	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3649 / 0 / 382	
Goodness-of-fit on F^2	1.080	
Final R indices [I>2sigma(I)]	R1 = 0.0448, wR2 = 0.1229	
R indices (all data)	R1 = 0.0465, wR2 = 0.1273	
Largest diff. peak and hole	0.591 and -0.789 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $Mo(CO)_2(Tp)(C_{12}H_{16}NO_4)(CH_2Cl_2)1/2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	1246(1)	1514(1)	20170(1)	50(1)
C(22)	2965(5)	1570(2)	19954(4)	60(1)
O(5)	4021(3)	1626(2)	19866(3)	82(1)
C(23)	1695(4)	703(2)	20638(3)	57(1)
O(6)	2020(3)	226(1)	20936(3)	72(1)
C(1)	1000(4)	1654(2)	17946(4)	58(1)
C(2)	26(4)	1389(2)	18359(4)	54(1)
C(3)	352(4)	809(2)	18827(3)	53(1)
C(4)	1182(4)	440(2)	18210(3)	54(1)
C(5)	515(4)	391(2)	16878(3)	61(1)
C(6)	992(5)	950(2)	16348(4)	70(1)
C(7)	1856(4)	1270(2)	17414(4)	59(1)
C(8)	3469(4)	521(2)	18078(4)	67(1)
C(9)	878(5)	-187(2)	16397(4)	69(1)
C(10)	328(6)	-734(2)	16797(5)	93(2)
C(11)	-246(5)	2527(2)	17375(5)	80(1)
C(12)	4747(7)	-323(3)	18480(8)	134(3)
N(1)	2350(3)	776(2)	18185(3)	57(1)
O(1)	4251(3)	763(2)	17670(4)	87(1)
O(2)	3594(3)	-21(2)	18538(3)	82(1)
O(3)	1567(4)	-212(2)	15745(4)	96(1)
O(4)	925(3)	2201(1)	17471(3)	67(1)
B(1)	114(6)	2448(2)	21902(5)	72(1)
N(2)	-707(4)	1593(2)	20562(3)	61(1)
N(3)	-941(3)	2035(2)	21264(3)	66(1)
N(4)	1835(3)	1675(2)	22079(3)	61(1)
N(5)	1220(4)	2065(2)	22626(3)	69(1)
N(6)	1220(3)	2505(2)	20245(3)	64(1)
N(7)	692(4)	2797(2)	21026(3)	68(1)
C(13)	1002(6)	3371(2)	21047(5)	83(2)

C(14)	1740(7)	3460(2)	20264(6)	85(2)
C(15)	1853(5)	2914(2)	19791(4)	72(1)
C(16)	1736(6)	2058(2)	23780(4)	80(1)
C(17)	2719(6)	1657(3)	24006(5)	85(2)
C(18)	2746(5)	1423(2)	22928(4)	69(1)
C(19)	-2166(5)	2021(2)	21310(5)	78(1)
C(20)	-2767(5)	1571(2)	20621(6)	82(2)
C(21)	-1829(4)	1312(2)	20168(4)	68(1)
Cl(1)	3328(4)	-47(2)	13737(3)	110(1)
C(24)	4470(30)	86(17)	15080(30)	154(14)
Cl(2)	5865(8)	-92(4)	15313(10)	149(3)

Table 3. Bond lengths [Å] and angles [°] for $Mo(CO)_2(Tp)(C_{12}H_{16}NO_4)(CH_2Cl_2)1/2$.

Mo(1)-C(22)	1.932(5)	N(4)-C(18)	1.349(6)
Mo(1)-C(23)	1.946(5)	N(4)-N(5)	1.357(5)
Mo(1)-N(4)	2.216(4)	N(5)-C(16)	1.340(6)
Mo(1)-C(2)	2.241(4)	N(6)-C(15)	1.336(6)
Mo(1)-N(6)	2.246(4)	N(6)-N(7)	1.362(5)
Mo(1)-N(2)	2.268(4)	N(7)-C(13)	1.340(6)
Mo(1)-C(3)	2.293(4)	C(13)-C(14)	1.369(9)
Mo(1)-C(1)	2.589(4)	C(14)-C(15)	1.373(7)
C(22)-O(5)	1.174(6)	C(16)-C(17)	1.374(8)
C(23)-O(6)	1.164(5)	C(17)-C(18)	1.382(7)
C(1)-O(4)	1.355(5)	C(19)-C(20)	1.364(8)
C(1)-C(2)	1.394(6)	C(20)-C(21)	1.382(7)
C(1)-C(7)	1.509(6)	Cl(1)-Cl(2)#1	1.282(10)
C(2)-C(3)	1.435(6)	Cl(1)-C(24)	1.78(3)
C(3)-C(4)	1.528(6)	C(24)-Cl(2)#1	0.51(3)
C(4)-N(1)	1.477(5)	C(24)-C(24)#1	1.25(7)
C(4)-C(5)	1.566(6)	C(24)-Cl(2)	1.51(2)
C(5)-C(9)	1.515(6)	Cl(2)-C(24)#1	0.51(3)
C(5)-C(6)	1.554(6)	Cl(2)-Cl(1)#1	1.282(10)
C(6)-C(7)	1.553(6)	Cl(2)-Cl(2)#1	1.879(17)
C(7)-N(1)	1.459(5)		
C(8)-O(1)	1.198(6)	C(22)-Mo(1)-C(23)	85.27(17)
C(8)-O(2)	1.335(6)	C(22)-Mo(1)-N(4)	94.12(17)
C(8)-N(1)	1.369(5)	C(23)-Mo(1)-N(4)	82.85(15)
C(9)-O(3)	1.190(6)	C(22)-Mo(1)-C(2)	104.24(18)
C(9)-C(10)	1.497(7)	C(23)-Mo(1)-C(2)	101.48(16)
C(11)-O(4)	1.442(5)	N(4)-Mo(1)-C(2)	161.38(16)
C(12)-O(2)	1.434(6)	C(22)-Mo(1)-N(6)	87.82(15)
B(1)-N(3)	1.525(7)	C(23)-Mo(1)-N(6)	159.52(14)
B(1)-N(7)	1.545(7)	N(4)-Mo(1)-N(6)	78.44(13)
B(1)-N(5)	1.554(7)	C(2)-Mo(1)-N(6)	98.90(14)
N(2)-C(21)	1.345(6)	C(22)-Mo(1)-N(2)	170.85(16)
N(2)-N(3)	1.361(5)	C(23)-Mo(1)-N(2)	101.28(15)
N(3)-C(19)	1.335(6)	N(4)-Mo(1)-N(2)	80.51(14)

C(2)-Mo(1)-N(2)	80.88(16)	N(1)-C(7)-C(1)	110.6(3)
N(6)-Mo(1)-N(2)	83.86(12)	N(1)-C(7)-C(6)	101.8(3)
C(22)-Mo(1)-C(3)	102.26(16)	C(1)-C(7)-C(6)	107.3(3)
C(23)-Mo(1)-C(3)	64.65(15)	O(1)-C(8)-O(2)	124.8(4)
N(4)-Mo(1)-C(3)	141.76(14)	O(1)-C(8)-N(1)	124.3(4)
C(2)-Mo(1)-C(3)	36.90(15)	O(2)-C(8)-N(1)	110.9(4)
N(6)-Mo(1)-C(3)	135.78(13)	O(3)-C(9)-C(10)	121.3(5)
N(2)-Mo(1)-C(3)	86.40(14)	O(3)-C(9)-C(5)	122.6(4)
C(22)-Mo(1)-C(1)	74.27(17)	C(10)-C(9)-C(5)	116.1(4)
C(23)-Mo(1)-C(1)	111.11(15)	C(8)-N(1)-C(7)	117.7(3)
N(4)-Mo(1)-C(1)	160.48(14)	C(8)-N(1)-C(4)	123.9(4)
C(2)-Mo(1)-C(1)	32.54(15)	C(7)-N(1)-C(4)	102.8(3)
N(6)-Mo(1)-C(1)	85.36(13)	C(8)-O(2)-C(12)	115.1(4)
N(2)-Mo(1)-C(1)	108.71(14)	C(1)-O(4)-C(11)	117.7(3)
C(3)-Mo(1)-C(1)	57.47(14)	N(3)-B(1)-N(7)	110.9(4)
O(5)-C(22)-Mo(1)	176.5(4)	N(3)-B(1)-N(5)	108.2(4)
O(6)-C(23)-Mo(1)	176.9(4)	N(7)-B(1)-N(5)	105.9(4)
O(4)-C(1)-C(2)	124.3(4)	C(21)-N(2)-N(3)	106.0(4)
O(4)-C(1)-C(7)	109.8(3)	C(21)-N(2)-Mo(1)	133.9(3)
C(2)-C(1)-C(7)	118.9(4)	N(3)-N(2)-Mo(1)	119.8(3)
O(4)-C(1)-Mo(1)	120.7(3)	C(19)-N(3)-N(2)	109.6(4)
C(2)-C(1)-Mo(1)	59.9(2)	C(19)-N(3)-B(1)	128.6(4)
C(7)-C(1)-Mo(1)	115.1(3)	N(2)-N(3)-B(1)	121.8(4)
C(1)-C(2)-C(3)	113.1(4)	C(18)-N(4)-N(5)	105.9(4)
C(1)-C(2)-Mo(1)	87.6(3)	C(18)-N(4)-Mo(1)	131.7(3)
C(3)-C(2)-Mo(1)	73.5(2)	N(5)-N(4)-Mo(1)	122.3(3)
C(2)-C(3)-C(4)	115.7(3)	C(16)-N(5)-N(4)	110.1(4)
C(2)-C(3)-Mo(1)	69.6(2)	C(16)-N(5)-B(1)	129.8(4)
C(4)-C(3)-Mo(1)	120.8(3)	N(4)-N(5)-B(1)	120.1(4)
N(1)-C(4)-C(3)	109.1(3)	C(15)-N(6)-N(7)	105.7(4)
N(1)-C(4)-C(5)	101.9(3)	C(15)-N(6)-Mo(1)	131.6(3)
C(3)-C(4)-C(5)	109.6(3)	N(7)-N(6)-Mo(1)	121.5(3)
C(9)-C(5)-C(6)	114.4(4)	C(13)-N(7)-N(6)	109.9(4)
C(9)-C(5)-C(4)	109.8(3)	C(13)-N(7)-B(1)	128.4(4)
C(6)-C(5)-C(4)	103.2(3)	N(6)-N(7)-B(1)	120.2(4)
C(7)-C(6)-C(5)	104.3(3)	N(7)-C(13)-C(14)	108.2(5)

C(13)-C(14)-C(15)	105.3(4)	C(24)#1-C(24)-Cl(2)	18(2)
N(6)-C(15)-C(14)	110.9(5)	Cl(2)#1-C(24)-Cl(1)	11(4)
N(5)-C(16)-C(17)	108.5(4)	C(24)#1-C(24)-Cl(1)	106(4)
C(16)-C(17)-C(18)	105.1(5)	Cl(2)-C(24)-Cl(1)	124(2)
N(4)-C(18)-C(17)	110.4(5)	C(24)#1-Cl(2)-Cl(1)#1	164(5)
N(3)-C(19)-C(20)	109.1(4)	C(24)#1-Cl(2)-C(24)	51(6)
C(19)-C(20)-C(21)	105.1(5)	Cl(1)#1-Cl(2)-C(24)	122.1(11)
N(2)-C(21)-C(20)	110.2(5)	C(24)#1-Cl(2)-Cl(2)#1	39(5)
Cl(2)#1-Cl(1)-C(24)	4.5(15)	Cl(1)#1-Cl(2)-Cl(2)#1	133.7(12)
Cl(2)#1-C(24)-C(24)#1	111(8)	C(24)-Cl(2)-Cl(2)#1	12.2(17)
Cl(2)#1-C(24)-Cl(2)	129(6)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+3

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $Mo(CO)_2(Tp)(C_{12}H_{16}NO_4)(CH_2Cl_2)1/2$. 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)	48(1)	52(1)	50(1)	-1(1)	15(1)	0(1)
C(22)	60(3)	57(2)	62(3)	-5(2)	14(2)	-2(2)
O(5)	50(2)	103(3)	97(3)	-22(2)	24(2)	-12(2)
C(23)	58(2)	63(3)	50(2)	-7(2)	13(2)	-6(2)
O(6)	84(2)	56(2)	75(2)	5(2)	14(2)	6(2)
C(1)	58(2)	60(2)	57(2)	5(2)	18(2)	-1(2)
C(2)	49(2)	64(2)	49(2)	-1(2)	11(2)	0(2)
C(3)	53(2)	62(2)	46(2)	-1(2)	15(2)	-9(2)
C(4)	55(2)	56(2)	52(2)	2(2)	16(2)	-5(2)
C(5)	66(3)	66(2)	51(2)	-1(2)	15(2)	-4(2)
C(6)	88(3)	73(3)	52(2)	4(2)	24(2)	4(2)
C(7)	59(2)	62(2)	62(2)	5(2)	28(2)	0(2)
C(8)	63(3)	71(3)	70(3)	-8(2)	23(2)	3(2)
C(9)	75(3)	79(3)	52(2)	-8(2)	15(2)	-5(2)
C(10)	133(5)	74(3)	72(3)	-11(2)	26(3)	-22(3)
C(11)	77(3)	78(3)	85(3)	19(2)	19(2)	15(2)
C(12)	108(5)	118(5)	199(8)	50(5)	81(5)	58(4)
N(1)	54(2)	59(2)	61(2)	-4(2)	22(2)	0(2)
O(1)	71(2)	86(2)	119(3)	5(2)	56(2)	6(2)
O(2)	73(2)	79(2)	102(2)	17(2)	35(2)	20(2)
O(3)	107(3)	90(2)	104(3)	-18(2)	52(2)	-7(2)
O(4)	70(2)	61(2)	76(2)	14(1)	30(2)	7(1)
B(1)	88(4)	68(3)	68(3)	-5(2)	33(3)	12(3)
N(2)	55(2)	67(2)	64(2)	-1(2)	21(2)	3(2)
N(3)	67(2)	73(2)	66(2)	0(2)	31(2)	13(2)
N(4)	62(2)	63(2)	59(2)	-3(2)	16(2)	-3(2)
N(5)	85(3)	66(2)	59(2)	-8(2)	20(2)	2(2)
N(6)	67(2)	58(2)	66(2)	-1(2)	15(2)	1(2)
N(7)	79(2)	55(2)	72(2)	-3(2)	24(2)	8(2)
C(13)	93(4)	59(3)	94(4)	-10(3)	16(3)	5(2)

C(14)	98(4)	56(3)	104(4)	1(2)	28(3)	-9(2)
C(15)	76(3)	64(3)	78(3)	6(2)	21(2)	-5(2)
C(16)	97(4)	82(3)	62(3)	-14(2)	21(3)	-9(3)
C(17)	91(4)	100(4)	58(3)	-6(3)	5(3)	-20(3)
C(18)	65(3)	74(3)	63(3)	3(2)	7(2)	-10(2)
C(19)	76(3)	79(3)	92(3)	10(3)	47(3)	19(3)
C(20)	58(3)	92(4)	108(4)	14(3)	40(3)	6(2)
C(21)	58(3)	74(3)	76(3)	2(2)	24(2)	-4(2)
Cl(1)	128(3)	98(2)	113(2)	23(2)	47(2)	12(2)
C(24)	54(10)	200(20)	190(30)	-90(20)	-8(14)	18(11)
Cl(2)	101(5)	123(4)	204(8)	11(4)	-1(5)	-1(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $Mo(CO)_2(Tp)(C_{12}H_{16}NO_4)(CH_2Cl_2)1/2$.

	x	y	z	U(eq)
H(3)	-310(40)	591(16)	19000(30)	44(9)
H(2)	-750(50)	1572(18)	18380(40)	62(13)
H(4A)	1380	51	18574	64
H(5A)	-415	410	16770	73
H(6A)	1476	843	15781	84
H(6B)	281	1198	15969	84
H(7A)	2540	1497	17199	71
H(10A)	615	-1074	16443	139
H(10B)	-588	-714	16571	139
H(10C)	604	-765	17632	139
H(11A)	-176	2905	17028	120
H(11B)	-398	2581	18138	120
H(11C)	-944	2311	16893	120
H(12A)	4756	-707	18829	201
H(12B)	5472	-100	18896	201
H(12C)	4783	-365	17678	201
H(1)	-220(60)	2740(30)	22400(60)	120(20)
H(13A)	759	3658	21514	100
H(14A)	2090	3814	20090	102
H(15A)	2310	2839	19229	87
H(16A)	1472	2287	24335	96
H(17A)	3252	1562	24728	102
H(18A)	3312	1134	22806	82
H(19A)	-2549	2276	21742	93
H(20A)	-3622	1463	20486	99
H(21A)	-1954	990	19663	82

Table 6. Torsion angles [°] for $Mo(CO)_2(Tp)(C_{12}H_{16}NO_4)(CH_2Cl_2)1/2$.

C(23)-Mo(1)-C(22)-O(5)	-120(7)	O(4)-C(1)-C(2)-C(3)	-179.5(4)
N(4)-Mo(1)-C(22)-O(5)	-37(7)	C(7)-C(1)-C(2)-C(3)	33.0(5)
C(2)-Mo(1)-C(22)-O(5)	140(7)	Mo(1)-C(1)-C(2)-C(3)	-70.9(3)
N(6)-Mo(1)-C(22)-O(5)	41(7)	O(4)-C(1)-C(2)-Mo(1)	-108.6(4)
N(2)-Mo(1)-C(22)-O(5)	17(8)	C(7)-C(1)-C(2)-Mo(1)	103.9(4)
C(3)-Mo(1)-C(22)-O(5)	178(100)	C(22)-Mo(1)-C(2)-C(1)	-23.4(3)
C(1)-Mo(1)-C(22)-O(5)	127(7)	C(23)-Mo(1)-C(2)-C(1)	-111.4(3)
C(22)-Mo(1)-C(23)-O(6)	30(7)	N(4)-Mo(1)-C(2)-C(1)	146.8(4)
N(4)-Mo(1)-C(23)-O(6)	-65(7)	N(6)-Mo(1)-C(2)-C(1)	66.6(3)
C(2)-Mo(1)-C(23)-O(6)	133(7)	N(2)-Mo(1)-C(2)-C(1)	148.8(3)
N(6)-Mo(1)-C(23)-O(6)	-41(7)	C(3)-Mo(1)-C(2)-C(1)	-115.0(4)
N(2)-Mo(1)-C(23)-O(6)	-144(7)	C(22)-Mo(1)-C(2)-C(3)	91.6(3)
C(3)-Mo(1)-C(23)-O(6)	136(7)	C(23)-Mo(1)-C(2)-C(3)	3.6(3)
C(1)-Mo(1)-C(23)-O(6)	101(7)	N(4)-Mo(1)-C(2)-C(3)	-98.3(5)
C(22)-Mo(1)-C(1)-O(4)	-89.3(3)	N(6)-Mo(1)-C(2)-C(3)	-178.4(2)
C(23)-Mo(1)-C(1)-O(4)	-167.7(3)	N(2)-Mo(1)-C(2)-C(3)	-96.2(2)
N(4)-Mo(1)-C(1)-O(4)	-34.1(6)	C(1)-Mo(1)-C(2)-C(3)	115.0(4)
C(2)-Mo(1)-C(1)-O(4)	114.3(4)	C(1)-C(2)-C(3)-C(4)	-35.3(5)
N(6)-Mo(1)-C(1)-O(4)	-0.2(3)	Mo(1)-C(2)-C(3)-C(4)	-115.3(3)
N(2)-Mo(1)-C(1)-O(4)	81.7(3)	C(1)-C(2)-C(3)-Mo(1)	80.0(3)
C(3)-Mo(1)-C(1)-O(4)	154.5(4)	C(22)-Mo(1)-C(3)-C(2)	-97.4(3)
C(22)-Mo(1)-C(1)-C(2)	156.4(3)	C(23)-Mo(1)-C(3)-C(2)	-176.1(3)
C(23)-Mo(1)-C(1)-C(2)	78.0(3)	N(4)-Mo(1)-C(3)-C(2)	149.3(3)
N(4)-Mo(1)-C(1)-C(2)	-148.4(4)	N(6)-Mo(1)-C(3)-C(2)	2.2(3)
N(6)-Mo(1)-C(1)-C(2)	-114.6(3)	N(2)-Mo(1)-C(3)-C(2)	79.6(3)
N(2)-Mo(1)-C(1)-C(2)	-32.7(3)	C(1)-Mo(1)-C(3)-C(2)	-35.3(2)
C(3)-Mo(1)-C(1)-C(2)	40.2(3)	C(22)-Mo(1)-C(3)-C(4)	11.1(3)
C(22)-Mo(1)-C(1)-C(7)	46.3(3)	C(23)-Mo(1)-C(3)-C(4)	-67.6(3)
C(23)-Mo(1)-C(1)-C(7)	-32.2(3)	N(4)-Mo(1)-C(3)-C(4)	-102.2(3)
N(4)-Mo(1)-C(1)-C(7)	101.4(5)	C(2)-Mo(1)-C(3)-C(4)	108.5(4)
C(2)-Mo(1)-C(1)-C(7)	-110.1(4)	N(6)-Mo(1)-C(3)-C(4)	110.7(3)
N(6)-Mo(1)-C(1)-C(7)	135.3(3)	N(2)-Mo(1)-C(3)-C(4)	-171.9(3)
N(2)-Mo(1)-C(1)-C(7)	-142.8(3)	C(1)-Mo(1)-C(3)-C(4)	73.2(3)
C(3)-Mo(1)-C(1)-C(7)	-69.9(3)	C(2)-C(3)-C(4)-N(1)	54.9(4)

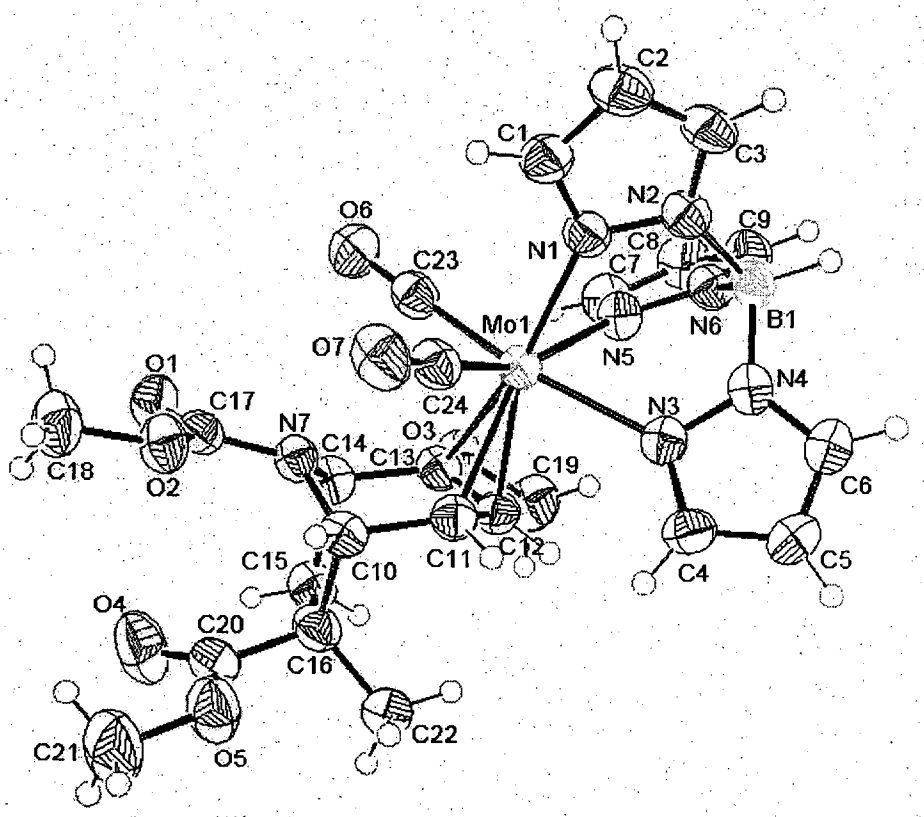
Mo(1)-C(3)-C(4)-N(1)	-25.7(4)	C(7)-C(1)-O(4)-C(11)	149.1(4)
C(2)-C(3)-C(4)-C(5)	-55.8(4)	Mo(1)-C(1)-O(4)-C(11)	-73.3(5)
Mo(1)-C(3)-C(4)-C(5)	-136.4(3)	C(22)-Mo(1)-N(2)-C(21)	163.7(9)
N(1)-C(4)-C(5)-C(9)	94.3(4)	C(23)-Mo(1)-N(2)-C(21)	-61.0(4)
C(3)-C(4)-C(5)-C(9)	-150.3(4)	N(4)-Mo(1)-N(2)-C(21)	-141.7(4)
N(1)-C(4)-C(5)-C(6)	-28.1(4)	C(2)-Mo(1)-N(2)-C(21)	39.0(4)
C(3)-C(4)-C(5)-C(6)	87.3(4)	N(6)-Mo(1)-N(2)-C(21)	139.0(4)
C(9)-C(5)-C(6)-C(7)	-120.3(4)	C(3)-Mo(1)-N(2)-C(21)	2.2(4)
C(4)-C(5)-C(6)-C(7)	-1.1(4)	C(1)-Mo(1)-N(2)-C(21)	56.1(4)
O(4)-C(1)-C(7)-N(1)	158.0(3)	C(22)-Mo(1)-N(2)-N(3)	-9.6(11)
C(2)-C(1)-C(7)-N(1)	-50.2(5)	C(23)-Mo(1)-N(2)-N(3)	125.6(3)
Mo(1)-C(1)-C(7)-N(1)	17.8(4)	N(4)-Mo(1)-N(2)-N(3)	44.9(3)
O(4)-C(1)-C(7)-C(6)	-91.8(4)	C(2)-Mo(1)-N(2)-N(3)	-134.4(3)
C(2)-C(1)-C(7)-C(6)	60.0(5)	N(6)-Mo(1)-N(2)-N(3)	-34.3(3)
Mo(1)-C(1)-C(7)-C(6)	128.0(3)	C(3)-Mo(1)-N(2)-N(3)	-171.1(3)
C(5)-C(6)-C(7)-N(1)	30.2(4)	C(1)-Mo(1)-N(2)-N(3)	-117.3(3)
C(5)-C(6)-C(7)-C(1)	-86.0(4)	C(21)-N(2)-N(3)-C(19)	0.8(5)
C(6)-C(5)-C(9)-O(3)	6.3(6)	Mo(1)-N(2)-N(3)-C(19)	175.8(3)
C(4)-C(5)-C(9)-O(3)	-109.1(5)	C(21)-N(2)-N(3)-B(1)	178.7(4)
C(6)-C(5)-C(9)-C(10)	-174.1(4)	Mo(1)-N(2)-N(3)-B(1)	-6.3(5)
C(4)-C(5)-C(9)-C(10)	70.4(5)	N(7)-B(1)-N(3)-C(19)	-121.2(5)
O(1)-C(8)-N(1)-C(7)	22.7(7)	N(5)-B(1)-N(3)-C(19)	123.2(5)
O(2)-C(8)-N(1)-C(7)	-160.2(4)	N(7)-B(1)-N(3)-N(2)	61.4(6)
O(1)-C(8)-N(1)-C(4)	153.6(4)	N(5)-B(1)-N(3)-N(2)	-54.3(5)
O(2)-C(8)-N(1)-C(4)	-29.3(6)	C(22)-Mo(1)-N(4)-C(18)	-50.6(4)
C(1)-C(7)-N(1)-C(8)	-155.9(4)	C(23)-Mo(1)-N(4)-C(18)	34.1(4)
C(6)-C(7)-N(1)-C(8)	90.3(4)	C(2)-Mo(1)-N(4)-C(18)	138.9(5)
C(1)-C(7)-N(1)-C(4)	64.1(4)	N(6)-Mo(1)-N(4)-C(18)	-137.5(4)
C(6)-C(7)-N(1)-C(4)	-49.6(4)	N(2)-Mo(1)-N(4)-C(18)	136.9(4)
C(3)-C(4)-N(1)-C(8)	156.6(4)	C(3)-Mo(1)-N(4)-C(18)	65.2(5)
C(5)-C(4)-N(1)-C(8)	-87.6(4)	C(1)-Mo(1)-N(4)-C(18)	-103.0(5)
C(3)-C(4)-N(1)-C(7)	-66.8(4)	C(22)-Mo(1)-N(4)-N(5)	132.9(3)
C(5)-C(4)-N(1)-C(7)	49.0(4)	C(23)-Mo(1)-N(4)-N(5)	-142.4(3)
O(1)-C(8)-O(2)-C(12)	-2.2(8)	C(2)-Mo(1)-N(4)-N(5)	-37.6(6)
N(1)-C(8)-O(2)-C(12)	-179.4(5)	N(6)-Mo(1)-N(4)-N(5)	46.0(3)
C(2)-C(1)-O(4)-C(11)	-0.9(6)	N(2)-Mo(1)-N(4)-N(5)	-39.6(3)

C(3)-Mo(1)-N(4)-N(5)	-111.3(3)	N(3)-B(1)-N(7)-N(6)	-58.0(6)
C(1)-Mo(1)-N(4)-N(5)	80.5(5)	N(5)-B(1)-N(7)-N(6)	59.0(5)
C(18)-N(4)-N(5)-C(16)	0.2(5)	N(6)-N(7)-C(13)-C(14)	0.4(6)
Mo(1)-N(4)-N(5)-C(16)	177.5(3)	B(1)-N(7)-C(13)-C(14)	166.5(5)
C(18)-N(4)-N(5)-B(1)	178.8(4)	N(7)-C(13)-C(14)-C(15)	-0.4(7)
Mo(1)-N(4)-N(5)-B(1)	-3.9(5)	N(7)-N(6)-C(15)-C(14)	0.0(6)
N(3)-B(1)-N(5)-C(16)	-120.7(5)	Mo(1)-N(6)-C(15)-C(14)	-167.2(4)
N(7)-B(1)-N(5)-C(16)	120.4(5)	C(13)-C(14)-C(15)-N(6)	0.2(7)
N(3)-B(1)-N(5)-N(4)	61.0(5)	N(4)-N(5)-C(16)-C(17)	0.3(6)
N(7)-B(1)-N(5)-N(4)	-57.9(5)	B(1)-N(5)-C(16)-C(17)	-178.1(5)
C(22)-Mo(1)-N(6)-C(15)	26.3(4)	N(5)-C(16)-C(17)-C(18)	-0.7(6)
C(23)-Mo(1)-N(6)-C(15)	96.6(6)	N(5)-N(4)-C(18)-C(17)	-0.6(5)
N(4)-Mo(1)-N(6)-C(15)	120.9(4)	Mo(1)-N(4)-C(18)-C(17)	-177.6(3)
C(2)-Mo(1)-N(6)-C(15)	-77.8(4)	C(16)-C(17)-C(18)-N(4)	0.8(6)
N(2)-Mo(1)-N(6)-C(15)	-157.5(4)	N(2)-N(3)-C(19)-C(20)	-0.9(6)
C(3)-Mo(1)-N(6)-C(15)	-79.1(4)	B(1)-N(3)-C(19)-C(20)	-178.6(5)
C(1)-Mo(1)-N(6)-C(15)	-48.1(4)	N(3)-C(19)-C(20)-C(21)	0.6(6)
C(22)-Mo(1)-N(6)-N(7)	-139.2(3)	N(3)-N(2)-C(21)-C(20)	-0.4(5)
C(23)-Mo(1)-N(6)-N(7)	-68.9(5)	Mo(1)-N(2)-C(21)-C(20)	-174.4(3)
N(4)-Mo(1)-N(6)-N(7)	-44.6(3)	C(19)-C(20)-C(21)-N(2)	-0.2(6)
C(2)-Mo(1)-N(6)-N(7)	116.7(3)	Cl(2)#1-Cl(1)-C(24)-C(24)#1	-115(25)
N(2)-Mo(1)-N(6)-N(7)	37.0(3)	Cl(2)#1-Cl(1)-C(24)-Cl(2)	-119(24)
C(3)-Mo(1)-N(6)-N(7)	115.4(3)	Cl(2)#1-C(24)-Cl(2)-C(24)#1	0.00(3)
C(1)-Mo(1)-N(6)-N(7)	146.4(3)	Cl(1)-C(24)-Cl(2)-C(24)#1	13(5)
C(15)-N(6)-N(7)-C(13)	-0.2(5)	Cl(2)#1-C(24)-Cl(2)-Cl(1)#1	163(7)
Mo(1)-N(6)-N(7)-C(13)	168.6(3)	C(24)#1-C(24)-Cl(2)-Cl(1)#1	163(7)
C(15)-N(6)-N(7)-B(1)	-167.7(4)	Cl(1)-C(24)-Cl(2)-Cl(1)#1	175(2)
Mo(1)-N(6)-N(7)-B(1)	1.1(5)	C(24)#1-C(24)-Cl(2)-Cl(2)#1	0.00(5)
N(3)-B(1)-N(7)-C(13)	137.1(5)	Cl(1)-C(24)-Cl(2)-Cl(2)#1	13(5)
N(5)-B(1)-N(7)-C(13)	-105.8(5)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+3

Ortep Drawing of Compound (±)-8



$C_{24}H_{28}BMoN_7O_7$

Crystal Structure Analysis

A suitable crystal of **HMB107c** 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 (±)-8

Table 1. Crystal data and structure refinement for $C_{24}H_{28}BMoN_7O_7$.

Identification code	hmb107c	
Empirical formula	C24 H28 B Mo N7 O7	
Formula weight	633.28	
Temperature	293(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 12.3960(6) Å	α= 90°.
	b = 13.5113(5) Å	β= 94.205(3)°.
	c = 15.9427(7) Å	γ = 90°.
Volume	2663.0(2) Å^3	
Z	4	
Density (calculated)	1.580 Mg/m^3	
Absorption coefficient	4.530 mm^{-1}	
F(000)	1296	
Crystal size	0.50 x 0.24 x 0.06 mm^3	
Theta range for data collection	3.58 to 56.74°.	
Index ranges	$-13 \le h \le 8$, $-14 \le k \le 1$, $-17 \le l \le 17$	
Reflections collected	4463	
Independent reflections	3494 [R(int) = 0.0648]	
Completeness to theta = 56.74°	98.2 %	
Absorption correction	Empirical	
Max. and min. transinission	0.1693 and 0.0479	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3494 / 0 / 365	
Goodness-of-fit on F^2	1.125	
Final R indices [I>2sigma(I)]	R1 = 0.0501, wR2 = 0.1326	
R indices (all data)	R1 = 0.0539, wR2 = 0.1364	
Largest diff. peak and hole	0.563 and -1.618 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $C_{24}H_{28}BMoN_7O_7$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	278(1)	2026(1)	1765(1)	37(1)
B(1)	-2361(4)	2615(4)	1868(3)	43(1)
N(1)	-1228(3)	1302(3)	1236(2)	44(1)
N(2)	-2228(3)	1657(3)	1365(2)	44(1)
N(3)	-760(3)	2243(3)	2897(2)	42(1)
N(4)	-1823(3)	2480(3)	2755(2)	43(1)
N(5)	-703(3)	3363(3)	1282(2)	42(1)
N(6)	-1766(3)	3434(3)	1411(2)	42(1)
N(7)	2916(3)	1533(3)	1728(2)	40(1)
O(1)	4084(3)	1272(2)	713(2)	52(1)
O(2)	3696(2)	50(2)	1606(2)	52(1)
O(3)	1943(2)	4038(2)	1515(2)	48(1)
O(4)	5426(3)	1370(3)	2710(3)	80(1)
O(5)	4626(3)	657(3)	3751(2)	70(1)
O(6)	1383(3)	1863(3)	91(2)	67(1)
O(7)	1012(3)	-166(3)	1926(2)	66(1)
C(1)	-1386(4)	476(4)	784(3)	50(1)
C(2)	-2478(4)	285(4)	628(3)	58(1)
C(3)	-2981(4)	1054(4)	1001(3)	52(1)
C(4)	-551(4)	2249(4)	3727(3)	49(1)
C(5)	-1482(4)	2470(4)	4130(3)	56(1)
C(6)	-2265(4)	2612(4)	3489(3)	51(1)
C(7)	-487(4)	4125(4)	788(3)	54(1)
C(8)	-1405(4)	4691(4)	609(3)	58(1)
C(9)	-2196(4)	4228(4)	1006(3)	51(1)
C(10)	2729(3)	1379(3)	2620(3)	43(1)
C(11)	1643(3)	1825(3)	2793(3)	42(1)
C(12)	1474(4)	2855(3)	2590(3)	43(1)
C(13)	1945(4)	3116(3)	1865(3)	42(1)
C(14)	3007(3)	2604(3)	1674(3)	41(1)
C(15)	3841(4)	2833(3)	2430(3)	48(1)

C(16)	3681(4)	2004(3)	3071(3)	46(1)
C(17)	3612(3)	981(3)	1298(3)	43(1)
C(18)	4469(4)	-561(4)	1232(4)	64(1)
C(19)	1589(4)	4849(4)	2008(3)	61(1)
C(20)	4686(3)	1339(4)	3141(3)	50(1)
C(21)	5550(5)	-2(5)	3869(4)	92(2)
C(22)	3462(4)	2363(4)	3950(3)	56(1)
C(23)	986(4)	1931(3)	725(3)	45(1)
C(24)	743(3)	660(4)	1893(3)	46(1)

Table 3. Bond lengths [Å] and angles [°] for $C_{24}H_{28}BMoN_7O_7$.

Mo(1)-C(23)	1.936(5)	C(2)-C(3)	1.370(7)
Mo(1)-C(24)	1.939(5)	C(4)-C(5)	1.394(7)
Mo(1)-C(12)	2.214(4)	C(5)-C(6)	1.370(7)
Mo(1)-N(1)	2.217(3)	C(7)-C(8)	1.383(7)
Mo(1)-N(5)	2.280(4)	C(8)-C(9)	1.358(7)
Mo(1)-C(11)	2.285(4)	C(10)-C(11)	1.519(6)
Mo(1)-N(3)	2.310(3)	C(10)-C(16)	1.581(6)
Mo(1)-C(13)	2.534(4)	C(11)-C(12)	1.441(6)
B(1)-N(4)	1.529(6)	C(12)-C(13)	1.379(7)
B(1)-N(2)	1.538(7)	C(13)-C(14)	1.537(6)
B(1)-N(6)	1.542(7)	C(14)-C(15)	1.561(6)
N(1)-C(1)	1.336(6)	C(15)-C(16)	1.539(7)
N(1)-N(2)	1.359(5)	C(16)-C(22)	1.527(7)
N(2)-C(3)	1.339(6)	C(16)-C(20)	1.533(7)
N(3)-C(4)	1.330(6)		
N(3)-N(4)	1.359(5)	C(23)-Mo(1)-C(24)	82.95(18)
N(4)-C(6)	1.339(6)	C(23)-Mo(1)-C(12)	102.49(18)
N(5)-C(7)	1.335(6)	C(24)-Mo(1)-C(12)	103.76(17)
N(5)-N(6)	1.352(5)	C(23)-Mo(1)-N(1)	93.85(17)
N(6)-C(9)	1.342(6)	C(24)-Mo(1)-N(1)	81.75(15)
N(7)-C(17)	1.364(6)	C(12)-Mo(1)-N(1)	163.23(15)
N(7)-C(14)	1.454(6)	C(23)-Mo(1)-N(5)	91.53(15)
N(7)-C(10)	1.472(5)	C(24)-Mo(1)-N(5)	159.50(16)
O(1)-C(17)	1.203(5)	C(12)-Mo(1)-N(5)	96.71(15)
O(2)-C(17)	1.352(5)	N(1)-Mo(1)-N(5)	78.93(13)
O(2)-C(18)	1.428(6)	C(23)-Mo(1)-C(11)	104.37(17)
O(3)-C(13)	1.365(5)	C(24)-Mo(1)-C(11)	67.18(17)
O(3)-C(19)	1.436(6)	C(12)-Mo(1)-C(11)	37.34(16)
O(4)-C(20)	1.187(5)	N(1)-Mo(1)-C(11)	141.16(15)
O(5)-C(20)	1.346(6)	N(5)-Mo(1)-C(11)	133.25(15)
O(5)-C(21)	1.451(7)	C(23)-Mo(1)-N(3)	172.11(16)
O(6)-C(23)	1.160(6)	C(24)-Mo(1)-N(3)	102.55(16)
O(7)-C(24)	1.165(6)	C(12)-Mo(1)-N(3)	81.86(15)
C(1)-C(2)	1.383(6)	N(1)-Mo(1)-N(3)	81.48(13)

N(5)-Mo(1)-N(3)	81.36(13)	N(1)-C(1)-C(2)	110.9(4)
C(11)-Mo(1)-N(3)	83.11(15)	C(3)-C(2)-C(1)	104.5(4)
C(23)-Mo(1)-C(13)	70.93(17)	N(2)-C(3)-C(2)	109.0(4)
C(24)-Mo(1)-C(13)	108.12(16)	N(3)-C(4)-C(5)	110.7(4)
C(12)-Mo(1)-C(13)	32.89(16)	C(6)-C(5)-C(4)	104.5(4)
N(1)-Mo(1)-C(13)	160.07(14)	N(4)-C(6)-C(5)	108.7(4)
N(5)-Mo(1)-C(13)	88.44(14)	N(5)-C(7)-C(8)	110.5(4)
C(11)-Mo(1)-C(13)	57.71(16)	C(9)-C(8)-C(7)	105.1(4)
N(3)-Mo(1)-C(13)	112.03(14)	N(6)-C(9)-C(8)	108.6(4)
N(4)-B(1)-N(2)	109.0(4)	N(7)-C(10)-C(11)	108.9(3)
N(4)-B(1)-N(6)	109.4(4)	N(7)-C(10)-C(16)	101.4(3)
N(2)-B(1)-N(6)	106.5(4)	C(11)-C(10)-C(16)	110.3(4)
C(1)-N(1)-N(2)	106.1(3)	C(12)-C(11)-C(10)	117.3(4)
C(1)-N(1)-Mo(1)	131.3(3)	C(12)-C(11)-Mo(1)	68.7(2)
N(2)-N(1)-Mo(1)	122.6(3)	C(10)-C(11)-Mo(1)	122.4(3)
C(3)-N(2)-N(1)	109.5(4)	C(13)-C(12)-C(11)	111.8(4)
C(3)-N(2)-B(1)	129.8(4)	C(13)-C(12)-Mo(1)	86.5(3)
N(1)-N(2)-B(1)	120.7(3)	C(11)-C(12)-Mo(1)	74.0(2)
C(4)-N(3)-N(4)	106.2(3)	O(3)-C(13)-C(12)	126.0(4)
C(4)-N(3)-Mo(1)	134.4(3)	O(3)-C(13)-C(14)	107.8(4)
N(4)-N(3)-Mo(1)	119.3(3)	C(12)-C(13)-C(14)	118.2(4)
C(6)-N(4)-N(3)	109.8(4)	O(3)-C(13)-Mo(1)	121.8(3)
C(6)-N(4)-B(1)	127.8(4)	C(12)-C(13)-Mo(1)	60.7(2)
N(3)-N(4)-B(1)	122.2(3)	C(14)-C(13)-Mo(1)	115.6(3)
C(7)-N(5)-N(6)	106.0(4)	N(7)-C(14)-C(13)	111.4(3)
C(7)-N(5)-Mo(1)	133.3(3)	N(7)-C(14)-C(15)	101.6(3)
N(6)-N(5)-Mo(1)	120.4(3)	C(13)-C(14)-C(15)	106.6(4)
C(9)-N(6)-N(5)	109.9(4)	C(16)-C(15)-C(14)	105.0(4)
C(9)-N(6)-B(1)	127.9(4)	C(22)-C(16)-C(20)	108.5(4)
N(5)-N(6)-B(1)	121.8(4)	C(22)-C(16)-C(15)	114.7(4)
C(17)-N(7)-C(14)	117.4(3)	C(20)-C(16)-C(15)	109.4(4)
C(17)-N(7)-C(10)	124.0(4)	C(22)-C(16)-C(10)	114.2(4)
C(14)-N(7)-C(10)	102.6(3)	C(20)-C(16)-C(10)	107.2(4)
C(17)-O(2)-C(18)	115.0(4)	C(15)-C(16)-C(10)	102.4(4)
C(13)-O(3)-C(19)	117.6(4)	O(1)-C(17)-O(2)	123.8(4)
C(20)-O(5)-C(21)	115.4(4)	O(1)-C(17)-N(7)	125.0(4)

O(2)-C(17)-N(7)	111.2(4)	O(5)-C(20)-C(16)	111.5(4)
O(4)-C(20)-O(5)	121.9(5)	O(6)-C(23)-Mo(1)	178.1(4)
O(4)-C(20)-C(16)	126.5(5)	O(7)-C(24)-Mo(1)	176.5(4)

Symmetry transformations used to generate equivalent atoms: