SUPPORTING INFORMATION

Alkylation of a Dimolybdenum SO Bridge, Subsequent Reactions, and Characterization of the Thioperoxide Bridge

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Crystallographic Studies for $BnS\{Mo_2\}SOEt^+$ (4^+) $CF_3SO_3^-$

A thin (0.25 x 0.20 x 0.02 mm^3) yellow plate crystal was mounted on a CryoLoop with Paratone oil for collection of x-ray data on a Bruker SMART APEX CCD diffractometer. The SMART[1] software package (v 5.632) was used to acquire a total of 1,868 sixty-second frame ω-scan exposures of data at 100K to a 2θ max = 52.26° using monochromated Mo Kα radiation (0.71073 Å) from a sealed tube and a monocapillary. Frame data were processed using SAINT[2] (v 6.45a) to determine final unit cell parameters a = 18.917(4) Å, b = 10.9062(18) Å, c = 24.231(4)) Å, β= 104.856(4)°, V = 4832.0(15)$Å^3$, Z = 4 and ρ_{calcd} = 1.623 Mgm^{-3} to produce raw hkl data that were then corrected for absorption (transmission min./max. = 0.716/0.964; μ = 0.951mm^{-1}) using SADABS[3] (v 2.10). The structure was solved by Patterson methods in the space group Cc using SHELXS-90[4] and refined by least squares methods on F^2 using SHELXL-99[5] incorporated into the SHELXTL[6] (v 6.14) suite of programs. The disordered triflate anion was accurately modeled using two, half-occupancy fluorine groups (F1a –F3a, and F1b –F3b) tetrahedrally coordinated to a full occupancy carbon atom in addition to two, half-occupancy oxygen groups (O10a –O12a, and O10b –O12b) and a full occupancy sulfur atom. The carbon atoms (C23a – C24a and C23b –C24b) of one OEt group were also modeled with a 50% disorder as was the methyl atom (C20a and C20b) of another OEt group. All non-hydrogen atoms except those involved in set b of the disordered anion were refined anisotropically. Hydrogen atoms were placed in their geometrically generated positions and refined as a riding model. Methyl H's were included as fixed contributions with U(H) = 1.5 x Ueq(attached C atom) while the torsion angle which defines its orientation was allowed to refine on the attached C atom. Methylene and phenyl H's were included as fixed contributions with U(H) = 1.2 x Ueq (attached C atom). For all 9175 unique reflections (R(int) = 0.045) the final anisotropic full matrix least-squares refinement on F^2 for 455 variables converged at R1 = 0.0505 and wR2 = 0.1175 with a GOF of

1.03.

References

1. SMART, V.5.632, Bruker Advanced X-ray Solutions, Inc., Madison, WI, 2005.

2. SAINT, V. 6.45a, Bruker Advanced X-ray Solutions, Inc., Madison, WI, 2003.

3. G. M. Sheldrick, SADABS, V. 2.10, Area Detector Absorption Correction, University of Göttingen, Göttingen, Germany, 2003.

4. G. M. Sheldrick, SHELXS-90., *Acta Crystallogr*. 1990, *A46*, 467.

5. G. M. Sheldrick, SHELXL-99, Program for the Refinement of Crystal Structures, University of Göttingen, Göttingen, Germany, 1997.

6. SHELXTL 6.14, Program Library for Structure Solution and Molecular graphics, Bruker Advanced X-ray Solutions, Madison, WI, 2000.

Table S1. Crystal data and structure refinement

Empirical formula	C34 H49 F3 Mo2 N2 O10 P2 S7	
Formula weight	1180.99	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	Cc	
Unit cell dimensions	a = 18.917(4) Å	α = 90°.
	b = 10.9062(18) Å	β = 104.856(4)°.
	c = 24.231(4) Å	γ = 90°.
Volume	4832.0(15) $Å^3$	
Z	4	
Density (calculated)	1.623 Mg/m^3	
Absorption coefficient	0.951 mm^{-1}	
F(000)	2400	
Crystal size	0.25 x 0.20 x 0.02 mm^3	
Theta range for data collection	1.74 to 26.13°	
Index ranges	-23<=h<=23, -13<=k<=13, -29<=l<=29	
Reflections collected	18147	
Independent reflections	9175 [R(int) = 0.0458]	
Completeness to theta = 26.13°	99.1 %	
Absorption correction	SADABS	
Max. and min. transmission	0.989 and 0.725	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9175 / 25 / 455	
Goodness-of-fit on F^2	1.032	
Final R indices [I>2sigma(I)]	R1 = 0.0505, wR2 = 0.1175	
R indices (all data)	R1 = 0.0619, wR2 = 0.1231	
Absolute structure parameter	0.050(4)	
Largest diff. peak and hole	1.276 and -1.189 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	90(1)	1658(1)	972(1)	19(1)
Mo(2)	1658(1)	1911(1)	1284(1)	23(1)
S(1)	785(1)	3272(2)	653(1)	26(1)
S(2)	966(1)	243(2)	1566(1)	20(1)
S(3)	-821(1)	481(2)	1341(1)	24(1)
S(4)	-1044(1)	2905(2)	570(1)	30(1)
S(6)	2601(1)	3530(2)	1319(1)	30(1)
S(5)	2685(1)	1087(2)	2058(1)	32(1)
P(1)	-1582(1)	1663(2)	913(1)	24(1)
P(2)	3274(1)	2535(2)	1936(1)	33(1)
O(1)	190(3)	2787(4)	1718(2)	22(1)
O(2)	1411(3)	2970(4)	1970(2)	27(1)
O(3)	-2215(2)	991(4)	463(2)	30(1)
O(4)	-2053(3)	2223(5)	1289(2)	34(1)
O(5)	4007(3)	2161(7)	1795(3)	58(2)
O(6)	3605(3)	3288(6)	2492(3)	57(2)
O(7)	696(3)	4522(4)	1017(2)	32(1)
N(1)	49(3)	853(5)	353(2)	24(1)
N(2)	1812(3)	1068(6)	728(2)	31(1)
C(1)	34(4)	248(5)	-166(2)	56(1)
C(2)	335(4)	769(5)	-572(2)	56(1)
C(3)	315(4)	148(5)	-1071(2)	56(1)
C(4)	-6(4)	-994(5)	-1165(2)	56(1)
C(5)	-308(4)	-1515(5)	-759(2)	56(1)
C(6)	-288(4)	-894(5)	-260(2)	56(1)
C(7)	-52(6)	-1659(8)	-1726(4)	56(1)
C(8)	1943(5)	270(8)	299(4)	48(1)
C(9)	2327(5)	679(9)	-84(4)	48(1)
C(10)	2416(5)	-96(8)	-516(4)	48(1)
C(11)	2123(5)	-1256(9)	-572(4)	48(1)
C(12)	1782(5)	-1656(8)	-170(4)	48(1)
C(13)	1679(5)	-937(8)	259(4)	48(1)
C(14)	2208(5)	-2097(8)	-1051(4)	48(1)
C(15)	783(4)	3245(6)	2018(3)	26(2)
C(16)	736(5)	4148(7)	2481(3)	37(2)
C(17)	-2048(4)	234(8)	31(3)	37(2)
C(18)	-2728(4)	-409(8)	-283(3)	44(2)
C(19)	-1681(5)	2909(8)	1812(4)	50(2)
C(20A)	-1830(12)	2150(20)	2342(9)	50(5)
C(20B)	-2105(11)	2850(20)	2221(9)	50(5)

Table S2, continued

C(21)	4017(6)	1239(11)	1299(6)	75(3)
C(22)	4139(6)	1894(11)	833(6)	80(4)
C(23A)	3033(12)	3720(30)	2780(9)	75(4)
C(24A)	3499(14)	4240(20)	3335(9)	75(4)
C(23B)	3201(15)	3510(20)	2924(10)	75(4)
C(24B)	2916(14)	4730(18)	2942(10)	75(4)
C(25)	968(4)	432(6)	2326(3)	24(2)
C(26)	1085(3)	-782(6)	2635(3)	21(1)
C(27)	501(4)	-1567(7)	2593(3)	31(2)
C(28)	603(5)	-2679(7)	2910(3)	38(1)
C(29)	1275(5)	-2950(7)	3240(3)	38(1)
C(30)	1858(5)	-2192(7)	3272(3)	38(1)
C(31)	1758(4)	-1105(7)	2982(3)	36(2)
C(32)	1042(4)	5611(7)	845(4)	40(2)
C(33)	1179(5)	6479(7)	1348(4)	52(2)
S(10)	4021(1)	45(2)	3513(1)	45(1)
O(10A)	4373(8)	-151(12)	3050(5)	57(2)
O(11A)	3612(8)	-914(11)	3666(6)	57(2)
O(12B)	3469(7)	994(10)	3534(5)	57(2)
O(10B)	4267(8)	214(13)	3028(6)	28(4)
O(11B)	3753(8)	-1173(11)	3638(7)	22(3)
O(12A)	3840(12)	1373(15)	3570(9)	76(6)
C(40)	4797(5)	254(8)	4131(4)	56(2)
F(1A)	5256(6)	-752(9)	4196(5)	56(2)
F(2A)	4502(7)	340(12)	4602(5)	56(2)
F(3A)	5313(6)	1121(10)	4143(4)	56(2)
F(1B)	5326(12)	-507(16)	4038(9)	143(10)
F(2B)	4694(7)	38(12)	4650(5)	63(4)
F(3B)	4966(7)	1465(10)	4081(6)	68(4)

Table S3. Bond lengths [Å]

Mo(1)-N(1)	1.721(6)
Mo(1)-O(1)	2.156(4)
Mo(1)-S(1)	2.4378(17)
Mo(1)-S(2)	2.4454(18)
Mo(1)-S(3)	2.4917(17)
Mo(1)-S(4)	2.5144(19)
Mo(1)-Mo(2)	2.8807(9)
Mo(2)-N(2)	1.718(6)
Mo(2)-O(2)	2.169(5)
Mo(2)-S(2)	2.4382(17)
Mo(2)-S(1)	2.4436(19)
Mo(2)-S(6)	2.495(2)
Mo(2)-S(5)	2.4969(19)
S(1)-O(7)	1.655(5)
S(2)-C(25)	1.853(7)
S(3)-P(1)	2.011(3)
S(4)-P(1)	1.998(2)
S(6)-P(2)	2.014(3)
S(5)-P(2)	1.998(3)
P(1)-O(4)	1.553(5)
P(1)-O(3)	1.579(5)
P(2)-O(6)	1.563(7)
P(2)-O(5)	1.567(7)
O(1)-C(15)	1.271(8)
O(2)-C(15)	1.260(9)
O(3)-C(17)	1.431(9)
O(4)-C(19)	1.485(10)
O(5)-C(21)	1.570(14)
O(6)-C(23B)	1.466(17)
O(6)-C(23A)	1.508(18)
O(7)-C(32)	1.466(8)
N(1)-C(1)	1.414(8)
N(2)-C(8)	1.424(11)
C(1)-C(2)	1.379(3)
C(1)-C(6)	1.379(3)
C(2)-C(3)	1.379(3)
C(2)-H(2)	0.95
C(3)-C(4)	1.379(3)
C(3)-H(3)	0.95
C(4)-C(5)	1.379(3)
C(4)-C(7)	1.522(9)
C(5)-C(6)	1.379(3)
C(5)-H(5)	0.95
C(6)-H(6)	0.95

Table S3, continued

C(7)-H(7A)	0.98
C(7)-H(7B)	0.98
C(7)-H(7C)	0.98
C(8)-C(9)	1.392(11)
C(8)-C(13)	1.402(12)
C(9)-C(10)	1.389(12)
C(9)-H(9)	0.95
C(10)-C(11)	1.374(13)
C(10)-H(10)	0.95
C(11)-C(12)	1.371(11)
C(11)-C(14)	1.520(12)
C(12)-C(13)	1.355(12)
C(12)-H(12)	0.95
C(13)-H(13)	0.95
C(14)-H(14A)	0.98
C(14)-H(14B)	0.98
C(14)-H(14C)	0.98
C(15)-C(16)	1.513(10)
C(16)-H(16A)	0.98
C(16)-H(16B)	0.98
C(16)-H(16C)	0.98
C(17)-C(18)	1.491(11)
C(17)-H(17A)	0.99
C(17)-H(17B)	0.99
C(18)-H(18A)	0.98
C(18)-H(18B)	0.98
C(18)-H(18C)	0.98
C(19)-C(20B)	1.43(2)
C(19)-C(20A)	1.61(2)
C(21)-C(22)	1.406(16)
C(21)-H(21A)	0.99
C(21)-H(21B)	0.99
C(22)-H(22A)	0.98
C(22)-H(22B)	0.98
C(22)-H(22C)	0.98
C(23A)-C(24A)	1.513(18)
C(25)-C(26)	1.509(9)
C(25)-H(25A)	0.99
C(25)-H(25B)	0.99
C(26)-C(31)	1.380(10)
C(26)-C(27)	1.381(10)
C(27)-C(28)	1.420(10)
C(27)-H(27)	0.95
C(28)-C(29)	1.350(11)

Table S3, continued

C(28)-H(28)	0.95
C(29)-C(30)	1.364(11)
C(29)-H(29)	0.95
C(30)-C(31)	1.366(10)
C(30)-H(30)	0.95
C(31)-H(31)	0.95
C(32)-C(33)	1.513(12)
C(32)-H(32A)	0.99
C(32)-H(32B)	0.99
C(33)-H(33A)	0.98
C(33)-H(33B)	0.98
C(33)-H(33C)	0.98
S(10)-O(10B)	1.382(12)
S(10)-O(11A)	1.407(11)
S(10)-O(10A)	1.461(11)
S(10)-O(11B)	1.480(12)
S(10)-O(12B)	1.482(9)
S(10)-O(12A)	1.503(15)
S(10)-C(40)	1.822(9)
O(12B)-O(12A)	0.80(2)
C(40)-F(2B)	1.340(12)
C(40)-F(3A)	1.354(11)

Table S4. Bond angles [°]

N(1)-Mo(1)-O(1)	175.1(2)
N(1)-Mo(1)-S(1)	90.04(19)
O(1)-Mo(1)-S(1)	85.10(12)
N(1)-Mo(1)-S(2)	93.59(19)
O(1)-Mo(1)-S(2)	88.02(13)
S(1)-Mo(1)-S(2)	107.60(6)
N(1)-Mo(1)-S(3)	99.70(19)
O(1)-Mo(1)-S(3)	85.03(12)
S(1)-Mo(1)-S(3)	164.71(6)
S(2)-Mo(1)-S(3)	83.69(6)
N(1)-Mo(1)-S(4)	95.51(19)
O(1)-Mo(1)-S(4)	84.20(14)
S(1)-Mo(1)-S(4)	87.90(6)
S(2)-Mo(1)-S(4)	162.01(6)
S(3)-Mo(1)-S(4)	79.50(6)
N(1)-Mo(1)-Mo(2)	95.23(19)
O(1)-Mo(1)-Mo(2)	82.02(12)
S(1)-Mo(1)-Mo(2)	53.93(5)
S(2)-Mo(1)-Mo(2)	53.74(4)
S(3)-Mo(1)-Mo(2)	135.66(5)
S(4)-Mo(1)-Mo(2)	140.23(5)
N(2)-Mo(2)-O(2)	177.5(2)
N(2)-Mo(2)-S(2)	91.8(2)
O(2)-Mo(2)-S(2)	86.95(13)
N(2)-Mo(2)-S(1)	93.3(2)
O(2)-Mo(2)-S(1)	84.97(14)
S(2)-Mo(2)-S(1)	107.65(6)
N(2)-Mo(2)-S(6)	98.1(2)
O(2)-Mo(2)-S(6)	83.64(13)
S(2)-Mo(2)-S(6)	161.52(6)
S(1)-Mo(2)-S(6)	87.36(7)
N(2)-Mo(2)-S(5)	98.1(2)
O(2)-Mo(2)-S(5)	83.97(14)
S(2)-Mo(2)-S(5)	83.76(6)
S(1)-Mo(2)-S(5)	163.64(7)
S(6)-Mo(2)-S(5)	79.47(7)
N(2)-Mo(2)-Mo(1)	96.5(2)
O(2)-Mo(2)-Mo(1)	80.99(13)
S(2)-Mo(2)-Mo(1)	53.97(4)
S(1)-Mo(2)-Mo(1)	53.74(4)
S(6)-Mo(2)-Mo(1)	139.07(6)
S(5)-Mo(2)-Mo(1)	135.54(5)
O(7)-S(1)-Mo(1)	106.87(18)
O(7)-S(1)-Mo(2)	108.18(19)

Table S4, continued

Mo(1)-S(1)-Mo(2)	72.33(5)
C(25)-S(2)-Mo(2)	109.3(2)
C(25)-S(2)-Mo(1)	110.1(2)
Mo(2)-S(2)-Mo(1)	72.30(5)
P(1)-S(3)-Mo(1)	87.35(8)
P(1)-S(4)-Mo(1)	87.01(8)
P(2)-S(6)-Mo(2)	87.39(9)
P(2)-S(5)-Mo(2)	87.71(9)
O(4)-P(1)-O(3)	98.0(3)
O(4)-P(1)-S(4)	114.0(2)
O(3)-P(1)-S(4)	113.9(2)
O(4)-P(1)-S(3)	113.1(2)
O(3)-P(1)-S(3)	112.0(2)
S(4)-P(1)-S(3)	105.99(11)
O(6)-P(2)-O(5)	98.2(4)
O(6)-P(2)-S(5)	113.8(3)
O(5)-P(2)-S(5)	112.6(3)
O(6)-P(2)-S(6)	113.2(3)
O(5)-P(2)-S(6)	113.9(3)
S(5)-P(2)-S(6)	105.40(12)
C(15)-O(1)-Mo(1)	125.4(4)
C(15)-O(2)-Mo(2)	126.2(4)
C(17)-O(3)-P(1)	120.2(4)
C(19)-O(4)-P(1)	118.7(5)
P(2)-O(5)-C(21)	121.3(5)
C(23B)-O(6)-P(2)	122.2(12)
C(23A)-O(6)-P(2)	112.8(10)
C(32)-O(7)-S(1)	113.7(5)
C(1)-N(1)-Mo(1)	176.7(5)
C(8)-N(2)-Mo(2)	174.6(6)
C(2)-C(1)-C(6)	120.0
C(2)-C(1)-N(1)	121.7(4)
C(6)-C(1)-N(1)	118.3(4)
C(1)-C(2)-C(3)	120.0
C(1)-C(2)-H(2)	120.0
C(3)-C(2)-H(2)	120.0
C(2)-C(3)-C(4)	120.0
C(2)-C(3)-H(3)	120.0
C(4)-C(3)-H(3)	120.0
C(5)-C(4)-C(3)	120.0
C(5)-C(4)-C(7)	120.0(5)
C(3)-C(4)-C(7)	119.9(5)
C(4)-C(5)-C(6)	120.0
C(4)-C(5)-H(5)	120.0

Table S4, continued

C(6)-C(5)-H(5)	120.0
C(5)-C(6)-C(1)	120.0
C(5)-C(6)-H(6)	120.0
C(1)-C(6)-H(6)	120.0
C(4)-C(7)-H(7A)	109.5
C(4)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(4)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(9)-C(8)-C(13)	119.5(8)
C(9)-C(8)-N(2)	120.5(8)
C(13)-C(8)-N(2)	120.0(7)
C(10)-C(9)-C(8)	119.6(9)
C(10)-C(9)-H(9)	120.2
C(8)-C(9)-H(9)	120.2
C(11)-C(10)-C(9)	120.7(8)
C(11)-C(10)-H(10)	119.7
C(9)-C(10)-H(10)	119.7
C(12)-C(11)-C(10)	118.3(8)
C(12)-C(11)-C(14)	120.9(9)
C(10)-C(11)-C(14)	120.8(8)
C(13)-C(12)-C(11)	123.2(9)
C(13)-C(12)-H(12)	118.4
C(11)-C(12)-H(12)	118.4
C(12)-C(13)-C(8)	118.5(8)
C(12)-C(13)-H(13)	120.7
C(8)-C(13)-H(13)	120.7
C(11)-C(14)-H(14A)	109.5
C(11)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(11)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
O(2)-C(15)-O(1)	124.6(7)
O(2)-C(15)-C(16)	117.3(6)
O(1)-C(15)-C(16)	118.0(7)
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
O(3)-C(17)-C(18)	108.7(6)

Table S4, continued

O(3)-C(17)-H(17A)	109.9
C(18)-C(17)-H(17A)	109.9
O(3)-C(17)-H(17B)	109.9
C(18)-C(17)-H(17B)	109.9
H(17A)-C(17)-H(17B)	108.3
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(20B)-C(19)-O(4)	110.1(10)
O(4)-C(19)-C(20A)	106.2(9)
C(22)-C(21)-O(5)	109.0(10)
C(22)-C(21)-H(21A)	109.9
O(5)-C(21)-H(21A)	109.9
C(22)-C(21)-H(21B)	109.9
O(5)-C(21)-H(21B)	109.9
H(21A)-C(21)-H(21B)	108.3
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
O(6)-C(23A)-C(24A)	101.9(17)
C(24B)-C(23B)-O(6)	116.2(19)
C(26)-C(25)-S(2)	111.0(5)
C(26)-C(25)-H(25A)	109.4
S(2)-C(25)-H(25A)	109.4
C(26)-C(25)-H(25B)	109.4
S(2)-C(25)-H(25B)	109.4
H(25A)-C(25)-H(25B)	108.0
C(31)-C(26)-C(27)	118.9(7)
C(31)-C(26)-C(25)	121.4(6)
C(27)-C(26)-C(25)	119.7(6)
C(26)-C(27)-C(28)	119.6(7)
C(26)-C(27)-H(27)	120.2
C(28)-C(27)-H(27)	120.2
C(29)-C(28)-C(27)	119.0(8)
C(29)-C(28)-H(28)	120.5
C(27)-C(28)-H(28)	120.5
C(28)-C(29)-C(30)	121.7(7)
C(28)-C(29)-H(29)	119.1

Table S4, continued

C(30)-C(29)-H(29)	119.1
C(29)-C(30)-C(31)	119.6(8)
C(29)-C(30)-H(30)	120.2
C(31)-C(30)-H(30)	120.2
C(30)-C(31)-C(26)	121.2(7)
C(30)-C(31)-H(31)	119.4
C(26)-C(31)-H(31)	119.4
O(7)-C(32)-C(33)	106.0(6)
O(7)-C(32)-H(32A)	110.5
C(33)-C(32)-H(32A)	110.5
O(7)-C(32)-H(32B)	110.5
C(33)-C(32)-H(32B)	110.5
H(32A)-C(32)-H(32B)	108.7
C(32)-C(33)-H(33A)	109.5
C(32)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(32)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
O(10A)-S(10)-O(11A)	119.0(8)
O(10A)-S(10)-O(12A)	111.8(10)
O(11A)-S(10)-O(12A)	122.6(10)
O(10B)-S(10)-O(11B)	120.1(8)
O(10B)-S(10)-O(12B)	109.3(7)
O(11B)-S(10)-O(12B)	109.7(7)
O(10A)-S(10)-C(40)	102.7(7)
O(11A)-S(10)-C(40)	105.0(7)
O(12A)-S(10)-C(40)	87.6(9)
O(10B)-S(10)-C(40)	107.8(7)
O(11B)-S(10)-C(40)	101.0(7)
O(12B)-S(10)-C(40)	108.1(6)
F(1B)-C(40)-F(2B)	109.7(11)
F(1B)-C(40)-F(3B)	111.9(11)
F(2B)-C(40)-F(3B)	110.2(9)
F(1A)-C(40)-F(2A)	109.4(9)
F(1A)-C(40)-F(3A)	97.1(9)
F(2A)-C(40)-F(3A)	111.9(9)
F(1A)-C(40)-S(10)	110.1(7)
F(2A)-C(40)-S(10)	105.9(7)
F(3A)-C(40)-S(10)	121.9(7)
F(1B)-C(40)-S(10)	105.0(12)
F(2B)-C(40)-S(10)	118.0(8)
F(3B)-C(40)-S(10)	101.8(7)

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	20(1)	20(1)	18(1)	3(1)	5(1)	-5(1)
Mo(2)	20(1)	28(1)	21(1)	7(1)	6(1)	-5(1)
S(1)	26(1)	28(1)	25(1)	8(1)	6(1)	-7(1)
S(2)	23(1)	21(1)	16(1)	2(1)	6(1)	-4(1)
S(3)	19(1)	25(1)	26(1)	6(1)	5(1)	-4(1)
S(4)	26(1)	26(1)	36(1)	11(1)	5(1)	-2(1)
S(6)	26(1)	30(1)	31(1)	11(1)	3(1)	-2(1)
S(5)	23(1)	32(1)	32(1)	12(1)	5(1)	-1(1)
P(1)	22(1)	22(1)	28(1)	3(1)	6(1)	-3(1)
P(2)	24(1)	38(1)	32(1)	20(1)	4(1)	-5(1)
O(1)	27(3)	17(2)	25(3)	-1(2)	11(2)	-5(2)
O(2)	31(3)	26(3)	25(3)	0(2)	5(2)	-6(2)
O(3)	22(3)	33(3)	34(3)	-6(2)	6(2)	-10(2)
O(4)	30(3)	34(3)	41(3)	-3(2)	14(2)	-6(2)
O(5)	30(3)	80(5)	61(4)	24(4)	8(3)	-18(3)
O(6)	51(4)	74(5)	38(4)	14(3)	-6(3)	-26(3)
O(7)	38(3)	19(2)	40(3)	4(2)	12(2)	-10(2)
N(1)	22(3)	26(3)	23(3)	6(2)	3(2)	-1(2)
N(2)	22(3)	51(4)	25(3)	8(3)	12(3)	0(3)
C(1)	96(3)	40(2)	46(2)	-8(2)	42(2)	-19(2)
C(2)	96(3)	40(2)	46(2)	-8(2)	42(2)	-19(2)
C(3)	96(3)	40(2)	46(2)	-8(2)	42(2)	-19(2)
C(4)	96(3)	40(2)	46(2)	-8(2)	42(2)	-19(2)
C(5)	96(3)	40(2)	46(2)	-8(2)	42(2)	-19(2)
C(6)	96(3)	40(2)	46(2)	-8(2)	42(2)	-19(2)
C(7)	96(3)	40(2)	46(2)	-8(2)	42(2)	-19(2)
C(8)	58(2)	49(2)	45(2)	12(2)	28(2)	13(2)
C(9)	58(2)	49(2)	45(2)	12(2)	28(2)	13(2)
C(10)	58(2)	49(2)	45(2)	12(2)	28(2)	13(2)
C(11)	58(2)	49(2)	45(2)	12(2)	28(2)	13(2)
C(12)	58(2)	49(2)	45(2)	12(2)	28(2)	13(2)
C(13)	58(2)	49(2)	45(2)	12(2)	28(2)	13(2)
C(14)	58(1)	49(1)	45(1)	12(1)	28(1)	13(1)
C(15)	31(4)	18(3)	27(4)	7(3)	4(3)	-11(3)
C(16)	63(5)	21(4)	28(4)	-6(3)	13(4)	-9(4)
C(17)	37(4)	48(5)	28(4)	-2(4)	12(3)	-10(4)
C(18)	41(5)	52(5)	33(5)	-5(4)	-2(4)	0(4)
C(19)	56(6)	46(5)	47(6)	-20(4)	15(5)	-14(4)
C(20A)	48(13)	56(13)	42(12)	-16(10)	5(9)	-17(10)
C(20B)	42(12)	62(14)	41(12)	-18(11)	4(9)	-14(10)

Table S5, continued

C(21)	48(6)	61(7)	129(11)	17(7)	46(7)	11(5)
C(22)	48(7)	82(8)	105(10)	14(7)	12(7)	-4(6)
C(23A)	100(10)	56(7)	60(8)	-9(6)	2(7)	-28(6)
C(24A)	100(10)	56(7)	60(8)	-9(6)	2(7)	-28(6)
C(23B)	100(10)	56(7)	60(8)	-9(6)	2(7)	-28(6)
C(24B)	100(10)	56(7)	60(8)	-9(6)	2(7)	-28(6)
C(25)	29(4)	23(3)	24(4)	3(3)	15(3)	-6(3)
C(26)	21(3)	28(4)	15(3)	-6(3)	6(3)	-4(3)
C(27)	36(4)	30(4)	27(4)	2(3)	11(3)	-1(3)
C(28)	56(3)	23(2)	30(3)	7(2)	6(2)	-1(2)
C(29)	56(3)	23(2)	30(3)	7(2)	6(2)	-1(2)
C(30)	56(3)	23(2)	30(3)	7(2)	6(2)	-1(2)
C(31)	36(4)	31(4)	33(4)	4(3)	-2(3)	-9(3)
C(32)	34(4)	36(5)	47(5)	11(4)	7(4)	-16(4)
C(33)	55(6)	33(5)	76(7)	-7(4)	30(5)	-21(4)
S(10)	60(1)	44(1)	28(1)	-2(1)	6(1)	4(1)
O(10A)	67(5)	42(4)	64(4)	-5(3)	23(4)	14(4)
O(11A)	67(5)	42(4)	64(4)	-5(3)	23(4)	14(4)
O(12B)	67(5)	42(4)	64(4)	-5(3)	23(4)	14(4)
C(40)	52(4)	59(4)	45(3)	6(3)	-5(3)	-24(3)
F(1A)	52(4)	59(4)	45(3)	6(3)	-5(3)	-24(3)
F(2A)	52(4)	59(4)	45(3)	6(3)	-5(3)	-24(3)
F(3A)	52(4)	59(4)	45(3)	6(3)	-5(3)	-24(3)

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

	x	y	z	U(eq)
H(2)	557	1556	-507	67
H(3)	523	506	-1351	67
H(5)	-530	-2301	-824	67
H(6)	-496	-1252	19	67
H(7A)	429	-1996	-1723	84
H(7B)	-206	-1081	-2044	84
H(7C)	-409	-2327	-1771	84
H(9)	2527	1482	-51	57
H(10)	2682	179	-776	57
H(12)	1609	-2477	-193	57
H(13)	1434	-1244	527	57
H(14A)	2323	-2929	-902	72
H(14B)	2605	-1795	-1207	72
H(14C)	1750	-2110	-1353	72
H(16A)	1064	3887	2844	56
H(16B)	233	4180	2518	56
H(16C)	883	4963	2381	56
H(17A)	-1669	-373	208	44
H(17B)	-1858	745	-237	44
H(18A)	-2918	-901	-14	67
H(18B)	-2617	-946	-574	67
H(18C)	-3096	197	-467	67
H(21A)	4410	626	1432	90
H(21B)	3544	800	1183	90
H(22A)	3737	2472	692	120
H(22B)	4166	1321	527	120
H(22C)	4601	2347	954	120
H(25A)	1361	1008	2512	29
H(25B)	495	787	2351	29
H(27)	33	-1366	2354	37
H(28)	205	-3223	2889	45
H(29)	1344	-3687	3455	45
H(30)	2330	-2418	3494	45
H(31)	2160	-561	3019	43
H(32A)	715	5994	503	48
H(32B)	1508	5389	755	48
H(33A)	711	6790	1393	78
H(33B)	1480	7167	1281	78
H(33C)	1435	6043	1695	78

Table S7. Torsion angles [°]

N(1)-Mo(1)-Mo(2)-N(2)	-3.1(3)
O(1)-Mo(1)-Mo(2)-N(2)	-179.1(2)
S(1)-Mo(1)-Mo(2)-N(2)	-89.3(2)
S(2)-Mo(1)-Mo(2)-N(2)	87.5(2)
S(3)-Mo(1)-Mo(2)-N(2)	106.5(2)
S(4)-Mo(1)-Mo(2)-N(2)	-108.2(2)
N(1)-Mo(1)-Mo(2)-O(2)	176.6(2)
O(1)-Mo(1)-Mo(2)-O(2)	0.62(17)
S(1)-Mo(1)-Mo(2)-O(2)	90.36(14)
S(2)-Mo(1)-Mo(2)-O(2)	-92.79(13)
S(3)-Mo(1)-Mo(2)-O(2)	-73.80(14)
S(4)-Mo(1)-Mo(2)-O(2)	71.48(15)
N(1)-Mo(1)-Mo(2)-S(2)	-90.63(19)
O(1)-Mo(1)-Mo(2)-S(2)	93.41(13)
S(1)-Mo(1)-Mo(2)-S(2)	-176.85(8)
S(3)-Mo(1)-Mo(2)-S(2)	18.99(8)
S(4)-Mo(1)-Mo(2)-S(2)	164.27(9)
N(1)-Mo(1)-Mo(2)-S(1)	86.23(19)
O(1)-Mo(1)-Mo(2)-S(1)	-89.74(13)
S(2)-Mo(1)-Mo(2)-S(1)	176.85(8)
S(3)-Mo(1)-Mo(2)-S(1)	-164.16(9)
S(4)-Mo(1)-Mo(2)-S(1)	-18.88(10)
N(1)-Mo(1)-Mo(2)-S(6)	107.3(2)
O(1)-Mo(1)-Mo(2)-S(6)	-68.64(15)
S(1)-Mo(1)-Mo(2)-S(6)	21.10(10)
S(2)-Mo(1)-Mo(2)-S(6)	-162.05(10)
S(3)-Mo(1)-Mo(2)-S(6)	-143.06(10)
S(4)-Mo(1)-Mo(2)-S(6)	2.22(13)
N(1)-Mo(1)-Mo(2)-S(5)	-111.7(2)
O(1)-Mo(1)-Mo(2)-S(5)	72.34(14)
S(1)-Mo(1)-Mo(2)-S(5)	162.08(10)
S(2)-Mo(1)-Mo(2)-S(5)	-21.07(9)
S(3)-Mo(1)-Mo(2)-S(5)	-2.08(11)
S(4)-Mo(1)-Mo(2)-S(5)	143.20(10)
N(1)-Mo(1)-S(1)-O(7)	159.3(3)
O(1)-Mo(1)-S(1)-O(7)	-20.5(2)
S(2)-Mo(1)-S(1)-O(7)	-106.88(19)
S(3)-Mo(1)-S(1)-O(7)	29.5(3)
S(4)-Mo(1)-S(1)-O(7)	63.8(2)
Mo(2)-Mo(1)-S(1)-O(7)	-104.2(2)
N(1)-Mo(1)-S(1)-Mo(2)	-96.44(19)
O(1)-Mo(1)-S(1)-Mo(2)	83.69(13)
S(2)-Mo(1)-S(1)-Mo(2)	-2.66(7)
S(3)-Mo(1)-S(1)-Mo(2)	133.7(2)

Table S7, continued

S(4)-Mo(1)-S(1)-Mo(2)	168.05(6)
N(2)-Mo(2)-S(1)-O(7)	-161.9(3)
O(2)-Mo(2)-S(1)-O(7)	20.0(2)
S(2)-Mo(2)-S(1)-O(7)	105.14(19)
S(6)-Mo(2)-S(1)-O(7)	-63.87(19)
S(5)-Mo(2)-S(1)-O(7)	-27.6(3)
Mo(1)-Mo(2)-S(1)-O(7)	102.47(19)
N(2)-Mo(2)-S(1)-Mo(1)	95.7(2)
O(2)-Mo(2)-S(1)-Mo(1)	-82.50(13)
S(2)-Mo(2)-S(1)-Mo(1)	2.67(7)
S(6)-Mo(2)-S(1)-Mo(1)	-166.34(7)
S(5)-Mo(2)-S(1)-Mo(1)	-130.1(2)
N(2)-Mo(2)-S(2)-C(25)	157.6(3)
O(2)-Mo(2)-S(2)-C(25)	-24.6(3)
S(1)-Mo(2)-S(2)-C(25)	-108.3(2)
S(6)-Mo(2)-S(2)-C(25)	34.8(3)
S(5)-Mo(2)-S(2)-C(25)	59.7(2)
Mo(1)-Mo(2)-S(2)-C(25)	-105.6(2)
N(2)-Mo(2)-S(2)-Mo(1)	-96.7(2)
O(2)-Mo(2)-S(2)-Mo(1)	81.07(13)
S(1)-Mo(2)-S(2)-Mo(1)	-2.66(7)
S(6)-Mo(2)-S(2)-Mo(1)	140.4(2)
S(5)-Mo(2)-S(2)-Mo(1)	165.33(6)
N(1)-Mo(1)-S(2)-C(25)	-161.5(3)
O(1)-Mo(1)-S(2)-C(25)	23.1(3)
S(1)-Mo(1)-S(2)-C(25)	107.3(2)
S(3)-Mo(1)-S(2)-C(25)	-62.1(2)
S(4)-Mo(1)-S(2)-C(25)	-41.2(3)
Mo(2)-Mo(1)-S(2)-C(25)	104.7(2)
N(1)-Mo(1)-S(2)-Mo(2)	93.85(19)
O(1)-Mo(1)-S(2)-Mo(2)	-81.56(12)
S(1)-Mo(1)-S(2)-Mo(2)	2.67(7)
S(3)-Mo(1)-S(2)-Mo(2)	-166.77(6)
S(4)-Mo(1)-S(2)-Mo(2)	-145.84(19)
N(1)-Mo(1)-S(3)-P(1)	-91.2(2)
O(1)-Mo(1)-S(3)-P(1)	87.69(15)
S(1)-Mo(1)-S(3)-P(1)	37.7(3)
S(2)-Mo(1)-S(3)-P(1)	176.24(9)
S(4)-Mo(1)-S(3)-P(1)	2.68(8)
Mo(2)-Mo(1)-S(3)-P(1)	160.93(6)
N(1)-Mo(1)-S(4)-P(1)	96.2(2)
O(1)-Mo(1)-S(4)-P(1)	-88.70(14)
S(1)-Mo(1)-S(4)-P(1)	-173.99(9)
S(2)-Mo(1)-S(4)-P(1)	-23.9(2)

Table S7, continued

S(3)-Mo(1)-S(4)-P(1)	-2.70(8)
Mo(2)-Mo(1)-S(4)-P(1)	-158.82(7)
N(2)-Mo(2)-S(6)-P(2)	-95.7(2)
O(2)-Mo(2)-S(6)-P(2)	86.08(16)
S(2)-Mo(2)-S(6)-P(2)	26.3(3)
S(1)-Mo(2)-S(6)-P(2)	171.31(11)
S(5)-Mo(2)-S(6)-P(2)	1.06(10)
Mo(1)-Mo(2)-S(6)-P(2)	154.42(9)
N(2)-Mo(2)-S(5)-P(2)	95.8(2)
O(2)-Mo(2)-S(5)-P(2)	-85.70(16)
S(2)-Mo(2)-S(5)-P(2)	-173.27(11)
S(1)-Mo(2)-S(5)-P(2)	-38.0(3)
S(6)-Mo(2)-S(5)-P(2)	-1.07(11)
Mo(1)-Mo(2)-S(5)-P(2)	-156.27(9)
Mo(1)-S(4)-P(1)-O(4)	128.5(2)
Mo(1)-S(4)-P(1)-O(3)	-120.1(2)
Mo(1)-S(4)-P(1)-S(3)	3.42(11)
Mo(1)-S(3)-P(1)-O(4)	-129.1(2)
Mo(1)-S(3)-P(1)-O(3)	121.3(2)
Mo(1)-S(3)-P(1)-S(4)	-3.45(11)
Mo(2)-S(5)-P(2)-O(6)	126.0(3)
Mo(2)-S(5)-P(2)-O(5)	-123.4(3)
Mo(2)-S(5)-P(2)-S(6)	1.36(13)
Mo(2)-S(6)-P(2)-O(6)	-126.4(3)
Mo(2)-S(6)-P(2)-O(5)	122.6(3)
Mo(2)-S(6)-P(2)-S(5)	-1.36(13)
S(1)-Mo(1)-O(1)-C(15)	-50.0(5)
S(2)-Mo(1)-O(1)-C(15)	57.8(5)
S(3)-Mo(1)-O(1)-C(15)	141.7(5)
S(4)-Mo(1)-O(1)-C(15)	-138.4(5)
Mo(2)-Mo(1)-O(1)-C(15)	4.2(5)
S(2)-Mo(2)-O(2)-C(15)	-59.9(5)
S(1)-Mo(2)-O(2)-C(15)	48.1(5)
S(6)-Mo(2)-O(2)-C(15)	136.0(5)
S(5)-Mo(2)-O(2)-C(15)	-144.0(5)
Mo(1)-Mo(2)-O(2)-C(15)	-5.9(5)
O(4)-P(1)-O(3)-C(17)	-175.4(5)
S(4)-P(1)-O(3)-C(17)	63.8(6)
S(3)-P(1)-O(3)-C(17)	-56.4(6)
O(3)-P(1)-O(4)-C(19)	176.2(6)
S(4)-P(1)-O(4)-C(19)	-63.1(6)
S(3)-P(1)-O(4)-C(19)	58.2(6)
O(6)-P(2)-O(5)-C(21)	172.9(7)
S(5)-P(2)-O(5)-C(21)	52.8(7)

Table S7, continued

S(6)-P(2)-O(5)-C(21)	-67.1(7)
O(5)-P(2)-O(6)-C(23B)	-158.0(12)
S(5)-P(2)-O(6)-C(23B)	-38.8(12)
S(6)-P(2)-O(6)-C(23B)	81.5(12)
O(5)-P(2)-O(6)-C(23A)	-175.5(13)
S(5)-P(2)-O(6)-C(23A)	-56.3(13)
S(6)-P(2)-O(6)-C(23A)	64.1(13)
Mo(1)-S(1)-O(7)-C(32)	-175.8(4)
Mo(2)-S(1)-O(7)-C(32)	107.8(4)
C(6)-C(1)-C(2)-C(3)	0.0
N(1)-C(1)-C(2)-C(3)	179.5(7)
C(1)-C(2)-C(3)-C(4)	0.0
C(2)-C(3)-C(4)-C(5)	0.0
C(2)-C(3)-C(4)-C(7)	177.8(8)
C(3)-C(4)-C(5)-C(6)	0.0
C(7)-C(4)-C(5)-C(6)	-177.8(8)
C(4)-C(5)-C(6)-C(1)	0.0
C(2)-C(1)-C(6)-C(5)	0.0
N(1)-C(1)-C(6)-C(5)	-179.5(7)
C(13)-C(8)-C(9)-C(10)	2.8(14)
N(2)-C(8)-C(9)-C(10)	-176.7(8)
C(8)-C(9)-C(10)-C(11)	0.6(14)
C(9)-C(10)-C(11)-C(12)	-4.1(14)
C(9)-C(10)-C(11)-C(14)	178.9(8)
C(10)-C(11)-C(12)-C(13)	4.3(15)
C(14)-C(11)-C(12)-C(13)	-178.7(9)
C(11)-C(12)-C(13)-C(8)	-0.9(14)
C(9)-C(8)-C(13)-C(12)	-2.7(14)
N(2)-C(8)-C(13)-C(12)	176.9(8)
Mo(2)-O(2)-C(15)-O(1)	11.4(9)
Mo(2)-O(2)-C(15)-C(16)	-171.0(4)
Mo(1)-O(1)-C(15)-O(2)	-10.3(9)
Mo(1)-O(1)-C(15)-C(16)	172.1(4)
P(1)-O(3)-C(17)-C(18)	172.7(5)
P(1)-O(4)-C(19)-C(20B)	-153.0(12)
P(1)-O(4)-C(19)-C(20A)	-116.3(10)
P(2)-O(5)-C(21)-C(22)	105.2(8)
C(23B)-O(6)-C(23A)-C(24A)	47(5)
P(2)-O(6)-C(23A)-C(24A)	171.9(13)
C(23A)-O(6)-C(23B)-C(24B)	-43(5)
P(2)-O(6)-C(23B)-C(24B)	-106(2)
Mo(2)-S(2)-C(25)-C(26)	-137.9(4)
Mo(1)-S(2)-C(25)-C(26)	144.5(4)
S(2)-C(25)-C(26)-C(31)	101.2(7)

Table S7, continued

S(2)-C(25)-C(26)-C(27)	-81.7(7)
C(31)-C(26)-C(27)-C(28)	0.6(10)
C(25)-C(26)-C(27)-C(28)	-176.5(6)
C(26)-C(27)-C(28)-C(29)	-0.9(11)
C(27)-C(28)-C(29)-C(30)	-0.8(13)
C(28)-C(29)-C(30)-C(31)	2.7(13)
C(29)-C(30)-C(31)-C(26)	-3.0(12)
C(27)-C(26)-C(31)-C(30)	1.3(11)
C(25)-C(26)-C(31)-C(30)	178.4(7)
S(1)-O(7)-C(32)-C(33)	-157.7(6)
O(10B)-S(10)-O(12B)-O(12A)	-66(2)
O(11A)-S(10)-O(12B)-O(12A)	158(2)
O(10A)-S(10)-O(12B)-O(12A)	-71(2)
O(11B)-S(10)-O(12B)-O(12A)	161(2)
C(40)-S(10)-O(12B)-O(12A)	51(2)
O(10B)-S(10)-O(12A)-O(12B)	120(2)
O(11A)-S(10)-O(12A)-O(12B)	-26(2)
O(10A)-S(10)-O(12A)-O(12B)	125.2(19)
O(11B)-S(10)-O(12A)-O(12B)	-28(3)
C(40)-S(10)-O(12A)-O(12B)	-132.1(19)
O(10B)-S(10)-C(40)-F(2B)	-175.0(10)
O(11A)-S(10)-C(40)-F(2B)	-32.4(10)
O(10A)-S(10)-C(40)-F(2B)	-157.5(10)
O(11B)-S(10)-C(40)-F(2B)	-48.2(10)
O(12B)-S(10)-C(40)-F(2B)	67.0(10)
O(12A)-S(10)-C(40)-F(2B)	90.8(12)
O(10B)-S(10)-C(40)-F(3A)	38.2(11)
O(11A)-S(10)-C(40)-F(3A)	-179.2(10)
O(10A)-S(10)-C(40)-F(3A)	55.7(10)
O(11B)-S(10)-C(40)-F(3A)	165.0(10)
O(12B)-S(10)-C(40)-F(3A)	-79.9(10)
O(12A)-S(10)-C(40)-F(3A)	-56.1(12)
O(10B)-S(10)-C(40)-F(1B)	-52.5(12)
O(11A)-S(10)-C(40)-F(1B)	90.2(11)
O(10A)-S(10)-C(40)-F(1B)	-35.0(11)
O(11B)-S(10)-C(40)-F(1B)	74.3(11)
O(12B)-S(10)-C(40)-F(1B)	-170.5(11)
O(12A)-S(10)-C(40)-F(1B)	-146.7(13)
O(10B)-S(10)-C(40)-F(3B)	64.3(9)
O(11A)-S(10)-C(40)-F(3B)	-153.0(8)
O(10A)-S(10)-C(40)-F(3B)	81.8(9)
O(11B)-S(10)-C(40)-F(3B)	-168.9(8)
O(12B)-S(10)-C(40)-F(3B)	-53.7(9)
O(12A)-S(10)-C(40)-F(3B)	-29.9(11)

Table S7, continued

O(10B)-S(10)-C(40)-F(1A)	-74.4(10)
O(11A)-S(10)-C(40)-F(1A)	68.3(9)
O(10A)-S(10)-C(40)-F(1A)	-56.8(9)
O(11B)-S(10)-C(40)-F(1A)	52.4(9)
O(12B)-S(10)-C(40)-F(1A)	167.6(9)
O(12A)-S(10)-C(40)-F(1A)	-168.6(11)
O(10B)-S(10)-C(40)-F(2A)	167.5(9)
O(11A)-S(10)-C(40)-F(2A)	-49.8(9)
O(10A)-S(10)-C(40)-F(2A)	-174.9(9)
O(11B)-S(10)-C(40)-F(2A)	-65.7(9)
O(12B)-S(10)-C(40)-F(2A)	49.5(9)
O(12A)-S(10)-C(40)-F(2A)	73.3(11)

Crystallographic Studies for Distal S{Mo_2}SOEt, 5

A red-orange needle (0.30 x 0.10 x 0.05 mm^3) crystal was mounted on a CryoLoop with Paratone oil for collection of x-ray data on a Bruker SMART APEX CCD diffractometer. The SMART[1] software package (v 5.632) was used to acquire a total of 1,868 eighty-second frame ω-scan exposures of data at 298K to a 2θ max = 50.30° using monochromated Mo Kα radiation (0.71073 Å) from a sealed tube and a monocapillary. Frame data were processed using SAINT[2] (v 6.45a) to determine final unit cell parameters a = 17.668(4) Å, b = 9.900(2) Å, c = 23.167(5) Å, β= 90.073(4)°, V = 4052.1(14) $Å^3$, Z = 4 and ρ_{calcd} = 1.542 Mgm^{-3} to produce raw hkl data that were then corrected for absorption (transmission min./max. = 0.672/0.927; μ = 1.047 mm^{-1}) using SADABS[3] (v 2.10). The structure was solved by Patterson methods in the space group $P2_1/c$ using SHELXS-90[4] and refined by least squares methods on F^2 using SHELXL-99[5] incorporated into the SHELXTL[6] (v 6.14) suite of programs. The disordered OEt group was modeled using two sets of 50% occupancy carbon atoms (C21a – C22a and C21b –C22b). All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed in their geometrically generated positions and refined as a riding model as described above for compound $\mathbf{4}^+$. For all 7235 unique reflections (R(int) = 0.047) the final anisotropic full matrix least-squares refinement on F^2 for 455 variables converged at R1 = 0.0455and wR2 = 0.0857 with a GOF of 1.03.

References

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Table S8. Crystal data and structure refinement

Empirical formula	C26 H42 Mo2 N2 O7 P2 S6	
Formula weight	940.80	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 17.668(4) Å	α = 90°.
	b = 9.900(2) Å	β = 90.073(4)°
	c = 23.167(5) Å	γ = 90°.
Volume	4052.1(14) $Å^3$	
Z	4	
Density (calculated)	1.542 Mg/m^3	
Absorption coefficient	1.047 mm^{-1}	
F(000)	1912	
Crystal color, habit	red-orange needle	
Crystal size	0.30 x 0.10 x 0.05 mm^3	
Theta range for data collection	2.10 to 25.15°	
Index ranges	-21<=h<=21, -11<=k<=11, -27<=l<=27	
Reflections collected	28618	
Independent reflections	7235 [R(int) = 0.0467]	
Completeness to theta = 25.15°	99.9 %	
Absorption correction	SADABS	
Max. and min. transmission	0.941 and 0.673	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7235 / 0 / 399	
Goodness-of-fit on F^2	1.028	
Final R indices [I>2sigma(I)]	R1 = 0.0455, wR2 = 0.0857	
R indices (all data)	R1 = 0.1029, wR2 = 0.0981	
Largest diff. peak and hole	0.425 and -0.427 $e.Å^{-3}$	

Table S9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	2314(1)	10332(1)	437(1)	40(1)
Mo(2)	3447(1)	9261(1)	1186(1)	42(1)
S(1)	2276(1)	8110(1)	892(1)	45(1)
S(2)	3426(1)	11398(1)	752(1)	48(1)
S(3)	2268(1)	12311(1)	-244(1)	51(1)
S(4)	1300(1)	9580(1)	-291(1)	56(1)
S(5)	4792(1)	9933(2)	1402(1)	68(1)
S(6)	4023(1)	7059(2)	1580(1)	67(1)
P(1)	1479(1)	11323(1)	-697(1)	48(1)
P(2)	5004(1)	8033(2)	1638(1)	66(1)
O(1)	3003(2)	9322(3)	-205(1)	46(1)
O(2)	3853(2)	8394(3)	385(2)	52(1)
O(3)	736(2)	12177(3)	-787(1)	55(1)
O(4)	1690(2)	11168(4)	-1350(1)	58(1)
O(5)	5391(2)	7905(5)	2249(2)	92(1)
O(6)	5669(2)	7384(4)	1282(2)	84(1)
O(7)	2404(2)	6956(3)	385(1)	56(1)
N(1)	1683(2)	10841(4)	965(2)	41(1)
N(2)	3024(2)	9551(4)	1852(2)	44(1)
C(1)	1183(3)	11015(5)	1421(2)	42(1)
C(2)	490(3)	10380(6)	1433(2)	68(2)
C(3)	29(3)	10484(7)	1900(3)	85(2)
C(4)	230(3)	11210(7)	2381(3)	70(2)
C(5)	918(4)	11852(6)	2369(2)	70(2)
C(6)	1387(3)	11791(5)	1893(2)	63(2)
C(7)	-260(4)	11239(8)	2916(3)	120(3)
C(8)	2671(3)	9468(5)	2379(2)	48(1)
C(9)	2090(4)	8566(6)	2473(2)	75(2)
C(10)	1730(4)	8502(6)	3007(3)	86(2)
C(11)	1950(4)	9295(6)	3460(2)	67(2)
C(12)	2535(4)	10186(7)	3369(2)	74(2)
C(13)	2886(3)	10294(6)	2844(2)	62(2)
C(14)	1564(4)	9186(7)	4042(2)	95(2)
C(17)	306(3)	12615(6)	-273(3)	77(2)
C(18)	-351(3)	13422(7)	-459(3)	86(2)
C(19)	2369(4)	10429(8)	-1519(3)	114(2)
C(20)	2504(4)	10438(8)	-2110(3)	114(2)
C(21A)	4887(9)	8122(17)	2772(6)	91(5)
C(21B)	5132(9)	8705(17)	2744(7)	92(5)
C(22A)	5271(11)	8590(20)	3287(9)	113(8)

Table S9, continued

C(22B)	5666(8)	8475(14)	3182(6)	81(4)
C(23)	5655(4)	7417(7)	659(3)	99(2)
C(24)	5725(4)	6067(7)	423(3)	99(2)
C(15)	3564(3)	8580(5)	-106(2)	49(1)
C(16)	3902(3)	7833(6)	-610(2)	71(2)
C(32)	2688(4)	5674(6)	569(3)	76(2)
C(33)	2240(4)	4972(6)	1010(3)	109(3)

Table S10. Bond lengths [Å]

Mo(1)-N(1)	1.731(4)
Mo(1)-O(1)	2.169(3)
Mo(1)-S(2)	2.3457(14)
Mo(1)-S(1)	2.4401(14)
Mo(1)-S(3)	2.5176(14)
Mo(1)-S(4)	2.5695(14)
Mo(1)-Mo(2)	2.8518(7)
Mo(2)-N(2)	1.737(4)
Mo(2)-O(2)	2.168(3)
Mo(2)-S(2)	2.3439(14)
Mo(2)-S(1)	2.4565(14)
Mo(2)-S(5)	2.5173(16)
Mo(2)-S(6)	2.5726(15)
S(1)-O(7)	1.654(3)
S(3)-P(1)	1.9983(19)
S(4)-P(1)	1.990(2)
S(5)-P(2)	1.994(2)
S(6)-P(2)	1.988(2)
P(1)-O(4)	1.567(3)
P(1)-O(3)	1.574(3)
P(2)-O(6)	1.574(4)
P(2)-O(5)	1.577(4)
O(1)-C(15)	1.254(6)
O(2)-C(15)	1.260(6)
O(3)-C(17)	1.479(6)
O(4)-C(19)	1.459(7)
O(5)-C(21B)	1.467(15)
O(5)-C(21A)	1.520(15)
O(6)-C(23)	1.443(7)
O(7)-C(32)	1.429(6)
N(1)-C(1)	1.388(6)
N(2)-C(8)	1.375(6)
C(1)-C(2)	1.376(7)
C(1)-C(6)	1.385(6)
C(2)-C(3)	1.359(7)
C(2)-H(2)	0.93
C(3)-C(4)	1.372(8)
C(3)-H(3)	0.93
C(4)-C(5)	1.371(8)
C(4)-C(7)	1.513(8)
C(5)-C(6)	1.381(7)
C(5)-H(5)	0.93
C(6)-H(6)	0.93
C(7)-H(7A)	0.96

Table S10, continued

C(7)-H(7B)	0.96
C(7)-H(7C)	0.96
C(8)-C(9)	1.377(7)
C(8)-C(13)	1.404(7)
C(9)-C(10)	1.393(8)
C(9)-H(9)	0.93
C(10)-C(11)	1.367(8)
C(10)-H(10)	0.93
C(11)-C(12)	1.373(8)
C(11)-C(14)	1.516(7)
C(12)-C(13)	1.370(7)
C(12)-H(12)	0.93
C(13)-H(13)	0.93
C(14)-H(14A)	0.96
C(14)-H(14B)	0.96
C(14)-H(14C)	0.96
C(17)-C(18)	1.472(7)
C(17)-H(15A)	0.97
C(17)-H(15B)	0.97
C(18)-H(16A)	0.96
C(18)-H(16B)	0.96
C(18)-H(16C)	0.96
C(19)-C(20)	1.391(8)
C(19)-H(17A)	0.97
C(19)-H(17B)	0.97
C(20)-H(18A)	0.96
C(20)-H(18B)	0.96
C(20)-H(18C)	0.96
C(21A)-C(22A)	1.45(2)
C(21A)-H(19A)	0.97
C(21A)-H(19B)	0.97
C(21B)-C(20B)	1.403(19)
C(21B)-H(19C)	0.97
C(21B)-H(19D)	0.97
C(22A)-H(20D)	0.96
C(22A)-H(20E)	0.96
C(22A)-H(20F)	0.96
C(22B)-H(20A)	0.96
C(22B)-H(20B)	0.96
C(22B)-H(20C)	0.96
C(23)-C(24)	1.449(8)
C(23)-H(21A)	0.97
C(23)-H(21B)	0.97
C(24)-H(22A)	0.96

Table S10, continued

C(24)-H(22B)	0.96
C(24)-H(22C)	0.96
C(15)-C(16)	1.507(7)
C(16)-H(24A)	0.96
C(16)-H(24B)	0.96
C(16)-H(24C)	0.96
C(32)-C(33)	1.468(8)
C(32)-H(25A)	0.97
C(32)-H(25B)	0.97
C(33)-H(26A)	0.96
C(33)-H(26B)	0.96
C(33)-H(26C)	0.96

Table S11. Bond angles [°]

N(1)-Mo(1)-O(1)	169.11(15)
N(1)-Mo(1)-S(2)	100.93(13)
O(1)-Mo(1)-S(2)	87.11(9)
N(1)-Mo(1)-S(1)	86.55(12)
O(1)-Mo(1)-S(1)	84.05(9)
S(2)-Mo(1)-S(1)	107.15(5)
N(1)-Mo(1)-S(3)	101.30(13)
O(1)-Mo(1)-S(3)	86.91(9)
S(2)-Mo(1)-S(3)	82.59(5)
S(1)-Mo(1)-S(3)	166.29(5)
N(1)-Mo(1)-S(4)	95.69(13)
O(1)-Mo(1)-S(4)	78.90(10)
S(2)-Mo(1)-S(4)	156.53(5)
S(1)-Mo(1)-S(4)	90.19(5)
S(3)-Mo(1)-S(4)	77.95(5)
N(1)-Mo(1)-Mo(2)	97.50(12)
O(1)-Mo(1)-Mo(2)	81.48(9)
S(2)-Mo(1)-Mo(2)	52.52(3)
S(1)-Mo(1)-Mo(2)	54.65(3)
S(3)-Mo(1)-Mo(2)	133.89(4)
S(4)-Mo(1)-Mo(2)	141.27(4)
N(2)-Mo(2)-O(2)	165.47(15)
N(2)-Mo(2)-S(2)	103.03(13)
O(2)-Mo(2)-S(2)	89.69(10)
N(2)-Mo(2)-S(1)	87.74(13)
O(2)-Mo(2)-S(1)	81.83(9)
S(2)-Mo(2)-S(1)	106.67(5)
N(2)-Mo(2)-S(5)	100.79(13)
O(2)-Mo(2)-S(5)	87.76(10)
S(2)-Mo(2)-S(5)	81.99(5)
S(1)-Mo(2)-S(5)	166.33(5)
N(2)-Mo(2)-S(6)	89.78(13)
O(2)-Mo(2)-S(6)	80.58(10)
S(2)-Mo(2)-S(6)	157.40(5)
S(1)-Mo(2)-S(6)	92.17(5)
S(5)-Mo(2)-S(6)	77.32(5)
N(2)-Mo(2)-Mo(1)	100.17(13)
O(2)-Mo(2)-Mo(1)	81.89(9)
S(2)-Mo(2)-Mo(1)	52.58(3)
S(1)-Mo(2)-Mo(1)	54.11(3)
S(5)-Mo(2)-Mo(1)	133.15(4)
S(6)-Mo(2)-Mo(1)	143.89(4)
O(7)-S(1)-Mo(1)	108.19(13)
O(7)-S(1)-Mo(2)	113.69(13)

Table S11, continued

Mo(1)-S(1)-Mo(2)	71.24(4)
Mo(2)-S(2)-Mo(1)	74.91(4)
P(1)-S(3)-Mo(1)	88.29(6)
P(1)-S(4)-Mo(1)	87.03(6)
P(2)-S(5)-Mo(2)	88.98(7)
P(2)-S(6)-Mo(2)	87.57(7)
O(4)-P(1)-O(3)	97.12(19)
O(4)-P(1)-S(4)	114.17(16)
O(3)-P(1)-S(4)	113.31(15)
O(4)-P(1)-S(3)	112.79(15)
O(3)-P(1)-S(3)	112.77(15)
S(4)-P(1)-S(3)	106.72(8)
O(6)-P(2)-O(5)	96.6(2)
O(6)-P(2)-S(6)	114.70(19)
O(5)-P(2)-S(6)	113.5(2)
O(6)-P(2)-S(5)	112.42(19)
O(5)-P(2)-S(5)	113.76(19)
S(6)-P(2)-S(5)	105.99(9)
C(15)-O(1)-Mo(1)	126.0(3)
C(15)-O(2)-Mo(2)	125.6(3)
C(17)-O(3)-P(1)	118.7(3)
C(19)-O(4)-P(1)	120.3(3)
C(21B)-O(5)-C(21A)	28.0(8)
C(21B)-O(5)-P(2)	121.6(7)
C(21A)-O(5)-P(2)	116.7(6)
C(23)-O(6)-P(2)	120.2(4)
C(32)-O(7)-S(1)	116.7(3)
C(1)-N(1)-Mo(1)	169.9(3)
C(8)-N(2)-Mo(2)	167.0(3)
C(2)-C(1)-C(6)	117.9(5)
C(2)-C(1)-N(1)	121.7(5)
C(6)-C(1)-N(1)	120.3(5)
C(3)-C(2)-C(1)	121.1(5)
C(3)-C(2)-H(2)	119.4
C(1)-C(2)-H(2)	119.4
C(2)-C(3)-C(4)	122.0(6)
C(2)-C(3)-H(3)	119.0
C(4)-C(3)-H(3)	119.0
C(5)-C(4)-C(3)	117.1(5)
C(5)-C(4)-C(7)	121.1(6)
C(3)-C(4)-C(7)	121.7(6)
C(4)-C(5)-C(6)	122.0(5)
C(4)-C(5)-H(5)	119.0
C(6)-C(5)-H(5)	119.0

Table S11, continued

C(5)-C(6)-C(1)	119.9(5)
C(5)-C(6)-H(6)	120.1
C(1)-C(6)-H(6)	120.1
C(4)-C(7)-H(7A)	109.5
C(4)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(4)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
N(2)-C(8)-C(9)	121.2(5)
N(2)-C(8)-C(13)	121.7(5)
C(9)-C(8)-C(13)	117.2(5)
C(8)-C(9)-C(10)	120.7(6)
C(8)-C(9)-H(9)	119.6
C(10)-C(9)-H(9)	119.6
C(11)-C(10)-C(9)	121.7(6)
C(11)-C(10)-H(10)	119.2
C(9)-C(10)-H(10)	119.2
C(10)-C(11)-C(12)	117.7(6)
C(10)-C(11)-C(14)	120.9(6)
C(12)-C(11)-C(14)	121.4(6)
C(13)-C(12)-C(11)	121.8(6)
C(13)-C(12)-H(12)	119.1
C(11)-C(12)-H(12)	119.1
C(12)-C(13)-C(8)	120.9(6)
C(12)-C(13)-H(13)	119.6
C(8)-C(13)-H(13)	119.6
C(11)-C(14)-H(14A)	109.5
C(11)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(11)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(18)-C(17)-O(3)	109.2(5)
C(18)-C(17)-H(15A)	109.8
O(3)-C(17)-H(15A)	109.8
C(18)-C(17)-H(15B)	109.8
O(3)-C(17)-H(15B)	109.8
H(15A)-C(17)-H(15B)	108.3
C(17)-C(18)-H(16A)	109.5
C(17)-C(18)-H(16B)	109.5
H(16A)-C(18)-H(16B)	109.5
C(17)-C(18)-H(16C)	109.5
H(16A)-C(18)-H(16C)	109.5

Table S11, continued

H(16B)-C(18)-H(16C)	109.5
C(20)-C(19)-O(4)	113.7(6)
C(20)-C(19)-H(17A)	108.8
O(4)-C(19)-H(17A)	108.8
C(20)-C(19)-H(17B)	108.8
O(4)-C(19)-H(17B)	108.8
H(17A)-C(19)-H(17B)	107.7
C(19)-C(20)-H(18A)	109.5
C(19)-C(20)-H(18B)	109.5
H(18A)-C(20)-H(18B)	109.5
C(19)-C(20)-H(18C)	109.5
H(18A)-C(20)-H(18C)	109.5
H(18B)-C(20)-H(18C)	109.5
C(22A)-C(21A)-O(5)	115.2(13)
C(22A)-C(21A)-H(19A)	108.5
O(5)-C(21A)-H(19A)	108.5
C(22A)-C(21A)-H(19B)	108.5
O(5)-C(21A)-H(19B)	108.5
H(19A)-C(21A)-H(19B)	107.5
C(20B)-C(21B)-O(5)	105.5(12)
C(20B)-C(21B)-H(19C)	110.6
O(5)-C(21B)-H(19C)	110.6
C(20B)-C(21B)-H(19D)	110.6
O(5)-C(21B)-H(19D)	110.6
H(19C)-C(21B)-H(19D)	108.8
C(21A)-C(22A)-H(20D)	109.5
C(21A)-C(22A)-H(20E)	109.5
H(20D)-C(22A)-H(20E)	109.5
C(21A)-C(22A)-H(20F)	109.5
H(20D)-C(22A)-H(20F)	109.5
H(20E)-C(22A)-H(20F)	109.5
C(19B)-C(22B)-H(20A)	109.5
C(19B)-C(22B)-H(20B)	109.5
H(20A)-C(22B)-H(20B)	109.5
C(19B)-C(22B)-H(20C)	109.5
H(20A)-C(22B)-H(20C)	109.5
H(20B)-C(22B)-H(20C)	109.5
O(6)-C(23)-C(24)	110.7(6)
O(6)-C(23)-H(21A)	109.5
C(24)-C(23)-H(21A)	109.5
O(6)-C(23)-H(21B)	109.5
C(24)-C(23)-H(21B)	109.5
H(21A)-C(23)-H(21B)	108.1
C(23)-C(24)-H(22A)	109.5

Table S11, continued

C(23)-C(24)-H(22B)	109.5
H(22A)-C(24)-H(22B)	109.5
C(23)-C(24)-H(22C)	109.5
H(22A)-C(24)-H(22C)	109.5
H(22B)-C(24)-H(22C)	109.5
O(1)-C(15)-O(2)	124.7(5)
O(1)-C(15)-C(16)	117.4(5)
O(2)-C(15)-C(16)	117.9(5)
C(15)-C(16)-H(24A)	109.5
C(15)-C(16)-H(24B)	109.5
H(24A)-C(16)-H(24B)	109.5
C(15)-C(16)-H(24C)	109.5
H(24A)-C(16)-H(24C)	109.5
H(24B)-C(16)-H(24C)	109.5
O(7)-C(32)-C(33)	116.0(5)
O(7)-C(32)-H(25A)	108.3
C(33)-C(32)-H(25A)	108.3
O(7)-C(32)-H(25B)	108.3
C(33)-C(32)-H(25B)	108.3
H(25A)-C(32)-H(25B)	107.4
C(32)-C(33)-H(26A)	109.5
C(32)-C(33)-H(26B)	109.5
H(26A)-C(33)-H(26B)	109.5
C(32)-C(33)-H(26C)	109.5
H(26A)-C(33)-H(26C)	109.5
H(26B)-C(33)-H(26C)	109.5

Table S12. Anisotropic displacement parameters ($Å^2 x\ 10^3$). The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	42(1)	41(1)	37(1)	-1(1)	0(1)	0(1)
Mo(2)	44(1)	43(1)	40(1)	0(1)	-1(1)	2(1)
S(1)	49(1)	43(1)	42(1)	-3(1)	3(1)	-2(1)
S(2)	48(1)	43(1)	54(1)	3(1)	-9(1)	-4(1)
S(3)	53(1)	47(1)	53(1)	6(1)	-10(1)	-7(1)
S(4)	59(1)	54(1)	56(1)	2(1)	-10(1)	-14(1)
S(5)	51(1)	66(1)	87(1)	4(1)	-13(1)	-3(1)
S(6)	71(1)	53(1)	77(1)	14(1)	-6(1)	8(1)
P(1)	44(1)	54(1)	44(1)	0(1)	-5(1)	-1(1)
P(2)	59(1)	75(1)	65(1)	2(1)	-11(1)	16(1)
O(1)	53(2)	46(2)	39(2)	-5(2)	6(2)	4(2)
O(2)	47(2)	57(2)	52(2)	-2(2)	5(2)	5(2)
O(3)	43(2)	72(3)	51(2)	4(2)	-3(2)	4(2)
O(4)	56(2)	83(3)	35(2)	-1(2)	2(2)	8(2)
O(5)	85(3)	119(4)	73(3)	4(3)	-23(3)	29(3)
O(6)	70(3)	103(3)	78(3)	-4(3)	-9(2)	36(2)
O(7)	71(3)	45(2)	52(2)	-8(2)	0(2)	-3(2)
N(1)	43(3)	37(2)	44(3)	-3(2)	-8(2)	-1(2)
N(2)	50(3)	45(3)	36(2)	-2(2)	-7(2)	2(2)
C(1)	35(3)	47(3)	43(3)	-6(3)	-5(3)	4(3)
C(2)	56(4)	91(5)	56(4)	-24(3)	3(3)	-12(3)
C(3)	42(4)	140(6)	73(5)	-28(4)	8(4)	-21(4)
C(4)	55(4)	107(5)	50(4)	-11(4)	9(3)	4(4)
C(5)	69(5)	87(5)	54(4)	-31(3)	1(3)	11(4)
C(6)	63(4)	61(4)	64(4)	-21(3)	3(3)	-12(3)
C(7)	98(6)	197(9)	65(5)	-17(5)	30(4)	1(6)
C(8)	57(4)	46(3)	42(3)	1(3)	-3(3)	4(3)
C(9)	107(5)	76(5)	41(4)	-10(3)	6(4)	-26(4)
C(10)	117(6)	83(5)	57(4)	0(4)	21(4)	-34(4)
C(11)	98(5)	58(4)	46(4)	-5(3)	17(4)	7(4)
C(12)	98(5)	86(5)	37(4)	-15(3)	1(4)	4(4)
C(13)	65(4)	70(4)	50(4)	-9(3)	-5(3)	-4(3)
C(14)	125(6)	97(5)	64(5)	-10(4)	34(4)	-6(4)
C(17)	58(4)	97(5)	74(5)	14(4)	12(4)	17(4)
C(18)	65(5)	105(6)	89(5)	-8(4)	7(4)	12(4)
C(19)	114(5)	169(5)	60(3)	-6(4)	13(3)	52(4)
C(20)	114(5)	169(5)	60(3)	-6(4)	13(3)	52(4)
C(23)	100(4)	104(4)	93(4)	-11(3)	3(3)	1(4)
C(24)	100(4)	104(4)	93(4)	-11(3)	3(3)	1(4)
C(15)	56(4)	40(3)	50(4)	-7(3)	12(3)	-5(3)

Table S12, continued

C(16)	85(5)	71(4)	57(4)	-8(3)	18(3)	15(3)
C(32)	85(5)	51(4)	93(5)	-17(4)	-12(4)	4(4)
C(33)	148(8)	60(5)	117(6)	22(4)	23(6)	7(4)

Table S13. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3)

	x	y	z	U(eq)
H(2)	336	9871	1117	81
H(3)	-438	10050	1894	102
H(5)	1072	12343	2690	84
H(6)	1840	12270	1890	75
H(7A)	-309	12153	3049	180
H(7B)	-31	10698	3212	180
H(7C)	-752	10884	2825	180
H(9)	1937	7994	2177	90
H(10)	1329	7905	3056	103
H(12)	2696	10730	3672	89
H(13)	3271	10923	2795	74
H(14A)	1037	8989	3987	143
H(14B)	1616	10026	4246	143
H(14C)	1795	8475	4262	143
H(15A)	135	11831	-58	92
H(15B)	628	13151	-23	92
H(16A)	-178	14244	-635	129
H(16B)	-659	13633	-130	129
H(16C)	-644	12915	-733	129
H(17A)	2802	10820	-1322	137
H(17B)	2322	9500	-1390	137
H(18A)	2071	10080	-2309	172
H(18B)	2940	9893	-2194	172
H(18C)	2594	11348	-2236	172
H(19A)	4499	8775	2671	109
H(19B)	4634	7277	2860	109
H(19C)	5112	9657	2646	110
H(19D)	4633	8415	2866	110
H(20D)	4910	8704	3592	214
H(20E)	5517	9432	3209	214
H(20F)	5643	7930	3402	214
H(20A)	5525	8972	3521	122
H(20B)	6156	8768	3054	122
H(20C)	5683	7528	3271	122
H(21A)	6068	7973	519	119
H(21B)	5184	7818	529	119
H(22A)	6186	5663	559	149
H(22B)	5732	6113	9	149
H(22C)	5302	5530	545	149
H(24A)	3636	6998	-666	107
H(24B)	4426	7649	-533	107

Table S13, continued

H(24C)	3860	8377	-952	107
H(25A)	3196	5802	718	92
H(25B)	2725	5091	233	92
H(26A)	2275	5455	1368	163
H(26B)	2433	4073	1061	163
H(26C)	1721	4930	889	163

Table S14. Torsion angles [°]

N(1)-Mo(1)-Mo(2)-N(2)	0.66(18)
O(1)-Mo(1)-Mo(2)-N(2)	-168.40(15)
S(2)-Mo(1)-Mo(2)-N(2)	98.70(13)
S(1)-Mo(1)-Mo(2)-N(2)	-79.68(13)
S(3)-Mo(1)-Mo(2)-N(2)	114.30(14)
S(4)-Mo(1)-Mo(2)-N(2)	-108.26(14)
N(1)-Mo(1)-Mo(2)-O(2)	166.08(15)
O(1)-Mo(1)-Mo(2)-O(2)	-2.97(12)
S(2)-Mo(1)-Mo(2)-O(2)	-95.87(10)
S(1)-Mo(1)-Mo(2)-O(2)	85.75(10)
S(3)-Mo(1)-Mo(2)-O(2)	-80.27(10)
S(4)-Mo(1)-Mo(2)-O(2)	57.17(11)
N(1)-Mo(1)-Mo(2)-S(2)	-98.04(13)
O(1)-Mo(1)-Mo(2)-S(2)	92.90(9)
S(1)-Mo(1)-Mo(2)-S(2)	-178.38(6)
S(3)-Mo(1)-Mo(2)-S(2)	15.60(6)
S(4)-Mo(1)-Mo(2)-S(2)	153.04(7)
N(1)-Mo(1)-Mo(2)-S(1)	80.33(13)
O(1)-Mo(1)-Mo(2)-S(1)	-88.72(9)
S(2)-Mo(1)-Mo(2)-S(1)	178.38(6)
S(3)-Mo(1)-Mo(2)-S(1)	-166.02(6)
S(4)-Mo(1)-Mo(2)-S(1)	-28.58(7)
N(1)-Mo(1)-Mo(2)-S(5)	-114.73(13)
O(1)-Mo(1)-Mo(2)-S(5)	76.22(10)
S(2)-Mo(1)-Mo(2)-S(5)	-16.69(7)
S(1)-Mo(1)-Mo(2)-S(5)	164.94(7)
S(3)-Mo(1)-Mo(2)-S(5)	-1.09(8)
S(4)-Mo(1)-Mo(2)-S(5)	136.36(8)
N(1)-Mo(1)-Mo(2)-S(6)	104.50(14)
O(1)-Mo(1)-Mo(2)-S(6)	-64.55(11)
S(2)-Mo(1)-Mo(2)-S(6)	-157.45(8)
S(1)-Mo(1)-Mo(2)-S(6)	24.17(8)
S(3)-Mo(1)-Mo(2)-S(6)	-141.85(8)
S(4)-Mo(1)-Mo(2)-S(6)	-4.41(10)
N(1)-Mo(1)-S(1)-O(7)	148.70(18)
O(1)-Mo(1)-S(1)-O(7)	-25.81(16)
S(2)-Mo(1)-S(1)-O(7)	-110.93(14)
S(3)-Mo(1)-S(1)-O(7)	23.2(3)
S(4)-Mo(1)-S(1)-O(7)	53.01(14)
Mo(2)-Mo(1)-S(1)-O(7)	-109.58(14)
N(1)-Mo(1)-S(1)-Mo(2)	-101.72(12)
O(1)-Mo(1)-S(1)-Mo(2)	83.76(9)
S(2)-Mo(1)-S(1)-Mo(2)	-1.35(5)
S(3)-Mo(1)-S(1)-Mo(2)	132.74(19)

Table S14, continued

S(4)-Mo(1)-S(1)-Mo(2)	162.58(4)
N(2)-Mo(2)-S(1)-O(7)	-153.54(19)
O(2)-Mo(2)-S(1)-O(7)	16.31(17)
S(2)-Mo(2)-S(1)-O(7)	103.53(15)
S(5)-Mo(2)-S(1)-O(7)	-24.5(3)
S(6)-Mo(2)-S(1)-O(7)	-63.85(15)
Mo(1)-Mo(2)-S(1)-O(7)	102.18(15)
N(2)-Mo(2)-S(1)-Mo(1)	104.28(13)
O(2)-Mo(2)-S(1)-Mo(1)	-85.87(10)
S(2)-Mo(2)-S(1)-Mo(1)	1.35(5)
S(5)-Mo(2)-S(1)-Mo(1)	-126.7(2)
S(6)-Mo(2)-S(1)-Mo(1)	-166.03(4)
N(2)-Mo(2)-S(2)-Mo(1)	-92.92(13)
O(2)-Mo(2)-S(2)-Mo(1)	80.00(10)
S(1)-Mo(2)-S(2)-Mo(1)	-1.37(5)
S(5)-Mo(2)-S(2)-Mo(1)	167.79(5)
S(6)-Mo(2)-S(2)-Mo(1)	143.98(12)
N(1)-Mo(1)-S(2)-Mo(2)	91.12(13)
O(1)-Mo(1)-S(2)-Mo(2)	-81.48(9)
S(1)-Mo(1)-S(2)-Mo(2)	1.39(5)
S(3)-Mo(1)-S(2)-Mo(2)	-168.73(5)
S(4)-Mo(1)-S(2)-Mo(2)	-134.60(11)
N(1)-Mo(1)-S(3)-P(1)	-94.06(14)
O(1)-Mo(1)-S(3)-P(1)	78.73(10)
S(2)-Mo(1)-S(3)-P(1)	166.21(7)
S(1)-Mo(1)-S(3)-P(1)	30.0(2)
S(4)-Mo(1)-S(3)-P(1)	-0.58(6)
Mo(2)-Mo(1)-S(3)-P(1)	153.79(5)
N(1)-Mo(1)-S(4)-P(1)	100.96(13)
O(1)-Mo(1)-S(4)-P(1)	-88.60(10)
S(2)-Mo(1)-S(4)-P(1)	-34.10(15)
S(1)-Mo(1)-S(4)-P(1)	-172.50(7)
S(3)-Mo(1)-S(4)-P(1)	0.58(6)
Mo(2)-Mo(1)-S(4)-P(1)	-149.53(5)
N(2)-Mo(2)-S(5)-P(2)	89.81(14)
O(2)-Mo(2)-S(5)-P(2)	-78.35(11)
S(2)-Mo(2)-S(5)-P(2)	-168.36(8)
S(1)-Mo(2)-S(5)-P(2)	-38.0(2)
S(6)-Mo(2)-S(5)-P(2)	2.49(7)
Mo(1)-Mo(2)-S(5)-P(2)	-155.05(6)
N(2)-Mo(2)-S(6)-P(2)	-103.61(14)
O(2)-Mo(2)-S(6)-P(2)	87.31(11)
S(2)-Mo(2)-S(6)-P(2)	21.69(17)
S(1)-Mo(2)-S(6)-P(2)	168.66(7)

Table S14, continued

S(5)-Mo(2)-S(6)-P(2)	-2.50(7)
Mo(1)-Mo(2)-S(6)-P(2)	149.27(6)
Mo(1)-S(4)-P(1)-O(4)	124.58(15)
Mo(1)-S(4)-P(1)-O(3)	-125.46(16)
Mo(1)-S(4)-P(1)-S(3)	-0.74(8)
Mo(1)-S(3)-P(1)-O(4)	-125.40(16)
Mo(1)-S(3)-P(1)-O(3)	125.81(15)
Mo(1)-S(3)-P(1)-S(4)	0.76(8)
Mo(2)-S(6)-P(2)-O(6)	-121.45(19)
Mo(2)-S(6)-P(2)-O(5)	128.78(19)
Mo(2)-S(6)-P(2)-S(5)	3.21(9)
Mo(2)-S(5)-P(2)-O(6)	122.78(19)
Mo(2)-S(5)-P(2)-O(5)	-128.7(2)
Mo(2)-S(5)-P(2)-S(6)	-3.27(10)
N(1)-Mo(1)-O(1)-C(15)	-79.6(9)
S(2)-Mo(1)-O(1)-C(15)	58.3(4)
S(1)-Mo(1)-O(1)-C(15)	-49.3(4)
S(3)-Mo(1)-O(1)-C(15)	141.0(4)
S(4)-Mo(1)-O(1)-C(15)	-140.6(4)
Mo(2)-Mo(1)-O(1)-C(15)	5.8(4)
N(2)-Mo(2)-O(2)-C(15)	101.4(7)
S(2)-Mo(2)-O(2)-C(15)	-50.0(4)
S(1)-Mo(2)-O(2)-C(15)	56.9(4)
S(5)-Mo(2)-O(2)-C(15)	-132.0(4)
S(6)-Mo(2)-O(2)-C(15)	150.5(4)
Mo(1)-Mo(2)-O(2)-C(15)	2.2(4)
O(4)-P(1)-O(3)-C(17)	-179.4(4)
S(4)-P(1)-O(3)-C(17)	60.4(4)
S(3)-P(1)-O(3)-C(17)	-61.0(4)
O(3)-P(1)-O(4)-C(19)	179.6(5)
S(4)-P(1)-O(4)-C(19)	-60.8(5)
S(3)-P(1)-O(4)-C(19)	61.3(5)
O(6)-P(2)-O(5)-C(21B)	161.7(9)
S(6)-P(2)-O(5)-C(21B)	-77.7(9)
S(5)-P(2)-O(5)-C(21B)	43.7(9)
O(6)-P(2)-O(5)-C(21A)	-166.5(8)
S(6)-P(2)-O(5)-C(21A)	-45.9(8)
S(5)-P(2)-O(5)-C(21A)	75.4(8)
O(5)-P(2)-O(6)-C(23)	-171.2(5)
S(6)-P(2)-O(6)-C(23)	69.1(5)
S(5)-P(2)-O(6)-C(23)	-52.1(5)
Mo(1)-S(1)-O(7)-C(32)	156.7(3)
Mo(2)-S(1)-O(7)-C(32)	79.7(4)
O(1)-Mo(1)-N(1)-C(1)	28(2)

Table S14, continued

S(2)-Mo(1)-N(1)-C(1)	-108.6(19)
S(1)-Mo(1)-N(1)-C(1)	-1.8(19)
S(3)-Mo(1)-N(1)-C(1)	166.9(19)
S(4)-Mo(1)-N(1)-C(1)	88(2)
Mo(2)-Mo(1)-N(1)-C(1)	-55(2)
O(2)-Mo(2)-N(2)-C(8)	12(2)
S(2)-Mo(2)-N(2)-C(8)	162.7(16)
S(1)-Mo(2)-N(2)-C(8)	56.1(16)
S(5)-Mo(2)-N(2)-C(8)	-113.1(16)
S(6)-Mo(2)-N(2)-C(8)	-36.1(16)
Mo(1)-Mo(2)-N(2)-C(8)	109.0(16)
Mo(1)-N(1)-C(1)-C(2)	-65(2)
Mo(1)-N(1)-C(1)-C(6)	111.6(19)
C(6)-C(1)-C(2)-C(3)	-1.5(9)
N(1)-C(1)-C(2)-C(3)	175.4(5)
C(1)-C(2)-C(3)-C(4)	-0.6(10)
C(2)-C(3)-C(4)-C(5)	1.0(10)
C(2)-C(3)-C(4)-C(7)	-175.5(7)
C(3)-C(4)-C(5)-C(6)	0.8(10)
C(7)-C(4)-C(5)-C(6)	177.3(6)
C(4)-C(5)-C(6)-C(1)	-2.9(9)
C(2)-C(1)-C(6)-C(5)	3.2(8)
N(1)-C(1)-C(6)-C(5)	-173.7(5)
Mo(2)-N(2)-C(8)-C(9)	-38.4(19)
Mo(2)-N(2)-C(8)-C(13)	141.5(14)
N(2)-C(8)-C(9)-C(10)	-179.2(5)
C(13)-C(8)-C(9)-C(10)	0.9(9)
C(8)-C(9)-C(10)-C(11)	-1.9(10)
C(9)-C(10)-C(11)-C(12)	1.2(10)
C(9)-C(10)-C(11)-C(14)	-178.5(6)
C(10)-C(11)-C(12)-C(13)	0.5(10)
C(14)-C(11)-C(12)-C(13)	-179.8(6)
C(11)-C(12)-C(13)-C(8)	-1.5(9)
N(2)-C(8)-C(13)-C(12)	-179.1(5)
C(9)-C(8)-C(13)-C(12)	0.8(8)
P(1)-O(3)-C(17)-C(18)	178.6(4)
P(1)-O(4)-C(19)-C(20)	-176.7(5)
C(21B)-O(5)-C(21A)-C(22A)	-46.4(19)
P(2)-O(5)-C(21A)-C(22A)	-154.0(12)
C(21A)-O(5)-C(21B)-C(22B)	100(3)
P(2)-O(5)-C(21B)-C(22B)	-171.9(9)
P(2)-O(6)-C(23)-C(24)	-124.7(5)
Mo(1)-O(1)-C(15)-O(2)	-6.2(7)
Mo(1)-O(1)-C(15)-C(16)	172.3(3)

Table S14, continued

Mo(2)-O(2)-C(15)-O(1)	1.5(7)
Mo(2)-O(2)-C(15)-C(16)	-177.0(3)
S(1)-O(7)-C(32)-C(33)	56.8(6)

Crystallographic Studies for Proximal S{Mo_2}SOEt, 5.

An orange prism (0.35 x 0.25 x 0.15 mm^3) crystal was mounted on a glass fiber oil for collection of x-ray data on a Bruker SMART APEX CCD diffractometer. The SMART[1] software package (v 5.632) was used to acquire a total of 1,868 thirty-second frame ω-scan exposures of data at 100K to a 2θ max = 56.18° using monochromated Mo Kα radiation (0.71073 Å) from a sealed tube and a monocapillary. Frame data were processed using SAINT[2] (v 6.45a) to determine final unit cell parameters a = 20.448(2) Å, b = 19.771(2) Å, c = 9.4698(10) Å, β= 97.819(2)°, V = 3792.8(7)$Å^3$, Z = 4 and ρ_{calcd} = 1.648Mgm^{-3} to produce raw hkl data that were then corrected for absorption (transmission min./max. = 0.733 /0.956; μ = 1.118 mm^{-1}) using SADABS[3] (v 2.10). The structure was solved by Patterson methods in the space group $P2_1/c$ using SHELXS-90[4] and refined by least squares methods on F^2 using SHELXL-99[5] incorporated into the SHELXTL[6] (v 6.14) suite of programs. The disordered OEt group was modeled using two sets of carbon atoms, C19a – C20a refined anisotropically at 80% occupancy and C19b –C20b isotropic at 20%. All other non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed in their geometrically generated positions and refined as a riding model as described above for compound $\mathbf{4}^+$. For all 8687 unique reflections (R(int) = 0.043) the final anisotropic full matrix least-squares refinement on F^2 for 423 variables converged at R1 = 0.0510 and wR2 = 0.1085 with a GOF of 1.06.

References

1. SMART, V.5.632, Bruker Advanced X-ray Solutions, Inc., Madison, WI, 2005.

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3. G. M. Sheldrick, SADABS, V. 2.10, Area Detector Absorption Correction, University of Göttingen, Göttingen, Germany, 2003.

4. G. M. Sheldrick, SHELXS-90., *Acta Crystallogr*. 1990, *A46*, 467.

5. G. M. Sheldrick, SHELXL-99, Program for the Refinement of Crystal Structures, University of Göttingen, Göttingen, Germany, 1997.

6. SHELXTL 6.14, Program Library for Structure Solution and Molecular graphics, Bruker Advanced X-ray Solutions, Madison, WI, 2000.

Table S15. Crystal data and structure refinement

Empirical formula	C26 H42 Mo2 N2 O7 P2 S6	
Formula weight	940.80	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 20.448(2) Å	α = 90°.
	b = 19.771(2) Å	β = 97.819(2)°.
	c = 9.4698(10) Å	γ = 90°.
Volume	3792.8(7) $Å^3$	
Z	4	
Density (calculated)	1.648 Mg/m^3	
Absorption coefficient	1.118 mm^{-1}	
F(000)	1912	
Crystal size	0.35 x 0.25 x 0.15 mm^3	
Crystal color, habit	orange rhomb prism	
Theta range for data collection	2.01 to 28.09°	
Index ranges	-27<=h<=26, -26<=k<=25, -12<=l<=12	
Reflections collected	32090	
Independent reflections	8687 [R(int) = 0.0429]	
Completeness to theta = 28.09°	94.0 %	
Absorption correction	SADABS	
Min. and max. transmission	0.733 and 0.895	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8687 / 1 / 423	
Goodness-of-fit on F^2	1.060	
Final R indices [I>2sigma(I)]	R1 = 0.0510, wR2 = 0.1085	
R indices (all data)	R1 = 0.0810, wR2 = 0.1174	
Largest diff. peak and hole	1.018 and -0.559 $e.Å^{-3}$	

Table S16. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	3079(1)	4252(1)	5693(1)	26(1)
Mo(2)	1758(1)	4220(1)	4295(1)	24(1)
S(1)	2753(1)	4107(1)	3159(1)	25(1)
S(2)	2108(1)	4213(1)	6771(1)	32(1)
S(3)	3639(1)	4022(1)	8182(1)	39(1)
S(4)	4248(1)	3939(1)	5251(1)	32(1)
S(5)	650(1)	3915(1)	4997(1)	32(1)
S(6)	1119(1)	3852(1)	1912(1)	30(1)
P(1)	4474(1)	3869(1)	7359(2)	34(1)
P(2)	361(1)	3661(1)	2964(1)	29(1)
O(1)	2982(2)	3149(2)	5469(4)	33(1)
O(2)	1951(2)	3125(2)	4354(4)	32(1)
O(3)	5061(2)	4357(2)	7966(4)	41(1)
O(4)	4821(2)	3188(2)	7896(5)	49(1)
O(5)	-299(2)	4014(2)	2291(4)	33(1)
O(6)	89(2)	2919(2)	2789(4)	34(1)
O(7)	2925(2)	4817(2)	2336(4)	39(1)
N(1)	3202(2)	5116(2)	5581(4)	30(1)
N(2)	1661(2)	5086(2)	4065(4)	27(1)
C(1)	3324(2)	5804(3)	5391(5)	29(1)
C(2)	3721(3)	6014(3)	4384(6)	37(1)
C(3)	3851(3)	6690(3)	4228(7)	41(1)
C(4)	3597(3)	7174(3)	5050(7)	42(1)
C(5)	3209(3)	6965(3)	6044(6)	44(2)
C(6)	3057(3)	6279(3)	6224(6)	38(1)
C(7)	3735(3)	7923(3)	4878(8)	58(2)
C(8)	1620(2)	5789(2)	4022(5)	26(1)
C(9)	1935(3)	6161(3)	3058(6)	34(1)
C(10)	1908(3)	6853(3)	3087(6)	32(1)
C(11)	1583(2)	7195(2)	4070(5)	30(1)
C(12)	1261(3)	6817(3)	5002(5)	33(1)
C(13)	1282(2)	6120(3)	4991(5)	30(1)
C(14)	1577(3)	7962(3)	4096(6)	39(1)
C(17)	5098(3)	5053(3)	7496(7)	48(2)
C(18)	4662(4)	5538(4)	8183(7)	61(2)
C(19A)	4480(5)	2563(4)	8116(11)	56(2)
C(20A)	4325(5)	2174(5)	6831(11)	63(3)
C(19B)	4320(30)	2570(30)	7280(80)	120(30)
C(20B)	4780(20)	1989(18)	7150(40)	61(10)

Table S16, continued

C(21)	-340(3)	4744(3)	2067(7)	41(1)
C(22)	-981(3)	4866(3)	1116(7)	49(2)
C(23)	503(3)	2336(3)	3268(7)	44(2)
C(24)	56(3)	1759(3)	3482(7)	46(2)
C(15)	2458(3)	2834(3)	4970(5)	30(1)
C(16)	2450(3)	2081(3)	5046(6)	37(1)
C(32)	2684(3)	4799(3)	837(6)	48(2)
C(33)	2946(4)	5405(3)	147(7)	55(2)

Table S17. Bond lengths [Å]

Mo(1)-N(1)	1.732(4)
Mo(1)-O(1)	2.196(3)
Mo(1)-S(2)	2.3543(14)
Mo(1)-S(1)	2.4176(13)
Mo(1)-S(3)	2.5175(14)
Mo(1)-S(4)	2.5580(14)
Mo(1)-Mo(2)	2.8419(7)
Mo(2)-N(2)	1.734(4)
Mo(2)-O(2)	2.199(3)
Mo(2)-S(2)	2.3564(13)
Mo(2)-S(1)	2.4370(13)
Mo(2)-S(5)	2.5208(14)
Mo(2)-S(6)	2.5547(13)
S(1)-O(7)	1.666(4)
S(3)-P(1)	1.994(2)
S(4)-P(1)	1.9923(19)
S(5)-P(2)	2.0003(19)
S(6)-P(2)	1.9897(19)
P(1)-O(4)	1.573(4)
P(1)-O(3)	1.585(4)
P(2)-O(6)	1.569(4)
P(2)-O(5)	1.575(4)
O(1)-C(15)	1.273(6)
O(2)-C(15)	1.258(6)
O(3)-C(17)	1.451(7)
O(4)-C(19A)	1.447(9)
O(4)-C(19B)	1.65(7)
O(5)-C(21)	1.459(6)
O(6)-C(23)	1.465(6)
O(7)-C(32)	1.438(6)
N(1)-C(1)	1.400(6)
N(2)-C(8)	1.394(6)
C(1)-C(6)	1.385(7)
C(1)-C(2)	1.397(7)
C(2)-C(3)	1.376(8)
C(2)-H(2)	0.95
C(3)-C(4)	1.379(8)
C(3)-H(3)	0.95
C(4)-C(5)	1.374(9)
C(4)-C(7)	1.521(8)
C(5)-C(6)	1.407(8)
C(5)-H(5)	0.95
C(6)-H(6)	0.95
C(7)-H(7A)	0.98

Table S17, continued

C(7)-H(7B)	0.98
C(7)-H(7C)	0.98
C(8)-C(13)	1.386(7)
C(8)-C(9)	1.395(7)
C(9)-C(10)	1.369(7)
C(9)-H(9)	0.95
C(10)-C(11)	1.391(7)
C(10)-H(10)	0.95
C(11)-C(12)	1.389(7)
C(11)-C(14)	1.516(7)
C(12)-C(13)	1.378(7)
C(12)-H(12)	0.95
C(13)-H(13)	0.95
C(14)-H(14A)	0.98
C(14)-H(14B)	0.98
C(14)-H(14C)	0.98
C(17)-C(18)	1.514(9)
C(17)-H(15A)	0.99
C(17)-H(15B)	0.99
C(18)-H(16A)	0.98
C(18)-H(16B)	0.98
C(18)-H(16C)	0.98
C(19A)-C(20A)	1.437(14)
C(19A)-H(17A)	0.99
C(19A)-H(17B)	0.99
C(20A)-H(18A)	0.98
C(20A)-H(18B)	0.98
C(20A)-H(18C)	0.98
C(19B)-C(20B)	1.51(2)
C(19B)-H(17C)	0.99
C(19B)-H(17D)	0.99
C(20B)-H(18D)	0.98
C(20B)-H(18E)	0.98
C(20B)-H(18F)	0.98
C(21)-C(22)	1.504(8)
C(21)-H(19A)	0.99
C(21)-H(19B)	0.99
C(22)-H(20A)	0.98
C(22)-H(20B)	0.98
C(22)-H(20C)	0.98
C(23)-C(24)	1.494(8)
C(23)-H(21A)	0.99
C(23)-H(21B)	0.99
C(24)-H(22A)	0.98

Table S17, continued

C(24)-H(22B)	0.98
C(24)-H(22C)	0.98
C(15)-C(16)	1.492(7)
C(16)-H(24A)	0.98
C(16)-H(24B)	0.98
C(16)-H(24C)	0.98
C(32)-C(33)	1.499(8)
C(32)-H(25A)	0.99
C(32)-H(25B)	0.99
C(33)-H(26A)	0.98
C(33)-H(26B)	0.98
C(33)-H(26C)	0.98

Table S18. Bond angles [°]

N(1)-Mo(1)-O(1)	170.05(17)
N(1)-Mo(1)-S(2)	101.32(14)
O(1)-Mo(1)-S(2)	86.53(10)
N(1)-Mo(1)-S(1)	94.52(14)
O(1)-Mo(1)-S(1)	77.20(10)
S(2)-Mo(1)-S(1)	106.96(5)
N(1)-Mo(1)-S(3)	100.57(14)
O(1)-Mo(1)-S(3)	86.26(10)
S(2)-Mo(1)-S(3)	83.73(5)
S(1)-Mo(1)-S(3)	159.49(5)
N(1)-Mo(1)-S(4)	94.66(14)
O(1)-Mo(1)-S(4)	79.56(10)
S(2)-Mo(1)-S(4)	157.72(5)
S(1)-Mo(1)-S(4)	86.95(4)
S(3)-Mo(1)-S(4)	78.10(5)
N(1)-Mo(1)-Mo(2)	97.49(14)
O(1)-Mo(1)-Mo(2)	82.28(9)
S(2)-Mo(1)-Mo(2)	52.93(3)
S(1)-Mo(1)-Mo(2)	54.49(3)
S(3)-Mo(1)-Mo(2)	135.57(4)
S(4)-Mo(1)-Mo(2)	140.22(3)
N(2)-Mo(2)-O(2)	172.72(17)
N(2)-Mo(2)-S(2)	98.31(14)
O(2)-Mo(2)-S(2)	86.58(10)
N(2)-Mo(2)-S(1)	97.04(14)
O(2)-Mo(2)-S(1)	76.34(10)
S(2)-Mo(2)-S(1)	106.26(5)
N(2)-Mo(2)-S(5)	100.22(14)
O(2)-Mo(2)-S(5)	85.58(10)
S(2)-Mo(2)-S(5)	84.17(5)
S(1)-Mo(2)-S(5)	158.32(4)
N(2)-Mo(2)-S(6)	97.70(14)
O(2)-Mo(2)-S(6)	79.10(10)
S(2)-Mo(2)-S(6)	157.96(5)
S(1)-Mo(2)-S(6)	86.65(4)
S(5)-Mo(2)-S(6)	78.15(4)
N(2)-Mo(2)-Mo(1)	97.00(13)
O(2)-Mo(2)-Mo(1)	81.61(9)
S(2)-Mo(2)-Mo(1)	52.86(3)
S(1)-Mo(2)-Mo(1)	53.85(3)
S(5)-Mo(2)-Mo(1)	135.59(4)
S(6)-Mo(2)-Mo(1)	139.21(3)
O(7)-S(1)-Mo(1)	108.54(14)
O(7)-S(1)-Mo(2)	111.85(15)

Table S18, continued

Mo(1)-S(1)-Mo(2)	71.66(4)
Mo(1)-S(2)-Mo(2)	74.21(4)
P(1)-S(3)-Mo(1)	88.06(6)
P(1)-S(4)-Mo(1)	86.96(6)
P(2)-S(5)-Mo(2)	87.96(6)
P(2)-S(6)-Mo(2)	87.24(6)
O(4)-P(1)-O(3)	96.8(2)
O(4)-P(1)-S(4)	114.63(19)
O(3)-P(1)-S(4)	112.39(16)
O(4)-P(1)-S(3)	112.10(18)
O(3)-P(1)-S(3)	114.34(17)
S(4)-P(1)-S(3)	106.68(8)
O(6)-P(2)-O(5)	95.77(19)
O(6)-P(2)-S(6)	114.43(16)
O(5)-P(2)-S(6)	113.37(15)
O(6)-P(2)-S(5)	112.99(16)
O(5)-P(2)-S(5)	113.70(15)
S(6)-P(2)-S(5)	106.62(8)
C(15)-O(1)-Mo(1)	125.5(3)
C(15)-O(2)-Mo(2)	126.6(3)
C(17)-O(3)-P(1)	122.3(4)
C(19A)-O(4)-P(1)	125.0(5)
C(19A)-O(4)-C(19B)	30(3)
P(1)-O(4)-C(19B)	106.6(18)
C(21)-O(5)-P(2)	121.8(3)
C(23)-O(6)-P(2)	121.4(3)
C(32)-O(7)-S(1)	112.0(3)
C(1)-N(1)-Mo(1)	175.4(4)
C(8)-N(2)-Mo(2)	174.0(4)
C(6)-C(1)-N(1)	119.7(5)
C(6)-C(1)-C(2)	119.9(5)
N(1)-C(1)-C(2)	120.4(5)
C(3)-C(2)-C(1)	120.1(5)
C(3)-C(2)-H(2)	120.0
C(1)-C(2)-H(2)	120.0
C(2)-C(3)-C(4)	121.3(6)
C(2)-C(3)-H(3)	119.3
C(4)-C(3)-H(3)	119.3
C(5)-C(4)-C(3)	118.4(5)
C(5)-C(4)-C(7)	120.0(6)
C(3)-C(4)-C(7)	121.7(6)
C(4)-C(5)-C(6)	122.0(5)
C(4)-C(5)-H(5)	119.0
C(6)-C(5)-H(5)	119.0

Table S18, continued

C(1)-C(6)-C(5)	118.3(5)
C(1)-C(6)-H(6)	120.9
C(5)-C(6)-H(6)	120.9
C(4)-C(7)-H(7A)	109.5
C(4)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(4)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(13)-C(8)-N(2)	119.1(4)
C(13)-C(8)-C(9)	120.0(5)
N(2)-C(8)-C(9)	120.9(4)
C(10)-C(9)-C(8)	119.3(5)
C(10)-C(9)-H(9)	120.3
C(8)-C(9)-H(9)	120.3
C(9)-C(10)-C(11)	121.6(5)
C(9)-C(10)-H(10)	119.2
C(11)-C(10)-H(10)	119.2
C(12)-C(11)-C(10)	118.3(5)
C(12)-C(11)-C(14)	121.5(5)
C(10)-C(11)-C(14)	120.2(5)
C(13)-C(12)-C(11)	121.0(5)
C(13)-C(12)-H(12)	119.5
C(11)-C(12)-H(12)	119.5
C(12)-C(13)-C(8)	119.7(5)
C(12)-C(13)-H(13)	120.1
C(8)-C(13)-H(13)	120.1
C(11)-C(14)-H(14A)	109.5
C(11)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(11)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
O(3)-C(17)-C(18)	114.3(5)
O(3)-C(17)-H(15A)	108.7
C(18)-C(17)-H(15A)	108.7
O(3)-C(17)-H(15B)	108.7
C(18)-C(17)-H(15B)	108.7
H(15A)-C(17)-H(15B)	107.6
C(17)-C(18)-H(16A)	109.5
C(17)-C(18)-H(16B)	109.5
H(16A)-C(18)-H(16B)	109.5
C(17)-C(18)-H(16C)	109.5
H(16A)-C(18)-H(16C)	109.5

Table S18, continued

H(16B)-C(18)-H(16C)	109.5
O(4)-C(19A)-C(20A)	113.0(8)
O(4)-C(19A)-H(17A)	109.0
C(20A)-C(19A)-H(17A)	109.0
O(4)-C(19A)-H(17B)	109.0
C(20A)-C(19A)-H(17B)	109.0
H(17A)-C(19A)-H(17B)	107.8
C(19A)-C(20A)-H(18A)	109.5
C(19A)-C(20A)-H(18B)	109.5
H(18A)-C(20A)-H(18B)	109.5
C(19A)-C(20A)-H(18C)	109.5
H(18A)-C(20A)-H(18C)	109.5
H(18B)-C(20A)-H(18C)	109.5
C(20B)-C(19B)-O(4)	103.(4)
C(20B)-C(19B)-H(17C)	111.2
O(4)-C(19B)-H(17C)	111.2
C(20B)-C(19B)-H(17D)	111.2
O(4)-C(19B)-H(17D)	111.2
H(17C)-C(19B)-H(17D)	109.1
C(19B)-C(20B)-H(18D)	109.5
C(19B)-C(20B)-H(18E)	109.5
H(18D)-C(20B)-H(18E)	109.5
C(19B)-C(20B)-H(18F)	109.5
H(18D)-C(20B)-H(18F)	109.5
H(18E)-C(20B)-H(18F)	109.5
O(5)-C(21)-C(22)	105.8(5)
O(5)-C(21)-H(19A)	110.6
C(22)-C(21)-H(19A)	110.6
O(5)-C(21)-H(19B)	110.6
C(22)-C(21)-H(19B)	110.6
H(19A)-C(21)-H(19B)	108.7
C(21)-C(22)-H(20A)	109.5
C(21)-C(22)-H(20B)	109.5
H(20A)-C(22)-H(20B)	109.5
C(21)-C(22)-H(20C)	109.5
H(20A)-C(22)-H(20C)	109.5
H(20B)-C(22)-H(20C)	109.5
O(6)-C(23)-C(24)	107.8(5)
O(6)-C(23)-H(21A)	110.1
C(24)-C(23)-H(21A)	110.1
O(6)-C(23)-H(21B)	110.1
C(24)-C(23)-H(21B)	110.2
H(21A)-C(23)-H(21B)	108.5
C(23)-C(24)-H(22A)	109.5

Table S18, continued

C(23)-C(24)-H(22B)	109.5
H(22A)-C(24)-H(22B)	109.5
C(23)-C(24)-H(22C)	109.5
H(22A)-C(24)-H(22C)	109.5
H(22B)-C(24)-H(22C)	109.5
O(2)-C(15)-O(1)	123.2(5)
O(2)-C(15)-C(16)	117.7(5)
O(1)-C(15)-C(16)	119.0(5)
C(15)-C(16)-H(24A)	109.5
C(15)-C(16)-H(24B)	109.5
H(24A)-C(16)-H(24B)	109.5
C(15)-C(16)-H(24C)	109.5
H(24A)-C(16)-H(24C)	109.5
H(24B)-C(16)-H(24C)	109.5
O(7)-C(32)-C(33)	108.4(5)
O(7)-C(32)-H(25A)	110.0
C(33)-C(32)-H(25A)	110.0
O(7)-C(32)-H(25B)	110.0
C(33)-C(32)-H(25B)	110.0
H(25A)-C(32)-H(25B)	108.4
C(32)-C(33)-H(26A)	109.5
C(32)-C(33)-H(26B)	109.5
H(26A)-C(33)-H(26B)	109.5
C(32)-C(33)-H(26C)	109.5
H(26A)-C(33)-H(26C)	109.5
H(26B)-C(33)-H(26C)	109.5

Table 19. Anisotropic displacement parameters ($Å^2 x\ 10^3$). The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	31(1)	26(1)	20(1)	-1(1)	2(1)	-2(1)
Mo(2)	30(1)	20(1)	22(1)	1(1)	4(1)	1(1)
S(1)	32(1)	22(1)	22(1)	1(1)	2(1)	-2(1)
S(2)	38(1)	33(1)	24(1)	-4(1)	5(1)	-2(1)
S(3)	40(1)	54(1)	23(1)	2(1)	3(1)	-5(1)
S(4)	33(1)	38(1)	26(1)	1(1)	5(1)	2(1)
S(5)	36(1)	32(1)	28(1)	1(1)	8(1)	-2(1)
S(6)	34(1)	33(1)	23(1)	1(1)	3(1)	1(1)
P(1)	34(1)	38(1)	30(1)	7(1)	0(1)	-2(1)
P(2)	32(1)	25(1)	29(1)	2(1)	2(1)	2(1)
O(1)	33(2)	29(2)	34(2)	1(2)	-2(2)	3(2)
O(2)	34(2)	20(2)	40(2)	2(2)	-3(2)	1(2)
O(3)	40(2)	47(2)	35(2)	8(2)	-4(2)	-6(2)
O(4)	46(2)	44(2)	55(3)	21(2)	0(2)	2(2)
O(5)	33(2)	27(2)	38(2)	4(2)	-1(2)	6(2)
O(6)	34(2)	24(2)	42(2)	-3(2)	-1(2)	2(2)
O(7)	59(3)	29(2)	28(2)	1(2)	7(2)	-6(2)
N(1)	31(2)	31(2)	26(2)	-9(2)	1(2)	-3(2)
N(2)	27(2)	24(2)	29(2)	0(2)	3(2)	-1(2)
C(1)	28(3)	25(2)	33(3)	-7(2)	1(2)	0(2)
C(2)	33(3)	32(3)	47(3)	-4(3)	8(2)	0(2)
C(3)	33(3)	36(3)	55(4)	-1(3)	3(3)	-7(2)
C(4)	37(3)	32(3)	50(4)	-1(3)	-14(3)	2(2)
C(5)	53(4)	30(3)	42(3)	-16(3)	-16(3)	21(3)
C(6)	35(3)	44(3)	32(3)	-6(3)	-1(2)	5(3)
C(7)	57(4)	30(3)	79(5)	-4(3)	-18(4)	-5(3)
C(8)	26(2)	23(2)	28(3)	3(2)	-2(2)	1(2)
C(9)	40(3)	32(3)	32(3)	-2(2)	12(2)	3(2)
C(10)	36(3)	27(3)	34(3)	6(2)	9(2)	0(2)
C(11)	31(3)	21(2)	34(3)	2(2)	-7(2)	2(2)
C(12)	36(3)	34(3)	28(3)	-3(2)	1(2)	11(2)
C(13)	33(3)	30(3)	27(3)	5(2)	8(2)	2(2)
C(14)	49(3)	24(3)	42(3)	2(2)	-2(3)	6(2)
C(17)	58(4)	42(3)	44(4)	-9(3)	6(3)	-12(3)
C(18)	81(5)	56(4)	44(4)	-9(3)	-1(3)	5(4)
C(19A)	65(6)	36(5)	70(7)	5(4)	19(5)	-7(4)
C(20A)	67(6)	40(5)	84(7)	11(5)	13(5)	6(5)
C(21)	47(3)	27(3)	49(4)	9(3)	10(3)	3(2)
C(22)	51(4)	42(3)	52(4)	17(3)	3(3)	9(3)
C(23)	37(3)	28(3)	65(4)	-3(3)	-2(3)	7(2)

Table S19, continued

C(24)	53(4)	35(3)	47(4)	11(3)	-2(3)	0(3)
C(15)	37(3)	27(2)	27(3)	3(2)	8(2)	2(2)
C(16)	39(3)	25(3)	46(3)	6(2)	5(3)	1(2)
C(32)	73(4)	44(3)	26(3)	5(3)	7(3)	-7(3)
C(33)	94(5)	37(3)	42(4)	7(3)	33(4)	6(3)

Table S20. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3).

	x	y	z	U(eq)
H(2)	3902	5689	3808	44
H(3)	4122	6827	3539	50
H(5)	3039	7294	6627	53
H(6)	2779	6145	6900	45
H(7A)	3320	8161	4564	87
H(7B)	4037	7982	4166	87
H(7C)	3938	8109	5793	87
H(9)	2165	5937	2387	41
H(10)	2117	7105	2421	39
H(12)	1022	7042	5657	39
H(13)	1066	5868	5645	36
H(14A)	1252	8130	3319	59
H(14B)	2016	8133	3976	59
H(14C)	1459	8118	5011	59
H(15A)	4971	5069	6449	58
H(15B)	5561	5208	7705	58
H(16A)	4201	5396	7964	92
H(16B)	4713	5995	7811	92
H(16C)	4792	5537	9218	92
H(17A)	4067	2668	8505	67
H(17B)	4760	2286	8831	67
H(18A)	4002	2421	6162	95
H(18B)	4139	1737	7058	95
H(18C)	4727	2100	6396	95
H(17C)	4000	2464	7956	147
H(17D)	4066	2690	6344	147
H(18D)	4968	2031	6258	91
H(18E)	4534	1562	7148	91
H(18F)	5132	1994	7958	91
H(19A)	37	4906	1606	49
H(19B)	-337	4984	2987	49
H(20A)	-977	4623	216	73
H(20B)	-1035	5351	926	73
H(20C)	-1348	4702	1589	73
H(21A)	787	2444	4172	53
H(21B)	790	2217	2544	53
H(22A)	-217	1876	4221	68
H(22B)	321	1357	3779	68
H(22C)	-230	1663	2587	68
H(24A)	2149	1937	5710	55
H(24B)	2896	1915	5381	55

Table S20, continued

H(24C)	2300	1896	4098	55
H(25A)	2196	4805	690	57
H(25B)	2834	4379	409	57
H(26A)	2841	5815	652	83
H(26B)	2743	5432	-850	83
H(26C)	3426	5365	188	83

Table S21. Torsion angles [°]

O(1)-Mo(1)-Mo(2)-N(2)	-173.37(17)
S(2)-Mo(1)-Mo(2)-N(2)	95.14(14)
S(1)-Mo(1)-Mo(2)-N(2)	-93.62(14)
S(3)-Mo(1)-Mo(2)-N(2)	110.07(15)
S(4)-Mo(1)-Mo(2)-N(2)	-110.03(15)
N(1)-Mo(1)-Mo(2)-O(2)	169.39(17)
O(1)-Mo(1)-Mo(2)-O(2)	-0.57(14)
S(2)-Mo(1)-Mo(2)-O(2)	-92.06(11)
S(1)-Mo(1)-Mo(2)-O(2)	79.17(10)
S(3)-Mo(1)-Mo(2)-O(2)	-77.14(11)
S(4)-Mo(1)-Mo(2)-O(2)	62.77(11)
N(1)-Mo(1)-Mo(2)-S(2)	-98.55(14)
O(1)-Mo(1)-Mo(2)-S(2)	91.49(10)
S(1)-Mo(1)-Mo(2)-S(2)	171.24(6)
S(3)-Mo(1)-Mo(2)-S(2)	14.93(7)
S(4)-Mo(1)-Mo(2)-S(2)	154.83(7)
N(1)-Mo(1)-Mo(2)-S(1)	90.21(14)
O(1)-Mo(1)-Mo(2)-S(1)	-79.75(10)
S(2)-Mo(1)-Mo(2)-S(1)	-171.24(6)
S(3)-Mo(1)-Mo(2)-S(1)	-156.31(7)
S(4)-Mo(1)-Mo(2)-S(1)	-16.40(6)
N(1)-Mo(1)-Mo(2)-S(5)	-115.79(14)
O(1)-Mo(1)-Mo(2)-S(5)	74.25(11)
S(2)-Mo(1)-Mo(2)-S(5)	-17.24(6)
S(1)-Mo(1)-Mo(2)-S(5)	154.00(6)
S(3)-Mo(1)-Mo(2)-S(5)	-2.31(8)
S(4)-Mo(1)-Mo(2)-S(5)	137.59(7)
N(1)-Mo(1)-Mo(2)-S(6)	107.01(15)
O(1)-Mo(1)-Mo(2)-S(6)	-62.95(11)
S(2)-Mo(1)-Mo(2)-S(6)	-154.44(7)
S(1)-Mo(1)-Mo(2)-S(6)	16.79(6)
S(3)-Mo(1)-Mo(2)-S(6)	-139.52(7)
S(4)-Mo(1)-Mo(2)-S(6)	0.39(8)
N(1)-Mo(1)-S(1)-O(7)	11.6(2)
O(1)-Mo(1)-S(1)-O(7)	-162.80(18)
S(2)-Mo(1)-S(1)-O(7)	114.90(16)
S(3)-Mo(1)-S(1)-O(7)	-125.80(19)
S(4)-Mo(1)-S(1)-O(7)	-82.82(16)
Mo(2)-Mo(1)-S(1)-O(7)	107.60(16)
N(1)-Mo(1)-S(1)-Mo(2)	-95.99(14)
O(1)-Mo(1)-S(1)-Mo(2)	89.59(10)
S(2)-Mo(1)-S(1)-Mo(2)	7.30(5)
S(3)-Mo(1)-S(1)-Mo(2)	126.60(13)
S(4)-Mo(1)-S(1)-Mo(2)	169.58(4)

Table S21, continued

N(2)-Mo(2)-S(1)-O(7)	-9.6(2)
O(2)-Mo(2)-S(1)-O(7)	167.31(18)
S(2)-Mo(2)-S(1)-O(7)	-110.44(15)
S(5)-Mo(2)-S(1)-O(7)	132.98(17)
S(6)-Mo(2)-S(1)-O(7)	87.72(15)
Mo(1)-Mo(2)-S(1)-O(7)	-103.18(15)
N(2)-Mo(2)-S(1)-Mo(1)	93.55(14)
O(2)-Mo(2)-S(1)-Mo(1)	-89.52(10)
S(2)-Mo(2)-S(1)-Mo(1)	-7.27(5)
S(5)-Mo(2)-S(1)-Mo(1)	-123.85(11)
S(6)-Mo(2)-S(1)-Mo(1)	-169.10(4)
N(1)-Mo(1)-S(2)-Mo(2)	90.89(14)
O(1)-Mo(1)-S(2)-Mo(2)	-82.94(9)
S(1)-Mo(1)-S(2)-Mo(2)	-7.45(5)
S(3)-Mo(1)-S(2)-Mo(2)	-169.55(5)
S(4)-Mo(1)-S(2)-Mo(2)	-134.14(11)
N(2)-Mo(2)-S(2)-Mo(1)	-92.51(14)
O(2)-Mo(2)-S(2)-Mo(1)	82.06(10)
S(1)-Mo(2)-S(2)-Mo(1)	7.36(5)
S(5)-Mo(2)-S(2)-Mo(1)	167.97(4)
S(6)-Mo(2)-S(2)-Mo(1)	131.32(12)
N(1)-Mo(1)-S(3)-P(1)	-89.61(15)
O(1)-Mo(1)-S(3)-P(1)	83.09(11)
S(2)-Mo(1)-S(3)-P(1)	170.01(7)
S(1)-Mo(1)-S(3)-P(1)	47.06(16)
S(4)-Mo(1)-S(3)-P(1)	2.98(6)
Mo(2)-Mo(1)-S(3)-P(1)	158.07(5)
N(1)-Mo(1)-S(4)-P(1)	96.85(15)
O(1)-Mo(1)-S(4)-P(1)	-91.32(11)
S(2)-Mo(1)-S(4)-P(1)	-39.04(15)
S(1)-Mo(1)-S(4)-P(1)	-168.86(7)
S(3)-Mo(1)-S(4)-P(1)	-2.98(6)
Mo(2)-Mo(1)-S(4)-P(1)	-155.55(5)
N(2)-Mo(2)-S(5)-P(2)	96.99(15)
O(2)-Mo(2)-S(5)-P(2)	-78.59(11)
S(2)-Mo(2)-S(5)-P(2)	-165.59(6)
S(1)-Mo(2)-S(5)-P(2)	-45.24(14)
S(6)-Mo(2)-S(5)-P(2)	1.18(6)
Mo(1)-Mo(2)-S(5)-P(2)	-151.85(5)
N(2)-Mo(2)-S(6)-P(2)	-100.08(14)
O(2)-Mo(2)-S(6)-P(2)	86.54(11)
S(2)-Mo(2)-S(6)-P(2)	36.17(15)
S(1)-Mo(2)-S(6)-P(2)	163.26(6)
S(5)-Mo(2)-S(6)-P(2)	-1.19(6)

Table S21, continued

Mo(1)-Mo(2)-S(6)-P(2)	149.75(5)
Mo(1)-S(4)-P(1)-O(4)	128.56(18)
Mo(1)-S(4)-P(1)-O(3)	-122.22(18)
Mo(1)-S(4)-P(1)-S(3)	3.85(8)
Mo(1)-S(3)-P(1)-O(4)	-130.15(19)
Mo(1)-S(3)-P(1)-O(3)	120.98(17)
Mo(1)-S(3)-P(1)-S(4)	-3.91(8)
Mo(2)-S(6)-P(2)-O(6)	-124.15(16)
Mo(2)-S(6)-P(2)-O(5)	127.40(16)
Mo(2)-S(6)-P(2)-S(5)	1.53(7)
Mo(2)-S(5)-P(2)-O(6)	124.99(16)
Mo(2)-S(5)-P(2)-O(5)	-127.22(16)
Mo(2)-S(5)-P(2)-S(6)	-1.55(8)
N(1)-Mo(1)-O(1)-C(15)	-93.7(10)
S(2)-Mo(1)-O(1)-C(15)	48.7(4)
S(1)-Mo(1)-O(1)-C(15)	-59.6(4)
S(3)-Mo(1)-O(1)-C(15)	132.6(4)
S(4)-Mo(1)-O(1)-C(15)	-148.8(4)
Mo(2)-Mo(1)-O(1)-C(15)	-4.4(4)
N(2)-Mo(2)-O(2)-C(15)	85.5(14)
S(2)-Mo(2)-O(2)-C(15)	-46.9(4)
S(1)-Mo(2)-O(2)-C(15)	60.8(4)
S(5)-Mo(2)-O(2)-C(15)	-131.3(4)
S(6)-Mo(2)-O(2)-C(15)	149.9(4)
Mo(1)-Mo(2)-O(2)-C(15)	6.0(4)
O(4)-P(1)-O(3)-C(17)	164.1(4)
S(4)-P(1)-O(3)-C(17)	43.9(5)
S(3)-P(1)-O(3)-C(17)	-77.9(4)
O(3)-P(1)-O(4)-C(19A)	158.1(6)
S(4)-P(1)-O(4)-C(19A)	-83.5(6)
S(3)-P(1)-O(4)-C(19A)	38.3(6)
O(3)-P(1)-O(4)-C(19B)	-176(3)
S(4)-P(1)-O(4)-C(19B)	-57(3)
S(3)-P(1)-O(4)-C(19B)	64(3)
O(6)-P(2)-O(5)-C(21)	-175.8(4)
S(6)-P(2)-O(5)-C(21)	-56.0(4)
S(5)-P(2)-O(5)-C(21)	66.0(4)
O(5)-P(2)-O(6)-C(23)	-179.3(4)
S(6)-P(2)-O(6)-C(23)	61.7(4)
S(5)-P(2)-O(6)-C(23)	-60.5(4)
Mo(1)-S(1)-O(7)-C(32)	-174.0(4)
Mo(2)-S(1)-O(7)-C(32)	-96.9(4)
O(1)-Mo(1)-N(1)-C(1)	-6(5)
S(2)-Mo(1)-N(1)-C(1)	-148(5)

Table S21, continued

S(1)-Mo(1)-N(1)-C(1)	-39(5)
S(3)-Mo(1)-N(1)-C(1)	127(5)
S(4)-Mo(1)-N(1)-C(1)	48(5)
Mo(2)-Mo(1)-N(1)-C(1)	-94(5)
O(2)-Mo(2)-N(2)-C(8)	-118(3)
S(2)-Mo(2)-N(2)-C(8)	14(4)
S(1)-Mo(2)-N(2)-C(8)	-94(4)
S(5)-Mo(2)-N(2)-C(8)	99(4)
S(6)-Mo(2)-N(2)-C(8)	179(100)
Mo(1)-Mo(2)-N(2)-C(8)	-39(4)
Mo(1)-N(1)-C(1)-C(6)	169(4)
Mo(1)-N(1)-C(1)-C(2)	-12(5)
C(6)-C(1)-C(2)-C(3)	0.4(8)
N(1)-C(1)-C(2)-C(3)	-178.4(5)
C(1)-C(2)-C(3)-C(4)	0.1(9)
C(2)-C(3)-C(4)-C(5)	0.3(9)
C(2)-C(3)-C(4)-C(7)	-179.6(5)
C(3)-C(4)-C(5)-C(6)	-1.1(8)
C(7)-C(4)-C(5)-C(6)	178.8(5)
N(1)-C(1)-C(6)-C(5)	177.6(5)
C(2)-C(1)-C(6)-C(5)	-1.2(8)
C(4)-C(5)-C(6)-C(1)	1.6(8)
Mo(2)-N(2)-C(8)-C(13)	-63(4)
Mo(2)-N(2)-C(8)-C(9)	114(3)
C(13)-C(8)-C(9)-C(10)	0.4(8)
N(2)-C(8)-C(9)-C(10)	-177.2(5)
C(8)-C(9)-C(10)-C(11)	0.9(8)
C(9)-C(10)-C(11)-C(12)	-2.3(8)
C(9)-C(10)-C(11)-C(14)	178.5(5)
C(10)-C(11)-C(12)-C(13)	2.3(8)
C(14)-C(11)-C(12)-C(13)	-178.5(5)
C(11)-C(12)-C(13)-C(8)	-1.0(8)
N(2)-C(8)-C(13)-C(12)	177.3(4)
C(9)-C(8)-C(13)-C(12)	-0.4(7)
P(1)-O(3)-C(17)-C(18)	79.6(6)
P(1)-O(4)-C(19A)-C(20A)	84.1(9)
C(19B)-O(4)-C(19A)-C(20A)	26(3)
C(19A)-O(4)-C(19B)-C(20B)	-75(4)
P(1)-O(4)-C(19B)-C(20B)	152(3)
P(2)-O(5)-C(21)-C(22)	167.1(4)
P(2)-O(6)-C(23)-C(24)	158.4(4)
Mo(2)-O(2)-C(15)-O(1)	-11.4(7)
Mo(2)-O(2)-C(15)-C(16)	171.8(3)
Mo(1)-O(1)-C(15)-O(2)	10.4(7)

Table S21, continued

Mo(1)-O(1)-C(15)-C(16)	-172.8(3)
S(1)-O(7)-C(32)-C(33)	-171.6(4)

Crystallographic Studies for BnS{Mo_2(P=O)}SOEt, 6.

An orange crystal 0.29 x 0.22 x 0.08 mm^3 was mounted on a CryoLoop with Paratone oil for collection of x-ray data on a Bruker SMART APEX CCD diffractometer. The SMART[1] software package (v 5.632) was used to acquire a total of 1,818 sixty-second frame ω-scan exposures of data at 100K to a 2θ max = 51.19° using monochromated Mo Kα radiation (0.71073 Å) from a sealed tube and a monocapillary. Frame data were processed using SAINT[2] (v 6.45a) to determine final unit cell parameters a = 12.940(3) Å, b = 13.775(3) Å, c = 23.200(5) Å, β = 94.521(4)°, V = 4122.6(14) $Å^3$, Z = 4 and ρ_{calcd} = 1.616 Mgm^{-3} to produce raw hkl data that were then corrected for absorption (transmission min./max. = 0.487/0.932; μ = 1.035 mm^{-1}) using SADABS[3] (v 2.10). The structure was solved by Patterson methods in the space group $P2_1/n$ using SHELXS-90[4] and refined by least squares methods on F^2 using SHELXL-99[5] incorporated into the SHELXTL[6] (v 6.14) suite of programs. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed in their geometrically generated positions and refined as a riding model. Methyl H's were included as fixed contributions with U(H) = 1.5 x Ueq (attached C atom) while the torsion angle which defines its orientation was allowed to refine on the attached C atom. Methylene and phenyl H's were included as fixed contributions with U(H) = 1.2 x Ueq (attached C atom). For all 7717 unique reflections (R(int) = 0.045) the final anisotropic full matrix least-squares refinement on F^2 for 422 variables converged at R1 = 0.0355 and wR2 = 0.0753 with a GOF of 1.02.

References

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3. G. M. Sheldrick, SADABS, V. 2.10, Area Detector Absorption Correction, University of

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5. G. M. Sheldrick, SHELXL-99, Program for the Refinement of Crystal Structures, University of Göttingen, Göttingen, Germany, 1997.

6. SHELXTL 6.14, Program Library for Structure Solution and Molecular graphics, Bruker Advanced X-ray Solutions, Madison, WI, 2000.

Table S22. Crystal data and structure refinement

Empirical formula	C31 H44 Mo2 N2 O7 P2 S6	
Formula weight	1002.86	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 12.940(3) Å	a= 90°.
	b = 13.775(3) Å	b= 94.521(4)°.
	c = 23.200(5) Å	γ = 90°.
Volume	4122.6(14) $Å^3$	
Z	4	
Density (calculated)	1.616 Mg/m^3	
Absorption coefficient	1.035 mm^{-1}	
F(000)	2040	
Crystal size	0.29 x 0.22 x 0.08 mm^3	
Crystal color, habit	orange plate	
Theta range for data collection	1.75 to 25.59°	
Index ranges	-15<=h<=15, -16<=k<=16, -28<=l<=27	
Reflections collected	30515	
Independent reflections	7717 [R(int) = 0.0453]	
Completeness to theta = 25.59°	99.7 %	
Absorption correction	SADABS	
Max. and min. transmission	0.914 and 0.787	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7717 / 0 / 422	
Goodness-of-fit on F^2	1.018	
Final R indices [I>2sigma(I)]	R1 = 0.0355, wR2 = 0.0753	
R indices (all data)	R1 = 0.0500, wR2 = 0.0806	
Largest diff. peak and hole	1.585 and -1.886 $e.Å^{-3}$	

Table S23. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	7693(1)	8939(1)	1606(1)	13(1)
Mo(2)	7349(1)	8442(1)	386(1)	13(1)
S(1)	6995(1)	10010(1)	822(1)	16(1)
S(2)	8007(1)	7362(1)	1172(1)	15(1)
S(3)	8719(1)	8258(1)	2476(1)	20(1)
S(4)	7875(1)	10411(1)	2264(1)	20(1)
S(6)	7078(1)	9285(1)	-549(1)	18(1)
S(5)	7980(1)	7196(1)	-269(1)	20(1)
P(1)	8815(1)	9612(1)	2794(1)	19(1)
P(2)	7616(1)	8091(1)	-964(1)	20(1)
O(1)	9160(2)	9385(2)	1335(1)	16(1)
O(2)	8931(2)	8973(2)	406(1)	16(1)
O(3)	8586(2)	9689(2)	3445(1)	26(1)
O(4)	9959(2)	9998(2)	2886(1)	23(1)
O(5)	6686(2)	7604(2)	-1354(1)	27(1)
O(6)	8442(2)	8281(2)	-1350(1)	27(1)
O(7)	7920(2)	10731(2)	615(1)	23(1)
N(1)	6445(2)	8659(2)	1775(1)	16(1)
N(2)	6104(2)	8005(2)	441(1)	15(1)
C(1)	5428(3)	8488(3)	1890(1)	15(1)
C(6)	5217(3)	7809(2)	2314(2)	16(1)
C(5)	4199(3)	7629(3)	2420(2)	19(1)
C(4)	3378(3)	8091(3)	2105(2)	21(1)
C(3)	3601(3)	8775(3)	1693(2)	20(1)
C(2)	4618(3)	8986(3)	1590(2)	18(1)
C(7)	2278(3)	7827(3)	2204(2)	31(1)
C(8)	5147(3)	7587(3)	508(2)	33(1)
C(13)	5107(3)	6688(3)	784(2)	33(1)
C(12)	4151(3)	6275(4)	851(2)	33(1)
C(11)	3242(3)	6747(3)	659(2)	33(1)
C(10)	3295(3)	7636(3)	390(2)	33(1)
C(9)	4244(3)	8057(4)	305(2)	33(1)
C(14)	2205(3)	6287(3)	745(2)	33(1)
C(15)	9480(3)	9312(2)	831(2)	15(1)
C(16)	10573(3)	9608(3)	759(2)	22(1)
C(17)	7590(3)	9386(3)	3641(2)	28(1)
C(18)	7716(3)	9405(3)	4292(2)	36(1)
C(19)	10636(3)	10054(3)	2411(2)	23(1)
C(20)	11718(3)	10223(3)	2677(2)	30(1)

Table S23, continued

C(21)	5744(3)	7249(3)	-1127(2)	37(1)
C(22)	4886(4)	7960(4)	-1235(2)	48(1)
C(25)	9419(3)	7188(3)	1151(2)	18(1)
C(26)	9736(3)	6155(3)	1256(2)	16(1)
C(27)	10090(3)	5842(3)	1807(2)	19(1)
C(28)	10457(3)	4910(3)	1895(2)	22(1)
C(29)	10486(3)	4273(3)	1438(2)	23(1)
C(30)	10114(3)	4571(3)	890(2)	23(1)
C(31)	9738(3)	5501(3)	800(2)	20(1)
C(32)	8031(4)	11642(3)	932(2)	36(1)
C(33)	9038(4)	12080(3)	781(3)	60(2)

Table S24. Bond lengths [Å]

Mo(1)-N(1)	1.735(3)
Mo(1)-O(1)	2.135(2)
Mo(1)-S(2)	2.4416(10)
Mo(1)-S(1)	2.4566(9)
Mo(1)-S(3)	2.5092(10)
Mo(1)-S(4)	2.5386(10)
Mo(1)-Mo(2)	2.9109(7)
Mo(2)-N(2)	1.734(3)
Mo(2)-O(2)	2.171(2)
Mo(2)-S(1)	2.4433(10)
Mo(2)-S(2)	2.4542(10)
Mo(2)-S(6)	2.4616(10)
Mo(2)-S(5)	2.4725(10)
S(1)-O(7)	1.655(3)
S(2)-C(25)	1.847(3)
S(3)-P(1)	2.0068(14)
S(4)-P(1)	1.9912(13)
S(6)-P(2)	2.0550(14)
S(5)-P(2)	2.0560(14)
P(1)-O(3)	1.566(3)
P(1)-O(4)	1.572(3)
P(2)-O(6)	1.470(3)
P(2)-O(5)	1.595(3)
O(1)-C(15)	1.275(4)
O(2)-C(15)	1.258(4)
O(3)-C(17)	1.461(5)
O(4)-C(19)	1.463(4)
O(5)-C(21)	1.451(5)
O(7)-C(32)	1.456(5)
N(1)-C(1)	1.384(4)
N(2)-C(8)	1.385(5)
C(1)-C(2)	1.392(5)
C(1)-C(6)	1.399(5)
C(6)-C(5)	1.382(5)
C(6)-H(2)	0.9500
C(5)-C(4)	1.395(5)
C(5)-H(3)	0.9500
C(4)-C(3)	1.388(5)
C(4)-C(7)	1.505(5)
C(3)-C(2)	1.386(5)
C(3)-H(5)	0.9500
C(2)-H(6)	0.9500
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800

Table S24, continued

C(7)-H(7C)	0.9800
C(8)-C(9)	1.386(6)
C(8)-C(13)	1.397(6)
C(13)-C(12)	1.382(5)
C(13)-H(9)	0.9500
C(12)-C(11)	1.386(6)
C(12)-H(10)	0.9500
C(11)-C(10)	1.379(6)
C(11)-C(14)	1.511(5)
C(10)-C(9)	1.386(5)
C(10)-H(12)	0.9500
C(9)-H(13)	0.9500
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-C(16)	1.493(5)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-C(18)	1.508(5)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-C(20)	1.503(5)
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-C(22)	1.487(6)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(25)-C(26)	1.495(5)
C(25)-H(23A)	0.9900
C(25)-H(23B)	0.9900
C(26)-C(31)	1.390(5)
C(26)-C(27)	1.391(5)
C(27)-C(28)	1.379(5)
C(27)-H(25)	0.9500

Table S24, continued

C(28)-C(29)	1.380(5)
C(28)-H(26)	0.9500
C(29)-C(30)	1.386(5)
C(29)-H(27)	0.9500
C(30)-C(31)	1.380(5)
C(30)-H(28)	0.9500
C(31)-H(29)	0.9500
C(32)-C(33)	1.502(6)
C(32)-H(30A)	0.9900
C(32)-H(30B)	0.9900
C(33)-H(31A)	0.9800
C(33)-H(31B)	0.9800
C(33)-H(31C)	0.9800

Table S25. Bond angles [°]

N(1)-Mo(1)-O(1)	174.20(11)
N(1)-Mo(1)-S(2)	94.82(10)
O(1)-Mo(1)-S(2)	87.37(7)
N(1)-Mo(1)-S(1)	90.36(10)
O(1)-Mo(1)-S(1)	83.86(7)
S(2)-Mo(1)-S(1)	107.04(3)
N(1)-Mo(1)-S(3)	100.26(10)
O(1)-Mo(1)-S(3)	85.29(7)
S(2)-Mo(1)-S(3)	84.48(3)
S(1)-Mo(1)-S(3)	163.74(3)
N(1)-Mo(1)-S(4)	94.87(10)
O(1)-Mo(1)-S(4)	84.53(7)
S(2)-Mo(1)-S(4)	161.47(3)
S(1)-Mo(1)-S(4)	88.65(3)
S(3)-Mo(1)-S(4)	78.28(3)
N(1)-Mo(1)-Mo(2)	95.39(9)
O(1)-Mo(1)-Mo(2)	81.56(6)
S(2)-Mo(1)-Mo(2)	53.72(2)
S(1)-Mo(1)-Mo(2)	53.34(2)
S(3)-Mo(1)-Mo(2)	136.45(3)
S(4)-Mo(1)-Mo(2)	140.56(2)
N(2)-Mo(2)-O(2)	174.55(11)
N(2)-Mo(2)-S(1)	94.09(10)
O(2)-Mo(2)-S(1)	84.30(7)
N(2)-Mo(2)-S(2)	90.29(9)
O(2)-Mo(2)-S(2)	85.22(6)
S(1)-Mo(2)-S(2)	107.07(3)
N(2)-Mo(2)-S(6)	99.18(9)
O(2)-Mo(2)-S(6)	85.93(6)
S(1)-Mo(2)-S(6)	85.98(3)
S(2)-Mo(2)-S(6)	163.38(3)
N(2)-Mo(2)-S(5)	99.06(10)
O(2)-Mo(2)-S(5)	83.71(7)
S(1)-Mo(2)-S(5)	161.72(3)
S(2)-Mo(2)-S(5)	85.61(3)
S(6)-Mo(2)-S(5)	79.46(3)
N(2)-Mo(2)-Mo(1)	94.73(9)
O(2)-Mo(2)-Mo(1)	80.10(6)
S(1)-Mo(2)-Mo(1)	53.76(2)
S(2)-Mo(2)-Mo(1)	53.32(2)
S(6)-Mo(2)-Mo(1)	138.26(3)
S(5)-Mo(2)-Mo(1)	136.68(3)
O(7)-S(1)-Mo(2)	104.30(10)
O(7)-S(1)-Mo(1)	110.07(10)

Table S25, continued

Mo(2)-S(1)-Mo(1)	72.89(3)
C(25)-S(2)-Mo(1)	108.86(12)
C(25)-S(2)-Mo(2)	110.21(12)
Mo(1)-S(2)-Mo(2)	72.96(3)
P(1)-S(3)-Mo(1)	87.78(4)
P(1)-S(4)-Mo(1)	87.30(4)
P(2)-S(6)-Mo(2)	90.32(5)
P(2)-S(5)-Mo(2)	89.99(5)
O(3)-P(1)-O(4)	95.31(14)
O(3)-P(1)-S(4)	113.94(12)
O(4)-P(1)-S(4)	114.88(11)
O(3)-P(1)-S(3)	113.98(12)
O(4)-P(1)-S(3)	113.24(11)
S(4)-P(1)-S(3)	105.68(6)
O(6)-P(2)-O(5)	106.39(15)
O(6)-P(2)-S(6)	115.61(12)
O(5)-P(2)-S(6)	109.52(11)
O(6)-P(2)-S(5)	116.87(12)
O(5)-P(2)-S(5)	107.95(12)
S(6)-P(2)-S(5)	100.19(5)
C(15)-O(1)-Mo(1)	127.4(2)
C(15)-O(2)-Mo(2)	128.0(2)
C(17)-O(3)-P(1)	121.3(2)
C(19)-O(4)-P(1)	121.9(2)
C(21)-O(5)-P(2)	123.6(2)
C(32)-O(7)-S(1)	114.6(2)
C(1)-N(1)-Mo(1)	176.4(3)
C(8)-N(2)-Mo(2)	175.1(3)
N(1)-C(1)-C(2)	120.6(3)
N(1)-C(1)-C(6)	119.4(3)
C(2)-C(1)-C(6)	120.0(3)
C(5)-C(6)-C(1)	119.2(3)
C(5)-C(6)-H(2)	120.4
C(1)-C(6)-H(2)	120.4
C(6)-C(5)-C(4)	121.4(3)
C(6)-C(5)-H(3)	119.3
C(4)-C(5)-H(3)	119.3
C(3)-C(4)-C(5)	118.7(3)
C(3)-C(4)-C(7)	121.3(3)
C(5)-C(4)-C(7)	120.0(3)
C(2)-C(3)-C(4)	120.8(3)
C(2)-C(3)-H(5)	119.6
C(4)-C(3)-H(5)	119.6
C(3)-C(2)-C(1)	119.9(3)

Table S25, continued

C(3)-C(2)-H(6)	120.1
C(1)-C(2)-H(6)	120.1
C(4)-C(7)-H(7A)	109.5
C(4)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(4)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
N(2)-C(8)-C(9)	120.3(4)
N(2)-C(8)-C(13)	119.1(4)
C(9)-C(8)-C(13)	120.6(4)
C(12)-C(13)-C(8)	118.8(4)
C(12)-C(13)-H(9)	120.6
C(8)-C(13)-H(9)	120.6
C(13)-C(12)-C(11)	121.0(4)
C(13)-C(12)-H(10)	119.5
C(11)-C(12)-H(10)	119.5
C(10)-C(11)-C(12)	119.4(4)
C(10)-C(11)-C(14)	120.6(4)
C(12)-C(11)-C(14)	120.0(4)
C(11)-C(10)-C(9)	120.8(4)
C(11)-C(10)-H(12)	119.6
C(9)-C(10)-H(12)	119.6
C(10)-C(9)-C(8)	119.3(4)
C(10)-C(9)-H(13)	120.3
C(8)-C(9)-H(13)	120.3
C(11)-C(14)-H(14A)	109.5
C(11)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(11)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
O(2)-C(15)-O(1)	122.9(3)
O(2)-C(15)-C(16)	119.6(3)
O(1)-C(15)-C(16)	117.4(3)
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
O(3)-C(17)-C(18)	106.2(3)
O(3)-C(17)-H(17A)	110.5
C(18)-C(17)-H(17A)	110.5

Table S25, continued

O(3)-C(17)-H(17B)	110.5
C(18)-C(17)-H(17B)	110.5
H(17A)-C(17)-H(17B)	108.7
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
O(4)-C(19)-C(20)	107.0(3)
O(4)-C(19)-H(19A)	110.3
C(20)-C(19)-H(19A)	110.3
O(4)-C(19)-H(19B)	110.3
C(20)-C(19)-H(19B)	110.3
H(19A)-C(19)-H(19B)	108.6
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
O(5)-C(21)-C(22)	110.8(4)
O(5)-C(21)-H(21A)	109.5
C(22)-C(21)-H(21A)	109.5
O(5)-C(21)-H(21B)	109.5
C(22)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	108.1
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(26)-C(25)-S(2)	112.2(2)
C(26)-C(25)-H(23A)	109.2
S(2)-C(25)-H(23A)	109.2
C(26)-C(25)-H(23B)	109.2
S(2)-C(25)-H(23B)	109.2
H(23A)-C(25)-H(23B)	107.9
C(31)-C(26)-C(27)	118.5(3)
C(31)-C(26)-C(25)	120.7(3)
C(27)-C(26)-C(25)	120.7(3)
C(28)-C(27)-C(26)	120.7(3)
C(28)-C(27)-H(25)	119.6

Table S25, continued

C(26)-C(27)-H(25)	119.6
C(27)-C(28)-C(29)	120.5(3)
C(27)-C(28)-H(26)	119.8
C(29)-C(28)-H(26)	119.8
C(28)-C(29)-C(30)	119.2(3)
C(28)-C(29)-H(27)	120.4
C(30)-C(29)-H(27)	120.4
C(31)-C(30)-C(29)	120.4(4)
C(31)-C(30)-H(28)	119.8
C(29)-C(30)-H(28)	119.8
C(30)-C(31)-C(26)	120.6(3)
C(30)-C(31)-H(29)	119.7
C(26)-C(31)-H(29)	119.7
O(7)-C(32)-C(33)	106.4(4)
O(7)-C(32)-H(30A)	110.5
C(33)-C(32)-H(30A)	110.5
O(7)-C(32)-H(30B)	110.5
C(33)-C(32)-H(30B)	110.5
H(30A)-C(32)-H(30B)	108.6
C(32)-C(33)-H(31A)	109.5
C(32)-C(33)-H(31B)	109.5
H(31A)-C(33)-H(31B)	109.5
C(32)-C(33)-H(31C)	109.5
H(31A)-C(33)-H(31C)	109.5
H(31B)-C(33)-H(31C)	109.5

Table S26. Anisotropic displacement parameters ($Å^2 x\ 10^3$). The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	12(1)	14(1)	13(1)	1(1)	1(1)	0(1)
Mo(2)	11(1)	15(1)	14(1)	0(1)	0(1)	-1(1)
S(1)	16(1)	15(1)	17(1)	2(1)	-1(1)	0(1)
S(2)	12(1)	15(1)	19(1)	2(1)	1(1)	0(1)
S(3)	21(1)	19(1)	18(1)	3(1)	-2(1)	2(1)
S(4)	23(1)	18(1)	18(1)	-1(1)	0(1)	3(1)
S(6)	17(1)	22(1)	15(1)	2(1)	-1(1)	-1(1)
S(5)	20(1)	22(1)	20(1)	-4(1)	2(1)	2(1)
P(1)	19(1)	22(1)	15(1)	0(1)	1(1)	0(1)
P(2)	16(1)	28(1)	15(1)	-4(1)	1(1)	-2(1)
O(1)	13(1)	18(1)	15(1)	1(1)	0(1)	-2(1)
O(2)	15(1)	18(1)	15(1)	3(1)	-1(1)	-2(1)
O(3)	23(1)	37(2)	17(1)	-2(1)	2(1)	-1(1)
O(4)	21(1)	29(2)	20(1)	-6(1)	-1(1)	-2(1)
O(5)	22(2)	37(2)	21(1)	-8(1)	-2(1)	-4(1)
O(6)	24(2)	39(2)	19(1)	-4(1)	6(1)	-4(1)
O(7)	22(1)	17(1)	29(2)	3(1)	2(1)	-5(1)
N(1)	19(2)	15(2)	14(2)	-1(1)	-2(1)	2(1)
N(2)	14(2)	18(2)	13(2)	0(1)	1(1)	1(1)
C(1)	14(2)	19(2)	14(2)	-3(1)	5(1)	-1(2)
C(6)	17(2)	16(2)	15(2)	0(1)	0(1)	1(2)
C(5)	25(2)	17(2)	16(2)	-2(2)	6(2)	-5(2)
C(4)	18(2)	20(2)	25(2)	-5(2)	6(2)	-3(2)
C(3)	21(2)	24(2)	15(2)	-4(2)	-3(2)	3(2)
C(2)	20(2)	19(2)	13(2)	0(2)	1(2)	0(2)
C(7)	19(2)	32(2)	42(3)	-2(2)	7(2)	-1(2)
C(8)	24(1)	56(1)	19(1)	-2(1)	1(1)	-14(1)
C(13)	24(1)	56(1)	19(1)	-2(1)	1(1)	-14(1)
C(12)	24(1)	56(1)	19(1)	-2(1)	1(1)	-14(1)
C(11)	24(1)	56(1)	19(1)	-2(1)	1(1)	-14(1)
C(10)	24(1)	56(1)	19(1)	-2(1)	1(1)	-14(1)
C(9)	24(1)	56(1)	19(1)	-2(1)	1(1)	-14(1)
C(14)	24(1)	56(1)	19(1)	-2(1)	1(1)	-14(1)
C(15)	14(2)	11(2)	19(2)	7(1)	1(2)	1(1)
C(16)	16(2)	31(2)	20(2)	6(2)	1(2)	-7(2)
C(17)	23(2)	38(2)	24(2)	3(2)	4(2)	0(2)
C(18)	35(3)	48(3)	26(2)	5(2)	6(2)	3(2)
C(19)	22(2)	26(2)	21(2)	-3(2)	3(2)	-1(2)
C(20)	21(2)	36(2)	31(2)	-4(2)	-1(2)	-3(2)
C(21)	26(2)	51(3)	33(2)	-12(2)	2(2)	-15(2)

Table S26, continued

C(22)	30(3)	57(3)	55(3)	-26(3)	-1(2)	-4(2)
C(25)	11(2)	20(2)	23(2)	2(2)	1(2)	0(2)
C(26)	11(2)	16(2)	22(2)	2(2)	2(1)	-1(1)
C(27)	17(2)	21(2)	20(2)	-1(2)	2(2)	-2(2)
C(28)	21(2)	24(2)	20(2)	7(2)	0(2)	3(2)
C(29)	22(2)	17(2)	29(2)	5(2)	7(2)	3(2)
C(30)	24(2)	21(2)	24(2)	-3(2)	8(2)	0(2)
C(31)	17(2)	25(2)	18(2)	4(2)	3(2)	1(2)
C(32)	55(3)	22(2)	29(2)	3(2)	-8(2)	-14(2)
C(33)	33(3)	25(3)	22(5)	3(3)	-2(3)	-7(2)

Table S27. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3)

	x	y	z	U(eq)
H(2)	5767	7477	2525	19
H(3)	4056	7181	2715	23
H(5)	3050	9103	1479	24
H(6)	4761	9469	1316	21
H(7A)	1804	8300	2009	46
H(7B)	2190	7833	2620	46
H(7C)	2122	7178	2049	46
H(9)	5727	6366	923	40
H(10)	4116	5658	1031	40
H(12)	2673	7963	260	40
H(13)	4274	8662	111	40
H(14A)	1661	6619	502	50
H(14B)	2060	6344	1152	50
H(14C)	2222	5599	637	50
H(16A)	11044	9088	900	34
H(16B)	10734	10202	981	34
H(16C)	10657	9728	349	34
H(17A)	7411	8724	3500	34
H(17B)	7034	9837	3495	34
H(18A)	8321	9016	4428	54
H(18B)	7094	9136	4447	54
H(18C)	7816	10076	4425	54
H(19A)	10418	10595	2148	27
H(19B)	10603	9442	2187	27
H(20A)	11731	10809	2916	44
H(20B)	12190	10304	2370	44
H(20C)	11939	9664	2918	44
H(21A)	5870	7135	-706	44
H(21B)	5543	6623	-1313	44
H(22A)	5044	8549	-1008	71
H(22B)	4239	7675	-1121	71
H(22C)	4810	8125	-1647	71
H(23A)	9629	7394	769	21
H(23B)	9787	7605	1449	21
H(25)	10079	6274	2125	23
H(26)	10692	4705	2274	26
H(27)	10757	3637	1498	27
H(28)	10118	4133	574	27
H(29)	9478	5696	423	24
H(30A)	8044	11523	1353	43
H(30B)	7446	12082	817	43

Table S27, continued

H(31A)	9611	11646	909	90
H(31B)	9137	12710	975	90
H(31C)	9023	12172	362	90

Table S28. Torsion angles [°]

N(1)-Mo(1)-Mo(2)-N(2)	-5.19(13)
O(1)-Mo(1)-Mo(2)-N(2)	179.78(11)
S(2)-Mo(1)-Mo(2)-N(2)	86.83(10)
S(1)-Mo(1)-Mo(2)-N(2)	-91.61(10)
S(3)-Mo(1)-Mo(2)-N(2)	105.84(10)
S(4)-Mo(1)-Mo(2)-N(2)	-109.61(10)
N(1)-Mo(1)-Mo(2)-O(2)	176.58(11)
O(1)-Mo(1)-Mo(2)-O(2)	1.55(9)
S(2)-Mo(1)-Mo(2)-O(2)	-91.40(7)
S(1)-Mo(1)-Mo(2)-O(2)	90.16(7)
S(3)-Mo(1)-Mo(2)-O(2)	-72.39(7)
S(4)-Mo(1)-Mo(2)-O(2)	72.16(7)
N(1)-Mo(1)-Mo(2)-S(1)	86.42(10)
O(1)-Mo(1)-Mo(2)-S(1)	-88.61(7)
S(2)-Mo(1)-Mo(2)-S(1)	178.44(4)
S(3)-Mo(1)-Mo(2)-S(1)	-162.55(5)
S(4)-Mo(1)-Mo(2)-S(1)	-18.00(5)
N(1)-Mo(1)-Mo(2)-S(2)	-92.03(10)
O(1)-Mo(1)-Mo(2)-S(2)	92.95(7)
S(1)-Mo(1)-Mo(2)-S(2)	-178.44(4)
S(3)-Mo(1)-Mo(2)-S(2)	19.01(4)
S(4)-Mo(1)-Mo(2)-S(2)	163.56(5)
N(1)-Mo(1)-Mo(2)-S(6)	104.27(10)
O(1)-Mo(1)-Mo(2)-S(6)	-70.76(7)
S(2)-Mo(1)-Mo(2)-S(6)	-163.71(4)
S(1)-Mo(1)-Mo(2)-S(6)	17.85(4)
S(3)-Mo(1)-Mo(2)-S(6)	-144.70(5)
S(4)-Mo(1)-Mo(2)-S(6)	-0.15(6)
N(1)-Mo(1)-Mo(2)-S(5)	-113.73(10)
O(1)-Mo(1)-Mo(2)-S(5)	71.24(7)
S(2)-Mo(1)-Mo(2)-S(5)	-21.71(4)
S(1)-Mo(1)-Mo(2)-S(5)	159.85(5)
S(3)-Mo(1)-Mo(2)-S(5)	-2.70(5)
S(4)-Mo(1)-Mo(2)-S(5)	141.85(5)
N(2)-Mo(2)-S(1)-O(7)	-160.15(13)
O(2)-Mo(2)-S(1)-O(7)	25.08(12)
S(2)-Mo(2)-S(1)-O(7)	108.28(10)
S(6)-Mo(2)-S(1)-O(7)	-61.22(10)
S(5)-Mo(2)-S(1)-O(7)	-24.11(15)
Mo(1)-Mo(2)-S(1)-O(7)	106.98(10)
N(2)-Mo(2)-S(1)-Mo(1)	92.87(9)
O(2)-Mo(2)-S(1)-Mo(1)	-81.90(6)
S(2)-Mo(2)-S(1)-Mo(1)	1.31(3)
S(6)-Mo(2)-S(1)-Mo(1)	-168.20(3)

Table S28, continued

S(5)-Mo(2)-S(1)-Mo(1)	-131.09(10)
N(1)-Mo(1)-S(1)-O(7)	164.18(14)
O(1)-Mo(1)-S(1)-O(7)	-15.33(12)
S(2)-Mo(1)-S(1)-O(7)	-100.68(10)
S(3)-Mo(1)-S(1)-O(7)	33.09(17)
S(4)-Mo(1)-S(1)-O(7)	69.31(11)
Mo(2)-Mo(1)-S(1)-O(7)	-99.36(11)
N(1)-Mo(1)-S(1)-Mo(2)	-96.46(9)
O(1)-Mo(1)-S(1)-Mo(2)	84.03(7)
S(2)-Mo(1)-S(1)-Mo(2)	-1.31(3)
S(3)-Mo(1)-S(1)-Mo(2)	132.45(11)
S(4)-Mo(1)-S(1)-Mo(2)	168.68(3)
N(1)-Mo(1)-S(2)-C(25)	-160.75(15)
O(1)-Mo(1)-S(2)-C(25)	24.63(14)
S(1)-Mo(1)-S(2)-C(25)	107.39(13)
S(3)-Mo(1)-S(2)-C(25)	-60.88(13)
S(4)-Mo(1)-S(2)-C(25)	-39.44(17)
Mo(2)-Mo(1)-S(2)-C(25)	106.09(13)
N(1)-Mo(1)-S(2)-Mo(2)	93.16(9)
O(1)-Mo(1)-S(2)-Mo(2)	-81.46(6)
S(1)-Mo(1)-S(2)-Mo(2)	1.31(3)
S(3)-Mo(1)-S(2)-Mo(2)	-166.97(3)
S(4)-Mo(1)-S(2)-Mo(2)	-145.53(9)
N(2)-Mo(2)-S(2)-C(25)	159.99(16)
O(2)-Mo(2)-S(2)-C(25)	-23.11(14)
S(1)-Mo(2)-S(2)-C(25)	-105.64(13)
S(6)-Mo(2)-S(2)-C(25)	34.91(18)
S(5)-Mo(2)-S(2)-C(25)	60.93(13)
Mo(1)-Mo(2)-S(2)-C(25)	-104.33(13)
N(2)-Mo(2)-S(2)-Mo(1)	-95.68(9)
O(2)-Mo(2)-S(2)-Mo(1)	81.22(7)
S(1)-Mo(2)-S(2)-Mo(1)	-1.31(3)
S(6)-Mo(2)-S(2)-Mo(1)	139.24(10)
S(5)-Mo(2)-S(2)-Mo(1)	165.26(3)
N(1)-Mo(1)-S(3)-P(1)	-99.45(10)
O(1)-Mo(1)-S(3)-P(1)	78.83(7)
S(2)-Mo(1)-S(3)-P(1)	166.64(4)
S(1)-Mo(1)-S(3)-P(1)	30.56(13)
S(4)-Mo(1)-S(3)-P(1)	-6.55(4)
Mo(2)-Mo(1)-S(3)-P(1)	151.34(4)
N(1)-Mo(1)-S(4)-P(1)	106.09(10)
O(1)-Mo(1)-S(4)-P(1)	-79.70(7)
S(2)-Mo(1)-S(4)-P(1)	-15.21(12)

Table S28, continued

S(1)-Mo(1)-S(4)-P(1)	-163.66(4)
S(3)-Mo(1)-S(4)-P(1)	6.60(4)
Mo(2)-Mo(1)-S(4)-P(1)	-149.31(4)
N(2)-Mo(2)-S(6)-P(2)	-96.20(10)
O(2)-Mo(2)-S(6)-P(2)	85.74(7)
S(1)-Mo(2)-S(6)-P(2)	170.30(4)
S(2)-Mo(2)-S(6)-P(2)	27.81(13)
S(5)-Mo(2)-S(6)-P(2)	1.39(4)
Mo(1)-Mo(2)-S(6)-P(2)	155.95(3)
N(2)-Mo(2)-S(5)-P(2)	96.34(10)
O(2)-Mo(2)-S(5)-P(2)	-88.40(7)
S(1)-Mo(2)-S(5)-P(2)	-39.14(12)
S(2)-Mo(2)-S(5)-P(2)	-174.06(4)
S(6)-Mo(2)-S(5)-P(2)	-1.39(4)
Mo(1)-Mo(2)-S(5)-P(2)	-156.75(3)
Mo(1)-S(4)-P(1)-O(3)	-134.31(12)
Mo(1)-S(4)-P(1)-O(4)	117.18(11)
Mo(1)-S(4)-P(1)-S(3)	-8.41(5)
Mo(1)-S(3)-P(1)-O(3)	134.38(12)
Mo(1)-S(3)-P(1)-O(4)	-118.09(11)
Mo(1)-S(3)-P(1)-S(4)	8.51(5)
Mo(2)-S(6)-P(2)-O(6)	-128.21(13)
Mo(2)-S(6)-P(2)-O(5)	111.66(12)
Mo(2)-S(6)-P(2)-S(5)	-1.67(5)
Mo(2)-S(5)-P(2)-O(6)	127.36(13)
Mo(2)-S(5)-P(2)-O(5)	-112.86(11)
Mo(2)-S(5)-P(2)-S(6)	1.67(5)
N(1)-Mo(1)-O(1)-C(15)	-61.0(12)
S(2)-Mo(1)-O(1)-C(15)	51.3(3)
S(1)-Mo(1)-O(1)-C(15)	-56.2(3)
S(3)-Mo(1)-O(1)-C(15)	136.0(3)
S(4)-Mo(1)-O(1)-C(15)	-145.4(3)
Mo(2)-Mo(1)-O(1)-C(15)	-2.4(3)
N(2)-Mo(2)-O(2)-C(15)	-20.7(13)
S(1)-Mo(2)-O(2)-C(15)	52.3(3)
S(2)-Mo(2)-O(2)-C(15)	-55.4(3)
S(6)-Mo(2)-O(2)-C(15)	138.7(3)
S(5)-Mo(2)-O(2)-C(15)	-141.5(3)
Mo(1)-Mo(2)-O(2)-C(15)	-1.8(3)
O(4)-P(1)-O(3)-C(17)	-178.2(3)
S(4)-P(1)-O(3)-C(17)	61.6(3)
S(3)-P(1)-O(3)-C(17)	-59.8(3)
O(3)-P(1)-O(4)-C(19)	177.0(3)

Table S28, continued

S(4)-P(1)-O(4)-C(19)	-63.5(3)
S(3)-P(1)-O(4)-C(19)	58.1(3)
O(6)-P(2)-O(5)-C(21)	176.0(3)
S(6)-P(2)-O(5)-C(21)	-58.4(3)
S(5)-P(2)-O(5)-C(21)	49.8(3)
Mo(2)-S(1)-O(7)-C(32)	-165.7(2)
Mo(1)-S(1)-O(7)-C(32)	-89.0(3)
O(1)-Mo(1)-N(1)-C(1)	-13(5)
S(2)-Mo(1)-N(1)-C(1)	-125(4)
S(1)-Mo(1)-N(1)-C(1)	-18(4)
S(3)-Mo(1)-N(1)-C(1)	150(4)
S(4)-Mo(1)-N(1)-C(1)	71(4)
Mo(2)-Mo(1)-N(1)-C(1)	-71(4)
O(2)-Mo(2)-N(2)-C(8)	-54(4)
S(1)-Mo(2)-N(2)-C(8)	-127(3)
S(2)-Mo(2)-N(2)-C(8)	-20(3)
S(6)-Mo(2)-N(2)-C(8)	147(3)
S(5)-Mo(2)-N(2)-C(8)	66(3)
Mo(1)-Mo(2)-N(2)-C(8)	-73(3)
Mo(1)-N(1)-C(1)-C(2)	13(4)
Mo(1)-N(1)-C(1)-C(6)	-167(4)
N(1)-C(1)-C(6)-C(5)	-178.9(3)
C(2)-C(1)-C(6)-C(5)	1.3(5)
C(1)-C(6)-C(5)-C(4)	1.7(5)
C(6)-C(5)-C(4)-C(3)	-2.8(5)
C(6)-C(5)-C(4)-C(7)	175.9(3)
C(5)-C(4)-C(3)-C(2)	1.1(5)
C(7)-C(4)-C(3)-C(2)	-177.6(3)
C(4)-C(3)-C(2)-C(1)	1.8(5)
N(1)-C(1)-C(2)-C(3)	177.2(3)
C(6)-C(1)-C(2)-C(3)	-3.0(5)
Mo(2)-N(2)-C(8)-C(9)	179(100)
Mo(2)-N(2)-C(8)-C(13)	0(3)
N(2)-C(8)-C(13)-C(12)	179.9(4)
C(9)-C(8)-C(13)-C(12)	0.0(6)
C(8)-C(13)-C(12)-C(11)	-1.2(6)
C(13)-C(12)-C(11)-C(10)	1.0(6)
C(13)-C(12)-C(11)-C(14)	-179.1(4)
C(12)-C(11)-C(10)-C(9)	0.5(6)
C(14)-C(11)-C(10)-C(9)	-179.5(4)
C(11)-C(10)-C(9)-C(8)	-1.6(6)
N(2)-C(8)-C(9)-C(10)	-178.5(4)
C(13)-C(8)-C(9)-C(10)	1.4(6)

Table S28, continued

Mo(2)-O(2)-C(15)-O(1)	0.7(5)
Mo(2)-O(2)-C(15)-C(16)	177.8(2)
Mo(1)-O(1)-C(15)-O(2)	1.8(5)
Mo(1)-O(1)-C(15)-C(16)	-175.4(2)
P(1)-O(3)-C(17)-C(18)	170.8(3)
P(1)-O(4)-C(19)-C(20)	-166.9(3)
P(2)-O(5)-C(21)-C(22)	100.5(4)
Mo(1)-S(2)-C(25)-C(26)	144.1(2)
Mo(2)-S(2)-C(25)-C(26)	-137.6(2)
S(2)-C(25)-C(26)-C(31)	88.0(4)
S(2)-C(25)-C(26)-C(27)	-95.6(3)
C(31)-C(26)-C(27)-C(28)	1.5(5)
C(25)-C(26)-C(27)-C(28)	-175.0(3)
C(26)-C(27)-C(28)-C(29)	0.4(6)
C(27)-C(28)-C(29)-C(30)	-1.8(6)
C(28)-C(29)-C(30)-C(31)	1.3(6)
C(29)-C(30)-C(31)-C(26)	0.7(6)
C(27)-C(26)-C(31)-C(30)	-2.0(5)
C(25)-C(26)-C(31)-C(30)	174.5(3)
S(1)-O(7)-C(32)-C(33)	167.5(3)