- Supplementary material –

Carbon-sulfur and carbon-halogen bond cleavage of acyclic or cyclic thioethers, thiophenes, and dihaloalkanes with the trithiolato-bridged cation $[Mo_2Cp_2(\mu\text{-}SMe)_3(MeCN)_2]^+$.

Wilfried-Solo Ojo, François Y. Pétillon*, P. Schollhammer*,
and Jean Talarmin.

2. X-ray crystallographic data for 4'

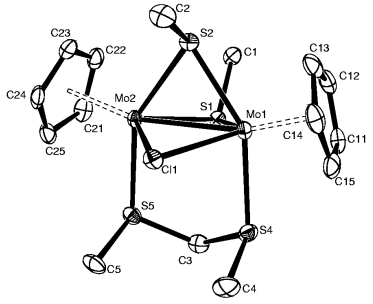


Table 1. Crystal data and structure refinement for 4'

Identification code	**4'**
Empirical formula	C15 H24 Cl F6 Mo2 P S4
Formula weight	704.88
Temperature	170(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P212121
Unit cell dimensions	a = 12.7338(3) A alpha = 90 deg. b = 13.3930(3) A beta = 90 deg. c = 13.9952(4) A gamma = 90 deg.
Volume	2386.79(10) A^3
Z, Calculated density	4, 1.962 Mg/m^3
Absorption coefficient	1.628 mm^-1
F(000)	1392
Crystal size	0.18 x 0.10 x 0.02 mm
Theta range for data collection	2.64 to 24.71 deg.
Limiting indices	-14<=h<=14, -15<=k<=15, -14<=l<=13
Reflections collected / unique	15187 / 3842 [R(int) = 0.0320]
Completeness to theta = 24.71	94.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9682 and 0.7582
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3842 / 190 / 266
Goodness-of-fit on F^2	0.990
Final R indices [I>2sigma(I)]	R1 = 0.0254, wR2 = 0.0491
R indices (all data)	R1 = 0.0371, wR2 = 0.0528
Absolute structure parameter	-0.04(4)
Largest diff. peak and hole	0.524 and -0.329 e.A^-3

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

	x	y	z	U(eq)
C(1)	1722(4)	3920(3)	5306(3)	35(1)
C(2)	-624(4)	1525(4)	3546(3)	45(1)
C(3)	4345(4)	2311(3)	3180(3)	38(1)
C(4)	4064(4)	268(4)	2869(4)	51(2)
C(5)	3645(4)	2150(4)	1288(3)	45(1)
C(11)	2713(4)	904(4)	5655(3)	41(1)
C(12)	1715(4)	1266(4)	5882(3)	43(1)
C(13)	970(5)	648(4)	5434(3)	44(1)
C(14)	1515(5)	-98(4)	4941(3)	45(1)
C(15)	2590(5)	40(4)	5079(4)	47(1)
C(21)	1769(5)	4537(3)	2457(4)	43(1)
C(22)	812(4)	4415(4)	2955(4)	43(1)
C(23)	161(4)	3794(4)	2415(4)	43(1)
C(24)	696(4)	3523(4)	1587(3)	42(1)
C(25)	1673(5)	3968(4)	1608(3)	43(1)
S(1)	2514(1)	3207(1)	4460(1)	27(1)
S(2)	363(1)	2327(1)	4087(1)	29(1)
S(4)	3880(1)	1215(1)	3779(1)	35(1)
S(5)	3503(1)	2920(1)	2337(1)	33(1)
Cl(1)	1597(1)	1128(1)	2587(1)	30(1)
Mo(1)	2015(1)	1459(1)	4299(1)	26(1)
Mo(2)	1640(1)	2947(1)	2943(1)	24(1)
P(1)	2009(1)	2858(1)	8705(1)	36(1)
F(1)	1168(3)	3696(3)	8909(4)	112(2)
F(2)	2823(3)	2017(3)	8537(3)	108(1)
F(3)	2108(4)	3238(3)	7663(2)	111(2)
F(4)	2883(3)	3589(3)	9051(2)	89(1)
F(5)	1869(4)	2457(3)	9749(2)	101(1)
F(6)	1092(3)	2128(2)	8375(2)	62(1)

Table 3. Bond lengths [A] and angles [deg] for 4'.

C(1)-S(1)	1.825(5)
C(2)-S(2)	1.818(4)
C(3)-S(4)	1.790(5)
C(3)-S(5)	1.791(5)
C(4)-S(4)	1.813(5)
C(5)-S(5)	1.804(4)
C(11)-C(12)	1.397(7)
C(11)-C(15)	1.418(7)
C(11)-Mo(1)	2.223(5)
C(12)-C(13)	1.407(7)
C(12)-Mo(1)	2.262(4)
C(13)-C(14)	1.398(7)
C(13)-Mo(1)	2.339(5)
C(14)-C(15)	1.395(8)
C(14)-Mo(1)	2.358(5)
C(15)-Mo(1)	2.311(5)
C(21)-C(22)	1.413(7)
C(21)-C(25)	1.417(6)
C(21)-Mo(2)	2.241(4)
C(22)-C(23)	1.397(7)
C(22)-Mo(2)	2.231(5)
C(23)-C(24)	1.393(7)
C(23)-Mo(2)	2.319(5)
C(24)-C(25)	1.380(7)
C(24)-Mo(2)	2.376(4)
C(25)-Mo(2)	2.316(4)
S(1)-Mo(2)	2.4219(12)
S(1)-Mo(1)	2.4365(12)
S(2)-Mo(1)	2.4221(13)
S(2)-Mo(2)	2.4275(12)
S(4)-Mo(1)	2.5061(13)
S(5)-Mo(2)	2.5194(12)
Cl(1)-Mo(2)	2.4878(11)
Cl(1)-Mo(1)	2.4944(11)
Mo(1)-Mo(2)	2.7929(5)
P(1)-F(2)	1.549(4)
P(1)-F(3)	1.550(3)
P(1)-F(4)	1.559(3)
P(1)-F(5)	1.567(3)
P(1)-F(1)	1.577(4)
P(1)-F(6)	1.591(3)

S(4)-C(3)-S(5)	118.9(3)
C(12)-C(11)-C(15)	108.2(5)
C(12)-C(11)-Mo(1)	73.4(3)
C(15)-C(11)-Mo(1)	75.2(3)
C(11)-C(12)-C(13)	107.9(5)
C(11)-C(12)-Mo(1)	70.3(3)
C(13)-C(12)-Mo(1)	75.2(3)
C(14)-C(13)-C(12)	107.8(5)
C(14)-C(13)-Mo(1)	73.4(3)
C(12)-C(13)-Mo(1)	69.2(3)
C(15)-C(14)-C(13)	108.9(5)
C(15)-C(14)-Mo(1)	70.8(3)
C(13)-C(14)-Mo(1)	72.0(3)
C(14)-C(15)-C(11)	107.1(5)
C(14)-C(15)-Mo(1)	74.5(3)
C(11)-C(15)-Mo(1)	68.4(3)
C(22)-C(21)-C(25)	106.1(5)
C(22)-C(21)-Mo(2)	71.2(3)
C(25)-C(21)-Mo(2)	74.8(3)
C(23)-C(22)-C(21)	108.3(5)
C(23)-C(22)-Mo(2)	75.6(3)
C(21)-C(22)-Mo(2)	72.0(3)
C(24)-C(23)-C(22)	108.4(5)
C(24)-C(23)-Mo(2)	75.0(3)
C(22)-C(23)-Mo(2)	68.7(3)
C(25)-C(24)-C(23)	108.0(5)
C(25)-C(24)-Mo(2)	70.5(3)
C(23)-C(24)-Mo(2)	70.5(3)
C(24)-C(25)-C(21)	109.2(5)
C(24)-C(25)-Mo(2)	75.3(3)
C(21)-C(25)-Mo(2)	69.0(2)
C(1)-S(1)-Mo(2)	112.97(15)
C(1)-S(1)-Mo(1)	114.73(16)
Mo(2)-S(1)-Mo(1)	70.18(3)
C(2)-S(2)-Mo(1)	111.56(19)
C(2)-S(2)-Mo(2)	112.99(16)
Mo(1)-S(2)-Mo(2)	70.33(4)
C(3)-S(4)-C(4)	101.7(2)
C(3)-S(4)-Mo(1)	110.05(17)
C(4)-S(4)-Mo(1)	114.67(19)
C(3)-S(5)-C(5)	102.5(2)
C(3)-S(5)-Mo(2)	110.41(16)
C(5)-S(5)-Mo(2)	112.16(17)
Mo(2)-Cl(1)-Mo(1)	68.19(3)
C(11)-Mo(1)-C(12)	36.29(18)
C(11)-Mo(1)-C(15)	36.40(18)

C(12)-Mo(1)-C(15)	59.83(19)
C(11)-Mo(1)-C(13)	59.54(19)
C(12)-Mo(1)-C(13)	35.56(17)
C(15)-Mo(1)-C(13)	58.5(2)
C(11)-Mo(1)-C(14)	59.16(19)
C(12)-Mo(1)-C(14)	58.71(18)
C(15)-Mo(1)-C(14)	34.77(19)
C(13)-Mo(1)-C(14)	34.62(18)
C(11)-Mo(1)-S(2)	127.80(14)
C(12)-Mo(1)-S(2)	91.63(15)
C(15)-Mo(1)-S(2)	136.76(16)
C(13)-Mo(1)-S(2)	79.19(14)
C(14)-Mo(1)-S(2)	103.70(17)
C(11)-Mo(1)-S(1)	97.94(14)
C(12)-Mo(1)-S(1)	93.63(13)
C(15)-Mo(1)-S(1)	131.60(16)
C(13)-Mo(1)-S(1)	122.15(13)
C(14)-Mo(1)-S(1)	152.25(12)
S(2)-Mo(1)-S(1)	77.09(4)
C(11)-Mo(1)-Cl(1)	147.73(14)
C(12)-Mo(1)-Cl(1)	152.16(14)
C(15)-Mo(1)-Cl(1)	112.02(14)
C(13)-Mo(1)-Cl(1)	116.63(14)
C(14)-Mo(1)-Cl(1)	98.69(13)
S(2)-Mo(1)-Cl(1)	77.42(4)
S(1)-Mo(1)-Cl(1)	108.38(4)
C(11)-Mo(1)-S(4)	79.95(14)
C(12)-Mo(1)-S(4)	115.47(15)
C(15)-Mo(1)-S(4)	74.32(16)
C(13)-Mo(1)-S(4)	132.54(14)
C(14)-Mo(1)-S(4)	104.58(16)
S(2)-Mo(1)-S(4)	148.21(4)
S(1)-Mo(1)-S(4)	84.53(4)
Cl(1)-Mo(1)-S(4)	84.23(4)
C(11)-Mo(1)-Mo(2)	152.46(14)
C(12)-Mo(1)-Mo(2)	135.87(14)
C(15)-Mo(1)-Mo(2)	164.14(14)
C(13)-Mo(1)-Mo(2)	134.06(14)
C(14)-Mo(1)-Mo(2)	147.53(15)
S(2)-Mo(1)-Mo(2)	54.93(3)
S(1)-Mo(1)-Mo(2)	54.67(3)
Cl(1)-Mo(1)-Mo(2)	55.79(3)
S(4)-Mo(1)-Mo(2)	93.28(3)
C(22)-Mo(2)-C(21)	36.83(19)
C(22)-Mo(2)-C(25)	59.60(19)
C(21)-Mo(2)-C(25)	36.17(16)

C(22)-Mo(2)-C(23)	35.69(17)
C(21)-Mo(2)-C(23)	59.9(2)
C(25)-Mo(2)-C(23)	57.90(19)
C(22)-Mo(2)-C(24)	58.73(18)
C(21)-Mo(2)-C(24)	59.09(19)
C(25)-Mo(2)-C(24)	34.18(18)
C(23)-Mo(2)-C(24)	34.49(17)
C(22)-Mo(2)-S(1)	94.80(13)
C(21)-Mo(2)-S(1)	95.49(13)
C(25)-Mo(2)-S(1)	127.87(14)
C(23)-Mo(2)-S(1)	125.59(13)
C(24)-Mo(2)-S(1)	152.40(14)
C(22)-Mo(2)-S(2)	88.86(14)
C(21)-Mo(2)-S(2)	125.03(15)
C(25)-Mo(2)-S(2)	138.22(15)
C(23)-Mo(2)-S(2)	80.41(14)
C(24)-Mo(2)-S(2)	107.37(14)
S(1)-Mo(2)-S(2)	77.26(4)
C(22)-Mo(2)-Cl(1)	148.71(14)
C(21)-Mo(2)-Cl(1)	150.60(13)
C(25)-Mo(2)-Cl(1)	114.65(13)
C(23)-Mo(2)-Cl(1)	113.43(14)
C(24)-Mo(2)-Cl(1)	98.43(14)
S(1)-Mo(2)-Cl(1)	109.06(4)
S(2)-Mo(2)-Cl(1)	77.45(4)
C(22)-Mo(2)-S(5)	117.38(15)
C(21)-Mo(2)-S(5)	80.93(16)
C(25)-Mo(2)-S(5)	73.73(15)
C(23)-Mo(2)-S(5)	131.61(14)
C(24)-Mo(2)-S(5)	102.24(13)
S(1)-Mo(2)-S(5)	82.22(4)
S(2)-Mo(2)-S(5)	147.97(4)
Cl(1)-Mo(2)-S(5)	86.49(4)
C(22)-Mo(2)-Mo(1)	134.80(13)
C(21)-Mo(2)-Mo(1)	150.64(13)
C(25)-Mo(2)-Mo(1)	165.12(14)
C(23)-Mo(2)-Mo(1)	134.78(13)
C(24)-Mo(2)-Mo(1)	149.43(14)
S(1)-Mo(2)-Mo(1)	55.15(3)
S(2)-Mo(2)-Mo(1)	54.75(3)
Cl(1)-Mo(2)-Mo(1)	56.02(3)
S(5)-Mo(2)-Mo(1)	93.30(3)
F(2)-P(1)-F(3)	92.4(2)
F(2)-P(1)-F(4)	91.4(2)
F(3)-P(1)-F(4)	91.6(2)
F(2)-P(1)-F(5)	88.2(3)

F(3)-P(1)-F(5)	177.9(3)
F(4)-P(1)-F(5)	90.4(2)
F(2)-P(1)-F(1)	178.0(3)
F(3)-P(1)-F(1)	89.5(3)
F(4)-P(1)-F(1)	89.0(2)
F(5)-P(1)-F(1)	89.9(3)
F(2)-P(1)-F(6)	90.0(2)
F(3)-P(1)-F(6)	89.31(19)
F(4)-P(1)-F(6)	178.2(2)
F(5)-P(1)-F(6)	88.7(2)
F(1)-P(1)-F(6)	89.5(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 4'.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	37(3)	34(3)	35(3)	-7(2)	-6(2)	3(2)
C(2)	36(3)	53(4)	46(3)	-16(3)	-2(2)	-18(3)
C(3)	35(3)	40(3)	38(3)	-10(2)	0(2)	-4(2)
C(4)	59(4)	38(3)	57(3)	-19(3)	4(3)	12(3)
C(5)	45(4)	61(4)	29(3)	-19(3)	7(2)	-5(3)
C(11)	56(3)	41(3)	26(3)	12(2)	-7(2)	-5(2)
C(12)	68(4)	40(3)	21(2)	1(2)	5(2)	0(3)
C(13)	58(3)	35(3)	39(3)	13(2)	14(2)	-5(2)
C(14)	75(4)	27(3)	34(3)	7(2)	0(3)	-14(3)
C(15)	66(3)	32(3)	42(3)	16(2)	0(3)	10(3)
C(21)	58(4)	22(2)	48(3)	4(2)	-12(3)	-6(2)
C(22)	57(3)	36(3)	36(3)	1(2)	-9(3)	18(2)
C(23)	37(3)	48(3)	44(3)	12(2)	-4(2)	12(2)
C(24)	51(3)	49(3)	25(2)	1(2)	-16(2)	9(3)
C(25)	58(3)	42(3)	29(2)	12(2)	5(2)	8(3)
S(1)	30(1)	25(1)	27(1)	-6(1)	-4(1)	-2(1)
S(2)	27(1)	27(1)	31(1)	-6(1)	1(1)	-3(1)
S(4)	35(1)	35(1)	36(1)	-4(1)	-3(1)	10(1)
S(5)	34(1)	36(1)	30(1)	-4(1)	2(1)	-5(1)
Cl(1)	36(1)	27(1)	28(1)	-10(1)	-2(1)	-2(1)
Mo(1)	34(1)	21(1)	23(1)	-1(1)	-1(1)	0(1)

Mo(2)	30(1)	21(1)	22(1)	-1(1)	-3(1)	0(1)
P(1)	43(1)	35(1)	28(1)	2(1)	-6(1)	-4(1)
F(1)	80(3)	60(3)	196(4)	-36(3)	-8(3)	23(2)
F(2)	58(3)	76(3)	190(4)	0(3)	20(3)	22(2)
F(3)	178(4)	107(3)	49(2)	32(2)	-12(2)	-58(3)
F(4)	78(3)	76(2)	113(3)	12(2)	-45(2)	-35(2)
F(5)	157(4)	101(3)	44(2)	12(2)	-9(2)	-42(3)
F(6)	61(2)	44(2)	81(2)	-2(2)	-20(2)	-9(2)

2. X-ray crystallographic data for 6'.

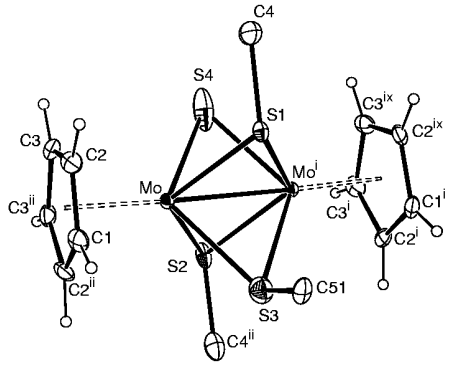


Table 1. Crystal data and structure refinement for 6'.

Identification code	**6'**
Empirical formula	C37 H39 B Mo2 S4
Formula weight	814.61
Temperature	170(2) K
Wavelength	0.71073 Å
Crystal system	Tetragonal
Space group	P -4 21 m
Unit cell dimensions	a = 14.6955(4) Å
	c = 7.7749(4) Å
Volume	1679.05(11) Å^3
Z	2
Density (calculated)	1.611 Mg/m^3
Absorption coefficient	1.023 mm^{-1}
F(000)	828
Crystal size	0.20 x 0.20 x 0.20 mm^3
Theta range for data collection	3.82 to 33.05°.
Index ranges	-22<=h<=19, -22<=k<=21, -11<=l<=11
Reflections collected	19843
Independent reflections	3185 [R(int) = 0.0497]
Completeness to theta = 33.05°	97.4 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3185 / 0 / 125
Goodness-of-fit on F^2	1.085
Final R indices [I>2sigma(I)]	R1 = 0.0500, wR2 = 0.1214
R indices (all data)	R1 = 0.0571, wR2 = 0.1248
Absolute structure parameter	0.13(8)
Largest diff. peak and hole	2.107 and -1.872 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for 6'. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo	5609(1)	9391(1)	6661(1)	19(1)
S(1)	4110(1)	9110(1)	7972(3)	25(1)
S(2)	5901(2)	10900(2)	5440(5)	37(1)
S(3)	5472(2)	10472(2)	9057(6)	55(1)
S(4)	4538(4)	9538(4)	4440(7)	84(2)
C(1)	6597(3)	8403(3)	8061(8)	36(1)
C(2)	6029(3)	7880(3)	7006(7)	36(1)
C(3)	6213(3)	8113(3)	5266(6)	37(1)
C(4)	3385(4)	8385(4)	6757(12)	53(2)
C(51)	5000	10000	11170(20)	45(6)
C(52)	5000	10000	12210(40)	63(6)
B	0	10000	5000	22(1)
C(11)	12(2)	9116(2)	6288(4)	22(1)
C(12)	669(3)	9062(3)	7593(5)	29(1)
C(13)	673(3)	8365(3)	8830(5)	36(1)
C(14)	8(3)	7692(3)	8779(5)	32(1)
C(15)	-641(3)	7730(2)	7522(5)	32(1)
C(16)	-636(3)	8419(2)	6282(4)	25(1)

Table 3. Bond lengths [Å] and angles [°] for 6'.

Mo-C(2)#1	2.320(4)
Mo-C(2)	2.320(4)
Mo-C(1)	2.325(5)
Mo-C(3)	2.344(4)
Mo-C(3)#1	2.344(4)
Mo-S(4)	2.347(6)
Mo-S(4)#2	2.347(6)
Mo-S(2)#2	2.450(2)
Mo-S(2)	2.450(2)
Mo-S(3)	2.456(4)
Mo-S(3)#2	2.456(4)
Mo-S(1)#2	2.462(2)
Mo-S(1)	2.462(2)
Mo-Mo#2	2.5304(7)
S(1)-S(3)#2	1.211(6)
S(1)-C(4)	1.779(8)
S(1)-S(2)#2	1.969(4)
S(1)-Mo#2	2.462(2)
S(2)-S(4)#2	1.197(6)
S(2)-C(4)#2	1.804(10)
S(2)-S(1)#2	1.969(4)
S(2)-Mo#2	2.450(2)
S(3)-S(1)#2	1.211(6)
S(3)-C(51)	1.911(14)
S(3)-S(3)#2	1.961(9)
S(3)-Mo#2	2.456(4)
S(4)-S(2)#2	1.197(6)
S(4)-S(4)#2	1.922(15)
S(4)-C(52)#3	1.98(2)
S(4)-Mo#2	2.347(6)
C(1)-C(2)	1.400(6)
C(1)-C(2)#1	1.400(6)
C(1)-H(1)	0.9500
C(2)-C(3)	1.421(7)
C(2)-H(2)	0.9500
C(3)-C(3)#1	1.402(9)
C(3)-H(3)	0.9500
C(4)-S(2)#2	1.804(10)
C(51)-C(52)	0.81(3)
C(51)-S(3)#2	1.911(14)
C(52)-S(4)#4	1.98(2)
C(52)-S(4)#5	1.98(2)
B-C(11)#6	1.640(3)
B-C(11)#7	1.640(3)
B-C(11)	1.640(3)
B-C(11)#8	1.640(3)
C(11)-C(16)	1.398(5)
C(11)-C(12)	1.404(5)
C(12)-C(13)	1.405(5)
C(12)-H(12)	0.9500

C(13)-C(14)	1.391(6)
C(13)-H(13)	0.9500
C(14)-C(15)	1.367(6)
C(14)-H(14)	0.9500
C(15)-C(16)	1.399(5)
C(15)-H(15)	0.9500
C(16)-H(16)	0.9500
C(2)#1-Mo-C(2)	58.5(2)
C(2)#1-Mo-C(1)	35.09(15)
C(2)-Mo-C(1)	35.09(15)
C(2)#1-Mo-C(3)	58.52(16)
C(2)-Mo-C(3)	35.47(18)
C(1)-Mo-C(3)	58.61(19)
C(2)#1-Mo-C(3)#1	35.47(18)
C(2)-Mo-C(3)#1	58.52(16)
C(1)-Mo-C(3)#1	58.61(19)
C(3)-Mo-C(3)#1	34.8(2)
C(2)#1-Mo-S(4)	138.71(16)
C(2)-Mo-S(4)	110.56(18)
C(1)-Mo-S(4)	145.18(17)
C(3)-Mo-S(4)	89.26(15)
C(3)#1-Mo-S(4)	103.41(14)
C(2)#1-Mo-S(4)#2	110.56(18)
C(2)-Mo-S(4)#2	138.71(16)
C(1)-Mo-S(4)#2	145.18(17)
C(3)-Mo-S(4)#2	103.41(14)
C(3)#1-Mo-S(4)#2	89.26(15)
S(4)-Mo-S(4)#2	48.3(3)
C(2)#1-Mo-S(2)#2	149.83(13)
C(2)-Mo-S(2)#2	96.78(12)
C(1)-Mo-S(2)#2	129.62(7)
C(3)-Mo-S(2)#2	91.34(12)
C(3)#1-Mo-S(2)#2	118.69(13)
S(4)-Mo-S(2)#2	28.80(16)
S(4)#2-Mo-S(2)#2	75.48(18)
C(2)#1-Mo-S(2)	96.78(12)
C(2)-Mo-S(2)	149.83(13)
C(1)-Mo-S(2)	129.62(7)
C(3)-Mo-S(2)	118.69(13)
C(3)#1-Mo-S(2)	91.34(11)
S(4)-Mo-S(2)	75.48(18)
S(4)#2-Mo-S(2)	28.80(16)
S(2)#2-Mo-S(2)	99.59(14)
C(2)#1-Mo-S(3)	99.37(15)
C(2)-Mo-S(3)	123.57(16)
C(1)-Mo-S(3)	95.74(16)
C(3)-Mo-S(3)	154.18(13)
C(3)#1-Mo-S(3)	131.42(14)
S(4)-Mo-S(3)	116.35(11)
S(4)#2-Mo-S(3)	96.72(12)

S(2)#2-Mo-S(3)	109.44(9)
S(2)-Mo-S(3)	73.92(13)
C(2)#1-Mo-S(3)#2	123.57(16)
C(2)-Mo-S(3)#2	99.37(15)
C(1)-Mo-S(3)#2	95.74(16)
C(3)-Mo-S(3)#2	131.42(14)
C(3)#1-Mo-S(3)#2	154.18(13)
S(4)-Mo-S(3)#2	96.72(12)
S(4)#2-Mo-S(3)#2	116.35(11)
S(2)#2-Mo-S(3)#2	73.92(13)
S(2)-Mo-S(3)#2	109.44(9)
S(3)-Mo-S(3)#2	47.1(2)
C(2)#1-Mo-S(1)#2	91.68(12)
C(2)-Mo-S(1)#2	139.79(14)
C(1)-Mo-S(1)#2	105.08(11)
C(3)-Mo-S(1)#2	147.68(12)
C(3)#1-Mo-S(1)#2	113.32(12)
S(4)-Mo-S(1)#2	109.59(13)
S(4)#2-Mo-S(1)#2	73.74(12)
S(2)#2-Mo-S(1)#2	117.96(4)
S(2)-Mo-S(1)#2	47.26(10)
S(3)-Mo-S(1)#2	28.51(13)
S(3)#2-Mo-S(1)#2	73.81(12)
C(2)#1-Mo-S(1)	139.79(14)
C(2)-Mo-S(1)	91.68(12)
C(1)-Mo-S(1)	105.08(11)
C(3)-Mo-S(1)	113.32(12)
C(3)#1-Mo-S(1)	147.68(12)
S(4)-Mo-S(1)	73.74(12)
S(4)#2-Mo-S(1)	109.59(13)
S(2)#2-Mo-S(1)	47.26(10)
S(2)-Mo-S(1)	117.96(4)
S(3)-Mo-S(1)	73.81(12)
S(3)#2-Mo-S(1)	28.51(13)
S(1)#2-Mo-S(1)	97.41(11)
C(2)#1-Mo-Mo#2	149.85(11)
C(2)-Mo-Mo#2	149.85(11)
C(1)-Mo-Mo#2	152.08(16)
C(3)-Mo-Mo#2	146.58(11)
C(3)#1-Mo-Mo#2	146.58(11)
S(4)-Mo-Mo#2	57.37(9)
S(4)#2-Mo-Mo#2	57.37(9)
S(2)#2-Mo-Mo#2	58.91(3)
S(2)-Mo-Mo#2	58.91(3)
S(3)-Mo-Mo#2	58.99(6)
S(3)#2-Mo-Mo#2	58.99(6)
S(1)#2-Mo-Mo#2	59.08(3)
S(1)-Mo-Mo#2	59.08(3)
S(3)#2-S(1)-C(4)	168.0(4)
S(3)#2-S(1)-S(2)#2	134.8(3)

C(4)-S(1)-S(2)#2	57.3(3)
S(3)#2-S(1)-Mo	75.5(2)
C(4)-S(1)-Mo	114.6(3)
S(2)#2-S(1)-Mo	66.06(11)
S(3)#2-S(1)-Mo#2	75.5(2)
C(4)-S(1)-Mo#2	114.6(3)
S(2)#2-S(1)-Mo#2	66.06(11)
Mo-S(1)-Mo#2	61.85(6)
S(4)#2-S(2)-C(4)#2	174.1(5)
S(4)#2-S(2)-S(1)#2	129.9(4)
C(4)#2-S(2)-S(1)#2	56.1(3)
S(4)#2-S(2)-Mo#2	70.8(3)
C(4)#2-S(2)-Mo#2	114.1(3)
S(1)#2-S(2)-Mo#2	66.68(11)
S(4)#2-S(2)-Mo	70.8(3)
C(4)#2-S(2)-Mo	114.1(3)
S(1)#2-S(2)-Mo	66.68(11)
Mo#2-S(2)-Mo	62.17(7)
S(1)#2-S(3)-C(51)	165.0(5)
S(1)#2-S(3)-S(3)#2	135.9(3)
C(51)-S(3)-S(3)#2	59.1(3)
S(1)#2-S(3)-Mo	76.0(2)
C(51)-S(3)-Mo	116.5(3)
S(3)#2-S(3)-Mo	66.47(11)
S(1)#2-S(3)-Mo#2	76.0(2)
C(51)-S(3)-Mo#2	116.5(3)
S(3)#2-S(3)-Mo#2	66.47(11)
Mo-S(3)-Mo#2	62.02(12)
S(2)#2-S(4)-S(4)#2	139.5(4)
S(2)#2-S(4)-C(52)#3	159.5(7)
S(4)#2-S(4)-C(52)#3	61.0(5)
S(2)#2-S(4)-Mo#2	80.4(3)
S(4)#2-S(4)-Mo#2	65.83(15)
C(52)#3-S(4)-Mo#2	116.4(4)
S(2)#2-S(4)-Mo	80.4(3)
S(4)#2-S(4)-Mo	65.83(15)
C(52)#3-S(4)-Mo	116.4(4)
Mo#2-S(4)-Mo	65.25(19)
C(2)-C(1)-C(2)#1	108.2(6)
C(2)-C(1)-Mo	72.3(3)
C(2)#1-C(1)-Mo	72.3(3)
C(2)-C(1)-H(1)	125.9
C(2)#1-C(1)-H(1)	125.9
Mo-C(1)-H(1)	121.2
C(1)-C(2)-C(3)	108.2(4)
C(1)-C(2)-Mo	72.6(3)
C(3)-C(2)-Mo	73.2(2)
C(1)-C(2)-H(2)	125.9
C(3)-C(2)-H(2)	125.9
Mo-C(2)-H(2)	120.1

C(3)#1-C(3)-C(2)	107.8(3)
C(3)#1-C(3)-Mo	72.61(11)
C(2)-C(3)-Mo	71.3(2)
C(3)#1-C(3)-H(3)	126.1
C(2)-C(3)-H(3)	126.1
Mo-C(3)-H(3)	121.7
S(1)-C(4)-S(2)#2	66.7(3)
C(52)-C(51)-S(3)#2	149.1(3)
C(52)-C(51)-S(3)	149.1(3)
S(3)#2-C(51)-S(3)	61.7(6)
C(51)-C(52)-S(4)#4	151.0(5)
C(51)-C(52)-S(4)#5	151.0(4)
S(4)#4-C(52)-S(4)#5	58.1(9)
C(11)#6-B-C(11)#7	111.88(12)
C(11)#6-B-C(11)	104.8(2)
C(11)#7-B-C(11)	111.88(12)
C(11)#6-B-C(11)#8	111.88(12)
C(11)#7-B-C(11)#8	104.8(2)
C(11)-B-C(11)#8	111.88(12)
C(16)-C(11)-C(12)	115.4(3)
C(16)-C(11)-B	124.8(3)
C(12)-C(11)-B	119.6(3)
C(11)-C(12)-C(13)	122.6(4)
C(11)-C(12)-H(12)	118.7
C(13)-C(12)-H(12)	118.7
C(14)-C(13)-C(12)	119.7(4)
C(14)-C(13)-H(13)	120.1
C(12)-C(13)-H(13)	120.1
C(15)-C(14)-C(13)	118.8(4)
C(15)-C(14)-H(14)	120.6
C(13)-C(14)-H(14)	120.6
C(14)-C(15)-C(16)	121.2(4)
C(14)-C(15)-H(15)	119.4
C(16)-C(15)-H(15)	119.4
C(11)-C(16)-C(15)	122.1(4)
C(11)-C(16)-H(16)	118.9
C(15)-C(16)-H(16)	118.9

Symmetry transformations used to generate equivalent atoms: #1 -y+3/2,-x+3/2,z #2 -x+1,-y+2,z #3 x,y,z-1
#4 -x+1,-y+2,z+1 #5 x,y,z+1 #6 -x,-y+2,z #7 y-1,-x+1,-z+1 #8 -y+1,x+1,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$)for 6'. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo	18(1)	18(1)	21(1)	0(1)	0(1)	2(1)
S(1)	23(1)	23(1)	28(1)	6(1)	6(1)	4(1)
S(2)	30(1)	30(1)	51(2)	19(1)	19(1)	8(1)
S(3)	49(1)	49(1)	68(2)	1(1)	1(1)	4(2)
S(4)	85(2)	85(2)	81(3)	44(2)	44(2)	50(3)
C(1)	35(2)	35(2)	39(3)	9(2)	-9(2)	9(2)
C(2)	35(2)	20(2)	54(3)	11(2)	-5(2)	1(1)
C(3)	36(2)	31(2)	44(2)	-13(2)	4(2)	5(2)
C(4)	45(2)	45(2)	70(5)	-13(3)	-13(3)	10(3)
C(51)	67(9)	67(9)	1(5)	0	0	37(11)
C(52)	72(11)	72(11)	46(14)	0	0	-1(14)
B	19(2)	19(2)	28(3)	0	0	0
C(11)	23(1)	19(1)	23(2)	-2(1)	1(1)	1(1)
C(12)	28(2)	26(2)	33(2)	4(1)	-9(2)	-6(2)
C(13)	41(2)	36(2)	29(2)	9(1)	-8(2)	-3(2)
C(14)	42(2)	25(2)	29(2)	7(1)	0(2)	-1(2)
C(15)	32(2)	23(2)	40(2)	-1(1)	6(2)	-10(2)
C(16)	21(1)	25(2)	30(2)	-2(1)	0(1)	-2(1)

Table 5. Hydrogen coordinates ($x 10^4$) and isotropic displacement parameters ($Å^2 x 10^3$) for 6'.

	x	y	z	U(eq)
H(1)	6623	8377	9281	43
H(2)	5595	7445	7387	44
H(3)	5930	7857	4280	44
H(12)	1130	9515	7642	35
H(13)	1128	8353	9698	43
H(14)	5	7215	9604	38
H(15)	-1104	7279	7489	38
H(16)	-1087	8414	5407	30

3. X-ray crystallographic data for 7'

Table 1. Crystal data and structure refinement for 7' at 170 K.

Identification code	**7'**
Empirical formula	C37 H39 B Mo2 O S3
Formula weight	798.55
Temperature	170(2) K
Wavelength	0.71073 A
Crystal system, space group	Tetragonal, P -4 21 m
Unit cell dimensions	a = 14.6783(4) A
	b = 14.6783(4) A
	c = 7.7906(4) A
Volume	1678.50(11) A^3
Z, Calculated density	2, 1.580 Mg/m^3
Absorption coefficient	0.963 mm^-1
F(000)	812
Crystal size	0.33 x 0.19 x 0.08 mm
Cystal description	trapezoidal plate, main faces {0 0 1}
Crystal colour	black
Theta range for data collection	3.10 to 26.37 deg.
Limiting indices	-18<=h<=15, -18<=k<=18, -9<=l<=9
Reflections collected / unique	13619 / 1809 [R(int) = 0.0342]
Completeness to theta = 26.37	99.6 %
Absorption correction	Analytical
Max. and min. transmission	0.9269 and 0.7416
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1809 / 28 / 124
Goodness-of-fit on F^2	1.181
Final R indices [I>2sigma(I)]	R1 = 0.0304, wR2 = 0.0751
R indices (all data)	R1 = 0.0310, wR2 = 0.0754
Absolute structure parameter	-0.09(7)
Largest diff. peak and hole	0.537 and -0.356 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 7'.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	3371(3)	-1629(3)	1819(11)	54(2)
C(2)	5000	0	6072(14)	31(4)
O(1)	4747(7)	-253(7)	-70(20)	21(4)
S(1)	4098(2)	-902(2)	453(5)	35(1)
S(2)	4520(3)	-480(3)	4052(6)	16(1)
S(3)	4114(1)	-886(1)	2992(3)	24(1)
Mo(1)	4392(1)	608(1)	1660(1)	17(1)
C(51)	3371(3)	-1629(3)	1819(11)	54(2)
C(52)	5000	0	-2663(17)	64(7)
O(51)	4694(8)	-306(8)	3410(20)	30(4)
S(51)	4098(2)	-902(2)	453(5)	35(1)
S(52)	4479(3)	-521(3)	-618(6)	26(1)
S(53)	4114(1)	-886(1)	2992(3)	24(1)
Mo(51)	4392(1)	608(1)	1660(1)	17(1)
C(11)	3399(3)	1601(3)	3048(9)	36(2)
C(12)	3963(3)	2125(3)	1991(7)	35(1)
C(13)	3781(3)	1889(3)	265(6)	36(1)
B(1)	5000	5000	0	20(2)
C(30)	4113(2)	5012(3)	1294(4)	21(1)
C(31)	4056(3)	5667(3)	2603(5)	28(1)
C(32)	3373(3)	5678(3)	3815(5)	33(1)
C(33)	2695(3)	5014(3)	3785(5)	31(1)
C(34)	2733(3)	4357(3)	2513(5)	29(1)
C(35)	3419(2)	4365(3)	1281(4)	23(1)

Table 3. Bond lengths [A] and angles [deg] for 7'.

C(1)-S(3)	1.792(8)
C(1)-S(1)	1.846(8)
C(2)-S(2)	1.863(10)
C(2)-S(2)#1	1.863(10)
O(1)-O(1)#1	1.05(3)
O(1)-S(1)	1.406(15)
O(1)-Mo(1)#1	1.919(12)
O(1)-Mo(1)	1.919(12)
S(1)-S(3)	1.979(4)
S(1)-Mo(1)#1	2.446(3)
S(1)-Mo(1)	2.446(3)
S(2)-S(3)	1.180(6)
S(2)-S(2)#1	1.994(11)
S(2)-Mo(1)#1	2.462(4)
S(2)-Mo(1)	2.462(4)
S(3)-Mo(1)#1	2.461(2)
S(3)-Mo(1)	2.461(2)
Mo(1)-O(1)#1	1.919(12)
Mo(1)-C(11)	2.327(6)
Mo(1)-C(12)	2.327(4)
Mo(1)-C(12)#2	2.327(4)
Mo(1)-C(13)	2.350(4)
Mo(1)-C(13)#2	2.350(4)
Mo(1)-S(1)#1	2.446(3)
Mo(1)-S(3)#1	2.461(2)
Mo(1)-S(2)#1	2.462(4)
C(52)-S(52)#1	1.926(11)
C(52)-S(52)	1.926(11)
O(51)-O(51)#1	1.27(3)
O(51)-Mo(51)#1	1.966(13)
S(52)-S(52)#1	2.162(14)
S(52)-Mo(51)#1	2.431(5)
C(11)-C(12)#2	1.398(6)
C(11)-C(12)	1.398(6)
C(12)-C(13)	1.414(7)
C(13)-C(13)#2	1.391(9)
B(1)-C(30)#3	1.646(3)
B(1)-C(30)#4	1.646(3)
B(1)-C(30)	1.646(3)
B(1)-C(30)#5	1.646(3)
C(30)-C(35)	1.393(5)
C(30)-C(31)	1.404(5)
C(31)-C(32)	1.378(5)
C(32)-C(33)	1.392(6)
C(33)-C(34)	1.384(6)
C(34)-C(35)	1.391(5)

S(3)-C(1)-S(1) 65.9(3)
S(2)-C(2)-S(2)#1 64.7(5)
O(1)#1-O(1)-S(1) 163.2(6)
O(1)#1-O(1)-Mo(1)#1 74.1(4)
S(1)-O(1)-Mo(1)#1 93.5(7)
O(1)#1-O(1)-Mo(1) 74.1(4)
S(1)-O(1)-Mo(1) 93.5(7)
Mo(1)#1-O(1)-Mo(1) 82.3(6)
O(1)-S(1)-C(1) 161.5(7)
O(1)-S(1)-S(3) 105.8(7)
C(1)-S(1)-S(3) 55.7(3)
O(1)-S(1)-Mo(1)#1 51.5(5)
C(1)-S(1)-Mo(1)#1 113.8(2)
S(3)-S(1)-Mo(1)#1 66.61(11)
O(1)-S(1)-Mo(1) 51.5(5)
C(1)-S(1)-Mo(1) 113.8(2)
S(3)-S(1)-Mo(1) 66.61(11)
Mo(1)#1-S(1)-Mo(1) 62.14(7)
S(3)-S(2)-C(2) 166.8(5)
S(3)-S(2)-S(2)#1 135.6(3)
C(2)-S(2)-S(2)#1 57.6(2)
S(3)-S(2)-Mo(1)#1 76.1(2)
C(2)-S(2)-Mo(1)#1 115.0(3)
S(2)#1-S(2)-Mo(1)#1 66.12(12)
S(3)-S(2)-Mo(1) 76.1(2)
C(2)-S(2)-Mo(1) 115.0(3)
S(2)#1-S(2)-Mo(1) 66.12(12)
Mo(1)#1-S(2)-Mo(1) 61.70(12)
S(2)-S(3)-C(1) 166.3(4)
S(2)-S(3)-S(1) 135.4(3)
C(1)-S(3)-S(1) 58.4(3)
S(2)-S(3)-Mo(1)#1 76.2(2)
C(1)-S(3)-Mo(1)#1 115.3(2)
S(1)-S(3)-Mo(1)#1 65.83(11)
S(2)-S(3)-Mo(1) 76.2(2)
C(1)-S(3)-Mo(1) 115.3(2)
S(1)-S(3)-Mo(1) 65.83(11)
Mo(1)#1-S(3)-Mo(1) 61.73(7)
O(1)#1-Mo(1)-O(1) 31.8(9)
O(1)#1-Mo(1)-C(11) 155.3(3)
O(1)-Mo(1)-C(11) 155.3(3)
O(1)#1-Mo(1)-C(12) 121.0(4)
O(1)-Mo(1)-C(12) 141.4(4)
C(11)-Mo(1)-C(12) 34.96(15)
O(1)#1-Mo(1)-C(12)#2 141.4(4)
O(1)-Mo(1)-C(12)#2 121.0(4)
C(11)-Mo(1)-C(12)#2 34.96(15)
C(12)-Mo(1)-C(12)#2 58.0(2)
O(1)#1-Mo(1)-C(13) 98.3(3)

O(1)-Mo(1)-C(13)	107.9(4)
C(11)-Mo(1)-C(13)	58.33(19)
C(12)-Mo(1)-C(13)	35.18(17)
C(12)#2-Mo(1)-C(13)	57.99(15)
O(1)#1-Mo(1)-C(13)#2	107.9(4)
O(1)-Mo(1)-C(13)#2	98.3(3)
C(11)-Mo(1)-C(13)#2	58.33(19)
C(12)-Mo(1)-C(13)#2	57.99(15)
C(12)#2-Mo(1)-C(13)#2	35.18(17)
C(13)-Mo(1)-C(13)#2	34.4(2)
O(1)#1-Mo(1)-S(1)#1	35.0(5)
O(1)-Mo(1)-S(1)#1	66.5(4)
C(11)-Mo(1)-S(1)#1	129.47(6)
C(12)-Mo(1)-S(1)#1	96.84(12)
C(12)#2-Mo(1)-S(1)#1	149.50(12)
C(13)-Mo(1)-S(1)#1	91.55(11)
C(13)#2-Mo(1)-S(1)#1	118.71(13)
O(1)#1-Mo(1)-S(1)	66.5(4)
O(1)-Mo(1)-S(1)	35.0(5)
C(11)-Mo(1)-S(1)	129.47(6)
C(12)-Mo(1)-S(1)	149.50(12)
C(12)#2-Mo(1)-S(1)	96.84(12)
C(13)-Mo(1)-S(1)	118.71(13)
C(13)#2-Mo(1)-S(1)	91.55(11)
S(1)#1-Mo(1)-S(1)	99.89(14)
O(1)#1-Mo(1)-S(3)#1	75.7(4)
O(1)-Mo(1)-S(3)#1	99.4(3)
C(11)-Mo(1)-S(3)#1	104.95(11)
C(12)-Mo(1)-S(3)#1	92.04(11)
C(12)#2-Mo(1)-S(3)#1	139.54(13)
C(13)-Mo(1)-S(3)#1	113.73(12)
C(13)#2-Mo(1)-S(3)#1	147.69(12)
S(1)#1-Mo(1)-S(3)#1	47.56(10)
S(1)-Mo(1)-S(3)#1	118.01(5)
O(1)#1-Mo(1)-S(3)	99.4(3)
O(1)-Mo(1)-S(3)	75.7(4)
C(11)-Mo(1)-S(3)	104.95(11)
C(12)-Mo(1)-S(3)	139.54(13)
C(12)#2-Mo(1)-S(3)	92.04(11)
C(13)-Mo(1)-S(3)	147.69(12)
C(13)#2-Mo(1)-S(3)	113.73(12)
S(1)#1-Mo(1)-S(3)	118.01(5)
S(1)-Mo(1)-S(3)	47.56(10)
S(3)#1-Mo(1)-S(3)	96.76(12)
O(1)#1-Mo(1)-S(2)#1	94.7(4)
O(1)-Mo(1)-S(2)#1	107.7(3)
C(11)-Mo(1)-S(2)#1	95.85(17)
C(12)-Mo(1)-S(2)#1	99.46(14)
C(12)#2-Mo(1)-S(2)#1	123.86(15)
C(13)-Mo(1)-S(2)#1	131.20(15)

C(13)#2-Mo(1)-S(2)#1	153.96(13)
S(1)#1-Mo(1)-S(2)#1	73.53(14)
S(1)-Mo(1)-S(2)#1	109.65(10)
S(3)#1-Mo(1)-S(2)#1	27.74(14)
S(3)-Mo(1)-S(2)#1	73.76(14)
S(52)#1-C(52)-S(52)	68.3(6)
O(51)#1-O(51)-Mo(51)#1	71.1(5)
C(52)-S(52)-S(52)#1	55.9(3)
C(52)-S(52)-Mo(51)#1	110.8(3)
S(52)#1-S(52)-Mo(51)#1	63.60(15)
C(12)#2-C(11)-C(12)	107.7(6)
C(12)#2-C(11)-Mo(1)	72.5(3)
C(12)-C(11)-Mo(1)	72.5(3)
C(11)-C(12)-C(13)	108.3(4)
C(11)-C(12)-Mo(1)	72.5(3)
C(13)-C(12)-Mo(1)	73.3(2)
C(13)#2-C(13)-C(12)	107.8(3)
C(13)#2-C(13)-Mo(1)	72.78(11)
C(12)-C(13)-Mo(1)	71.6(2)
C(30)#3-B(1)-C(30)#4	112.02(12)
C(30)#3-B(1)-C(30)	112.02(12)
C(30)#4-B(1)-C(30)	104.5(2)
C(30)#3-B(1)-C(30)#5	104.5(2)
C(30)#4-B(1)-C(30)#5	112.02(12)
C(30)-B(1)-C(30)#5	112.02(12)
C(35)-C(30)-C(31)	115.4(3)
C(35)-C(30)-B(1)	124.6(3)
C(31)-C(30)-B(1)	119.9(3)
C(32)-C(31)-C(30)	123.3(4)
C(31)-C(32)-C(33)	120.0(4)
C(34)-C(33)-C(32)	118.1(4)
C(33)-C(34)-C(35)	121.1(4)
C(34)-C(35)-C(30)	122.1(4)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,z #2 -y+1/2,-x+1/2,z #3 -y+1,x,-z
#4 -x+1,-y+1,z #5 y,-x+1,-z

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 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
S(1)	30(1)	30(1)	47(2)	-15(1)	-15(1)	8(1)
S(2)	17(2)	17(2)	16(2)	8(2)	8(2)	6(2)
S(3)	25(1)	25(1)	23(2)	8(1)	8(1)	9(1)
Mo(1)	17(1)	17(1)	19(1)	0(1)	0(1)	2(1)
S(51)	30(1)	30(1)	47(2)	-15(1)	-15(1)	8(1)
S(52)	30(2)	30(2)	18(2)	-1(2)	-1(2)	9(3)
S(53)	25(1)	25(1)	23(2)	8(1)	8(1)	9(1)
Mo(51)	17(1)	17(1)	19(1)	0(1)	0(1)	2(1)
C(11)	33(2)	33(2)	43(4)	-9(2)	9(2)	7(2)
C(12)	29(2)	18(2)	58(3)	-7(2)	-2(2)	5(2)
C(13)	34(2)	24(2)	49(3)	15(2)	-5(2)	6(2)
B(1)	19(2)	19(2)	23(4)	0	0	0
C(30)	19(2)	22(2)	20(2)	2(1)	0(1)	1(1)
C(31)	26(2)	29(2)	31(2)	-4(2)	6(2)	-7(2)
C(32)	34(2)	37(2)	27(2)	-10(2)	7(2)	0(2)
C(33)	24(2)	41(2)	27(2)	3(2)	9(2)	0(2)
C(34)	22(2)	27(2)	38(2)	10(2)	-2(2)	-7(2)
C(35)	22(2)	20(2)	27(2)	1(2)	-3(1)	0(2)

To solve the disorder observed in **7'**, the cation was built from two structurally equivalent entities (A and B) (see enclosed Figures 3a,3b,3c). In this model, the oxo bridge occupies four sites accounting for 25% each. The S(1)Me and S(51)Me, and S(3)Me and S(53)Me groups occupy two sites accounting for 50% each, whereas S(2)Me and S(52)Me occupy four sites accounting for 25% each. In order to simplify the model, Mo(51), S(51), S(53), …were superposed upon Mo(1), S(1), S(3),…, respectively. Finally, the use of PARST program allows to obtain distances and angles (see enclosed **7'A**.txt and **7'B**.txt)

Figure 3a : Cation of 7'-Entities A & B with 4-fold symmetry, [1-10] axis view

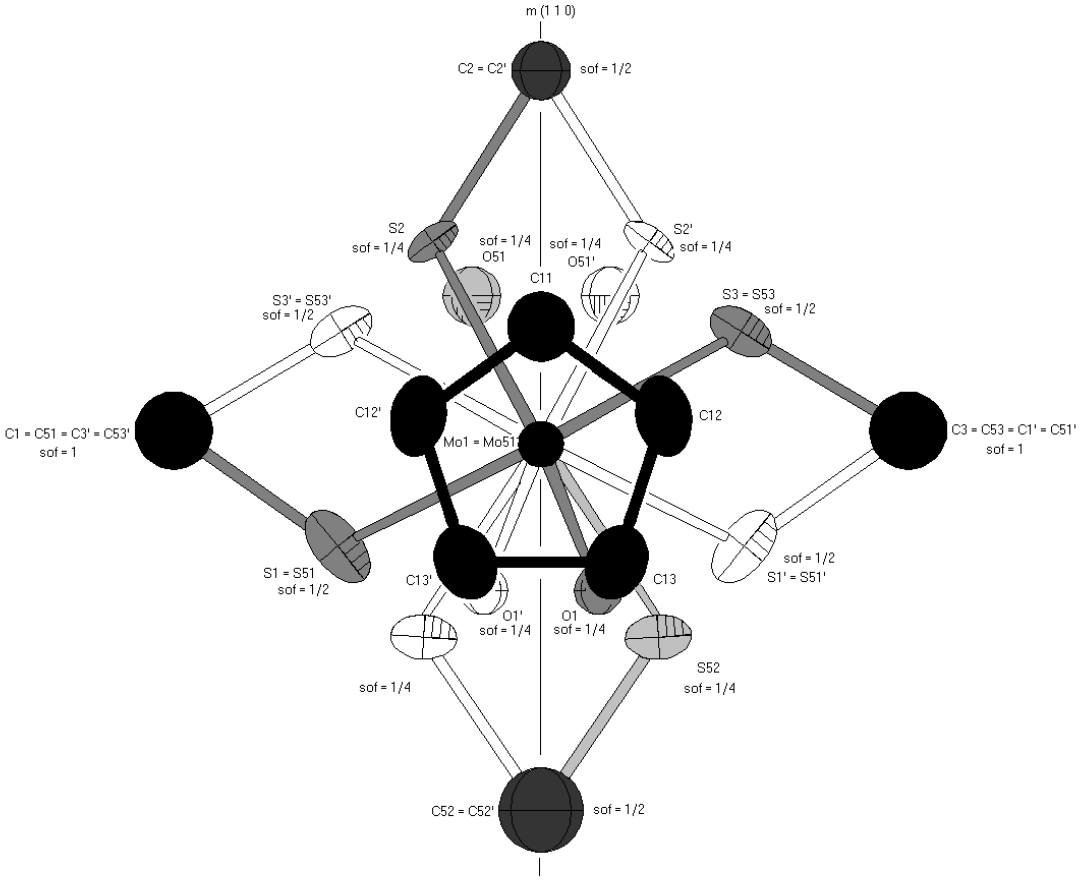
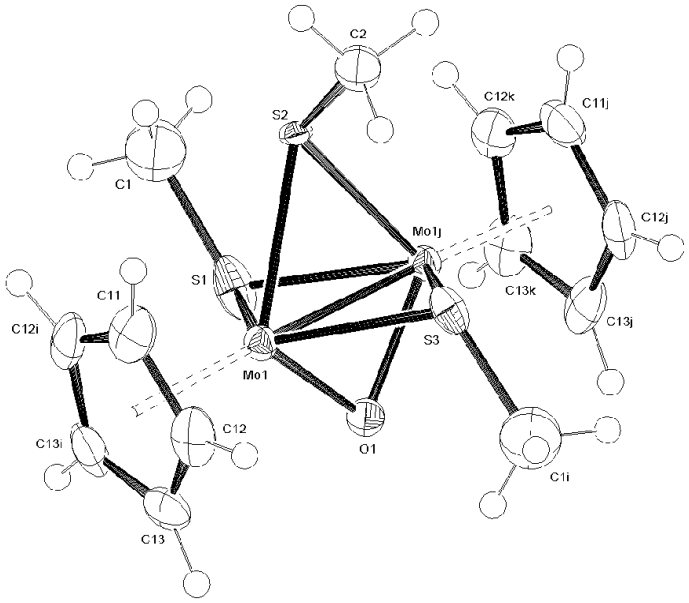


Figure 3b : Cation of 7'A



7' at 170 K in P-42(1)m / Cation A rebuilt

Crystal data

a = 14.6783(0.0004)	alpha= 90.00(0.00)
b = 14.6783(0.0004)	beta = 90.00(0.00)
c = 7.7906(0.0004)	gamma= 90.00(0.00)

V = 1678.50(0.11) cubic-Angstrom

Niggli reduced cell: 7.791 14.678 14.678 90.00 90.00 90.00

Niggli matrix: 60.6934 215.4525 215.4525
0.0000 0.0000 0.0000

Transformation matrix: 0.00 0.00 1.00
1.00 0.00 0.00
0.00 1.00 0.00

C 37. H 39. O 1. S 3. Mo 2. B 1.
M = 798.584 (Atomic weights 1977)
Z = 2.00
D(calc.)= 1.5801 Mg/m**3
F(000) = 812.0
mu = 9.634 cm**-1 (Int.Tab. Vol.C, Table 4.2.4.2, p.193)
Lambda = 0.7107300 Angstrom

Number of atoms: 38

Atomic coordinates

Atom	X/a	Y/b	Z/c
C1	0.33711(0)	-0.16288(0)	0.18188(0)
H1A	0.32818(0)	-0.22204(0)	0.12603(0)
H1B	0.27793(0)	-0.13330(0)	0.19871(0)
H1C	0.36666(0)	-0.17189(0)	0.29340(0)
C1I	0.66289(0)	0.16288(0)	0.18188(0)
H1I1	0.72038(0)	0.16985(0)	0.24447(0)
H1I2	0.63387(0)	0.22260(0)	0.16864(0)
H1I3	0.67502(0)	0.13681(0)	0.06835(0)
C2	0.50000(0)	0.00000(0)	0.60716(0)
H2A	0.50261(0)	-0.04776(0)	0.69492(0)
H2B	0.46112(0)	0.04987(0)	0.64752(0)
H2C	0.56154(0)	0.02316(0)	0.58531(0)
C11	0.66006(0)	-0.16006(0)	0.30483(0)
H11I	0.66234(0)	-0.16234(0)	0.42662(0)
C11J	0.33994(0)	0.16006(0)	0.30483(0)
H11J	0.33766(0)	0.16234(0)	0.42662(0)
C12	0.71246(0)	-0.10369(0)	0.19911(0)
H12	0.75636(0)	-0.06053(0)	0.23679(0)
C12I	0.60369(0)	-0.21246(0)	0.19911(0)
H12I	0.56053(0)	-0.25636(0)	0.23679(0)
C12J	0.39631(0)	0.21246(0)	0.19911(0)
H12J	0.43947(0)	0.25636(0)	0.23679(0)
C12K	0.28754(0)	0.10369(0)	0.19911(0)
H12K	0.24364(0)	0.06053(0)	0.23679(0)
C13	0.68894(0)	-0.12191(0)	0.02653(0)
H13	0.71438(0)	-0.09345(0)	-0.07194(0)
C13I	0.62191(0)	-0.18894(0)	0.02653(0)
H13I	0.59345(0)	-0.21438(0)	-0.07194(0)
C13J	0.37809(0)	0.18894(0)	0.02653(0)
H13J	0.40655(0)	0.21438(0)	-0.07194(0)
C13K	0.31106(0)	0.12191(0)	0.02653(0)
H13K	0.28562(0)	0.09345(0)	-0.07194(0)
O1	0.52535(0)	0.02534(0)	-0.00677(0)
S1	0.40979(0)	-0.09020(0)	0.04525(0)
S2	0.45198(0)	-0.04802(0)	0.40521(0)
S3	0.58863(0)	0.08863(0)	0.29920(0)
Mo1	0.56082(0)	-0.06082(0)	0.1659(0)
Mo1J	0.43918(0)	0.06082(0)	0.16596(0)

Orthogonal coordinates (Angstrom)

Orthogonalization matrix:

a b cosgamma c cosbeta 14.67830 0.00000 0.00000

0 b singamma -c sinbeta cosalpha* 0.00000 14.67830 0.00000

0 0 c sinbeta sinalpha* 0.00000 0.00000 7.79060

Atom	X	Y	Z
C1	4.9482(0.0000)	-2.3908(0.0000)	1.4170(0.0000)
H1A	4.8171(0.0000)	-3.2592(0.0000)	0.9818(0.0000)

H1B	4.0795(0.0000)	-1.9566(0.0000)	1.5481(0.0000)
H1C	5.3819(0.0000)	-2.5231(0.0000)	2.2858(0.0000)
C1I	9.7301(0.0000)	2.3908(0.0000)	1.4170(0.0000)
H1I1	10.5740(0.0000)	2.4931(0.0000)	1.9046(0.0000)
H1I2	9.3041(0.0000)	3.2674(0.0000)	1.3138(0.0000)
H1I3	9.9081(0.0000)	2.0081(0.0000)	0.5325(0.0000)
C2	7.3391(0.0000)	0.0000(0.0000)	4.7301(0.0000)
H2A	7.3775(0.0000)	-0.7010(0.0000)	5.4138(0.0000)
H2B	6.7685(0.0000)	0.7320(0.0000)	5.0446(0.0000)
H2C	8.2425(0.0000)	0.3399(0.0000)	4.5599(0.0000)
C11	9.6886(0.0000)	-2.3494(0.0000)	2.3748(0.0000)
H11I	9.7220(0.0000)	-2.3829(0.0000)	3.3236(0.0000)
C11J	4.9897(0.0000)	2.3494(0.0000)	2.3748(0.0000)
H11J	4.9563(0.0000)	2.3829(0.0000)	3.3236(0.0000)
C12	10.4577(0.0000)	-1.5220(0.0000)	1.5512(0.0000)
H12	11.1021(0.0000)	-0.8885(0.0000)	1.8447(0.0000)
C12I	8.8611(0.0000)	-3.1186(0.0000)	1.5512(0.0000)
H12I	8.2276(0.0000)	-3.7629(0.0000)	1.8447(0.0000)
C12J	5.8172(0.0000)	3.1186(0.0000)	1.5512(0.0000)
H12J	6.4507(0.0000)	3.7629(0.0000)	1.8447(0.0000)
C12K	4.2206(0.0000)	1.5220(0.0000)	1.5512(0.0000)
H12K	3.5762(0.0000)	0.8885(0.0000)	1.8447(0.0000)
C13	10.1125(0.0000)	-1.7894(0.0000)	0.2067(0.0000)
H13	10.4859(0.0000)	-1.3717(0.0000)	-0.5605(0.0000)
C13I	9.1286(0.0000)	-2.7733(0.0000)	0.2067(0.0000)
H13I	8.7108(0.0000)	-3.1467(0.0000)	-0.5605(0.0000)
C13J	5.5497(0.0000)	2.7733(0.0000)	0.2067(0.0000)
H13J	5.9675(0.0000)	3.1467(0.0000)	-0.5605(0.0000)
C13K	4.5658(0.0000)	1.7894(0.0000)	0.2067(0.0000)
H13K	4.1924(0.0000)	1.3717(0.0000)	-0.5605(0.0000)
O1	7.7112(0.0000)	0.3719(0.0000)	-0.0527(0.0000)
S1	6.0150(0.0000)	-1.3240(0.0000)	0.3525(0.0000)
S2	6.6343(0.0000)	-0.7049(0.0000)	3.1568(0.0000)
S3	8.6401(0.0000)	1.3009(0.0000)	2.3309(0.0000)
Mo1	8.2319(0.0000)	-0.8927(0.0000)	1.2929(0.0000)
Mo1J	6.4464(0.0000)	0.8927(0.0000)	1.2929(0.0000)

Displacement parameters, U(I,J)x10**4
exp(-2*pi**2(U11*h**2*(a*)**2+...+2*U12*h*k*(a*)*(b*)+...)

Atom	U11	U22	U33	U23	U13	U12
C1	537(0)					
H1A	*****(0)					
H1B	*****(0)					
H1C	*****(0)					
C1I	537(0)					
H1I1	*****(0)					
H1I2	*****(0)					
H1I3	*****(0)					
C2	306(0)					
H2A	*****(0)					

H2B *****(0)
H2C *****(0)
C11 327(0) 327(0) 430(0) 89(0) -89(0) 75(0)
H11I *****(0)
C11J 327(0) 327(0) 430(0) -89(0) 89(0) 75(0)
H11J *****(0)
C12 177(0) 295(0) 584(0) -16(0) -75(0) 47(0)
H12 *****(0)
C12I 295(0) 177(0) 584(0) 75(0) 16(0) 47(0)
H12I *****(0)
C12J 295(0) 177(0) 584(0) -75(0) -16(0) 47(0)
H12J *****(0)
C12K 177(0) 295(0) 584(0) 16(0) 75(0) 47(0)
H12K *****(0)
C13 244(0) 340(0) 489(0) -52(0) 150(0) 64(0)
H13 *****(0)
C13I 340(0) 244(0) 489(0) -150(0) 52(0) 64(0)
H13I *****(0)
C13J 340(0) 244(0) 489(0) 150(0) -52(0) 64(0)
H13J *****(0)
C13K 244(0) 340(0) 489(0) 52(0) -150(0) 64(0)
H13K *****(0)
O1 206(0)
S1 296(0) 296(0) 470(0) -152(0) -152(0) 80(0)
S2 167(0) 167(0) 155(0) 76(0) 76(0) 58(0)
S3 252(0) 252(0) 231(0) -81(0) -81(0) 87(0)
Mo1 166(0) 166(0) 185(0) 1(0) -1(0) 17(0)
Mo1J 166(0) 166(0) 185(0) -1(0) 1(0) 17(0)

Principal axes of the thermal ellipsoids, Uequiv. (x10**4 A**2) and Bequiv.(A**2)

Atom	R1	R2	R3	Uequiv.	Bequiv.	Rmax/Rmin
C11	495(0)	401(0)	186(0)	361(0)	2.85(0.00)	2.66
C11J	495(0)	401(0)	186(0)	361(0)	2.85(0.00)	2.66
C12	599(0)	306(0)	150(0)	352(0)	2.78(0.00)	3.99
C12I	599(0)	306(0)	150(0)	352(0)	2.78(0.00)	3.99
C12J	599(0)	306(0)	150(0)	352(0)	2.78(0.00)	3.99
C12K	599(0)	306(0)	150(0)	352(0)	2.78(0.00)	3.99
C13	562(0)	370(0)	140(0)	358(0)	2.82(0.00)	4.01
C13I	562(0)	370(0)	140(0)	358(0)	2.82(0.00)	4.01
C13J	562(0)	370(0)	140(0)	358(0)	2.82(0.00)	4.01
C13K	562(0)	370(0)	140(0)	358(0)	2.82(0.00)	4.01
S1	643(0)	216(0)	202(0)	354(0)	2.79(0.00)	3.18
S2	303(0)	108(0)	77(0)	163(0)	1.29(0.00)	3.95
S3	412(0)	165(0)	158(0)	245(0)	1.93(0.00)	2.61
Mo1	185(0)	183(0)	149(0)	172(0)	1.36(0.00)	1.25
Mo1J	185(0)	183(0)	149(0)	172(0)	1.36(0.00)	1.25

Bond distances (Angstrom)
(Corrections following Busing & Levy, Acta Cryst.(1964).17,142)

	uncorrected distance	lower bound	upper bound	riding motion	non-correlated motion
C1 - H1A	0.9801(0)				
C1 - H1B	0.9799(0)				
C1 - H1C	0.9800(0)				
C1 - S1	1.8464(0)				
C1I - H1I1	0.9800(0)				
C1I - H1I2	0.9800(0)				
C1I - H1I3	0.9800(0)				
C1I - S3	1.7920(0)				
C2 - H2A	0.9800(0)				
C2 - H2B	0.9800(0)				
C2 - H2C	0.9800(0)				
C2 - S2	1.8625(1)				
C11 - H11I	0.9500(0)				
C11 - C12	1.3981(0)	1.3981	1.4896	1.4006	1.4439
C11 - C12I	1.3981(0)	1.3981	1.4896	1.4006	1.4439
C11 - MO1	2.3269(0)	2.3294	2.3784	2.3384	2.3539
C11J - H11J	0.9500(0)				
C11J - C12J	1.3981(0)	1.3981	1.4896	1.4006	1.4439
C11J - C12K	1.3981(0)	1.3981	1.4896	1.4006	1.4439
C11J - MO1J	2.3269(0)	2.3294	2.3784	2.3384	2.3539
C12 - H12	0.9501(0)				
C12 - C13	1.4136(1)	1.4136	1.4907	1.4138	1.4522
C12 - MO1	2.3274(1)	2.3301	2.3791	2.3391	2.3546
C12I - H12I	0.9501(0)				
C12I - C13I	1.4136(1)	1.4136	1.4907	1.4138	1.4522
C12I - MO1	2.3274(1)	2.3301	2.3791	2.3391	2.3546
C12J - H12J	0.9501(0)				
C12J - C13J	1.4136(1)	1.4136	1.4907	1.4138	1.4522
C12J - MO1J	2.3274(1)	2.3301	2.3791	2.3391	2.3546
C12K - H12K	0.9501(0)				
C12K - C13K	1.4136(1)	1.4136	1.4907	1.4138	1.4522
C12K - MO1J	2.3274(1)	2.3301	2.3791	2.3391	2.3546
C13 - H13	0.9500(0)				
C13 - C13I	1.3914(0)	1.3914	1.4944	1.3914	1.4429
C13 - MO1	2.3496(0)	2.3525	2.4015	2.3618	2.3770
C13I - H13I	0.9500(0)				
C13I - MO1	2.3496(0)	2.3525	2.4015	2.3618	2.3770
C13J - H13J	0.9500(0)				
C13J - C13K	1.3914(0)	1.3914	1.4944	1.3914	1.4429
C13J - MO1J	2.3496(0)	2.3525	2.4015	2.3618	2.3770
C13K - H13K	0.9500(0)				
C13K - MO1J	2.3496(0)	2.3525	2.4015	2.3618	2.3770
O1 - MO1	1.9187(1)				
O1 - MO1J	1.9188(1)				
S1 - MO1	2.4464(1)	2.4486	2.4926	2.4566	2.4706
S1 - MO1J	2.4463(1)	2.4485	2.4924	2.4565	2.4705

S2	- MO1	2.4621(1)	2.4621	2.4921	2.4633	2.4771
S2	- MO1J	2.4621(1)	2.4621	2.4921	2.4633	2.4771
S3	- MO1	2.4610(1)	2.4614	2.4961	2.4648	2.4787
S3	- MO1J	2.4610(1)	2.4614	2.4961	2.4648	2.4787
Mo1	- Mo1J	2.5250(0)	2.5250	2.5542	2.5250	2.5396

Number of bond distances: 51

Bond angles (deg)
(s.u. following Cruickshank, Internat. Tables, II, 1959, p.331)

			Angle	s.u.
H1A	- C1	- H1B	109.48	0.00
H1A	- C1	- H1C	109.46	0.00
H1A	- C1	- S1	109.47	0.00
H1B	- C1	- H1C	109.48	0.00
H1B	- C1	- S1	109.47	0.00
H1C	- C1	- S1	109.47	0.00
H1I1	- C1I	- H1I2	109.47	0.00
H1I1	- C1I	- H1I3	109.47	0.00
H1I1	- C1I	- S3	109.48	0.00
H1I2	- C1I	- H1I3	109.46	0.00
H1I2	- C1I	- S3	109.47	0.00
H1I3	- C1I	- S3	109.47	0.00
H2A	- C2	- H2B	109.47	0.00
H2A	- C2	- H2C	109.47	0.00
H2A	- C2	- S2	109.48	0.00
H2B	- C2	- H2C	109.47	0.00
H2B	- C2	- S2	109.47	0.00
H2C	- C2	- S2	109.47	0.00
H11I	- C11	- C12	126.15	0.00
H11I	- C11	- C12I	126.15	0.00
H11I	- C11	- Mo1	120.56	0.00
C12	- C11	- C12I	107.71	0.00
C12	- C11	- Mo1	72.54	0.00
C12I	- C11	- Mo1	72.54	0.00
H11J	- C11J	- C12J	126.15	0.00
H11J	- C11J	- C12K	126.15	0.00
H11J	- C11J	- Mo1J	120.56	0.00
C12J	- C11J	- C12K	107.71	0.00
C12J	- C11J	- Mo1J	72.54	0.00
C12K	- C11J	- Mo1J	72.54	0.00
C11	- C12	- H12	125.85	0.00
C11	- C12	- C13	108.30	0.00
C11	- C12	- Mo1	72.50	0.00
H12	- C12	- C13	125.85	0.00
H12	- C12	- Mo1	120.17	0.00
C13	- C12	- Mo1	73.27	0.00
C11	- C12I	- H12I	125.85	0.00
C11	- C12I	- C13I	108.30	0.00
C11	- C12I	- Mo1	72.50	0.00

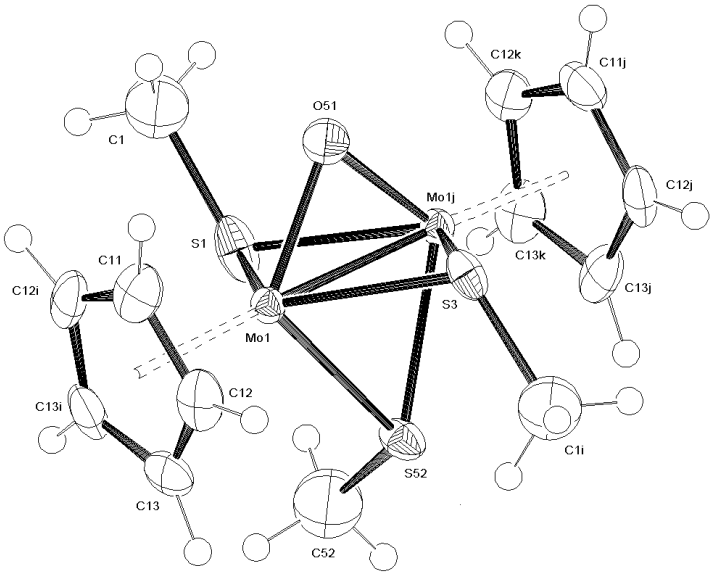
H12I - C12I - C13I	125.85	0.00
H12I - C12I - Mo1	120.17	0.00
C13I - C12I - Mo1	73.27	0.00
C11J - C12J - H12J	125.85	0.00
C11J - C12J - C13J	108.30	0.00
C11J - C12J - Mo1J	72.50	0.00
H12J - C12J - C13J	125.85	0.00
H12J - C12J - Mo1J	120.17	0.00
C13J - C12J - Mo1J	73.27	0.00
C11J - C12K - H12K	125.85	0.00
C11J - C12K - C13K	108.30	0.00
C11J - C12K - Mo1J	72.50	0.00
H12K - C12K - C13K	125.85	0.00
H12K - C12K - Mo1J	120.17	0.00
C13K - C12K - Mo1J	73.27	0.00
C12 - C13 - H13	126.08	0.00
C12 - C13 - C13I	107.85	0.00
C12 - C13 - Mo1	71.55	0.00
H13 - C13 - C13I	126.08	0.00
H13 - C13 - Mo1	121.34	0.00
C13I - C13 - Mo1	72.78	0.00
C12I - C13I - C13	107.85	0.00
C12I - C13I - H13I	126.08	0.00
C12I - C13I - Mo1	71.55	0.00
C13 - C13I - H13I	126.08	0.00
C13 - C13I - Mo1	72.78	0.00
H13I - C13I - Mo1	121.34	0.00
C12J - C13J - H13J	126.08	0.00
C12J - C13J - C13K	107.85	0.00
C12J - C13J - Mo1J	71.55	0.00
H13J - C13J - C13K	126.08	0.00
H13J - C13J - Mo1J	121.34	0.00
C13K - C13J - Mo1J	72.78	0.00
C12K - C13K - C13J	107.85	0.00
C12K - C13K - H13K	126.08	0.00
C12K - C13K - Mo1J	71.55	0.00
C13J - C13K - H13K	126.08	0.00
C13J - C13K - Mo1J	72.78	0.00
H13K - C13K - Mo1J	121.34	0.00
Mo1 - O1 - Mo1J	82.29	0.00
C1 - S1 - Mo1	113.82	0.00
C1 - S1 - Mo1J	113.82	0.00
Mo1 - S1 - Mo1J	62.14	0.00
C2 - S2 - Mo1	115.01	0.00
C2 - S2 - Mo1J	115.01	0.00
Mo1 - S2 - Mo1J	61.70	0.00
C1I - S3 - Mo1	115.33	0.00
C1I - S3 - Mo1J	115.34	0.00
Mo1 - S3 - Mo1J	61.73	0.00
C11 - Mo1 - C12	34.96	0.00

C11	- Mo1	- C12I	34.96	0.00
C11	- Mo1	- C13	58.33	0.00
C11	- Mo1	- C13I	58.33	0.00
C11	- Mo1	- O1	155.31	0.00
C11	- Mo1	- S1	129.47	0.00
C11	- Mo1	- S2	95.85	0.00
C11	- Mo1	- S3	104.96	0.00
C11	- Mo1	- Mo1J	152.29	0.00
C12	- Mo1	- C12I	58.03	0.00
C12	- Mo1	- C13	35.18	0.00
C12	- Mo1	- C13I	57.99	0.00
C12	- Mo1	- O1	121.03	0.00
C12	- Mo1	- S1	149.50	0.00
C12	- Mo1	- S2	123.86	0.00
C12	- Mo1	- S3	92.04	0.00
C12	- Mo1	- Mo1J	150.16	0.00
C12I	- Mo1	- C13	57.99	0.00
C12I	- Mo1	- C13I	35.18	0.00
C12I	- Mo1	- O1	141.40	0.00
C12I	- Mo1	- S1	96.84	0.00
C12I	- Mo1	- S2	99.46	0.00
C12I	- Mo1	- S3	139.54	0.00
C12I	- Mo1	- Mo1J	150.16	0.00
C13	- Mo1	- C13I	34.45	0.00
C13	- Mo1	- O1	98.31	0.00
C13	- Mo1	- S1	118.71	0.00
C13	- Mo1	- S2	153.96	0.00
C13	- Mo1	- S3	113.73	0.00
C13	- Mo1	- Mo1J	146.70	0.00
C13I	- Mo1	- O1	107.87	0.00
C13I	- Mo1	- S1	91.55	0.00
C13I	- Mo1	- S2	131.20	0.00
C13I	- Mo1	- S3	147.69	0.00
C13I	- Mo1	- Mo1J	146.70	0.00
O1	- Mo1	- S1	66.47	0.00
O1	- Mo1	- S2	107.73	0.00
O1	- Mo1	- S3	75.72	0.00
O1	- Mo1	- Mo1J	48.86	0.00
S1	- Mo1	- S2	73.53	0.00
S1	- Mo1	- S3	118.01	0.00
S1	- Mo1	- Mo1J	58.93	0.00
S2	- Mo1	- S3	73.76	0.00
S2	- Mo1	- Mo1J	59.15	0.00
S3	- Mo1	- Mo1J	59.13	0.00
C11J	- Mo1J	- C12J	34.96	0.00
C11J	- Mo1J	- C12K	34.96	0.00
C11J	- Mo1J	- C13J	58.33	0.00
C11J	- Mo1J	- C13K	58.33	0.00
C11J	- Mo1J	- O1	155.32	0.00
C11J	- Mo1J	- S1	129.47	0.00

C11J - Mo1J - S2	95.85	0.00
C11J - Mo1J - S3	104.96	0.00
C11J - Mo1J - Mo1	152.29	0.00
C12J - Mo1J - C12K	58.03	0.00
C12J - Mo1J - C13J	35.18	0.00
C12J - Mo1J - C13K	57.99	0.00
C12J - Mo1J - O1	121.04	0.00
C12J - Mo1J - S1	149.49	0.00
C12J - Mo1J - S2	123.86	0.00
C12J - Mo1J - S3	92.04	0.00
C12J - Mo1J - Mo1	150.16	0.00
C12K - Mo1J - C13J	57.99	0.00
C12K - Mo1J - C13K	35.18	0.00
C12K - Mo1J - O1	141.41	0.00
C12K - Mo1J - S1	96.83	0.00
C12K - Mo1J - S2	99.46	0.00
C12K - Mo1J - S3	139.54	0.00
C12K - Mo1J - Mo1	150.16	0.00
C13J - Mo1J - C13K	34.45	0.00
C13J - Mo1J - O1	98.31	0.00
C13J - Mo1J - S1	118.70	0.00
C13J - Mo1J - S2	153.96	0.00
C13J - Mo1J - S3	113.73	0.00
C13J - Mo1J - Mo1	146.70	0.00
C13K - Mo1J - O1	107.88	0.00
C13K - Mo1J - S1	91.54	0.00
C13K - Mo1J - S2	131.20	0.00
C13K - Mo1J - S3	147.69	0.00
C13K - Mo1J - Mo1	146.70	0.00
O1 - Mo1J - S1	66.47	0.00
O1 - Mo1J - S2	107.73	0.00
O1 - Mo1J - S3	75.71	0.00
O1 - Mo1J - Mo1	48.85	0.00
S1 - Mo1J - S2	73.53	0.00
S1 - Mo1J - S3	118.01	0.00
S1 - Mo1J - Mo1	58.93	0.00
S2 - Mo1J - S3	73.76	0.00
S2 - Mo1J - Mo1	59.15	0.00
S3 - Mo1J - Mo1	59.13	0.00

Number of angles: 178

Figure 3c : Cation of 7'B



7' at 170 K in P-42(1)m, :cationB rebuilt

Crystal data
a = 14.6783(0.0004) alpha= 90.00(0.00)
b = 14.6783(0.0004) beta = 90.00(0.00)
c = 7.7906(0.0004) gamma= 90.00(0.00)
V = 1678.50(0.11) cubic-Angstrom

Niggli reduced cell: 7.791 14.678 14.678 90.00 90.00 90.00
Niggli matrix: 60.6934 215.4525 215.4525
0.0000 0.0000 0.0000
Transformation matrix: 0.00 0.00 1.00
1.00 0.00 0.00
0.00 1.00 0.00

C 37. H 39. O 1. S 3. Mo 2. B 1.
M = 798.584 (Atomic weights 1977)
Z = 2.00
D(calc.)= 1.5801 Mg/m**3
F(000) = 812.0
mu = 9.634 cm**-1 (Int.Tab. Vol.C, Table 4.2.4.2, p.193)
Lambda = 0.7107300 Angstrom

Number of atoms: 38

Atomic coordinates

Atom	X/a	Y/b	Z/c
C1	0.33711(0)	-0.16288(0)	0.18188(0)
H1A	0.32815(0)	-0.22204(0)	0.12606(0)
H1B	0.27794(0)	-0.13329(0)	0.19876(0)
H1C	0.36669(0)	-0.17188(0)	0.29337(0)
C3	0.66289(0)	0.16288(0)	0.18188(0)
H3A	0.72038(0)	0.16985(0)	0.24447(0)
H3B	0.63387(0)	0.22260(0)	0.16864(0)
H3C	0.67502(0)	0.13681(0)	0.06835(0)
C52	0.50000(0)	0.00000(0)	-0.26637(0)
H52A	0.49708(0)	0.04654(0)	-0.35639(0)
H52B	0.43844(0)	-0.02220(0)	-0.24142(0)
H52C	0.53800(0)	-0.05083(0)	-0.30544(0)
C11	0.66006(0)	-0.16006(0)	0.30483(0)
H11I	0.66234(0)	-0.16234(0)	0.42662(0)
C11J	0.33994(0)	0.16006(0)	0.30483(0)
H11J	0.33766(0)	0.16234(0)	0.42662(0)
C12	0.71246(0)	-0.10369(0)	0.19911(0)
H12	0.75636(0)	-0.06053(0)	0.23679(0)
C12I	0.60369(0)	-0.21246(0)	0.19911(0)
H12I	0.56053(0)	-0.25636(0)	0.23679(0)
C12J	0.39631(0)	0.21246(0)	0.19911(0)
H12J	0.43947(0)	0.25636(0)	0.23679(0)
C12K	0.28754(0)	0.10369(0)	0.19911(0)
H12K	0.24364(0)	0.06053(0)	0.23679(0)
C13	0.68894(0)	-0.12191(0)	0.02653(0)
H13	0.71438(0)	-0.09345(0)	-0.07194(0)
C13I	0.62191(0)	-0.18894(0)	0.02653(0)
H13I	0.59345(0)	-0.21438(0)	-0.07194(0)
C13J	0.37809(0)	0.18894(0)	0.02653(0)
H13J	0.40655(0)	0.21438(0)	-0.07194(0)
C13K	0.31106(0)	0.12191(0)	0.02653(0)
H13K	0.28562(0)	0.09345(0)	-0.07194(0)
O51	0.46968(0)	-0.03032(0)	0.34153(0)
S3	0.58863(0)	0.08863(0)	0.29920(0)
S1	0.40981(0)	-0.09019(0)	0.04508(0)
S52	0.55202(0)	0.05202(0)	-0.06177(0)
Mo1	0.56082(0)	-0.06082(0)	0.16596(0)
Mo1J	0.43918(0)	0.06082(0)	0.16596(0)

Orthogonal coordinates (Angstrom)

Orthogonalization matrix:

a b cosgamma c cosbeta 14.67830 0.00000 0.00000

0 b singamma -c sinbeta cosalpha* 0.00000 14.67830 0.00000

0 0 c sinbeta sinalpha* 0.00000 0.00000 7.79060

Atom	X	Y	Z
C1	4.9482(0.0000)	-2.3908(0.0000)	1.4170(0.0000)
H1A	4.8167(0.0000)	-3.2592(0.0000)	0.9821(0.0000)

H1B	4.0797(0.0000)	-1.9565(0.0000)	1.5485(0.0000)
H1C	5.3824(0.0000)	-2.5229(0.0000)	2.2855(0.0000)
C3	9.7301(0.0000)	2.3908(0.0000)	1.4170(0.0000)
H3A	10.5740(0.0000)	2.4931(0.0000)	1.9046(0.0000)
H3B	9.3041(0.0000)	3.2674(0.0000)	1.3138(0.0000)
H3C	9.9081(0.0000)	2.0081(0.0000)	0.5325(0.0000)
C52	7.3391(0.0000)	0.0000(0.0000)	-2.0752(0.0000)
H52A	7.2963(0.0000)	0.6831(0.0000)	-2.7765(0.0000)
H52B	6.4356(0.0000)	-0.3259(0.0000)	-1.8808(0.0000)
H52C	7.8969(0.0000)	-0.7461(0.0000)	-2.3796(0.0000)
C11	9.6886(0.0000)	-2.3494(0.0000)	2.3748(0.0000)
H11I	9.7220(0.0000)	-2.3829(0.0000)	3.3236(0.0000)
C11J	4.9897(0.0000)	2.3494(0.0000)	2.3748(0.0000)
H11J	4.9563(0.0000)	2.3829(0.0000)	3.3236(0.0000)
C12	10.4577(0.0000)	-1.5220(0.0000)	1.5512(0.0000)
H12	11.1021(0.0000)	-0.8885(0.0000)	1.8447(0.0000)
C12I	8.8611(0.0000)	-3.1186(0.0000)	1.5512(0.0000)
H12I	8.2276(0.0000)	-3.7629(0.0000)	1.8447(0.0000)
C12J	5.8172(0.0000)	3.1186(0.0000)	1.5512(0.0000)
H12J	6.4507(0.0000)	3.7629(0.0000)	1.8447(0.0000)
C12K	4.2206(0.0000)	1.5220(0.0000)	1.5512(0.0000)
H12K	3.5762(0.0000)	0.8885(0.0000)	1.8447(0.0000)
C13	10.1125(0.0000)	-1.7894(0.0000)	0.2067(0.0000)
H13	10.4859(0.0000)	-1.3717(0.0000)	-0.5605(0.0000)
C13I	9.1286(0.0000)	-2.7733(0.0000)	0.2067(0.0000)
H13I	8.7108(0.0000)	-3.1467(0.0000)	-0.5605(0.0000)
C13J	5.5497(0.0000)	2.7733(0.0000)	0.2067(0.0000)
H13J	5.9675(0.0000)	3.1467(0.0000)	-0.5605(0.0000)
C13K	4.5658(0.0000)	1.7894(0.0000)	0.2067(0.0000)
H13K	4.1924(0.0000)	1.3717(0.0000)	-0.5605(0.0000)
O51	6.8941(0.0000)	-0.4450(0.0000)	2.6607(0.0000)
S3	8.6401(0.0000)	1.3009(0.0000)	2.3309(0.0000)
S1	6.0153(0.0000)	-1.3238(0.0000)	0.3512(0.0000)
S52	8.1027(0.0000)	0.7636(0.0000)	-0.4812(0.0000)
Mo1	8.2319(0.0000)	-0.8927(0.0000)	1.2929(0.0000)
Mo1J	6.4464(0.0000)	0.8927(0.0000)	1.2929(0.0000)

Displacement parameters, U(I,J)x10**4
exp(-2*pi**2(U11*h**2*(a*)**2+...+2*U12*h*k*(a*)*(b*)+...)

Atom	U11	U22	U33	U23	U13	U12
C1	537(0)					
H1A	*****(0)					
H1B	*****(0)					
H1C	*****(0)					
C3	537(0)					
H3A	*****(0)					
H3B	*****(0)					
H3C	*****(0)					
C52	638(0)					
H52A	*****(0)					

H52B *****(0)
H52C *****(0)
C11 327(0) 327(0) 430(0) 89(0) -89(0) 75(0)
H11I *****(0)
C11J 327(0) 327(0) 430(0) -89(0) 89(0) 75(0)
H11J *****(0)
C12 177(0) 295(0) 584(0) -16(0) -75(0) 47(0)
H12 *****(0)
C12I 295(0) 177(0) 584(0) 75(0) 16(0) 47(0)
H12I *****(0)
C12J 295(0) 177(0) 584(0) -75(0) -16(0) 47(0)
H12J *****(0)
C12K 177(0) 295(0) 584(0) 16(0) 75(0) 47(0)
H12K *****(0)
C13 244(0) 340(0) 489(0) -52(0) 150(0) 64(0)
H13 *****(0)
C13I 340(0) 244(0) 489(0) -150(0) 52(0) 64(0)
H13I *****(0)
C13J 340(0) 244(0) 489(0) 150(0) -52(0) 64(0)
H13J *****(0)
C13K 244(0) 340(0) 489(0) 52(0) -150(0) 64(0)
H13K *****(0)
O51 290(0)
S3 252(0) 252(0) 231(0) -81(0) -81(0) 87(0)
S1 297(0) 297(0) 471(0) -154(0) -154(0) 83(0)
S52 305(0) 305(0) 170(0) -1(0) -1(0) 96(0)
Mo1 166(0) 166(0) 185(0) 1(0) -1(0) 17(0)
Mo1J 166(0) 166(0) 185(0) -1(0) 1(0) 17(0)

Principal axes of the thermal ellipsoids, Uequiv. (x10**4 A**2) and Bequiv.(A**2)

Atom	R1	R2	R3	Uequiv.	Bequiv.	Rmax/Rmin
C11	495(0)	401(0)	186(0)	361(0)	2.85(0.00)	2.66
C11J	495(0)	401(0)	186(0)	361(0)	2.85(0.00)	2.66
C12	599(0)	306(0)	150(0)	352(0)	2.78(0.00)	3.99
C12I	599(0)	306(0)	150(0)	352(0)	2.78(0.00)	3.99
C12J	599(0)	306(0)	150(0)	352(0)	2.78(0.00)	3.99
C12K	599(0)	306(0)	150(0)	352(0)	2.78(0.00)	3.99
C13	562(0)	370(0)	140(0)	358(0)	2.82(0.00)	4.01
C13I	562(0)	370(0)	140(0)	358(0)	2.82(0.00)	4.01
C13J	562(0)	370(0)	140(0)	358(0)	2.82(0.00)	4.01
C13K	562(0)	370(0)	140(0)	358(0)	2.82(0.00)	4.01
S3	412(0)	165(0)	158(0)	245(0)	1.93(0.00)	2.61
S1	649(0)	214(0)	202(0)	355(0)	2.80(0.00)	3.21
S52	401(0)	208(0)	170(0)	260(0)	2.05(0.00)	2.36
Mo1	185(0)	183(0)	149(0)	172(0)	1.36(0.00)	1.25
Mo1J	185(0)	183(0)	149(0)	172(0)	1.36(0.00)	1.25

Bond distances (Angstrom)
(Corrections following Busing & Levy, Acta Cryst.(1964).17,142)

	uncorrected distance	lower bound	upper bound	riding motion	non-correlated motion
C1 - H1A	0.9800(0)				
C1 - H1B	0.9799(0)				
C1 - H1C	0.9800(0)				
C1 - S1	1.8474(0)				
C3 - H3A	0.9800(0)				
C3 - H3B	0.9800(0)				
C3 - H3C	0.9800(0)				
C3 - S3	1.7920(0)				
C52 - H52A	0.9800(0)				
C52 - H52B	0.9800(0)				
C52 - H52C	0.9800(0)				
C52 - S52	1.9253(1)				
C11 - H11I	0.9500(0)				
C11 - C12	1.3981(0)	1.3981	1.4896	1.4006	1.4439
C11 - C12I	1.3981(0)	1.3981	1.4896	1.4006	1.4439
C11 - MO1	2.3269(0)	2.3294	2.3784	2.3384	2.3539
C11J - H11J	0.9500(0)				
C11J - C12J	1.3981(0)	1.3981	1.4896	1.4006	1.4439
C11J - C12K	1.3981(0)	1.3981	1.4896	1.4006	1.4439
C11J - MO1J	2.3269(0)	2.3294	2.3784	2.3384	2.3539
C12 - H12	0.9501(0)				
C12 - C13	1.4136(1)	1.4136	1.4907	1.4138	1.4522
C12 - MO1	2.3274(1)	2.3301	2.3791	2.3391	2.3546
C12I - H12I	0.9501(0)				
C12I - C13I	1.4136(1)	1.4136	1.4907	1.4138	1.4522
C12I - MO1	2.3274(1)	2.3301	2.3791	2.3391	2.3546
C12J - H12J	0.9501(0)				
C12J - C13J	1.4136(1)	1.4136	1.4907	1.4138	1.4522
C12J - MO1J	2.3274(1)	2.3301	2.3791	2.3391	2.3546
C12K - H12K	0.9501(0)				
C12K - C13K	1.4136(1)	1.4136	1.4907	1.4138	1.4522
C12K - MO1J	2.3274(1)	2.3301	2.3791	2.3391	2.3546
C13 - H13	0.9500(0)				
C13 - C13I	1.3914(0)	1.3914	1.4944	1.3914	1.4429
C13 - MO1	2.3496(0)	2.3525	2.4015	2.3618	2.3770
C13I - H13I	0.9500(0)				
C13I - MO1	2.3496(0)	2.3525	2.4015	2.3618	2.3770
C13J - H13J	0.9500(0)				
C13J - C13K	1.3914(0)	1.3914	1.4944	1.3914	1.4429
C13J - MO1J	2.3496(0)	2.3525	2.4015	2.3618	2.3770
C13K - H13K	0.9500(0)				
C13K - MO1J	2.3496(0)	2.3525	2.4015	2.3618	2.3770
O51 - MO1	1.9649(1)				
O51 - MO1J	1.9649(1)				
S3 - MO1	2.4610(1)	2.4614	2.4961	2.4648	2.4787
S3 - MO1J	2.4610(1)	2.4614	2.4961	2.4648	2.4787
S1 - MO1	2.4466(1)	2.4489	2.4929	2.4569	2.4709
S1 - MO1J	2.4466(1)	2.4489	2.4929	2.4569	2.4709

S52	- MO1	2.4306(1)	2.4311	2.4669	2.4349 2.4490
S52	- MO1J	2.4306(1)	2.4311	2.4669	2.4349 2.4490
Mo1	- Mo1J	2.5250(0)	2.5250	2.5542	2.5250 2.5396

Number of bond distances: 51

Bond angles (deg)
(s.u. following Cruickshank, Internat. Tables, II, 1959, p.331)

			Angle	s.u.
H1A	- C1	- H1B	109.47	0.00
H1A	- C1	- H1C	109.47	0.00
H1A	- C1	- S1	109.47	0.00
H1B	- C1	- H1C	109.48	0.00
H1B	- C1	- S1	109.47	0.00
H1C	- C1	- S1	109.47	0.00
H3A	- C3	- H3B	109.47	0.00
H3A	- C3	- H3C	109.47	0.00
H3A	- C3	- S3	109.48	0.00
H3B	- C3	- H3C	109.46	0.00
H3B	- C3	- S3	109.47	0.00
H3C	- C3	- S3	109.47	0.00
H52A	- C52	- H52B	109.48	0.00
H52A	- C52	- H52C	109.47	0.00
H52A	- C52	- S52	109.47	0.00
H52B	- C52	- H52C	109.46	0.00
H52B	- C52	- S52	109.47	0.00
H52C	- C52	- S52	109.47	0.00
H11I	- C11	- C12	126.15	0.00
H11I	- C11	- C12I	126.15	0.00
H11I	- C11	- Mo1	120.56	0.00
C12	- C11	- C12I	107.71	0.00
C12	- C11	- Mo1	72.54	0.00
C12I	- C11	- Mo1	72.54	0.00
H11J	- C11J	- C12J	126.15	0.00
H11J	- C11J	- C12K	126.15	0.00
H11J	- C11J	- Mo1J	120.56	0.00
C12J	- C11J	- C12K	107.71	0.00
C12J	- C11J	- Mo1J	72.54	0.00
C12K	- C11J	- Mo1J	72.54	0.00
C11	- C12	- H12	125.85	0.00
C11	- C12	- C13	108.30	0.00
C11	- C12	- Mo1	72.50	0.00
H12	- C12	- C13	125.85	0.00
H12	- C12	- Mo1	120.17	0.00
C13	- C12	- Mo1	73.27	0.00
C11	- C12I	- H12I	125.85	0.00
C11	- C12I	- C13I	108.30	0.00
C11	- C12I	- Mo1	72.50	0.00
H12I	- C12I	- C13I	125.85	0.00
H12I	- C12I	- Mo1	120.17	0.00

C13I - C12I - Mo1	73.27	0.00
C11J - C12J - H12J	125.85	0.00
C11J - C12J - C13J	108.30	0.00
C11J - C12J - Mo1J	72.50	0.00
H12J - C12J - C13J	125.85	0.00
H12J - C12J - Mo1J	120.17	0.00
C13J - C12J - Mo1J	73.27	0.00
C11J - C12K - H12K	125.85	0.00
C11J - C12K - C13K	108.30	0.00
C11J - C12K - Mo1J	72.50	0.00
H12K - C12K - C13K	125.85	0.00
H12K - C12K - Mo1J	120.17	0.00
C13K - C12K - Mo1J	73.27	0.00
C12 - C13 - H13	126.08	0.00
C12 - C13 - C13I	107.85	0.00
C12 - C13 - Mo1	71.55	0.00
H13 - C13 - C13I	126.08	0.00
H13 - C13 - Mo1	121.34	0.00
C13I - C13 - Mo1	72.78	0.00
C12I - C13I - C13	107.85	0.00
C12I - C13I - H13I	126.08	0.00
C12I - C13I - Mo1	71.55	0.00
C13 - C13I - H13I	126.08	0.00
C13 - C13I - Mo1	72.78	0.00
H13I - C13I - Mo1	121.34	0.00
C12J - C13J - H13J	126.08	0.00
C12J - C13J - C13K	107.85	0.00
C12J - C13J - Mo1J	71.55	0.00
H13J - C13J - C13K	126.08	0.00
H13J - C13J - Mo1J	121.34	0.00
C13K - C13J - Mo1J	72.78	0.00
C12K - C13K - C13J	107.85	0.00
C12K - C13K - H13K	126.08	0.00
C12K - C13K - Mo1J	71.55	0.00
C13J - C13K - H13K	126.08	0.00
C13J - C13K - Mo1J	72.78	0.00
H13K - C13K - Mo1J	121.34	0.00
Mo1 - O51 - Mo1J	79.96	0.00
C3 - S3 - Mo1	115.33	0.00
C3 - S3 - Mo1J	115.34	0.00
Mo1 - S3 - Mo1J	61.73	0.00
C1 - S1 - Mo1	113.77	0.00
C1 - S1 - Mo1J	113.76	0.00
Mo1 - S1 - Mo1J	62.13	0.00
C52 - S52 - Mo1	110.80	0.00
C52 - S52 - Mo1J	110.80	0.00
Mo1 - S52 - Mo1J	62.59	0.00
C11 - Mo1 - C12	34.96	0.00
C11 - Mo1 - C12I	34.96	0.00
C11 - Mo1 - C13	58.33	0.00

C11	- Mo1	- C13I	58.33	0.00
C11	- Mo1	- O51	104.19	0.00
C11	- Mo1	- S3	104.96	0.00
C11	- Mo1	- S1	129.48	0.00
C11	- Mo1	- S52	143.06	0.00
C11	- Mo1	- Mo1J	152.29	0.00
C12	- Mo1	- C12I	58.03	0.00
C12	- Mo1	- C13	35.18	0.00
C12	- Mo1	- C13I	57.99	0.00
C12	- Mo1	- O51	129.45	0.00
C12	- Mo1	- S3	92.04	0.00
C12	- Mo1	- S1	149.48	0.00
C12	- Mo1	- S52	108.42	0.00
C12	- Mo1	- Mo1J	150.16	0.00
C12I	- Mo1	- C13	57.99	0.00
C12I	- Mo1	- C13I	35.18	0.00
C12I	- Mo1	- O51	108.95	0.00
C12I	- Mo1	- S3	139.54	0.00
C12I	- Mo1	- S1	96.84	0.00
C12I	- Mo1	- S52	138.34	0.00
C12I	- Mo1	- Mo1J	150.16	0.00
C13	- Mo1	- C13I	34.45	0.00
C13	- Mo1	- O51	162.50	0.00
C13	- Mo1	- S3	113.73	0.00
C13	- Mo1	- S1	118.68	0.00
C13	- Mo1	- S52	88.00	0.00
C13	- Mo1	- Mo1J	146.70	0.00
C13I	- Mo1	- O51	139.82	0.00
C13I	- Mo1	- S3	147.69	0.00
C13I	- Mo1	- S1	91.53	0.00
C13I	- Mo1	- S52	103.19	0.00
C13I	- Mo1	- Mo1J	146.70	0.00
O51	- Mo1	- S3	67.43	0.00
O51	- Mo1	- S1	72.02	0.00
O51	- Mo1	- S52	108.46	0.00
O51	- Mo1	- Mo1J	50.02	0.00
S3	- Mo1	- S1	118.01	0.00
S3	- Mo1	- S52	73.10	0.00
S3	- Mo1	- Mo1J	59.13	0.00
S1	- Mo1	- S52	77.93	0.00
S1	- Mo1	- Mo1J	58.93	0.00
S52	- Mo1	- Mo1J	58.71	0.00
C11J	- Mo1J	- C12J	34.96	0.00
C11J	- Mo1J	- C12K	34.96	0.00
C11J	- Mo1J	- C13J	58.33	0.00
C11J	- Mo1J	- C13K	58.33	0.00
C11J	- Mo1J	- O51	104.19	0.00
C11J	- Mo1J	- S3	104.96	0.00
C11J	- Mo1J	- S1	129.48	0.00
C11J	- Mo1J	- S52	143.06	0.00

C11J - Mo1J - Mo1	152.29	0.00
C12J - Mo1J - C12K	58.03	0.00
C12J - Mo1J - C13J	35.18	0.00
C12J - Mo1J - C13K	57.99	0.00
C12J - Mo1J - O51	129.45	0.00
C12J - Mo1J - S3	92.04	0.00
C12J - Mo1J - S1	149.48	0.00
C12J - Mo1J - S52	108.42	0.00
C12J - Mo1J - Mo1	150.16	0.00
C12K - Mo1J - C13J	57.99	0.00
C12K - Mo1J - C13K	35.18	0.00
C12K - Mo1J - O51	108.95	0.00
C12K - Mo1J - S3	139.54	0.00
C12K - Mo1J - S1	96.84	0.00
C12K - Mo1J - S52	138.34	0.00
C12K - Mo1J - Mo1	150.16	0.00
C13J - Mo1J - C13K	34.45	0.00
C13J - Mo1J - O51	162.50	0.00
C13J - Mo1J - S3	113.73	0.00
C13J - Mo1J - S1	118.68	0.00
C13J - Mo1J - S52	88.00	0.00
C13J - Mo1J - Mo1	146.70	0.00
C13K - Mo1J - O51	139.82	0.00
C13K - Mo1J - S3	147.69	0.00
C13K - Mo1J - S1	91.53	0.00
C13K - Mo1J - S52	103.19	0.00
C13K - Mo1J - Mo1	146.70	0.00
O51 - Mo1J - S3	67.43	0.00
O51 - Mo1J - S1	72.02	0.00
O51 - Mo1J - S52	108.46	0.00
O51 - Mo1J - Mo1	50.02	0.00
S3 - Mo1J - S1	118.01	0.00
S3 - Mo1J - S52	73.10	0.00
S3 - Mo1J - Mo1	59.13	0.00
S1 - Mo1J - S52	77.93	0.00
S1 - Mo1J - Mo1	58.93	0.00
S52 - Mo1J - Mo1	58.71	0.00

Number of angles: 178

4. X-ray crystallographic data for 8'

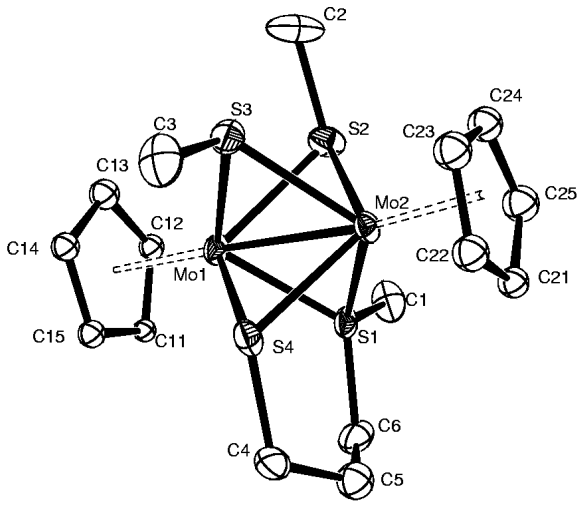


Table 1. Crystal data and structure refinement for 8'.

Identification code	**8'**
Empirical formula	C40 H47 B Mo2 O S4
Formula weight	874.71
Temperature	170(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 1 21/c 1
Unit cell dimensions	a = 17.8598(12) A alpha = 90 deg.
	b = 10.0786(6) A beta = 107.308(8) deg.
	c = 22.2717(19) A gamma = 90 deg.
Volume	3827.4(5) A^3
Z, Calculated density	4, 1.518 Mg/m^3
Absorption coefficient	0.905 mm^-1
F(000)	1792
Crystal size	0.21 x 0.17 x 0.02 mm
Theta range for data collection	2.67 to 20.82 deg.
Limiting indices	-17<=h<=17, -10<=k<=9, -22<=l<=22
Reflections collected / unique	11385 / 3863 [R(int) = 0.0503]
Completeness to theta = 20.82	96.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9821 and 0.8327
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3863 / 133 / 353
Goodness-of-fit on F^2	1.029
Final R indices [I>2sigma(I)]	R1 = 0.0529, wR2 = 0.1422
R indices (all data)	R1 = 0.0829, wR2 = 0.1539
Largest diff. peak and hole	1.364 and -0.367 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 8'.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1A)	4968(5)	9535(10)	560(4)	51(2)
O(1D)	4840(14)	8790(30)	267(12)	41(7)
C(1A)	1759(7)	1072(12)	2873(5)	60(3)
C(2A)	4599(6)	1606(13)	3441(6)	79(4)
C(3A)	4418(7)	2597(12)	1329(5)	68(3)
C(4A)	1608(6)	2144(11)	706(5)	58(3)
C(5A)	1052(8)	2480(15)	1053(6)	52(4)
C(6A)	1072(6)	1583(11)	1629(6)	59(3)
C(11A)	2492(6)	-1350(15)	1715(8)	22(5)
C(12A)	3104(12)	-1474(15)	2289(5)	28(5)
C(13A)	3827(7)	-1250(16)	2162(7)	39(5)
C(14A)	3662(9)	-987(15)	1509(8)	32(5)
C(15A)	2836(10)	-1049(14)	1233(4)	30(5)
C(21A)	2270(6)	5070(20)	2184(9)	34(7)
C(22A)	2821(13)	5377(19)	1858(6)	44(6)
C(23A)	3585(9)	5269(19)	2289(11)	48(7)
C(24A)	3506(9)	4900(19)	2883(7)	43(7)
C(25A)	2694(11)	4780(20)	2818(8)	50(9)
S(1A)	2020(2)	1583(3)	2194(2)	35(1)
S(2A)	3545(2)	1592(4)	3065(2)	46(1)
S(3A)	4209(2)	2216(4)	2057(2)	47(1)
S(4A)	2671(2)	2255(3)	1149(2)	40(1)
Mo(1A)	3138(1)	661(1)	1985(1)	34(1)
Mo(2A)	3019(1)	3185(1)	2206(1)	32(1)
C(1D)	1608(6)	2144(11)	706(5)	58(3)
C(2D)	4418(7)	2597(12)	1329(5)	68(3)
C(3D)	4599(6)	1606(13)	3441(6)	79(4)
C(4D)	1759(7)	1072(12)	2873(5)	60(3)
C(5D)	1200(30)	1860(50)	2440(20)	62(13)
C(6D)	1072(6)	1583(11)	1629(6)	59(3)
C(11D)	2606(8)	-1217(15)	1504(9)	45(6)
C(12D)	3327(14)	-984(16)	1374(6)	53(7)
C(13D)	3943(7)	-1111(15)	1946(11)	47(7)
C(14D)	3603(12)	-1421(16)	2430(5)	58(6)
C(15D)	2777(10)	-1486(16)	2157(10)	51(7)
C(21D)	2267(7)	4950(20)	2368(10)	45(8)
C(22D)	2941(12)	4814(19)	2899(6)	35(7)
C(23D)	3613(7)	5067(19)	2701(8)	39(6)
C(24D)	3355(10)	5357(18)	2047(8)	33(5)

C(25D)	2523(10)	5283(19)	1842(6)	42(7)
S(1D)	1957(6)	1943(10)	1499(5)	39(3)
S(2D)	3420(6)	2450(11)	1272(5)	43(3)
S(3D)	4240(6)	1968(11)	2585(5)	40(3)
S(4D)	2790(6)	1427(11)	2854(5)	41(3)
Mo(1D)	3138(1)	661(1)	1985(1)	34(1)
Mo(2D)	3019(1)	3185(1)	2206(1)	32(1)
C(30)	1157(3)	7793(6)	3662(2)	35(2)
C(31)	1248(4)	7264(6)	3108(3)	51(3)
C(32)	819(5)	7671(7)	2516(2)	67(3)
C(33)	247(4)	8606(7)	2440(3)	67(3)
C(34)	141(3)	9205(6)	2967(4)	60(3)
C(35)	580(4)	8792(6)	3551(3)	41(2)
C(40)	2500(3)	8246(7)	4563(3)	39(2)
C(41)	2875(4)	8606(8)	4122(2)	64(3)
C(42)	3582(4)	9324(9)	4297(4)	88(4)
C(43)	3885(4)	9717(9)	4917(4)	92(5)
C(44)	3539(4)	9359(9)	5353(3)	85(4)
C(45)	2860(4)	8660(8)	5172(3)	56(3)
C(50)	1205(3)	7521(6)	4868(3)	37(2)
C(51)	858(3)	6472(5)	5097(3)	36(2)
C(52)	432(3)	6656(6)	5503(3)	46(3)
C(53)	321(4)	7920(7)	5709(3)	55(3)
C(54)	666(4)	8955(6)	5510(3)	62(3)
C(55)	1095(4)	8770(5)	5099(3)	53(3)
C(60)	1941(4)	5769(5)	4327(3)	35(2)
C(61)	1418(3)	4785(6)	4037(3)	42(2)
C(62)	1601(4)	3471(6)	4041(3)	50(3)
C(63)	2340(4)	3014(5)	4336(3)	55(3)
C(64)	2897(3)	3957(7)	4630(3)	58(3)
C(65)	2697(3)	5293(6)	4615(3)	49(3)
B	1701(6)	7321(12)	4340(5)	38(2)

Table 3. Bond lengths [A] and angles [deg] for 8'.

C(1A)-S(1A)	1.786(11)
C(2A)-S(2A)	1.820(11)
C(3A)-S(3A)	1.810(11)
C(4A)-C(5A)	1.468(17)
C(4A)-S(4A)	1.864(11)
C(5A)-C(6A)	1.562(18)
C(6A)-S(1A)	1.783(10)
C(11A)-C(12A)	1.4200
C(11A)-C(15A)	1.4200
C(11A)-Mo(1A)	2.321(13)
C(12A)-C(13A)	1.4200
C(12A)-Mo(1A)	2.262(14)
C(13A)-C(14A)	1.4200
C(13A)-Mo(1A)	2.257(15)
C(14A)-C(15A)	1.4200
C(14A)-Mo(1A)	2.312(14)
C(15A)-Mo(1A)	2.351(13)
C(21A)-C(22A)	1.4200
C(21A)-C(25A)	1.4200
C(21A)-Mo(2A)	2.318(18)
C(22A)-C(23A)	1.4200
C(22A)-Mo(2A)	2.333(17)
C(23A)-C(24A)	1.4200
C(23A)-Mo(2A)	2.314(17)
C(24A)-C(25A)	1.4200
C(24A)-Mo(2A)	2.287(17)
C(25A)-Mo(2A)	2.290(18)
S(1A)-Mo(1A)	2.371(3)
S(1A)-Mo(2A)	2.402(3)
S(2A)-Mo(2A)	2.460(4)
S(2A)-Mo(1A)	2.482(4)
S(3A)-Mo(1A)	2.441(3)
S(3A)-Mo(2A)	2.450(4)
S(4A)-Mo(1A)	2.413(4)
S(4A)-Mo(2A)	2.438(3)
Mo(1A)-Mo(2A)	2.6126(12)
C(11D)-C(15D)	1.4200
C(11D)-C(12D)	1.4200
C(12D)-C(13D)	1.4200
C(13D)-C(14D)	1.4200
C(14D)-C(15D)	1.4200
C(21D)-C(22D)	1.4200
C(21D)-C(25D)	1.4200
C(22D)-C(23D)	1.4200
C(23D)-C(24D)	1.4200
C(24D)-C(25D)	1.4200

C(30)-C(31)	1.3987
C(30)-C(35)	1.4089
C(30)-B	1.605(12)
C(31)-C(32)	1.3752
C(32)-C(33)	1.3631
C(33)-C(34)	1.3820
C(34)-C(35)	1.3682
C(40)-C(45)	1.3821
C(40)-C(41)	1.3907
C(40)-B	1.654(12)
C(41)-C(42)	1.4057
C(42)-C(43)	1.3830
C(43)-C(44)	1.3439
C(44)-C(45)	1.3555
C(50)-C(55)	1.3953
C(50)-C(51)	1.3955
C(50)-B	1.683(12)
C(51)-C(52)	1.3567
C(52)-C(53)	1.3882
C(53)-C(54)	1.3523
C(54)-C(55)	1.3699
C(60)-C(61)	1.3840
C(60)-C(65)	1.3951
C(60)-B	1.625(13)
C(61)-C(62)	1.3634
C(62)-C(63)	1.3679
C(63)-C(64)	1.3912
C(64)-C(65)	1.3913

C(5A)-C(4A)-S(4A)	116.8(9)
C(4A)-C(5A)-C(6A)	116.4(11)
C(5A)-C(6A)-S(1A)	111.4(8)
C(12A)-C(11A)-C(15A)	108.0
C(12A)-C(11A)-Mo(1A)	69.7(5)
C(15A)-C(11A)-Mo(1A)	73.5(5)
C(11A)-C(12A)-C(13A)	108.0
C(11A)-C(12A)-Mo(1A)	74.2(5)
C(13A)-C(12A)-Mo(1A)	71.5(5)
C(14A)-C(13A)-C(12A)	108.0
C(14A)-C(13A)-Mo(1A)	74.0(5)
C(12A)-C(13A)-Mo(1A)	71.9(5)
C(15A)-C(14A)-C(13A)	108.0
C(15A)-C(14A)-Mo(1A)	73.8(5)
C(13A)-C(14A)-Mo(1A)	69.8(5)
C(14A)-C(15A)-C(11A)	108.0
C(14A)-C(15A)-Mo(1A)	70.8(5)
C(11A)-C(15A)-Mo(1A)	71.1(5)
C(22A)-C(21A)-C(25A)	108.0
C(22A)-C(21A)-Mo(2A)	72.8(7)
C(25A)-C(21A)-Mo(2A)	71.0(6)

C(23A)-C(22A)-C(21A)	108.0
C(23A)-C(22A)-Mo(2A)	71.5(6)
C(21A)-C(22A)-Mo(2A)	71.6(7)
C(22A)-C(23A)-C(24A)	108.0
C(22A)-C(23A)-Mo(2A)	72.9(6)
C(24A)-C(23A)-Mo(2A)	71.0(7)
C(25A)-C(24A)-C(23A)	108.0
C(25A)-C(24A)-Mo(2A)	72.0(7)
C(23A)-C(24A)-Mo(2A)	73.1(7)
C(24A)-C(25A)-C(21A)	108.0
C(24A)-C(25A)-Mo(2A)	71.8(7)
C(21A)-C(25A)-Mo(2A)	73.1(6)
C(6A)-S(1A)-C(1A)	99.5(6)
C(6A)-S(1A)-Mo(1A)	122.6(4)
C(1A)-S(1A)-Mo(1A)	120.1(4)
C(6A)-S(1A)-Mo(2A)	123.6(4)
C(1A)-S(1A)-Mo(2A)	124.4(4)
Mo(1A)-S(1A)-Mo(2A)	66.37(9)
C(2A)-S(2A)-Mo(2A)	117.1(4)
C(2A)-S(2A)-Mo(1A)	114.4(5)
Mo(2A)-S(2A)-Mo(1A)	63.82(9)
C(3A)-S(3A)-Mo(1A)	116.4(4)
C(3A)-S(3A)-Mo(2A)	117.1(4)
Mo(1A)-S(3A)-Mo(2A)	64.59(9)
C(4A)-S(4A)-Mo(1A)	115.6(4)
C(4A)-S(4A)-Mo(2A)	117.4(4)
Mo(1A)-S(4A)-Mo(2A)	65.18(9)
C(13A)-Mo(1A)-C(12A)	36.6(2)
C(13A)-Mo(1A)-C(14A)	36.2(2)
C(12A)-Mo(1A)-C(14A)	60.3(3)
C(13A)-Mo(1A)-C(11A)	60.2(3)
C(12A)-Mo(1A)-C(11A)	36.1(2)
C(14A)-Mo(1A)-C(11A)	59.5(2)
C(13A)-Mo(1A)-C(15A)	59.8(3)
C(12A)-Mo(1A)-C(15A)	59.7(3)
C(14A)-Mo(1A)-C(15A)	35.45(18)
C(11A)-Mo(1A)-C(15A)	35.39(18)
C(13A)-Mo(1A)-S(1A)	138.4(5)
C(12A)-Mo(1A)-S(1A)	102.4(4)
C(14A)-Mo(1A)-S(1A)	148.3(4)
C(11A)-Mo(1A)-S(1A)	90.6(3)
C(15A)-Mo(1A)-S(1A)	113.6(4)
C(13A)-Mo(1A)-S(4A)	138.5(5)
C(12A)-Mo(1A)-S(4A)	146.2(4)
C(14A)-Mo(1A)-S(4A)	102.7(4)
C(11A)-Mo(1A)-S(4A)	110.5(4)
C(15A)-Mo(1A)-S(4A)	89.2(3)
S(1A)-Mo(1A)-S(4A)	76.90(12)
C(13A)-Mo(1A)-S(3A)	99.2(4)
C(12A)-Mo(1A)-S(3A)	132.9(5)

C(14A)-Mo(1A)-S(3A)	94.3(3)
C(11A)-Mo(1A)-S(3A)	153.8(3)
C(15A)-Mo(1A)-S(3A)	121.8(4)
S(1A)-Mo(1A)-S(3A)	115.13(12)
S(4A)-Mo(1A)-S(3A)	72.96(13)
C(13A)-Mo(1A)-S(2A)	99.5(4)
C(12A)-Mo(1A)-S(2A)	95.5(3)
C(14A)-Mo(1A)-S(2A)	132.4(5)
C(11A)-Mo(1A)-S(2A)	124.1(4)
C(15A)-Mo(1A)-S(2A)	155.1(3)
S(1A)-Mo(1A)-S(2A)	71.42(12)
S(4A)-Mo(1A)-S(2A)	115.50(12)
S(3A)-Mo(1A)-S(2A)	72.28(13)
C(13A)-Mo(1A)-Mo(2A)	150.3(3)
C(12A)-Mo(1A)-Mo(2A)	149.2(3)
C(14A)-Mo(1A)-Mo(2A)	148.5(3)
C(11A)-Mo(1A)-Mo(2A)	146.9(3)
C(15A)-Mo(1A)-Mo(2A)	146.5(3)
S(1A)-Mo(1A)-Mo(2A)	57.37(8)
S(4A)-Mo(1A)-Mo(2A)	57.87(8)
S(3A)-Mo(1A)-Mo(2A)	57.87(9)
S(2A)-Mo(1A)-Mo(2A)	57.67(9)
C(24A)-Mo(2A)-C(25A)	36.1(3)
C(24A)-Mo(2A)-C(23A)	35.9(2)
C(25A)-Mo(2A)-C(23A)	59.9(3)
C(24A)-Mo(2A)-C(21A)	59.9(3)
C(25A)-Mo(2A)-C(21A)	35.9(3)
C(23A)-Mo(2A)-C(21A)	59.5(3)
C(24A)-Mo(2A)-C(22A)	59.6(3)
C(25A)-Mo(2A)-C(22A)	59.6(3)
C(23A)-Mo(2A)-C(22A)	35.6(2)
C(21A)-Mo(2A)-C(22A)	35.6(2)
C(24A)-Mo(2A)-S(1A)	130.6(6)
C(25A)-Mo(2A)-S(1A)	99.1(4)
C(23A)-Mo(2A)-S(1A)	156.4(3)
C(21A)-Mo(2A)-S(1A)	97.5(4)
C(22A)-Mo(2A)-S(1A)	126.5(6)
C(24A)-Mo(2A)-S(4A)	149.9(5)
C(25A)-Mo(2A)-S(4A)	143.9(5)
C(23A)-Mo(2A)-S(4A)	114.0(5)
C(21A)-Mo(2A)-S(4A)	108.4(5)
C(22A)-Mo(2A)-S(4A)	94.2(4)
S(1A)-Mo(2A)-S(4A)	75.86(11)
C(24A)-Mo(2A)-S(3A)	102.5(5)
C(25A)-Mo(2A)-S(3A)	138.1(5)
C(23A)-Mo(2A)-S(3A)	89.8(3)
C(21A)-Mo(2A)-S(3A)	147.5(5)
C(22A)-Mo(2A)-S(3A)	112.6(5)
S(1A)-Mo(2A)-S(3A)	113.70(11)
S(4A)-Mo(2A)-S(3A)	72.38(12)

C(24A)-Mo(2A)-S(2A)	89.9(4)
C(25A)-Mo(2A)-S(2A)	95.8(4)
C(23A)-Mo(2A)-S(2A)	118.3(6)
C(21A)-Mo(2A)-S(2A)	129.5(5)
C(22A)-Mo(2A)-S(2A)	149.5(4)
S(1A)-Mo(2A)-S(2A)	71.32(12)
S(4A)-Mo(2A)-S(2A)	115.41(12)
S(3A)-Mo(2A)-S(2A)	72.53(13)
C(24A)-Mo(2A)-Mo(1A)	145.5(3)
C(25A)-Mo(2A)-Mo(1A)	147.6(4)
C(23A)-Mo(2A)-Mo(1A)	147.3(3)
C(21A)-Mo(2A)-Mo(1A)	151.0(4)
C(22A)-Mo(2A)-Mo(1A)	150.7(3)
S(1A)-Mo(2A)-Mo(1A)	56.26(8)
S(4A)-Mo(2A)-Mo(1A)	56.95(8)
S(3A)-Mo(2A)-Mo(1A)	57.55(9)
S(2A)-Mo(2A)-Mo(1A)	58.51(9)
C(15D)-C(11D)-C(12D)	108.0
C(13D)-C(12D)-C(11D)	108.0
C(14D)-C(13D)-C(12D)	108.0
C(15D)-C(14D)-C(13D)	108.0
C(14D)-C(15D)-C(11D)	108.0
C(22D)-C(21D)-C(25D)	108.0
C(23D)-C(22D)-C(21D)	108.0
C(22D)-C(23D)-C(24D)	108.0
C(25D)-C(24D)-C(23D)	108.0
C(24D)-C(25D)-C(21D)	108.0
C(31)-C(30)-C(35)	112.8
C(31)-C(30)-B	121.4(6)
C(35)-C(30)-B	125.7(6)
C(32)-C(31)-C(30)	123.7
C(33)-C(32)-C(31)	120.6
C(32)-C(33)-C(34)	118.9
C(35)-C(34)-C(33)	119.3
C(34)-C(35)-C(30)	124.6
C(45)-C(40)-C(41)	115.7
C(45)-C(40)-B	124.9(6)
C(41)-C(40)-B	119.3(6)
C(40)-C(41)-C(42)	121.3
C(43)-C(42)-C(41)	118.5
C(44)-C(43)-C(42)	121.1
C(43)-C(44)-C(45)	119.2
C(44)-C(45)-C(40)	124.1
C(55)-C(50)-C(51)	115.0
C(55)-C(50)-B	121.7(6)
C(51)-C(50)-B	123.2(6)
C(52)-C(51)-C(50)	122.6
C(51)-C(52)-C(53)	120.6
C(54)-C(53)-C(52)	118.4
C(53)-C(54)-C(55)	121.0

C(54)-C(55)-C(50)	122.4
C(61)-C(60)-C(65)	113.3
C(61)-C(60)-B	123.5(6)
C(65)-C(60)-B	123.2(6)
C(62)-C(61)-C(60)	124.4
C(61)-C(62)-C(63)	121.7
C(62)-C(63)-C(64)	116.7
C(63)-C(64)-C(65)	120.5
C(64)-C(65)-C(60)	123.4
C(30)-B-C(60)	111.0(7)
C(30)-B-C(40)	110.0(8)
C(60)-B-C(40)	109.8(7)
C(30)-B-C(50)	109.0(7)
C(60)-B-C(50)	108.9(7)
C(40)-B-C(50)	108.0(7)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 8'.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1A)	65(8)	55(8)	75(7)	-13(6)	43(6)	-18(6)
C(2A)	55(7)	85(11)	71(8)	25(7)	-23(5)	-24(6)
C(3A)	73(8)	66(9)	81(8)	-2(7)	49(7)	-11(6)
C(4A)	61(6)	42(8)	55(6)	-14(5)	-9(4)	9(5)
C(6A)	32(4)	41(8)	93(7)	-11(6)	5(5)	-1(4)
S(1A)	37(2)	22(2)	48(2)	-7(2)	16(2)	1(1)
S(2A)	51(2)	39(2)	40(2)	7(2)	2(2)	-4(2)
S(3A)	36(2)	37(2)	69(3)	-9(2)	18(2)	-7(2)
S(4A)	56(2)	30(2)	34(2)	-6(2)	13(2)	3(2)
Mo(1A)	34(1)	21(1)	49(1)	-3(1)	14(1)	2(1)
Mo(2A)	41(1)	20(1)	35(1)	-4(1)	11(1)	-1(1)
C(1D)	61(6)	42(8)	55(6)	-14(5)	-9(4)	9(5)
C(2D)	73(8)	66(9)	81(8)	-2(7)	49(7)	-11(6)
C(3D)	55(7)	85(11)	71(8)	25(7)	-23(5)	-24(6)
C(4D)	65(8)	55(8)	75(7)	-13(6)	43(6)	-18(6)
C(6D)	32(4)	41(8)	93(7)	-11(6)	5(5)	-1(4)
Mo(1D)	34(1)	21(1)	49(1)	-3(1)	14(1)	2(1)
Mo(2D)	41(1)	20(1)	35(1)	-4(1)	11(1)	-1(1)
C(30)	42(5)	28(6)	34(5)	-2(4)	10(4)	-5(4)
C(31)	63(7)	53(8)	30(5)	0(5)	1(5)	14(5)
C(32)	114(10)	34(8)	35(6)	4(5)	-5(6)	-10(6)

C(33)	73(8)	48(8)	48(6)	21(5)	-31(6)	-24(5)
C(34)	33(6)	43(7)	95(8)	32(6)	6(6)	-1(5)
C(35)	31(6)	41(6)	54(6)	13(5)	16(5)	-4(4)
C(40)	40(5)	40(6)	38(5)	13(5)	12(4)	6(4)
C(41)	48(7)	94(10)	47(6)	26(6)	12(5)	-5(6)
C(42)	54(8)	123(13)	90(8)	50(9)	25(7)	-13(7)
C(43)	49(8)	102(12)	117(9)	12(9)	11(7)	-34(7)
C(44)	51(8)	112(12)	80(8)	-8(8)	1(6)	-31(7)
C(45)	44(6)	70(8)	50(6)	-6(6)	8(5)	-19(5)
C(50)	32(5)	45(6)	32(6)	-4(4)	5(4)	0(4)
C(51)	24(5)	45(6)	37(6)	-1(5)	5(4)	1(4)
C(52)	35(6)	63(6)	40(7)	3(5)	13(5)	-9(5)
C(53)	46(7)	81(8)	42(7)	-7(6)	20(5)	7(6)
C(54)	62(8)	57(7)	78(9)	-32(6)	36(6)	-13(6)
C(55)	58(7)	45(6)	61(8)	-14(5)	28(6)	-12(6)
C(60)	36(5)	48(5)	24(6)	-1(4)	11(4)	2(4)
C(61)	41(5)	42(5)	45(7)	-2(5)	16(5)	8(4)
C(62)	60(6)	40(6)	51(7)	-10(5)	19(5)	1(5)
C(63)	75(7)	45(6)	49(8)	13(5)	26(6)	19(5)
C(64)	56(6)	64(7)	50(8)	13(6)	12(6)	27(5)
C(65)	54(6)	59(6)	30(6)	-3(5)	3(5)	15(5)
B	35(6)	44(6)	33(5)	0(5)	7(4)	3(4)

5. X-ray crystallographic data for 10'.

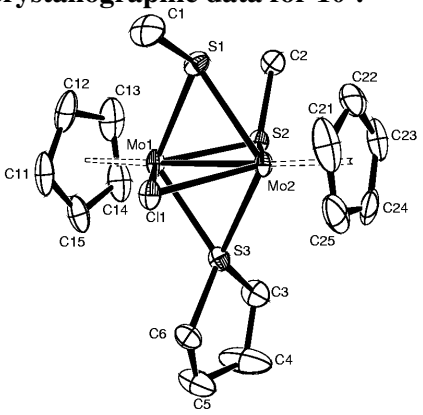


Table 1. Crystal data and structure refinement for 10'.

Identification code	**10'**
Empirical formula	C16 H24 Cl F6 Mo2 P S3
Formula weight	684.83
Temperature	170(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 10.8501(8) A alpha = 68.456(7) deg. b = 13.5873(15) A beta = 89.075(5) deg. c = 17.1418(10) A gamma = 81.857(8) deg.
Volume	2325.1(3) A^3
Z, Calculated density	4, 1.956 Mg/m^3
Absorption coefficient	1.581 mm^-1
F(000)	1352
Crystal size	0.55 x 0.41 x 0.14 mm
Theta range for data collection	2.66 to 23.26 deg.
Limiting indices	-12<=h<=12, -15<=k<=15, -16<=l<=17
Reflections collected / unique	12430 / 5776 [R(int) = 0.0212]
Completeness to theta = 23.26	86.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8090 and 0.4767
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5776 / 0 / 527
Goodness-of-fit on F^2	1.058
Final R indices [I>2sigma(I)]	R1 = 0.0514, wR2 = 0.1355
R indices (all data)	R1 = 0.0754, wR2 = 0.1507
Largest diff. peak and hole	1.966 and -1.013 e.A^-3

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

	x	y	z	U(eq)
C(1)	-398(11)	2797(9)	4198(7)	66(3)
C(2)	614(9)	4568(7)	1314(6)	46(3)
C(3)	4301(9)	5658(9)	2363(6)	57(3)
C(4)	5323(15)	5900(15)	2780(9)	133(8)
C(5)	5581(11)	5282(11)	3638(8)	77(4)
C(6)	4402(9)	4920(8)	4060(6)	46(2)
C(11)	3735(13)	1680(9)	3935(8)	69(4)
C(12)	2780(14)	1593(8)	3387(10)	85(4)
C(13)	2997(17)	2243(11)	2571(9)	84(4)
C(14)	4030(14)	2716(10)	2579(9)	79(4)
C(15)	4458(12)	2342(10)	3431(8)	66(3)
C(21)	-372(15)	5971(11)	3730(9)	82(5)
C(22)	-846(11)	6107(10)	2955(10)	68(4)
C(23)	-90(13)	6678(9)	2385(8)	69(4)
C(24)	833(13)	6917(9)	2781(13)	92(5)
C(25)	692(16)	6452(12)	3638(11)	88(5)
Cl(1)	1967(2)	3679(2)	4559(1)	40(1)
S(1)	281(2)	3552(2)	3202(2)	45(1)
S(2)	1807(2)	4827(2)	1920(1)	37(1)
S(3)	3388(2)	4923(2)	3216(2)	39(1)
Mo(1)	2550(1)	3378(1)	3233(1)	36(1)
Mo(2)	1137(1)	5116(1)	3194(1)	33(1)
C(51)	11259(10)	591(12)	1924(9)	89(4)
C(52)	7587(11)	3129(8)	2184(8)	71(4)
C(53)	5003(9)	592(9)	1677(8)	58(3)
C(54)	4437(13)	-99(13)	1327(11)	108(6)
C(55)	5210(15)	-1173(13)	1660(12)	123(7)
C(56)	6525(13)	-1063(9)	1476(8)	75(4)
C(61)	9030(16)	-1107(11)	3837(7)	88(5)
C(62)	9080(11)	-206(10)	3984(7)	61(3)
C(63)	7875(14)	294(9)	3961(6)	65(3)
C(64)	7058(12)	-317(14)	3793(7)	85(5)
C(65)	7810(20)	-1203(10)	3725(8)	98(6)
C(71)	9132(14)	1777(14)	-225(8)	86(5)
C(72)	9012(14)	2645(14)	-64(8)	83(4)
C(73)	7814(19)	3048(11)	-16(9)	92(5)
C(74)	7109(12)	2353(16)	-188(8)	104(6)
C(75)	7940(20)	1546(13)	-310(8)	102(5)
Cl(51)	9285(3)	-527(2)	1653(2)	71(1)

S(51)	9732(3)	1419(3)	2010(2)	64(1)
S(52)	6996(2)	2043(2)	1981(2)	44(1)
S(53)	6684(2)	174(2)	1663(2)	42(1)
Mo(51)	8169(1)	255(1)	2644(1)	37(1)
Mo(52)	8170(1)	1360(1)	1023(1)	41(1)
F(1)	2140(7)	8736(7)	4163(6)	123(3)
F(2)	4871(7)	7600(6)	4244(6)	106(3)
F(3)	3132(11)	7122(9)	4778(10)	232(9)
F(4)	3863(10)	9183(7)	3487(7)	152(4)
F(5)	3234(10)	7843(11)	3428(7)	166(5)
F(6)	3795(12)	8498(17)	4883(10)	294(12)
P(1)	3499(3)	8173(2)	4193(2)	57(1)
F(51)	7950(15)	7199(16)	-226(12)	285(10)
F(52)	5992(15)	6009(18)	786(10)	274(9)
F(53)	7691(13)	5593(9)	378(7)	183(6)
F(54)	6108(12)	7617(12)	340(10)	231(9)
F(55)	7647(11)	6580(13)	1114(9)	219(8)
F(56)	6329(10)	6804(8)	-506(5)	136(4)
P(51)	7002(3)	6685(3)	321(2)	66(1)

Table 3. Bond lengths [A] and angles [deg] for 10'.

C(1)-S(1)	1.843(10)
C(2)-S(2)	1.822(9)
C(3)-C(4)	1.467(16)
C(3)-S(3)	1.811(10)
C(4)-C(5)	1.408(17)
C(5)-C(6)	1.513(15)
C(6)-S(3)	1.830(9)
C(11)-C(15)	1.334(17)
C(11)-C(12)	1.454(18)
C(11)-Mo(1)	2.365(10)
C(12)-C(13)	1.390(18)
C(12)-Mo(1)	2.318(10)
C(13)-C(14)	1.370(18)
C(13)-Mo(1)	2.225(11)
C(14)-C(15)	1.420(17)
C(14)-Mo(1)	2.217(11)
C(15)-Mo(1)	2.286(11)
C(21)-C(22)	1.371(17)
C(21)-C(25)	1.385(19)
C(21)-Mo(2)	2.251(10)
C(22)-C(23)	1.352(17)
C(22)-Mo(2)	2.326(10)
C(23)-C(24)	1.358(18)
C(23)-Mo(2)	2.301(10)
C(24)-C(25)	1.386(19)
C(24)-Mo(2)	2.259(11)
C(25)-Mo(2)	2.204(11)
Cl(1)-Mo(1)	2.510(2)
Cl(1)-Mo(2)	2.512(2)
S(1)-Mo(2)	2.431(2)
S(1)-Mo(1)	2.439(3)
S(2)-Mo(1)	2.439(2)
S(2)-Mo(2)	2.439(2)
S(3)-Mo(1)	2.394(2)
S(3)-Mo(2)	2.419(2)
Mo(1)-Mo(2)	2.6069(10)
C(51)-S(51)	1.902(12)
C(52)-S(52)	1.833(10)
C(53)-C(54)	1.485(15)
C(53)-S(53)	1.834(10)
C(54)-C(55)	1.49(2)
C(55)-C(56)	1.473(17)
C(56)-S(53)	1.854(9)
C(61)-C(62)	1.346(17)
C(61)-C(65)	1.37(2)
C(61)-Mo(51)	2.296(10)

C(62)-C(63)	1.380(16)
C(62)-Mo(51)	2.343(11)
C(63)-C(64)	1.396(18)
C(63)-Mo(51)	2.294(10)
C(64)-C(65)	1.40(2)
C(64)-Mo(51)	2.237(11)
C(65)-Mo(51)	2.239(11)
C(71)-C(72)	1.295(19)
C(71)-C(75)	1.40(2)
C(71)-Mo(52)	2.279(12)
C(72)-C(73)	1.351(19)
C(72)-Mo(52)	2.315(12)
C(73)-C(74)	1.41(2)
C(73)-Mo(52)	2.314(12)
C(74)-C(75)	1.39(2)
C(74)-Mo(52)	2.244(11)
C(75)-Mo(52)	2.219(14)
Cl(51)-Mo(52)	2.516(3)
Cl(51)-Mo(51)	2.525(3)
S(51)-Mo(52)	2.444(3)
S(51)-Mo(51)	2.450(3)
S(52)-Mo(52)	2.429(3)
S(52)-Mo(51)	2.440(2)
S(53)-Mo(51)	2.389(3)
S(53)-Mo(52)	2.405(3)
Mo(51)-Mo(52)	2.6290(12)
F(1)-P(1)	1.553(7)
F(2)-P(1)	1.568(7)
F(3)-P(1)	1.516(10)
F(4)-P(1)	1.556(9)
F(5)-P(1)	1.577(10)
F(6)-P(1)	1.460(10)
F(51)-P(51)	1.455(13)
F(52)-P(51)	1.549(16)
F(53)-P(51)	1.533(10)
F(54)-P(51)	1.492(9)
F(55)-P(51)	1.489(10)
F(56)-P(51)	1.549(8)

C(4)-C(3)-S(3)	104.3(8)
C(5)-C(4)-C(3)	117.5(11)
C(4)-C(5)-C(6)	110.2(10)
C(5)-C(6)-S(3)	104.9(7)
C(15)-C(11)-C(12)	105.6(12)
C(15)-C(11)-Mo(1)	70.1(6)
C(12)-C(11)-Mo(1)	70.1(6)
C(13)-C(12)-C(11)	107.5(13)
C(13)-C(12)-Mo(1)	68.6(6)
C(11)-C(12)-Mo(1)	73.7(6)
C(14)-C(13)-C(12)	109.1(14)

C(14)-C(13)-Mo(1)	71.7(7)
C(12)-C(13)-Mo(1)	75.8(7)
C(13)-C(14)-C(15)	106.2(13)
C(13)-C(14)-Mo(1)	72.3(7)
C(15)-C(14)-Mo(1)	74.3(6)
C(11)-C(15)-C(14)	111.6(14)
C(11)-C(15)-Mo(1)	76.6(7)
C(14)-C(15)-Mo(1)	69.0(6)
C(22)-C(21)-C(25)	109.5(13)
C(22)-C(21)-Mo(2)	75.6(7)
C(25)-C(21)-Mo(2)	70.1(7)
C(23)-C(22)-C(21)	106.6(12)
C(23)-C(22)-Mo(2)	72.0(6)
C(21)-C(22)-Mo(2)	69.6(6)
C(22)-C(23)-C(24)	110.0(13)
C(22)-C(23)-Mo(2)	74.0(6)
C(24)-C(23)-Mo(2)	71.0(7)
C(23)-C(24)-C(25)	108.0(13)
C(23)-C(24)-Mo(2)	74.4(7)
C(25)-C(24)-Mo(2)	69.8(7)
C(21)-C(25)-C(24)	105.8(12)
C(21)-C(25)-Mo(2)	73.8(7)
C(24)-C(25)-Mo(2)	74.1(7)
Mo(1)-Cl(1)-Mo(2)	62.55(6)
C(1)-S(1)-Mo(2)	114.8(4)
C(1)-S(1)-Mo(1)	115.2(4)
Mo(2)-S(1)-Mo(1)	64.73(7)
C(2)-S(2)-Mo(1)	116.3(3)
C(2)-S(2)-Mo(2)	116.3(3)
Mo(1)-S(2)-Mo(2)	64.61(6)
C(3)-S(3)-C(6)	96.0(5)
C(3)-S(3)-Mo(1)	122.1(4)
C(6)-S(3)-Mo(1)	123.4(3)
C(3)-S(3)-Mo(2)	124.9(3)
C(6)-S(3)-Mo(2)	126.3(3)
Mo(1)-S(3)-Mo(2)	65.60(7)
C(14)-Mo(1)-C(13)	35.9(5)
C(14)-Mo(1)-C(15)	36.7(4)
C(13)-Mo(1)-C(15)	59.3(5)
C(14)-Mo(1)-C(12)	59.4(5)
C(13)-Mo(1)-C(12)	35.6(5)
C(15)-Mo(1)-C(12)	57.7(5)
C(14)-Mo(1)-C(11)	59.5(5)
C(13)-Mo(1)-C(11)	59.9(5)
C(15)-Mo(1)-C(11)	33.3(4)
C(12)-Mo(1)-C(11)	36.2(4)
C(14)-Mo(1)-S(3)	99.8(5)
C(13)-Mo(1)-S(3)	133.9(5)
C(15)-Mo(1)-S(3)	93.8(4)
C(12)-Mo(1)-S(3)	151.5(4)

C(11)-Mo(1)-S(3)	117.9(4)
C(14)-Mo(1)-S(1)	134.3(5)
C(13)-Mo(1)-S(1)	100.3(5)
C(15)-Mo(1)-S(1)	150.3(4)
C(12)-Mo(1)-S(1)	93.0(4)
C(11)-Mo(1)-S(1)	119.3(4)
S(3)-Mo(1)-S(1)	115.17(8)
C(14)-Mo(1)-S(2)	91.1(4)
C(13)-Mo(1)-S(2)	91.2(4)
C(15)-Mo(1)-S(2)	124.2(3)
C(12)-Mo(1)-S(2)	122.6(4)
C(11)-Mo(1)-S(2)	149.2(3)
S(3)-Mo(1)-S(2)	73.16(8)
S(1)-Mo(1)-S(2)	73.28(8)
C(14)-Mo(1)-Cl(1)	145.9(4)
C(13)-Mo(1)-Cl(1)	148.8(4)
C(15)-Mo(1)-Cl(1)	109.5(3)
C(12)-Mo(1)-Cl(1)	113.2(4)
C(11)-Mo(1)-Cl(1)	94.3(3)
S(3)-Mo(1)-Cl(1)	71.89(8)
S(1)-Mo(1)-Cl(1)	76.09(8)
S(2)-Mo(1)-Cl(1)	116.42(8)
C(14)-Mo(1)-Mo(2)	144.5(4)
C(13)-Mo(1)-Mo(2)	144.6(4)
C(15)-Mo(1)-Mo(2)	150.8(4)
C(12)-Mo(1)-Mo(2)	150.1(4)
C(11)-Mo(1)-Mo(2)	153.1(3)
S(3)-Mo(1)-Mo(2)	57.66(6)
S(1)-Mo(1)-Mo(2)	57.50(6)
S(2)-Mo(1)-Mo(2)	57.71(6)
Cl(1)-Mo(1)-Mo(2)	58.78(5)
C(25)-Mo(2)-C(21)	36.2(5)
C(25)-Mo(2)-C(24)	36.2(5)
C(21)-Mo(2)-C(24)	58.7(5)
C(25)-Mo(2)-C(23)	59.0(5)
C(21)-Mo(2)-C(23)	57.3(4)
C(24)-Mo(2)-C(23)	34.6(5)
C(25)-Mo(2)-C(22)	59.5(5)
C(21)-Mo(2)-C(22)	34.8(4)
C(24)-Mo(2)-C(22)	57.9(5)
C(23)-Mo(2)-C(22)	34.0(4)
C(25)-Mo(2)-S(3)	100.8(5)
C(21)-Mo(2)-S(3)	134.9(5)
C(24)-Mo(2)-S(3)	95.7(4)
C(23)-Mo(2)-S(3)	122.2(4)
C(22)-Mo(2)-S(3)	153.6(3)
C(25)-Mo(2)-S(1)	139.7(6)
C(21)-Mo(2)-S(1)	103.9(5)
C(24)-Mo(2)-S(1)	145.9(4)
C(23)-Mo(2)-S(1)	111.6(4)

C(22)-Mo(2)-S(1)	90.7(3)
S(3)-Mo(2)-S(1)	114.50(9)
C(25)-Mo(2)-S(2)	138.9(5)
C(21)-Mo(2)-S(2)	143.9(4)
C(24)-Mo(2)-S(2)	103.0(5)
C(23)-Mo(2)-S(2)	89.5(3)
C(22)-Mo(2)-S(2)	109.4(4)
S(3)-Mo(2)-S(2)	72.71(8)
S(1)-Mo(2)-S(2)	73.39(8)
C(25)-Mo(2)-Cl(1)	98.6(4)
C(21)-Mo(2)-Cl(1)	97.1(3)
C(24)-Mo(2)-Cl(1)	131.2(6)
C(23)-Mo(2)-Cl(1)	154.1(3)
C(22)-Mo(2)-Cl(1)	125.5(4)
S(3)-Mo(2)-Cl(1)	71.44(8)
S(1)-Mo(2)-Cl(1)	76.17(8)
S(2)-Mo(2)-Cl(1)	116.29(8)
C(25)-Mo(2)-Mo(1)	150.8(3)
C(21)-Mo(2)-Mo(1)	151.1(4)
C(24)-Mo(2)-Mo(1)	148.7(4)
C(23)-Mo(2)-Mo(1)	146.8(3)
C(22)-Mo(2)-Mo(1)	147.5(3)
S(3)-Mo(2)-Mo(1)	56.74(6)
S(1)-Mo(2)-Mo(1)	57.77(7)
S(2)-Mo(2)-Mo(1)	57.68(6)
Cl(1)-Mo(2)-Mo(1)	58.67(6)
C(54)-C(53)-S(53)	103.8(8)
C(53)-C(54)-C(55)	106.8(12)
C(56)-C(55)-C(54)	109.4(12)
C(55)-C(56)-S(53)	102.0(8)
C(62)-C(61)-C(65)	109.5(12)
C(62)-C(61)-Mo(51)	75.1(7)
C(65)-C(61)-Mo(51)	70.1(6)
C(61)-C(62)-C(63)	107.8(12)
C(61)-C(62)-Mo(51)	71.2(6)
C(63)-C(62)-Mo(51)	70.7(6)
C(62)-C(63)-C(64)	108.9(11)
C(62)-C(63)-Mo(51)	74.7(7)
C(64)-C(63)-Mo(51)	69.8(6)
C(63)-C(64)-C(65)	105.7(12)
C(63)-C(64)-Mo(51)	74.3(6)
C(65)-C(64)-Mo(51)	71.9(7)
C(61)-C(65)-C(64)	108.1(12)
C(61)-C(65)-Mo(51)	74.6(7)
C(64)-C(65)-Mo(51)	71.7(6)
C(72)-C(71)-C(75)	107.8(14)
C(72)-C(71)-Mo(52)	75.2(8)
C(75)-C(71)-Mo(52)	69.6(8)
C(71)-C(72)-C(73)	113.4(15)
C(71)-C(72)-Mo(52)	72.1(8)

C(73)-C(72)-Mo(52)	73.0(8)
C(72)-C(73)-C(74)	104.7(14)
C(72)-C(73)-Mo(52)	73.1(8)
C(74)-C(73)-Mo(52)	69.4(7)
C(75)-C(74)-C(73)	107.8(13)
C(75)-C(74)-Mo(52)	70.8(7)
C(73)-C(74)-Mo(52)	74.7(8)
C(74)-C(75)-C(71)	106.2(15)
C(74)-C(75)-Mo(52)	72.8(8)
C(71)-C(75)-Mo(52)	74.2(8)
Mo(52)-Cl(51)-Mo(51)	62.87(7)
C(51)-S(51)-Mo(52)	109.5(4)
C(51)-S(51)-Mo(51)	110.3(5)
Mo(52)-S(51)-Mo(51)	64.99(8)
C(52)-S(52)-Mo(52)	116.1(4)
C(52)-S(52)-Mo(51)	116.6(4)
Mo(52)-S(52)-Mo(51)	65.35(7)
C(53)-S(53)-C(56)	95.0(5)
C(53)-S(53)-Mo(51)	123.7(4)
C(56)-S(53)-Mo(51)	123.6(4)
C(53)-S(53)-Mo(52)	124.9(4)
C(56)-S(53)-Mo(52)	125.3(4)
Mo(51)-S(53)-Mo(52)	66.52(7)
C(64)-Mo(51)-C(65)	36.4(5)
C(64)-Mo(51)-C(63)	35.9(5)
C(65)-Mo(51)-C(63)	58.8(5)
C(64)-Mo(51)-C(61)	59.3(5)
C(65)-Mo(51)-C(61)	35.2(5)
C(63)-Mo(51)-C(61)	57.4(4)
C(64)-Mo(51)-C(62)	59.0(4)
C(65)-Mo(51)-C(62)	57.9(5)
C(63)-Mo(51)-C(62)	34.6(4)
C(61)-Mo(51)-C(62)	33.7(4)
C(64)-Mo(51)-S(53)	97.6(4)
C(65)-Mo(51)-S(53)	97.5(4)
C(63)-Mo(51)-S(53)	129.3(4)
C(61)-Mo(51)-S(53)	127.7(5)
C(62)-Mo(51)-S(53)	154.5(3)
C(64)-Mo(51)-S(52)	98.5(4)
C(65)-Mo(51)-S(52)	133.3(6)
C(63)-Mo(51)-S(52)	92.0(3)
C(61)-Mo(51)-S(52)	149.2(3)
C(62)-Mo(51)-S(52)	118.0(3)
S(53)-Mo(51)-S(52)	72.35(8)
C(64)-Mo(51)-S(51)	142.4(5)
C(65)-Mo(51)-S(51)	144.3(5)
C(63)-Mo(51)-S(51)	106.7(4)
C(61)-Mo(51)-S(51)	109.0(5)
C(62)-Mo(51)-S(51)	91.1(3)
S(53)-Mo(51)-S(51)	114.41(9)

S(52)-Mo(51)-S(51)	74.67(9)
C(64)-Mo(51)-Cl(51)	137.2(5)
C(65)-Mo(51)-Cl(51)	102.7(5)
C(63)-Mo(51)-Cl(51)	151.3(3)
C(61)-Mo(51)-Cl(51)	94.6(3)
C(62)-Mo(51)-Cl(51)	118.1(3)
S(53)-Mo(51)-Cl(51)	70.84(9)
S(52)-Mo(51)-Cl(51)	115.41(9)
S(51)-Mo(51)-Cl(51)	74.95(12)
C(64)-Mo(51)-Mo(52)	147.6(3)
C(65)-Mo(51)-Mo(52)	151.0(3)
C(63)-Mo(51)-Mo(52)	147.0(3)
C(61)-Mo(51)-Mo(52)	151.2(3)
C(62)-Mo(51)-Mo(52)	148.5(3)
S(53)-Mo(51)-Mo(52)	57.03(6)
S(52)-Mo(51)-Mo(52)	57.12(7)
S(51)-Mo(51)-Mo(52)	57.39(7)
Cl(51)-Mo(51)-Mo(52)	58.41(7)
C(75)-Mo(52)-C(74)	36.3(5)
C(75)-Mo(52)-C(71)	36.2(5)
C(74)-Mo(52)-C(71)	59.1(5)
C(75)-Mo(52)-C(73)	59.8(6)
C(74)-Mo(52)-C(73)	35.9(5)
C(71)-Mo(52)-C(73)	57.6(5)
C(75)-Mo(52)-C(72)	57.3(6)
C(74)-Mo(52)-C(72)	57.3(5)
C(71)-Mo(52)-C(72)	32.7(5)
C(73)-Mo(52)-C(72)	33.9(5)
C(75)-Mo(52)-S(53)	100.8(5)
C(74)-Mo(52)-S(53)	98.9(5)
C(71)-Mo(52)-S(53)	133.1(5)
C(73)-Mo(52)-S(53)	128.3(5)
C(72)-Mo(52)-S(53)	155.5(4)
C(75)-Mo(52)-S(52)	135.8(5)
C(74)-Mo(52)-S(52)	100.2(5)
C(71)-Mo(52)-S(52)	146.2(5)
C(73)-Mo(52)-S(52)	89.6(4)
C(72)-Mo(52)-S(52)	114.3(5)
S(53)-Mo(52)-S(52)	72.28(8)
C(75)-Mo(52)-S(51)	140.7(5)
C(74)-Mo(52)-S(51)	142.6(6)
C(71)-Mo(52)-S(51)	104.5(5)
C(73)-Mo(52)-S(51)	106.7(5)
C(72)-Mo(52)-S(51)	90.3(4)
S(53)-Mo(52)-S(51)	114.04(9)
S(52)-Mo(52)-S(51)	74.97(10)
C(75)-Mo(52)-Cl(51)	101.2(5)
C(74)-Mo(52)-Cl(51)	135.3(6)
C(71)-Mo(52)-Cl(51)	95.7(4)
C(73)-Mo(52)-Cl(51)	153.1(4)

C(72)-Mo(52)-Cl(51)	120.9(5)
S(53)-Mo(52)-Cl(51)	70.74(9)
S(52)-Mo(52)-Cl(51)	116.14(9)
S(51)-Mo(52)-Cl(51)	75.21(11)
C(75)-Mo(52)-Mo(51)	152.4(4)
C(74)-Mo(52)-Mo(51)	149.4(3)
C(71)-Mo(52)-Mo(51)	150.5(4)
C(73)-Mo(52)-Mo(51)	145.4(4)
C(72)-Mo(52)-Mo(51)	147.7(4)
S(53)-Mo(52)-Mo(51)	56.45(6)
S(52)-Mo(52)-Mo(51)	57.53(6)
S(51)-Mo(52)-Mo(51)	57.61(7)
Cl(51)-Mo(52)-Mo(51)	58.72(7)
F(6)-P(1)-F(3)	93.2(11)
F(6)-P(1)-F(1)	89.0(6)
F(3)-P(1)-F(1)	90.4(6)
F(6)-P(1)-F(4)	95.3(11)
F(3)-P(1)-F(4)	171.4(9)
F(1)-P(1)-F(4)	91.3(5)
F(6)-P(1)-F(2)	90.0(6)
F(3)-P(1)-F(2)	89.0(5)
F(1)-P(1)-F(2)	178.8(5)
F(4)-P(1)-F(2)	89.5(5)
F(6)-P(1)-F(5)	177.4(10)
F(3)-P(1)-F(5)	88.8(9)
F(1)-P(1)-F(5)	92.7(6)
F(4)-P(1)-F(5)	82.7(7)
F(2)-P(1)-F(5)	88.3(6)
F(51)-P(51)-F(55)	95.1(10)
F(51)-P(51)-F(54)	102.4(11)
F(55)-P(51)-F(54)	91.6(6)
F(51)-P(51)-F(53)	89.4(10)
F(55)-P(51)-F(53)	90.5(6)
F(54)-P(51)-F(53)	167.7(10)
F(51)-P(51)-F(52)	168.5(12)
F(55)-P(51)-F(52)	93.4(10)
F(54)-P(51)-F(52)	85.0(10)
F(53)-P(51)-F(52)	82.8(9)
F(51)-P(51)-F(56)	84.7(9)
F(55)-P(51)-F(56)	179.5(7)
F(54)-P(51)-F(56)	88.1(5)
F(53)-P(51)-F(56)	89.9(6)
F(52)-P(51)-F(56)	86.8(8)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 10'.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	72(8)	74(8)	43(8)	-4(6)	23(6)	-29(6)
C(2)	65(7)	49(6)	29(6)	-18(5)	2(5)	-10(5)
C(3)	49(6)	68(7)	45(7)	-6(5)	5(5)	-18(5)
C(4)	121(13)	220(20)	58(11)	-14(11)	10(9)	-127(14)
C(5)	57(8)	113(11)	61(10)	-25(8)	0(7)	-26(7)
C(6)	43(6)	61(6)	33(6)	-18(5)	-1(5)	-3(5)
C(11)	97(10)	33(6)	56(9)	-6(6)	-3(8)	29(6)
C(12)	107(11)	25(6)	117(13)	-24(7)	20(10)	-2(6)
C(13)	127(14)	63(9)	56(10)	-31(8)	3(9)	34(9)
C(14)	83(10)	64(8)	75(12)	-26(7)	29(8)	33(8)
C(15)	81(9)	65(8)	41(9)	-19(6)	-4(7)	28(7)
C(21)	84(10)	75(9)	57(10)	-13(7)	28(9)	44(8)
C(22)	40(7)	61(8)	99(12)	-35(8)	-19(8)	16(6)
C(23)	72(9)	54(7)	62(9)	-10(7)	-3(8)	22(7)
C(24)	63(9)	27(6)	166(17)	-18(8)	13(10)	4(6)
C(25)	98(12)	73(9)	105(13)	-64(10)	-47(10)	41(9)
Cl(1)	54(2)	38(1)	25(1)	-8(1)	7(1)	-1(1)
S(1)	54(2)	43(1)	39(2)	-11(1)	6(1)	-16(1)
S(2)	48(1)	37(1)	24(2)	-8(1)	7(1)	-8(1)
S(3)	41(1)	40(1)	32(2)	-10(1)	1(1)	-4(1)
Mo(1)	46(1)	31(1)	28(1)	-11(1)	5(1)	7(1)
Mo(2)	40(1)	28(1)	28(1)	-10(1)	3(1)	3(1)
C(51)	43(7)	134(12)	91(11)	-46(9)	-2(7)	2(7)
C(52)	81(9)	46(7)	91(10)	-22(6)	0(7)	-29(6)
C(53)	35(6)	61(7)	79(9)	-28(6)	14(6)	-9(5)
C(54)	63(9)	137(14)	176(17)	-113(13)	11(10)	-35(9)
C(55)	109(13)	137(15)	199(19)	-130(15)	85(13)	-83(12)
C(56)	109(11)	49(7)	89(10)	-48(7)	10(8)	-19(7)
C(61)	130(14)	79(10)	25(8)	-8(6)	-18(8)	57(9)
C(62)	66(8)	67(8)	42(8)	-7(6)	-3(6)	-17(7)
C(63)	106(11)	58(7)	23(7)	-14(5)	4(6)	8(7)
C(64)	56(8)	127(13)	33(8)	15(8)	15(6)	-17(9)
C(65)	196(19)	47(8)	39(8)	10(6)	-23(10)	-54(11)
C(71)	82(11)	102(12)	39(9)	7(8)	31(7)	4(9)
C(72)	66(10)	100(12)	57(10)	5(8)	14(7)	-28(9)
C(73)	130(15)	57(8)	63(10)	8(7)	28(10)	-16(10)
C(74)	44(8)	159(16)	37(9)	30(9)	-3(6)	34(10)
C(75)	146(17)	108(13)	40(9)	-7(8)	12(10)	-38(13)
Cl(51)	56(2)	77(2)	55(2)	-10(2)	10(1)	31(2)
S(51)	39(2)	83(2)	53(2)	-1(2)	1(1)	-17(1)

S(52)	42(1)	33(1)	53(2)	-12(1)	2(1)	-6(1)
S(53)	44(1)	38(1)	44(2)	-16(1)	8(1)	-1(1)
Mo(51)	37(1)	33(1)	27(1)	0(1)	3(1)	2(1)
Mo(52)	32(1)	47(1)	28(1)	1(1)	5(1)	-2(1)
F(1)	53(5)	128(7)	148(8)	-17(6)	4(5)	24(4)
F(2)	65(5)	82(5)	144(8)	-19(5)	7(5)	16(4)
F(3)	159(11)	129(9)	259(16)	85(10)	106(11)	17(8)
F(4)	147(9)	78(6)	180(11)	1(6)	45(8)	8(6)
F(5)	129(9)	249(14)	164(11)	-122(10)	-1(8)	-46(9)
F(6)	179(12)	530(30)	274(16)	-340(20)	-145(12)	178(16)
P(1)	49(2)	47(2)	68(2)	-15(2)	-4(2)	-1(1)
F(51)	213(15)	370(20)	280(20)	-67(17)	70(14)	-213(17)
F(52)	180(14)	410(30)	183(16)	-37(15)	74(12)	-70(16)
F(53)	230(13)	151(10)	124(9)	-44(7)	-41(9)	96(9)
F(54)	178(11)	277(15)	326(18)	-270(15)	-143(12)	140(11)
F(55)	161(11)	324(17)	209(13)	-189(13)	-127(10)	112(11)
F(56)	196(10)	139(8)	62(6)	-47(5)	-43(6)	42(7)
P(51)	50(2)	90(2)	56(2)	-34(2)	1(2)	14(2)

6. X-ray crystallographic data for 13'

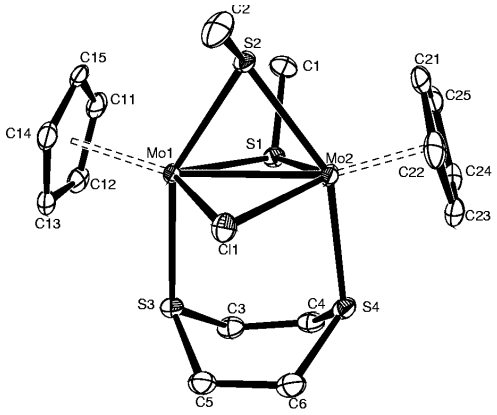


Table 1. Crystal data and structure refinement for 13'.

Identification code	**13'**
Empirical formula	C40 H44 B Cl Mo2 S4
Formula weight	891.13
Temperature	170(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P21/n
Unit cell dimensions	a = 9.4536(5) A alpha = 90 deg. b = 30.7462(12) A beta = 90.258(4) deg. c = 12.7894(6) A gamma = 90 deg.
Volume	3717.4(3) A^3
Z, Calculated density	4, 1.592 Mg/m^3
Absorption coefficient	1.001 mm^-1
F(000)	1816
Crystal size	0.17 x 0.14 x 0.08 mm
Theta range for data collection	2.67 to 25.35 deg.
Limiting indices	-11<=h<=11, -37<=k<=37, -12<=l<=12
Reflections collected / unique	23625 / 5876 [R(int) = 0.0283]
Completeness to theta = 25.35	86.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9242 and 0.8483
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5876 / 0 / 435
Goodness-of-fit on F^2	1.064
Final R indices [I>2sigma(I)]	R1 = 0.0286, wR2 = 0.0685
R indices (all data)	R1 = 0.0448, wR2 = 0.0750
Largest diff. peak and hole	0.672 and -0.338 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 13'
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	5114(4)	1052(1)	8108(3)	37(1)
C(2)	8688(5)	-74(1)	8894(4)	48(1)
C(3)	8322(4)	1599(1)	5249(3)	36(1)
C(4)	8668(4)	1875(1)	6206(3)	34(1)
C(5)	10814(4)	1164(1)	5362(3)	37(1)
C(6)	11244(4)	1468(1)	6263(3)	38(1)
C(11)	5838(4)	243(1)	6071(3)	35(1)
C(12)	6637(4)	395(1)	5215(3)	36(1)
C(13)	7913(4)	138(1)	5164(3)	35(1)
C(14)	7848(4)	-158(1)	5993(3)	35(1)
C(15)	6581(4)	-96(1)	6547(3)	31(1)
C(21)	8847(5)	972(1)	10127(3)	46(1)
C(22)	10240(5)	1067(1)	9844(3)	41(1)
C(23)	10271(4)	1476(1)	9369(3)	36(1)
C(24)	8865(4)	1640(1)	9361(3)	34(1)
C(25)	7987(4)	1327(1)	9838(3)	41(1)
C(30)	4523(3)	1751(1)	3450(3)	24(1)
C(31)	4977(4)	2163(1)	3771(3)	29(1)
C(32)	5191(4)	2272(1)	4815(3)	35(1)
C(33)	4950(4)	1974(1)	5583(3)	36(1)
C(34)	4490(3)	1561(1)	5314(3)	31(1)
C(35)	4283(3)	1458(1)	4279(3)	27(1)
C(40)	4744(3)	1921(1)	1325(3)	23(1)
C(41)	6073(4)	2120(1)	1369(3)	29(1)
C(42)	6624(4)	2361(1)	544(4)	41(1)
C(43)	5875(5)	2409(1)	-362(4)	45(1)
C(44)	4574(5)	2213(1)	-452(3)	41(1)
C(45)	4023(4)	1975(1)	384(3)	32(1)
C(50)	4887(3)	1121(1)	1993(3)	22(1)
C(51)	6003(3)	941(1)	2546(3)	24(1)
C(52)	6613(4)	545(1)	2283(3)	31(1)
C(53)	6129(4)	313(1)	1438(3)	35(1)
C(54)	5046(4)	488(1)	851(3)	34(1)
C(55)	4446(4)	881(1)	1127(3)	29(1)
C(60)	2418(3)	1568(1)	2243(2)	21(1)
C(61)	1679(4)	1185(1)	2445(3)	26(1)
C(62)	219(4)	1166(1)	2515(3)	30(1)
C(63)	-575(4)	1541(1)	2388(3)	31(1)
C(64)	115(4)	1926(1)	2195(3)	32(1)

C(65)	1572(4)	1938(1)	2127(3)	27(1)
B	4155(4)	1599(1)	2257(3)	22(1)
S(1)	6713(1)	1181(1)	7353(1)	26(1)
Cl(1)	10406(1)	535(1)	7322(1)	31(1)
S(2)	7589(1)	381(1)	8475(1)	27(1)
S(3)	8952(1)	1049(1)	5280(1)	29(1)
S(4)	9852(1)	1637(1)	7147(1)	29(1)
Mo(1)	7938(1)	549(1)	6636(1)	21(1)
Mo(2)	8888(1)	1059(1)	8305(1)	22(1)

Table 3. Bond lengths [A] and angles [deg] for 13'.

C(1)-S(1)	1.840(3)
C(2)-S(2)	1.820(4)
C(3)-C(4)	1.525(5)
C(3)-S(3)	1.793(4)
C(4)-S(4)	1.795(4)
C(5)-C(6)	1.539(5)
C(5)-S(3)	1.798(4)
C(6)-S(4)	1.814(4)
C(11)-C(15)	1.395(5)
C(11)-C(12)	1.413(5)
C(11)-Mo(1)	2.310(3)
C(12)-C(13)	1.445(5)
C(12)-Mo(1)	2.241(4)
C(13)-C(14)	1.398(5)
C(13)-Mo(1)	2.269(3)
C(14)-C(15)	1.408(5)
C(14)-Mo(1)	2.326(3)
C(15)-Mo(1)	2.365(3)
C(21)-C(22)	1.397(6)
C(21)-C(25)	1.411(6)
C(21)-Mo(2)	2.346(4)
C(22)-C(23)	1.398(5)
C(22)-Mo(2)	2.342(4)
C(23)-C(24)	1.422(5)
C(23)-Mo(2)	2.279(3)
C(24)-C(25)	1.410(5)
C(24)-Mo(2)	2.239(3)
C(25)-Mo(2)	2.295(4)
C(30)-C(31)	1.398(5)
C(30)-C(35)	1.411(5)
C(30)-B	1.632(5)
C(31)-C(32)	1.391(5)
C(32)-C(33)	1.362(5)
C(33)-C(34)	1.385(5)
C(34)-C(35)	1.375(5)

C(40)-C(45)	1.391(5)
C(40)-C(41)	1.399(5)
C(40)-B	1.647(5)
C(41)-C(42)	1.392(5)
C(42)-C(43)	1.363(6)
C(43)-C(44)	1.374(6)
C(44)-C(45)	1.398(5)
C(50)-C(51)	1.384(5)
C(50)-C(55)	1.393(5)
C(50)-B	1.659(5)
C(51)-C(52)	1.390(5)
C(52)-C(53)	1.371(5)
C(53)-C(54)	1.376(5)
C(54)-C(55)	1.383(5)
C(60)-C(61)	1.395(4)
C(60)-C(65)	1.397(5)
C(60)-B	1.645(5)
C(61)-C(62)	1.385(5)
C(62)-C(63)	1.385(5)
C(63)-C(64)	1.373(5)
C(64)-C(65)	1.381(5)
S(1)-Mo(2)	2.4134(9)
S(1)-Mo(1)	2.4410(9)
Cl(1)-Mo(1)	2.4884(9)
Cl(1)-Mo(2)	2.5002(9)
S(2)-Mo(2)	2.4301(9)
S(2)-Mo(1)	2.4318(9)
S(3)-Mo(1)	2.5108(9)
S(4)-Mo(2)	2.4894(9)
Mo(1)-Mo(2)	2.7924(4)

C(4)-C(3)-S(3)	116.0(3)
C(3)-C(4)-S(4)	116.1(3)
C(6)-C(5)-S(3)	114.8(3)
C(5)-C(6)-S(4)	116.8(3)
C(15)-C(11)-C(12)	108.4(4)
C(15)-C(11)-Mo(1)	74.8(2)
C(12)-C(11)-Mo(1)	69.2(2)
C(11)-C(12)-C(13)	107.7(3)
C(11)-C(12)-Mo(1)	74.6(2)
C(13)-C(12)-Mo(1)	72.4(2)
C(14)-C(13)-C(12)	106.4(3)
C(14)-C(13)-Mo(1)	74.5(2)
C(12)-C(13)-Mo(1)	70.3(2)
C(13)-C(14)-C(15)	109.6(4)
C(13)-C(14)-Mo(1)	70.1(2)
C(15)-C(14)-Mo(1)	74.1(2)
C(11)-C(15)-C(14)	108.0(3)
C(11)-C(15)-Mo(1)	70.50(19)
C(14)-C(15)-Mo(1)	71.02(19)

C(22)-C(21)-C(25)	108.2(4)
C(22)-C(21)-Mo(2)	72.5(2)
C(25)-C(21)-Mo(2)	70.3(2)
C(21)-C(22)-C(23)	108.8(4)
C(21)-C(22)-Mo(2)	72.8(2)
C(23)-C(22)-Mo(2)	69.9(2)
C(22)-C(23)-C(24)	107.5(4)
C(22)-C(23)-Mo(2)	74.9(2)
C(24)-C(23)-Mo(2)	70.13(19)
C(25)-C(24)-C(23)	107.9(4)
C(25)-C(24)-Mo(2)	74.1(2)
C(23)-C(24)-Mo(2)	73.2(2)
C(24)-C(25)-C(21)	107.5(4)
C(24)-C(25)-Mo(2)	69.7(2)
C(21)-C(25)-Mo(2)	74.3(2)
C(31)-C(30)-C(35)	114.1(3)
C(31)-C(30)-B	126.7(3)
C(35)-C(30)-B	119.0(3)
C(32)-C(31)-C(30)	122.9(3)
C(33)-C(32)-C(31)	120.4(4)
C(32)-C(33)-C(34)	119.4(4)
C(35)-C(34)-C(33)	119.6(4)
C(34)-C(35)-C(30)	123.5(3)
C(45)-C(40)-C(41)	114.7(3)
C(45)-C(40)-B	122.2(3)
C(41)-C(40)-B	122.7(3)
C(42)-C(41)-C(40)	122.9(4)
C(43)-C(42)-C(41)	120.4(4)
C(42)-C(43)-C(44)	119.1(4)
C(43)-C(44)-C(45)	120.1(4)
C(40)-C(45)-C(44)	122.9(4)
C(51)-C(50)-C(55)	114.8(3)
C(51)-C(50)-B	124.7(3)
C(55)-C(50)-B	120.5(3)
C(50)-C(51)-C(52)	123.0(3)
C(53)-C(52)-C(51)	120.6(3)
C(52)-C(53)-C(54)	118.2(3)
C(53)-C(54)-C(55)	120.5(3)
C(54)-C(55)-C(50)	123.0(3)
C(61)-C(60)-C(65)	114.8(3)
C(61)-C(60)-B	123.2(3)
C(65)-C(60)-B	121.7(3)
C(62)-C(61)-C(60)	123.2(3)
C(63)-C(62)-C(61)	119.8(3)
C(64)-C(63)-C(62)	118.7(3)
C(63)-C(64)-C(65)	120.6(3)
C(64)-C(65)-C(60)	122.8(3)
C(30)-B-C(60)	103.6(3)
C(30)-B-C(40)	115.7(3)
C(60)-B-C(40)	111.6(3)

C(30)-B-C(50)	110.9(3)
C(60)-B-C(50)	111.4(3)
C(40)-B-C(50)	104.0(3)
C(1)-S(1)-Mo(2)	113.70(13)
C(1)-S(1)-Mo(1)	114.72(13)
Mo(2)-S(1)-Mo(1)	70.23(2)
Mo(1)-Cl(1)-Mo(2)	68.08(2)
C(2)-S(2)-Mo(2)	113.38(14)
C(2)-S(2)-Mo(1)	111.60(16)
Mo(2)-S(2)-Mo(1)	70.11(2)
C(3)-S(3)-C(5)	98.06(18)
C(3)-S(3)-Mo(1)	117.66(13)
C(5)-S(3)-Mo(1)	117.18(14)
C(4)-S(4)-C(6)	98.70(18)
C(4)-S(4)-Mo(2)	117.46(12)
C(6)-S(4)-Mo(2)	115.76(13)
C(12)-Mo(1)-C(13)	37.37(14)
C(12)-Mo(1)-C(11)	36.13(13)
C(13)-Mo(1)-C(11)	60.50(14)
C(12)-Mo(1)-C(14)	59.76(14)
C(13)-Mo(1)-C(14)	35.41(13)
C(11)-Mo(1)-C(14)	58.56(14)
C(12)-Mo(1)-C(15)	59.20(13)
C(13)-Mo(1)-C(15)	59.25(13)
C(11)-Mo(1)-C(15)	34.69(12)
C(14)-Mo(1)-C(15)	34.91(13)
C(12)-Mo(1)-S(2)	131.54(10)
C(13)-Mo(1)-S(2)	133.09(10)
C(11)-Mo(1)-S(2)	95.48(10)
C(14)-Mo(1)-S(2)	97.95(10)
C(15)-Mo(1)-S(2)	78.01(9)
C(12)-Mo(1)-S(1)	102.29(11)
C(13)-Mo(1)-S(1)	138.75(10)
C(11)-Mo(1)-S(1)	91.89(10)
C(14)-Mo(1)-S(1)	149.25(10)
C(15)-Mo(1)-S(1)	115.28(10)
S(2)-Mo(1)-S(1)	74.90(3)
C(12)-Mo(1)-Cl(1)	142.39(11)
C(13)-Mo(1)-Cl(1)	106.78(11)
C(11)-Mo(1)-Cl(1)	154.95(10)
C(14)-Mo(1)-Cl(1)	98.11(10)
C(15)-Mo(1)-Cl(1)	120.66(10)
S(2)-Mo(1)-Cl(1)	77.70(3)
S(1)-Mo(1)-Cl(1)	109.10(3)
C(12)-Mo(1)-S(3)	77.19(10)
C(13)-Mo(1)-S(3)	76.70(10)
C(11)-Mo(1)-S(3)	111.29(10)
C(14)-Mo(1)-S(3)	109.93(10)
C(15)-Mo(1)-S(3)	133.50(9)
S(2)-Mo(1)-S(3)	148.48(3)

S(1)-Mo(1)-S(3)	87.47(3)
Cl(1)-Mo(1)-S(3)	83.92(3)
C(12)-Mo(1)-Mo(2)	155.75(10)
C(13)-Mo(1)-Mo(2)	161.68(10)
C(11)-Mo(1)-Mo(2)	137.78(10)
C(14)-Mo(1)-Mo(2)	143.72(10)
C(15)-Mo(1)-Mo(2)	132.87(9)
S(2)-Mo(1)-Mo(2)	54.92(2)
S(1)-Mo(1)-Mo(2)	54.42(2)
Cl(1)-Mo(1)-Mo(2)	56.16(2)
S(3)-Mo(1)-Mo(2)	93.57(2)
C(24)-Mo(2)-C(23)	36.67(13)
C(24)-Mo(2)-C(25)	36.22(14)
C(23)-Mo(2)-C(25)	60.10(14)
C(24)-Mo(2)-C(22)	59.46(14)
C(23)-Mo(2)-C(22)	35.19(13)
C(25)-Mo(2)-C(22)	58.77(15)
C(24)-Mo(2)-C(21)	59.46(14)
C(23)-Mo(2)-C(21)	58.86(14)
C(25)-Mo(2)-C(21)	35.37(15)
C(22)-Mo(2)-C(21)	34.68(15)
C(24)-Mo(2)-S(1)	99.79(10)
C(23)-Mo(2)-S(1)	134.38(10)
C(25)-Mo(2)-S(1)	93.24(11)
C(22)-Mo(2)-S(1)	151.95(11)
C(21)-Mo(2)-S(1)	120.06(12)
C(24)-Mo(2)-S(2)	128.59(10)
C(23)-Mo(2)-S(2)	135.90(10)
C(25)-Mo(2)-S(2)	92.40(10)
C(22)-Mo(2)-S(2)	101.96(10)
C(21)-Mo(2)-S(2)	78.59(10)
S(1)-Mo(2)-S(2)	75.43(3)
C(24)-Mo(2)-S(4)	78.10(10)
C(23)-Mo(2)-S(4)	75.09(10)
C(25)-Mo(2)-S(4)	112.95(11)
C(22)-Mo(2)-S(4)	107.03(11)
C(21)-Mo(2)-S(4)	132.85(10)
S(1)-Mo(2)-S(4)	84.42(3)
S(2)-Mo(2)-S(4)	148.51(3)
C(24)-Mo(2)-Cl(1)	145.53(10)
C(23)-Mo(2)-Cl(1)	109.51(10)
C(25)-Mo(2)-Cl(1)	151.33(12)
C(22)-Mo(2)-Cl(1)	96.72(11)
C(21)-Mo(2)-Cl(1)	115.96(12)
S(1)-Mo(2)-Cl(1)	109.61(3)
S(2)-Mo(2)-Cl(1)	77.51(3)
S(4)-Mo(2)-Cl(1)	87.06(3)
C(24)-Mo(2)-Mo(1)	154.76(10)
C(23)-Mo(2)-Mo(1)	162.57(10)
C(25)-Mo(2)-Mo(1)	137.32(10)

C(22)-Mo(2)-Mo(1)	145.09(10)
C(21)-Mo(2)-Mo(1)	133.47(10)
S(1)-Mo(2)-Mo(1)	55.35(2)
S(2)-Mo(2)-Mo(1)	54.97(2)
S(4)-Mo(2)-Mo(1)	93.66(2)
Cl(1)-Mo(2)-Mo(1)	55.76(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 13'
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	29(2)	46(2)	38(3)	2(2)	9(2)	1(2)
C(2)	64(3)	24(2)	56(3)	9(2)	-20(2)	-1(2)
C(3)	37(2)	29(2)	40(3)	10(2)	3(2)	0(2)
C(4)	34(2)	27(2)	40(3)	10(2)	8(2)	2(2)
C(5)	33(2)	34(2)	44(3)	0(2)	13(2)	-2(2)
C(6)	32(2)	33(2)	49(3)	2(2)	9(2)	-2(2)
C(11)	36(2)	34(2)	36(3)	-8(2)	-9(2)	-12(2)
C(12)	50(2)	34(2)	24(2)	1(2)	-17(2)	-14(2)
C(13)	54(3)	27(2)	24(2)	-9(2)	2(2)	-11(2)
C(14)	50(2)	23(2)	32(3)	-7(2)	-6(2)	-5(2)
C(15)	47(2)	21(2)	26(2)	-4(2)	-4(2)	-17(2)
C(21)	79(3)	44(3)	16(3)	-3(2)	-8(2)	-23(2)
C(22)	57(3)	39(2)	27(3)	-7(2)	-21(2)	5(2)
C(23)	42(2)	38(2)	27(2)	-8(2)	-8(2)	-13(2)
C(24)	43(2)	33(2)	28(2)	-12(2)	-7(2)	-2(2)
C(25)	42(2)	58(3)	24(2)	-18(2)	3(2)	-13(2)
C(30)	16(2)	28(2)	27(2)	-2(2)	-1(2)	4(1)
C(31)	31(2)	25(2)	32(3)	-4(2)	-4(2)	7(2)
C(32)	37(2)	29(2)	39(3)	-14(2)	-12(2)	9(2)
C(33)	35(2)	47(2)	25(2)	-13(2)	-8(2)	20(2)
C(34)	26(2)	41(2)	26(3)	2(2)	0(2)	6(2)
C(35)	23(2)	35(2)	23(3)	-2(2)	-2(2)	0(2)
C(40)	30(2)	16(2)	23(2)	-2(1)	5(2)	4(1)
C(41)	29(2)	21(2)	37(2)	0(2)	5(2)	4(2)
C(42)	37(2)	20(2)	65(3)	1(2)	21(2)	2(2)
C(43)	59(3)	30(2)	46(3)	10(2)	26(2)	4(2)
C(44)	68(3)	34(2)	23(2)	2(2)	6(2)	2(2)
C(45)	45(2)	23(2)	28(3)	-1(2)	4(2)	-2(2)
C(50)	25(2)	19(2)	22(2)	3(1)	5(2)	-6(1)
C(51)	26(2)	22(2)	24(2)	0(1)	4(2)	-6(1)

C(52)	32(2)	29(2)	31(2)	6(2)	3(2)	3(2)
C(53)	47(2)	20(2)	39(3)	-1(2)	12(2)	3(2)
C(54)	49(2)	25(2)	27(2)	-8(2)	5(2)	-7(2)
C(55)	37(2)	23(2)	25(2)	1(2)	-1(2)	-3(2)
C(60)	29(2)	24(2)	11(2)	-1(1)	-2(1)	-3(1)
C(61)	32(2)	25(2)	19(2)	3(1)	-3(2)	-3(2)
C(62)	34(2)	34(2)	23(2)	4(2)	-2(2)	-10(2)
C(63)	24(2)	50(2)	20(2)	1(2)	0(2)	-4(2)
C(64)	35(2)	29(2)	31(2)	0(2)	-2(2)	5(2)
C(65)	30(2)	25(2)	27(2)	-4(2)	0(2)	-5(2)
B	28(2)	19(2)	19(3)	-2(2)	1(2)	-3(2)
S(1)	26(1)	23(1)	28(1)	2(1)	0(1)	0(1)
Cl(1)	32(1)	27(1)	34(1)	-2(1)	-4(1)	4(1)
S(2)	38(1)	21(1)	22(1)	3(1)	-4(1)	-7(1)
S(3)	33(1)	27(1)	27(1)	2(1)	3(1)	-5(1)
S(4)	30(1)	22(1)	34(1)	1(1)	1(1)	-5(1)
Mo(1)	28(1)	18(1)	19(1)	0(1)	-3(1)	-4(1)
Mo(2)	28(1)	18(1)	21(1)	-1(1)	-3(1)	-3(1)