ORGANOMETALLICS
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Supplementary Material

Complex **4b**: 85% yield, mp 133-134 °C; IR (ν_{max}, CH_2Cl_2) 1945, 1865 cm^{-1}; ^1H NMR ($CDCl_3$, 300 MHz, 25 °C) δ 7.80-7.35 (10 H, m), 5.47 (5 H, s), 4.13 (1 H, dd, J = 5.4, 2.4 Hz), 3.55 (1 H, t, J = 2.4 Hz), 3.13 (1 H, dd, J = 7.1, 2.6 Hz), 2.56-2.54 (1 H, m), 1.88-1.85 (1 H, m), 1.64-1.57 (1 H, m), 0.76-0.71 (1 H, m); ^{13}C NMR ($CDCl_3$, 75 MHz, 25 °C) δ 234.0, 231.9, 138.8, 138.7, 133.3, 131.9, 129.0, 128.8(×2), 127.8, 94.1, 76.7, 67.2, 62.8, 51.6, 21.3, 17.9.; Anal. Calcd for $C_{25}H_{22}MoO_4S_2$: C, 54.94; H, 4.06. Found: C, 54.75; H, 4.09. Complex **4c**: R_f 0.35 (EtOAc/hexane, 1:6), 81% yield, mp 146-147 °C; IR (ν_{max}, CH_2Cl_2) 1930, 1860 cm^{-1}; ^1H NMR ($CDCl_3$, 300 MHz, 25 °C) δ 7.76-7.48 (5 H, m), 5.54 (5 H, s), 3.92 (1 H, dd, J = 5.1, 2.6 Hz), 3.60 (1 H, br s), 2.34-2.28 (1 H, m), 2.09 (1 H, d, J = 11.2 Hz), 1.80 (2 H, dt, J = 11.2, 2.2 Hz), 1.16-1.11 (1 H, m), 0.80-0.70 (1 H, m).; ^{13}C NMR ($CDCl_3$, 75 MHz, 25 °C) δ 231.2, 230.3, 140.3, 133.7, 129.8, 129.4, 112.7, 112.3, 93.6, 73.5, 64.8, 57.0, 37.4, 28.5, 21.0, 19.7.; HRMS calcd (^{98}Mo) 472.0145. Found 472.0153. Anal. Calcd for $C_{22}H_{18}MoN_2O_2S_2$: C,56.17; N, 5.96; H, 3.86. Found: C, 55.99; N, 6.12; H, 3.98. Complex **4d**: R_f 0.36 (EtOAc/hexane, 1:6), 68% yield, mp 141-142 °C; IR (ν_{max}, CH_2Cl_2) 1940, 1865 cm^{-1}; ^1H NMR ($CDCl_3$, 300 MHz, 25 °C) δ 7.59-7.39 (5 H, m), 5.47 (5 H, s), 3.93 (1 H, dd, J = 5.4, 2.7 Hz), 3.69 (1 H, dd, J = 5.9, 2.7 Hz), 3.57 (3 H, s), 3.55 (3 H, s), 2.56 (1 H, d, J = 11.6 Hz), 2.52-2.45 (1 H, m), 2.09-1.98 (1 H, m), 1.79-1.23 (1 H, m), 0.64-0.59 (2 H, m).; ^{13}C NMR ($CDCl_3$, 75 MHz, 25 °C) δ 231.9, 231.7, 168.7, 168.5, 141.0, 131.6, 129.1, 128.0, 93.2, 73.3, 66.0, 63.0, 58.0, 52.2, 52.5, 33.6, 21.6, 20.6.; HRMS calcd (^{98}Mo) 538.0342. Found 538.0350. Anal. Calcd for $C_{24}H_{24}MoO_6S$: C, 53.74; H, 4.51. Found: C, 53.87; H, 4.67. Complex **4e**: R_f 0.34, 0.3 (EtOAc/hexane, 1:6), 75 % yield, 1.3 : 1 mixture of diastereomers, IR (ν_{max}, CH_2Cl_2) 1946, 1872 cm^{-1}; major isomer: mp 146-148 °C; ^1H NMR ($CDCl_3$, 300 MHz, 25 °C) δ 7.66-7.36 (5 H, m), 5.45 (5 H, s), 3.98-3.97 (1 H, m), δ 3.43 (1 H, d, J = 12.0 Hz), 3.22 (3 H, s), 3.12 (1 H, t, J = 2.1 Hz), 2.54 (1 H, ddd, J = 12.0, 5.5, 3.1 Hz), 2.18-2.08 (1 H, m), 1.88-1.59 (2 H, m), 0.68-0.59 (1 H, m).; ^{13}C NMR ($CDCl_3$, 75 MHz, 25 °C) δ 231.4, 231.6, 166.6, 141.4, 138.0, 133.9, 130.4, 129.1(×2), 128.7, 127.4, 93.5, 75.8, 72.0, 67.4, 60.7, 52.3, 33.7, 20.6, 19.8.; HRMS calcd (^{98}Mo) 620.0219. Found 620.0228. Anal. Calcd for $C_{28}H_{26}MoO_6S_2$: C,54.37; H, 4.24. Found: C, 54.03; H, 4.29.; minor isomer: mp 152-153 °C (decomp); ^1H NMR ($CDCl_3$, 300 MHz, 25 °C) δ 7.81-7.51 (5 H, m), 5.53 (5 H, s), 4.25 (1 H, br s), 3.97-3.96 (1 H, m), 3.44 (1 H, d, J = 10.5 Hz), 3.33 (3 H, s), 2.68-2.64 (1 H, m), 1.99-1.93 (1 H, m), 1.77-1.72 (1 H, m), 0.77-0.67 (1 H, m), 0.53 (1 H, dd, J = 15.6, 5.3 Hz).; ^{13}C NMR ($CDCl_3$, 75 MHz, 25 °C) δ 231.6, 231.5, 166.2, 141.4, 137.5, 134.0, 131.9, 129.4, 139.3, 128.6, 127.7, 93.5, 77.0, 72.3, 66.4, 62.1, 52.3, 33.1, 22.9, 21.0.; HRMS calcd (^{98}Mo) 620.0219. Found 620.0218.; Anal. Calcd

for $C_{28}H_{26}MoO_6S_2$: C, 54.37; H, 4.24. Found: C, 54.10; H, 4.34. **4f**: R_f 0.38, 0.31 (EtOAc/hexane, 1:6), 81% yield, 1.3 : 1 mixture of diastereomers, IR (ν_{max}, CH_2Cl_2) 1945, 1870 cm^{-1}; major isomer: mp 137-138 °C; ^1H NMR ($CDCl_3$, 300 MHz, 25 °C) δ 7.67-7.37 (5 H, m), 5.45 (5 H, s), 4.21 (1H, dd, J = 5.4, 2.7 Hz), 3.58 (3 H, s), 3.35 (1 H, t, J = 2.4 Hz), 2.95-2.91 (1 H, m), 2.20-2.15(1 H, m), 2.05-2.02 (1 H, m), 1.89-1.77 (3 H, m), 1.45-1.41 (2 H, m), 0.94-0.93 (1 H, m), 0.65-0.60 (2 H, m).; ^{13}C NMR ($CDCl_3$, 75 MHz, 25 °C) δ 233.3, 232.7, 214.4, 169.8, 139.9, 132.1, 129.3, 128.3, 93.4, 68.5, 66.7, 66.6, 62.0, 52.7, 39.2, 38.4, 27.0, 22.7, 20.2, 19.9.; HRMS calcd (^{98}Mo) 548.0557. Found 548.0554.; Anal. Calcd for $C_{26}H_{26}MoO_5S$: C, 57.14; H, 4.80. Found: C, 56.93; H, 4.30. minor isomer: mp 135-136 °C; ^1H NMR ($CDCl_3$, 300 MHz, 25 °C) δ 7.69-7.38 (5 H, m), 5.46 (5 H, s), 4.10 (1 H, br s), 3.69 (3 H, s), 3.57 (1 H, br s), 2.85 (1 H, ddd, J = 4.8, 4.8, 3.0 Hz), 2.23-2.14 (2 H, m), 1.95-1.78 (2 H, m), 1.54-1.40 (3 H, m), 1.01-0.72 (1 H, m), 0.72-0.69 (1 H, m), 0.46-0.44 (1 H, m).; ^{13}C NMR ($CDCl_3$, 75 MHz, 25 °C) δ 233.2, 233.2, 213.3, 170.1, 140.1, 133.2, 128.9, 128.3, 93.2, 67.7, 64.5, 63.5, 52.6, 52.5, 39.9, 38.4, 27.2, 24.4, 20.1, 19.3.; HRMS calcd (^{98}Mo) 548.0557. Found 548.0562. Anal. Calcd for $C_{26}H_{26}MoO_5S$: C, 57.14; H, 4.80. Found: C, 56.89; H, 4.83. **4g**, **5g**: R_f 0.37, 0.35 (EtOAc/hexane, 1:6), 76% yield, 3.3 : 1 mixture of regioisomer, IR (ν_{max}, CH_2Cl_2) 1935, 1858 cm^{-1}; **4g**: ^1H NMR ($CDCl_3$, 300 MHz, 25 °C) δ 7.62-7.40 (10 H, m), 5.48 (5 H, s, Cp, minor), 5.47 (5 H, s, Cp, major), 3.96-3.94 (1 H, m, H-1, major), 3.93-3.91 (1 H, m, H-1, minor), 3.65-3.64 (1 H, m, H-3, minor), 3.59 (3 H, s, CO_2Me, major), 3.55 (3 H, s, CO_2Me, minor), 3.54 (1 H, br s, H-3, major), 2.97 (1 H, d, J = 11.4 Hz, CH(COMe)(CO_2Me), major), 2.68 (1 H, d, J = 11.6 Hz, CH(COMe)(CO_2Me), minor), 2.58-2.25 (2 H, m), 2.19-2.14 (1 H, m), 1.96 (3 H, s, COMe, major), 1.58 (3 H, s, COMe, minor), 1.83-1.76 (2 H, m), 0.64-0.54 (5 H, m).; ^{13}C NMR ($CDCl_3$, 75 MHz, 25 °C) δ 231.9, 231.8, 231.7 (CO), 202.4, 201.3, 169.0, 168.7, 142.0, 141.1, 131.7, 130.8, 129.4, 129.1, 128.0, 127.6, 93.3 (Cp), 73.1, 72.4, 66.6, 66.2, 66.0, 63.6, 63.0, 52.3, 52.0, 33.5, 32.7, 29.3, 28.6, 21.8, 20.9, 20.8, 20.7.; HRMS calcd (^{98}Mo) 522.0400. Found 522.0401.; Anal. Calcd for $C_{24}H_{24}MoO_5S$: C, 55.39; H, 4.65. Found: C, 55.30; H, 4.74.; **5g**: mp 152-153 °C; ^1H NMR ($CDCl_3$, 300 MHz, 25 °C) δ 7.69-7.38 (5 H, m), 5.32 (5 H, s), 4.90 (1 H, d, J = 7.4 Hz), 4.53 (1 H, d, J = 3.6Hz), 3.85-3.72 (1 H, m), 3.67 (3 H, s), 2.90 (1 H, dd, J = 7.4, 3.6 Hz), 2.22 (3 H, s), 1.94-1.83 (1 H, m), 1.55-1.49 (1 H, m), 1.45 (1 H, dd, J = 15.0, 5.8 Hz), 0.68-0.59 (1 H, m).; ^{13}C NMR ($CDCl_3$, 75 MHz, 25 °C) δ 238.1, 234.9, 202.8, 170.1, 135.4, 132.0, 129.0, 127.8, 94.5, 72.7, 66.4, 61.0, 55.4, 52.1, 38.2, 29.5, 22.0, 18.9.; HRMS calcd (^{98}Mo) 522.0400. Found 522.0389.

able. Crystal Data and Conditions for Crystallographic
Data Collection and Structure Refinement 2

	2
ITLE,	Mo S O4 C19 H18
ormula ,	438.35
W ,	Nonius
iffractometer used,	Triclinic P -1
pace Group,	7.738(3)
(angstron),	8.6647(17)
(angstron),	13.86760(0)
(angstron),	96.369(18)
lpha(deg.),	105.119(23)
eta(deg.),	91.642(21)
amma(deg.),	890.4(3)
(A**3),	2
,	1.635
calc(g.cm-3),	0.70930
ambda(Angstron),	444.
(000) ,	25;(19.00 - 23.12 deg.)
nit cell detn: #;(2theta range),	theta/2theta
can type,	2(0.65+0.35tan(theta))
can width (deg),	2.06-8.24
can Speed (deg/min),	50.0
Theta(max),	(-9; 9)(0; 10)(-16; 16)
k l ranges ,	8.504
u(cm-1),	0.40 X 0.50 X 0.60
rystal size(mm),	0.957; 1.000
ransmission,	298.00
emperature,	3145
of meas. reflns,	2857
of obsed relfns (I > 2.0sig(I)),	3130
of unique reflns,	0.025;0.026
F;RW ,	2.80
oF,	NRCVAX
efinement program,	43
of atoms,	227 (2857 out of 3130 reflns.)
of refined params,	SUM(w|Fo-Fc|**2)
inimize function,	(1/sigma**2)(Fo)
eights scheme,	0.000010
he weight modifier K in KFo**2 is,	1.12(10)
(2nd. ext. coeff.) x 10e4,	0.0036
delta/sigma)max ,	-0.460; 0.400
D -map)max.min e/A**3 ,	

NOTE :
RF = Sum(Fo-Fc)/Sum(Fo)
Rw = Sqrt[Sum(w(Fo-Fc)**2)/Sum(wFo**2)]
GoF = Sqrt[Sum(w(Fo-Fc)**2)/(No. of reflns - No. of params.)]
Standard Reflns : No. 3 ; Variation < 2 %, 4 sigma ; every 3600 seconds

Table . Atomic Parameters x,y,z and Beq.
E.S.Ds. refer to the last digit printed.

	x	y	z	Beq
Mo	0.27885(3)	0.19913(3)	0.141089(18)	2.905(10)
S	0.64156(10)	0.40428(8)	0.31323 (6)	3.65 (3)
C1	0.3143 (4)	0.0034 (4)	0.06720 (22)	3.92 (15)
C2	0.0974 (4)	0.0783 (3)	0.17957 (21)	3.68 (14)
C3	0.5622 (3)	0.1076 (3)	0.20971 (21)	3.43 (13)
C4	0.5074 (3)	0.2304 (3)	0.27014 (19)	2.86 (12)
C5	0.3682 (4)	0.1892 (3)	0.31433 (20)	3.21 (12)
C6	0.3765 (4)	0.0359 (4)	0.35790 (23)	4.39 (15)
C7	0.4296 (5)	-0.0964 (3)	0.2920 (3)	4.94 (17)
C8	0.5799 (4)	-0.0500 (4)	0.24809 (25)	4.69 (16)
C9	0.7906 (4)	0.3492 (3)	0.42272 (20)	3.36 (12)
C10	0.7483 (4)	0.3747 (4)	0.51345 (24)	4.75 (16)
C11	0.8607 (5)	0.3283 (4)	0.59781 (24)	5.31 (19)
C12	1.0136 (5)	0.2593 (4)	0.5924 (3)	5.14 (17)
C13	1.0544 (5)	0.2323 (5)	0.5023 (3)	6.12 (20)
C14	0.9438 (4)	0.2772 (4)	0.41652 (24)	5.04 (18)
C15	0.2559 (7)	0.3229 (5)	-0.0026 (3)	6.26 (23)
C16	0.3472 (5)	0.4276 (6)	0.0777 (4)	7.04 (24)
C17	0.2368 (9)	0.4664 (4)	0.1361 (3)	7.0 (3)
C18	0.0740 (6)	0.3872 (6)	0.0949 (4)	6.9 (3)
C19	0.0858 (5)	0.2971 (4)	0.0086 (3)	5.98 (19)
O1	0.3330 (3)	-0.1123 (3)	0.02228 (17)	5.74 (13)
O2	-0.0129 (3)	0.0091 (3)	0.20113 (17)	5.53 (12)
O3	0.5372 (3)	0.52404(23)	0.34510 (16)	4.77 (10)
O4	0.7408 (3)	0.4336 (3)	0.24227 (15)	5.00 (11)
H3	0.657	0.133	0.179	4.1
H5	0.323	0.272	0.353	4.1
H6A	0.262	0.008	0.369	5.0
H6B	0.463	0.048	0.423	5.0
H7A	0.463	-0.182	0.332	5.4
H7B	0.325	-0.133	0.239	5.4
H8A	0.586	-0.128	0.195	5.6
H8B	0.692	-0.048	0.300	5.6
H10	0.640	0.423	0.517	5.4
H11	0.831	0.350	0.662	6.1
H12	1.094	0.230	0.653	6.0
H13	1.161	0.181	0.497	6.6
H14	0.972	0.255	0.352	5.4
H15	0.301	0.271	-0.056	6.7
H16	0.472	0.465	0.091	6.8
H17	0.267	0.539	0.199	6.8
H18	-0.030	0.395	0.121	7.0
H19	-0.013	0.230	-0.037	6.3

Beq is the Mean of the Principal Axes of the Thermal Ellipsoid

complex 2

Table of u(i,j) or U values *100.
E.S.Ds. refer to the last digit printed

	u11(U)	u22	u33	u12	u13	u23
M0	3.590(14)	3.835(15)	3.795(15)	0.136(10)	1.127(10)	0.917(10)
S	4.64 (4)	4.18 (4)	4.82 (4)	-0.41 (3)	0.85 (4)	0.76 (3)
C1	4.34 (17)	5.79 (20)	5.00 (19)	-0.40 (15)	1.83 (15)	0.41 (16)
C2	4.39 (17)	4.73 (18)	4.98 (18)	0.39 (14)	1.43 (14)	0.61 (14)
C3	3.44 (15)	4.72 (17)	4.98 (17)	0.38 (13)	1.33 (13)	0.49 (14)
C4	3.44 (15)	3.37 (15)	4.05 (15)	0.23 (11)	0.91 (12)	0.63 (12)
C5	4.25 (16)	4.30 (16)	3.94 (16)	0.43 (13)	1.40 (13)	0.87 (13)
C6	6.34 (20)	5.52 (20)	5.32 (19)	0.13 (16)	1.76 (16)	2.37 (16)
C7	7.24 (23)	3.80 (18)	7.97 (24)	0.99 (16)	1.59 (19)	2.58 (17)
C8	5.63 (20)	4.64 (19)	7.42 (23)	1.75 (16)	1.42 (17)	0.59 (17)
C9	4.21 (16)	3.75 (16)	4.51 (17)	-0.66 (13)	0.88 (13)	0.07 (13)
C10	5.47 (20)	7.37 (23)	5.30 (20)	1.60 (17)	1.62 (16)	0.45 (17)
C11	7.15 (24)	8.4 (3)	4.75 (20)	0.75 (20)	1.60 (18)	1.22 (18)
C12	6.51 (23)	5.99 (22)	6.15 (23)	0.24 (18)	-0.19 (18)	1.51 (18)
C13	5.39 (22)	9.6 (3)	7.8 (3)	2.99 (20)	0.97 (20)	0.53 (23)
C14	5.17 (20)	8.7 (3)	5.29 (20)	1.64 (18)	1.52 (16)	0.13 (18)
C15	11.3 (4)	8.7 (3)	5.59 (23)	3.2 (3)	3.97 (24)	3.72 (22)
C16	6.8 (3)	8.9 (3)	10.7 (4)	-2.02 (23)	-0.5 (3)	6.8 (3)
C17	15.8 (5)	4.20 (21)	5.57 (24)	1.6 (3)	0.2 (3)	1.69 (18)
C18	9.2 (3)	9.1 (3)	10.8 (4)	5.4 (3)	5.4 (3)	6.3 (3)
C19	7.1 (3)	6.9 (3)	7.2 (3)	-0.65 (20)	-1.67 (21)	3.30 (21)
O1	7.76 (17)	6.29 (16)	7.64 (17)	-0.32 (13)	3.15 (14)	-2.13 (13)
O2	5.25 (14)	8.11 (17)	8.50 (17)	-1.34 (12)	3.35 (13)	1.37 (13)
O3	6.37 (14)	3.88 (12)	7.06 (15)	0.85 (10)	0.45 (11)	0.27 (10)
O4	6.04 (14)	7.47 (16)	5.41 (13)	-2.35 (12)	1.38 (11)	1.47 (11)
H3	5.2					
H5	5.2					
H6A	6.3					
H6B	6.3					
H7A	6.8					
H7B	6.8					
H8A	7.0					
H8B	7.0					
H10	6.8					
H11	7.7					
H12	7.6					
H13	8.4					
H14	6.8					
H15	8.4					
H16	8.7					
H17	8.7					
H18	8.9					
H19	8.0					

Anisotropic Temperature Factors are of the form
Temp=-2*Pi*Pi*(h*h*u11*astar*astar+---+2*h*k*u12*astar*bstar+---)

Table : Bond Distances and Bond Angles of **2**

Mo-C(1)	1.947(3)
Mo-C(2)	1.945(3)
Mo-C(3)	2.349(3)
Mo-C(4)	2.149(3)
Mo-C(5)	2.332(3)
Mo-C(15)	2.336(3)
Mo-C(16)	2.353(3)
Mo-C(17)	2.353(4)
Mo-C(18)	2.330(3)
Mo-C(19)	2.306(3)
S-C(4)	1.758(3)
S-C(9)	1.773(3)
S-O(3)	1.4339(22)
S-O(4)	1.4356(21)
C(1)-O(1)	1.154(4)
C(2)-O(2)	1.149(4)
C(3)-C(4)	1.424(4)
C(3)-C(8)	1.517(4)
C(4)-C(5)	1.426(4)
C(5)-C(6)	1.515(4)
C(6)-C(7)	1.520(5)
C(7)-C(8)	1.510(5)
C(9)-C(10)	1.377(4)
C(9)-C(14)	1.373(4)
C(10)-C(11)	1.371(5)
C(11)-C(12)	1.357(5)
C(12)-C(13)	1.364(6)
C(13)-C(14)	1.374(5)
C(15)-C(16)	1.375(7)
C(15)-C(19)	1.380(7)
C(16)-C(17)	1.347(9)
C(17)-C(18)	1.368(8)
C(18)-C(19)	1.380(7)

C(1)-Mo-C(2)	84.67(12)
C(1)-Mo-C(3)	68.30(11)
C(1)-Mo-C(4)	104.00(11)
C(1)-Mo-C(5)	111.13(11)
C(1)-Mo-C(15)	90.01(13)
C(1)-Mo-C(16)	116.41(18)
C(1)-Mo-C(17)	146.30(14)
C(1)-Mo-C(18)	130.49(17)
C(1)-Mo-C(19)	97.21(15)
C(2)-Mo-C(3)	109.23(11)
C(2)-Mo-C(4)	105.92(11)
C(2)-Mo-C(5)	70.88(11)
C(2)-Mo-C(15)	129.67(16)
C(2)-Mo-C(16)	146.20(14)
C(2)-Mo-C(17)	116.55(19)
C(2)-Mo-C(18)	89.88(14)
C(2)-Mo-C(19)	96.55(14)
C(3)-Mo-C(4)	36.56(10)
C(3)-Mo-C(5)	62.07(9)
C(3)-Mo-C(15)	114.92(13)
C(3)-Mo-C(16)	103.32(12)
C(3)-Mo-C(17)	121.62(17)
C(3)-Mo-C(18)	155.58(16)
C(3)-Mo-C(19)	148.41(14)
C(4)-Mo-C(5)	36.82(9)
C(4)-Mo-C(15)	123.82(15)
C(4)-Mo-C(16)	94.69(12)
C(4)-Mo-C(17)	95.22(14)
C(4)-Mo-C(18)	124.66(17)
C(4)-Mo-C(19)	150.22(11)
C(5)-Mo-C(15)	153.12(14)
C(5)-Mo-C(16)	119.01(15)
C(5)-Mo-C(17)	100.90(12)
C(5)-Mo-C(18)	113.23(14)
C(5)-Mo-C(19)	147.15(15)
C(15)-Mo-C(16)	34.11(18)
C(15)-Mo-C(17)	56.32(15)
C(4)-S-O(3)	109.88(13)
C(4)-S-O(4)	109.56(13)
C(9)-S-O(3)	107.52(13)
C(9)-S-O(4)	109.05(13)
O(3)-S-O(4)	119.17(14)
Mo-C(1)-O(1)	178.9(3)
Mo-C(2)-O(2)	178.3(3)
Mo-C(3)-C(4)	64.03(14)
Mo-C(3)-C(8)	120.93(19)
C(4)-C(3)-C(8)	117.36(24)
Mo-C(4)-S	124.71(13)
Mo-C(4)-C(3)	79.40(16)
Mo-C(4)-C(5)	78.60(15)
S-C(4)-C(3)	120.72(19)
S-C(4)-C(5)	121.48(20)
C(3)-C(4)-C(5)	115.77(23)
Mo-C(5)-C(4)	64.58(14)
Mo-C(5)-C(6)	121.52(19)
C(4)-C(5)-C(6)	117.84(23)
C(5)-C(6)-C(7)	113.20(24)
C(6)-C(7)-C(8)	113.4(3)
C(3)-C(8)-C(7)	113.82(23)
S-C(9)-C(10)	119.33(22)
S-C(9)-C(14)	120.29(23)
C(10)-C(9)-C(14)	120.3(3)
C(9)-C(10)-C(11)	119.5(3)
C(10)-C(11)-C(12)	120.4(3)
C(11)-C(12)-C(13)	120.1(3)
C(12)-C(13)-C(14)	120.7(3)
C(9)-C(14)-C(13)	118.9(3)
Mo-C(15)-C(16)	73.64(20)
Mo-C(15)-C(19)	71.52(20)
C(16)-C(15)-C(19)	107.0(4)
Mo-C(16)-C(15)	72.25(21)
Mo-C(16)-C(17)	73.37(22)
C(15)-C(16)-C(17)	108.7(4)
Mo-C(17)-C(16)	73.36(23)

C(15)-Mo-C(18)	57.22(14)	Mo-C(17)-C(18)	72.09(22)
C(15)-Mo-C(19)	34.59(17)	C(16)-C(17)-C(18)	109.0(4)
C(16)-Mo-C(17)	33.27(21)	Mo-C(18)-C(17)	73.95(22)
C(16)-Mo-C(18)	56.33(16)	Mo-C(18)-C(19)	71.72(20)
C(16)-Mo-C(19)	56.76(14)	C(17)-C(18)-C(19)	107.2(4)
C(17)-Mo-C(18)	33.96(21)	Mo-C(19)-C(15)	73.89(20)
C(17)-Mo-C(19)	56.67(15)	Mo-C(19)-C(18)	73.66(21)
C(18)-Mo-C(19)	34.62(18)	C(15)-C(19)-C(18)	108.1(4)
C(4)-S-C(9)	99.90(12)		

Table. Crystal Data and Conditions for Crystallographic Data Collection and Structure Refinement **4b**

TITLE,	**4b**
Formula ,	C25 H22 O4 S2 Mo
FW ,	546.50
Diffractometer used,	Nonius
Space Group,	Orthorhombic P na21
a(angstron),	16.896(3)
b(angstron),	8.0125(10)
c(angstron),	16.899(3)
V(A**3),	2287.8(6)
Z ,	4
Dcalc(g.cm-3),	1.587
lambda(Angstron),	0.7107
F(000) ,	1106.
Unit cell detn: #;(2theta range),	25;(17.00 - 30.80 deg.)
Scan type,	theta/2theta
Scan width (deg),	2(0.65+0.35tan(theta))
Scan Speed (deg/min),	2.06-8.24
2 Theta(max),	50.0
h k l ranges ,	(0; 20)(0; 9)(0; 20)
mu(cm-1),	7.632
Crystal size(mm),	0.13 X 0.35 X 0.40
Transmission,	0.905; 1.000
Temperature,	298.00
# of meas. reflns,	2082
# of obsed relfns (I > 2.0sig(I)),	1740
# of unique reflns,	2082
RF;RW ,	0.029;0.030
GoF,	1.47
Refinement program,	NRCVAX
# of atoms,	54
# of refined params,	289 (1740 out of 2082 reflns.)
Minimize function,	SUM(w|Fo-Fc|**2)
Weights scheme,	(1/sigma**2)(Fo)
The weight modifier K in KFo**2 is,	0.000050
g (2nd. ext. coeff.) x 10e4,	0.09(3)
(delta/sigma)max ,	0.0076
(D-map)max.min e/A**3 ,	-0.320; 0.250

NOTE :

RF = Sum(Fo-Fc)/Sum(Fo)

Rw = Sqrt[Sum(w(Fo-Fc)**2)/Sum(wFo**2)]

GoF = Sqrt[Sum(w(Fo-Fc)**2)/(No. of reflns - No. of params.)]

Standard Reflns : No. 3 ; Variation < 2 %, 4 sigma ; every 3600 seconds

complex **4b**

Table . Atomic Parameters x,y,z and Beq.
E.S.Ds. refer to the last digit printed.

	x	y	z	Beq
Mo	0.14869(3)	0.03210(6)	0.25000	2.683(22)
S1	0.05619(10)	-0.16430(22)	-0.01201(10)	2.94 (7)
S2	-0.00933(11)	0.23307(22)	0.17903(12)	3.40 (8)
C1	0.2329 (4)	-0.0844 (8)	0.1932 (4)	2.9 (3)
C2	0.1403 (4)	-0.1802 (9)	0.3065 (4)	3.0 (3)
C3	0.0266 (3)	-0.1002 (8)	0.2216 (4)	2.8 (3)
C4	0.0437 (3)	0.0417 (7)	0.1718 (4)	2.3 (3)
C5	0.1062 (4)	0.0149 (7)	0.1180 (4)	2.22 (24)
C6	0.1155 (3)	-0.1508 (7)	0.0770 (4)	2.22 (25)
C7	0.0936 (4)	-0.3039 (8)	0.1285 (4)	2.8 (3)
C8	0.0264 (4)	-0.2707 (8)	0.1853 (4)	2.8 (3)
C9	0.0754 (4)	0.0215 (8)	-0.0647 (4)	2.5 (3)
C10	0.1395 (4)	0.0277 (10)	-0.1161 (4)	3.9 (4)
C11	0.1548 (4)	0.1750 (11)	-0.1557 (5)	5.0 (4)
C12	0.1076 (5)	0.3122 (10)	-0.1463 (5)	4.8 (4)
C13	0.0444 (5)	0.3051 (9)	-0.0955 (4)	4.5 (4)
C14	0.0271 (4)	0.1593 (9)	-0.0555 (4)	3.4 (3)
C15	-0.0944 (4)	0.2025 (8)	0.1185 (4)	2.9 (3)
C16	-0.1362 (4)	0.0530 (10)	0.1159 (4)	3.9 (3)
C17	-0.2039 (4)	0.0437 (11)	0.0702 (5)	4.7 (4)
C18	-0.2300 (5)	0.1769 (12)	0.0287 (5)	5.3 (4)
C19	-0.1895 (5)	0.3219 (11)	0.0310 (4)	5.0 (4)
C20	-0.1210 (4)	0.3318 (10)	0.0751 (5)	4.2 (4)
C21	0.1595 (5)	0.3237 (8)	0.2588 (6)	4.7 (4)
C22	0.1126 (4)	0.2765 (9)	0.3223 (4)	3.9 (3)
C23	0.1563 (4)	0.1757 (9)	0.3710 (4)	3.4 (3)
C24	0.2331 (4)	0.1579 (9)	0.3387 (4)	3.4 (3)
C25	0.2346 (4)	0.2518 (9)	0.2698 (4)	4.2 (3)
O1	0.2844 (3)	-0.1502 (6)	0.1620 (3)	4.11 (23)
O2	0.1370 (3)	-0.3036 (6)	0.3395 (3)	4.10 (24)
O3	0.0863 (3)	-0.3022 (6)	-0.0578 (3)	4.3 (3)
O4	-0.0251 (3)	-0.1651 (7)	0.0104 (3)	3.88 (23)
H3	-0.020	-0.075	0.254	3.5
H5	0.123	0.111	0.088	3.0
H6	0.172	-0.162	0.059	2.7
H7a	0.139	-0.336	0.159	3.2
H7b	0.080	-0.393	0.094	3.2
H8a	0.028	-0.353	0.227	3.2
H8b	-0.023	-0.288	0.158	3.2
H10	0.171	-0.070	-0.126	4.3
H11	0.203	0.182	-0.191	5.4
H12	0.118	0.414	-0.175	5.4
H13	0.012	0.405	-0.087	4.8
H14	-0.021	0.153	-0.022	3.9
H16	-0.117	-0.040	0.144	4.2
H17	-0.234	-0.063	0.070	5.3
H18	-0.278	0.175	-0.001	5.8
H19	-0.209	0.417	0.002	5.2
H20	-0.091	0.433	0.070	4.5
H21	0.144	0.394	0.218	4.7
H22	0.058	0.313	0.330	4.3
H23	0.135	0.124	0.420	4.4
H24	0.277	0.092	0.361	4.0

H25	0.279	0.273	0.237	4.7

Beq is the Mean of the Principal Axes of the Thermal Ellipsoid

complex **4b**

Table of u(i,j) or U values *100.
E.S.Ds. refer to the last digit printed

	u11(U)	u22	u33	u12	u13	u23
Mo	3.602(22)	3.119(22)	3.474(21)	-0.140(24)	0.00(3)	0.22(4)
S1	4.58 (10)	3.34 (10)	3.24 (8)	-0.44 (8)	-0.19(8)	-0.48(8)
S2	4.32 (10)	3.18 (10)	5.43 (11)	1.08 (9)	-0.80(9)	-0.70(10)
C1	3.9 (4)	3.5 (4)	3.6 (4)	-0.4 (3)	-0.4 (3)	0.6 (3)
C2	3.5 (4)	4.6 (4)	3.2 (3)	0.3 (3)	-0.3 (3)	-0.1 (3)
C3	2.6 (3)	3.6 (4)	4.4 (4)	0.0 (3)	0.5 (3)	-0.5 (3)
C4	2.7 (3)	2.3 (3)	3.7 (4)	0.2 (3)	-0.2 (3)	-0.3 (3)
C5	2.9 (3)	2.6 (3)	2.9 (3)	-0.1 (3)	-0.2 (3)	0.6 (3)
C6	2.9 (3)	2.4 (3)	3.2 (3)	0.1 (3)	-0.2 (3)	0.1 (3)
C7	4.7 (4)	2.2 (3)	3.7 (4)	0.3 (3)	-0.9 (3)	-0.4 (3)
C8	4.0 (4)	3.0 (4)	3.8 (4)	-1.0 (3)	-0.6 (3)	0.9 (3)
C9	3.4 (4)	3.0 (4)	3.1 (3)	-0.2 (3)	-0.4 (3)	-0.8 (3)
C10	4.6 (4)	5.8 (5)	4.5 (4)	0.3 (4)	-0.1 (4)	-0.5 (4)
C11	4.3 (5)	8.5 (7)	6.3 (5)	-2.1 (5)	-0.6 (4)	2.7 (5)
C12	6.7 (5)	4.8 (5)	6.8 (5)	-3.4 (4)	-3.2 (5)	1.9 (4)
C13	8.0 (6)	3.6 (5)	5.5 (5)	1.0 (4)	-2.9 (5)	-1.1 (4)
C14	5.1 (4)	4.9 (5)	3.0 (4)	0.7 (4)	0.2 (3)	-0.8 (4)
C15	3.3 (4)	4.0 (4)	3.6 (4)	1.6 (3)	0.7 (3)	-0.4 (3)
C16	4.2 (4)	5.9 (5)	4.6 (4)	1.7 (4)	0.7 (4)	0.4 (4)
C17	3.8 (4)	7.5 (6)	6.7 (5)	0.0 (4)	0.5 (4)	-1.9 (5)
C18	4.6 (5)	10.1 (7)	5.5 (5)	2.8 (5)	-1.9 (4)	-1.8 (5)
C19	7.4 (6)	6.9 (6)	4.9 (5)	4.4 (5)	-0.4 (4)	0.3 (4)
C20	4.5 (4)	5.7 (5)	5.9 (5)	1.2 (4)	0.5 (4)	0.3 (4)
C21	9.6 (6)	2.7 (3)	5.7 (5)	-0.5 (4)	-2.7 (5)	-0.1 (5)
C22	5.4 (5)	3.7 (4)	5.7 (5)	0.5 (4)	-1.1 (4)	-1.9 (4)
C23	5.3 (4)	4.1 (4)	3.5 (4)	-0.9 (4)	-0.7 (3)	-0.6 (3)
C24	3.4 (4)	4.8 (5)	4.8 (4)	-0.1 (3)	-1.2 (3)	-1.0 (4)
C25	6.8 (5)	4.6 (4)	4.5 (5)	-3.4 (4)	1.6 (4)	-1.7 (4)
O1	3.9 (3)	5.6 (3)	6.1 (3)	1.7 (3)	1.0 (3)	0.0 (3)
O2	6.2 (3)	3.7 (3)	5.7 (3)	-0.4 (3)	-0.3 (3)	2.1 (3)
O3	7.8 (4)	3.9 (3)	4.8 (3)	-0.3 (3)	-0.1 (3)	-0.8 (3)
O4	3.7 (3)	6.8 (4)	4.2 (3)	-0.8 (3)	-0.61(24)	0.9 (3)
H3	4.5					
H5	3.8					
H6	3.5					
H7a	4.0					
H7b	4.0					
H8a	4.1					
H8b	4.1					
H10	5.4					
H11	6.8					
H12	6.8					
H13	6.1					
H14	5.0					
H16	5.3					
H17	6.7					
H18	7.4					
H19	6.5					
H20	5.7					
H21	5.9					
H22	5.5					
H23	5.6					

H24	5.1
H25	6.0 .

Anisotropic Temperature Factors are of the form
Temp=-2*Pi*Pi*(h*h*u11*astar*astar+---+2*h*k*u12*astar*bstar+---)

Table : Bond Distances and Bond Angles of **4b**

Mo-C1	1.953(7)	C5-C6	1.506(8)
Mo-C2	1.956(7)	C6-C7	1.550(9)
Mo-C3	2.368(6)	C7-C8	1.510(9)
Mo-C4	2.213(6)	C9-C10	1.388(9)
Mo-C5	2.347(6)	C9-C14	1.382(10)
Mo-C21	2.348(6)	C10-C11	1.381(11)
Mo-C22	2.388(7)	C11-C12	1.367(13)
Mo-C23	2.349(7)	C12-C13	1.372(12)
Mo-C24	2.302(6)	C13-C14	1.381(11)
Mo-C25	2.306(6)	C15-C16	1.392(10)
S1-C6	1.811(6)	C15-C20	1.346(10)
S1-C9	1.765(7)	C16-C17	1.383(11)
S1-O3	1.441(5)	C17-C18	1.351(12)
S1-O4	1.424(5)	C18-C19	1.349(14)
S2-C4	1.781(6)	C19-C20	1.378(11)
S2-C15	1.782(7)	C21-C22	1.387(12)
C1-O1	1.147(8)	C21-C25	1.406(11)
C2-O2	1.136(8)	C22-C23	1.370(10)
C3-C4	1.444(9)	C23-C24	1.414(10)
C3-C8	1.497(9)	C24-C25	1.386(10)
C4-C5	1.409(8)		

C1-Mo-C2	82.9(3)	C4-S2-C15	104.4(3)
C1-Mo-C3	108.71(24)	Mo-C1-O1	177.2(6)
C1-Mo-C4	107.86(24)	Mo-C2-O2	178.7(6)
C1-Mo-C5	74.22(24)	Mo-C3-C4	65.9(3)
C1-Mo-C21	116.7(3)	Mo-C3-C8	119.6(4)
C1-Mo-C22	146.1(3)	C4-C3-C8	118.6(5)
C1-Mo-C23	128.4(3)	Mo-C4-S2	113.1(3)
C1-Mo-C24	94.5(3)	Mo-C4-C3	77.6(3)
C1-Mo-C25	88.7(3)	Mo-C4-C5	77.3(3)
C2-Mo-C3	69.30(25)	S2-C4-C3	122.5(4)
C2-Mo-C4	105.30(24)	S2-C4-C5	123.5(5)
C2-Mo-C5	113.02(24)	C3-C4-C5	114.0(5)
C2-Mo-C21	147.2(3)	Mo-C5-C4	66.9(3)
C2-Mo-C22	116.4(3)	Mo-C5-C6	117.2(4)
C2-Mo-C23	90.3(3)	C4-C5-C6	120.6(5)
C2-Mo-C24	96.2(3)	S1-C6-C5	112.1(4)
C2-Mo-C25	129.7(3)	S1-C6-C7	106.7(4)
C3-Mo-C4	36.55(22)	C5-C6-C7	114.5(5)
C3-Mo-C5	60.99(21)	C6-C7-C8	113.4(5)
C3-Mo-C21	121.74(25)	C3-C8-C7	114.8(5)
C3-Mo-C22	104.37(23)	S1-C9-C10	119.3(5)
C3-Mo-C23	116.32(23)	S1-C9-C14	120.5(5)
C3-Mo-C24	150.19(23)	C10-C9-C14	120.2(6)
C3-Mo-C25	156.8(3)	C9-C10-C11	118.6(7)
C4-Mo-C5	35.84(21)	C10-C11-C12	121.5(7)
C4-Mo-C21	93.77(25)	C11-C12-C13	119.5(7)
C4-Mo-C22	94.14(23)	C12-C13-C14	120.4(7)
C4-Mo-C23	123.15(24)	C9-C14-C13	119.7(7)
C4-Mo-C24	150.51(23)	S2-C15-C16	123.1(5)
C4-Mo-C25	124.4(3)	S2-C15-C20	118.5(6)
C5-Mo-C21	98.2(3)	C16-C15-C20	118.4(6)
C5-Mo-C22	117.12(23)	C15-C16-C17	118.9(7)
C5-Mo-C23	150.73(23)	C16-C17-C18	121.2(8)

C5-Mo-C24	146.52(23)	C17-C18-C19	119.9(7)
C5-Mo-C25	112.05(22)	C18-C19-C20	119.5(7)
C21-Mo-C22	34.0(3)	C15-C20-C19	122.0(7)
C21-Mo-C23	56.9(3)	Mo-C21-C22	74.5(4)
C21-Mo-C24	58.3(3)	Mo-C21-C25	70.8(4)
C21-Mo-C25	35.1(3)	C22-C21-C25	107.5(7)
C22-Mo-C23	33.6(3)	Mo-C22-C21	71.4(4)
C22-Mo-C24	57.73(24)	Mo-C22-C23	71.7(4)
C22-Mo-C25	57.3(3)	C21-C22-C23	108.4(7)
C23-Mo-C24	35.39(25)	Mo-C23-C22	74.7(4)
C23-Mo-C25	57.65(24)	Mo-C23-C24	70.5(4)
C24-Mo-C25	35.0(3)	C22-C23-C24	108.9(6)
C6-S1-C9	105.5(3)	Mo-C24-C23	74.1(4)
C6-S1-O3	107.2(3)	Mo-C24-C25	72.7(4)
C6-S1-O4	108.3(3)	C23-C24-C25	106.6(6)
C9-S1-O3	108.1(3)	Mo-C25-C21	74.1(4)
C9-S1-O4	108.4(3)	Mo-C25-C24	72.3(4)
O3-S1-O4	118.6(3)	C21-C25-C24	108.5(7)