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Table S1. Fractional Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for *cis,trans*-MoOClL; e.s.d. values are given in parentheses.

Atom	x	y	z	B_{eq}[a]
Mo	0.3879(1)	0.32037(6)	0.2505(1)	2.94(1)
Cl	0.5544(3)	0.4231(2)	0.2260(3)	5.57(5)
S1	0.2371(5)	0.4355(4)	0.1522(6)	3.54(7)
S2	0.5254(5)	0.1839(5)	0.2923(6)	3.45(6)
O	0.3874(7)	0.3314(4)	0.3860(5)	5.1(1)
N1	0.2077(8)	0.2300(4)	0.2097(6)	2.9(1)
N2	0.3935(7)	0.2548(5)	0.0577(6)	2.5(1)
C1	0.088(1)	0.3789(7)	0.147(1)	3.5(1)
C2	-0.028(1)	0.4300(7)	0.123(1)	4.4(2)
C3	-0.149(1)	0.3898(8)	0.112(1)	4.7(2)
C4	-0.1554(8)	0.2898(9)	0.129(1)	4.7(2)
C5	-0.0408(8)	0.2389(6)	0.1573(7)	3.5(1)
C6	0.0824(8)	0.2819(6)	0.1686(7)	2.8(1)
C7	0.1991(7)	0.1746(6)	0.3154(6)	3.7(1)
C8	0.226(1)	0.1598(6)	0.1198(9)	3.3(1)
C9	0.2612(8)	0.2142(8)	0.0222(7)	3.3(1)
C10	0.409(1)	0.3306(6)	-0.0246(7)	4.3(2)
C11	0.4943(7)	0.1842(5)	0.0607(6)	2.6(1)
C12	0.5227(9)	0.1477(6)	-0.0385(6)	3.2(1)
C13	0.6241(9)	0.0818(6)	-0.0323(7)	3.8(1)
C14	0.6942(9)	0.0499(6)	0.0722(8)	3.9(2)
C15	0.6603(9)	0.0807(7)	0.1709(7)	3.5(1)
C16	0.5618(8)	0.1488(6)	0.1657(6)	2.8(1)
Mo'	0.4253(3)	0.3359(2)	0.2076(4)	3.71(5)
Cl'	0.4370(7)	0.3806(6)	0.3945(5)	6.1(2)
S1'	0.557(1)	0.202(1)	0.282(2)	4.1(2)
S2'	0.243(2)	0.434(1)	0.142(2)	6.3(3)
O'	0.529(2)	0.412(2)	0.165(2)	6.5(5)
N1'	0.389(2)	0.245(1)	0.042(1)	4.2(7)
N2'	0.224(1)	0.232(1)	0.212(1)	4.2(7)
C1'	0.567(2)	0.143(2)	0.147(1)	3.2(3)
C2'	0.668(2)	0.079(2)	0.147(1)	3.2(3)
C3'	0.688(2)	0.042(2)	0.045(1)	3.2(3)
C4'	0.606(2)	0.070(2)	-0.058(1)	3.2(3)
C5'	0.506(2)	0.134(2)	-0.059(1)	3.2(3)
C6'	0.486(2)	0.171(2)	0.044(1)	3.2(3)
C7'	0.398(3)	0.314(1)	-0.0511(7)	3.3(3)
C8'	0.253(2)	0.202(2)	0.017(1)	3.3(3)
C9'	0.225(3)	0.159(1)	0.122(2)	3.3(3)
C10'	0.242(1)	0.187(1)	0.327(2)	3.3(3)
C11'	0.099(1)	0.283(1)	0.185(2)	2.2(2)
C12'	-0.018(1)	0.235(1)	0.184(2)	2.2(2)
C13'	-0.138(1)	0.280(1)	0.144(2)	2.2(2)
C14'	-0.142(1)	0.373(1)	0.107(2)	2.2(2)
C15'	-0.025(1)	0.421(1)	0.109(2)	2.2(2)
C16'	0.096(1)	0.376(1)	0.148(2)	2.2(2)

Site Occupation Factor for the unprimed atoms is 0.722(5), for the primed atoms 0.278(5).

[a] $B_{eq} = (8\pi^2/3)\Sigma\Sigma U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$

Table S2. Interatomic Distances (Å) and Angles (°) for *cis,trans*-MoOClL.

Distances	Major Component	Minor (') component
Mo-Cl	2.341(3)	2.316(8)
Mo-S1	2.398(6)	2.41(1)
Mo-S2	2.405(7)	2.35(2)
Mo-O	1.640(6)	1.69(3)
Mo-N1	2.243(7)	2.34(1)
Mo-N2	2.515(8)	2.58(1)
S1-C1	1.74(1)	1.85(3)
S2-C16	1.73(1)	1.76(2)
N1-C6	1.49(1)	1.46(3)
N1-C7	1.52(1)	1.51(2)
N1-C8	1.52(1)	1.52(3)
N2-C9	1.47(1)	1.50(3)
N2-C10	1.50(1)	1.50(3)
N2-C11	1.45(1)	1.47(2)
C1-C2	1.39(1)	1.40(4)
C1-C6	1.41(1)	1.40(2)
C2-C3	1.37(2)	1.39(2)
C3-C4	1.44(2)	1.40(2)
C4-C5	1.38(1)	1.39(4)
C5-C6	1.40(1)	1.40(2)
C8-C9	1.52(2)	1.49(3)
C11-C12	1.39(1)	1.40(2)
C11-C16	1.40(1)	1.40(2)
C12-C13	1.40(1)	1.40(2)
C13-C14	1.39(1)	1.40(2)
C14-C15	1.38(1)	1.40(2)
C15-C16	1.41(1)	1.40(2)
Angles		
Cl-Mo-S1	86.2(2)	87.3(6)
Cl-Mo-S2	96.2(3)	91.6(7)
Cl-Mo-O	103.4(3)	103(1)
Cl-Mo-N1	160.4(3)	160.9(6)
Cl-Mo-N2	87.0(3)	90.4(5)
S1-Mo-S2	162.5(3)	161.7(9)
S1-Mo-O	106.2(3)	106(1)
S1-Mo-N1	81.8(3)	81.3(8)
S1-Mo-N2	86.9(3)	86.4(7)
S2-Mo-O	90.1(3)	92(1)
S2-Mo-N1	90.8(3)	94.4(9)
S2-Mo-N2	76.0(3)	75.3(8)
O-Mo-N1	94.9(3)	95(1)
O-Mo-N2	163.6(3)	162(1)
N1-Mo-N2	76.9(3)	73.7(7)
Mo-S1-C1	100.6(5)	100(1)
Mo-S2-C16	106.7(5)	111(1)
Mo-N1-C6	114.8(5)	114(1)
Mo-N1-C7	108.5(5)	104(1)
Mo-N1-C8	107.7(6)	111(1)
C6-N1-C7	109.1(5)	109(1)
C6-N1-C8	109.3(6)	109(1)

Table S2, contd. Interatomic Distances (Å) and Angles (°) for *cis,trans*-MoOClL.

C7-N1-C8	107.2(6)	109(1)
Mo-N2-C9	101.7(6)	104(1)
Mo-N2-C10	111.7(6)	109(1)
Mo-N2-C11	113.5(5)	114(1)
C9-N2-C10	108.9(6)	111(1)
C9-N2-C11	111.3(6)	109(1)
C10-N2-C11	109.5(5)	110(1)
S1-C1-C2	119.7(8)	119(2)
S1-C1-C6	121.4(7)	121(2)
C2-C1-C6	118.9(8)	120(2)
C1-C2-C3	123.0(8)	120(2)
C2-C3-C4	118.1(8)	119(2)
C3-C4-C5	119.4(8)	121(2)
C4-C5-C6	121.4(7)	120(2)
N1-C6-C1	118.6(6)	120(2)
N1-C6-C5	122.3(6)	120(2)
C1-C6-C5	119.0(7)	120(2)
N1-C8-C9	107.8(7)	110(2)
N2-C9-C8	110.4(7)	111(2)
N2-C11-C12	121.9(6)	120(1)
N2-C11-C16	119.4(5)	120(1)
C12-C11-C16	118.7(6)	120(1)
C11-C12-C13	120.3(6)	120(1)
C12-C13-C14	120.6(7)	120(1)
C13-C14-C15	119.4(7)	120(1)
C14-C15-C16	120.3(7)	120(1)
S2-C16-C11	121.9(6)	120(1)
S2-C16-C15	117.6(6)	120(1)
C11-C16-C15	120.5(6)	120(1)

Table S3. Anisotropic and Isotropic Displacement Parameters ($Å^2$) for *cis,trans*-MoOClL
The anisotropic temperature factor is given by:

$$T = \exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2hka^*b^*U_{12} + 2hla^*c^*U_{13} + 2klb^*c^*U_{23})]$$

The aromatic and aliphatic carbon atoms of the minor (') component were assigned common isotropic Displacement Parameters.

Atom	U_{11}/U_{iso}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mo	0.0348(4)	0.0370(3)	0.0380(5)	-0.0021(3)	0.0041(3)	-0.0073(3)
Cl	0.047(1)	0.070(1)	0.093(2)	-0.024(1)	0.012(1)	-0.014(1)
S1	0.038(2)	0.028(2)	0.068(2)	-0.006(2)	0.011(2)	0.001(2)
S2	0.037(2)	0.052(2)	0.037(1)	0.007(2)	-0.003(1)	-0.003(1)
O	0.073(4)	0.065(4)	0.053(3)	-0.003(3)	0.011(3)	-0.018(3)
N1	0.044(4)	0.027(3)	0.038(4)	0.005(2)	0.007(2)	-0.001(2)
N2	0.035(3)	0.029(3)	0.031(3)	0.004(2)	0.004(2)	-0.002(2)
C1	0.051(4)	0.039(3)	0.042(4)	0.000(3)	0.008(3)	0.002(3)
C2	0.071(5)	0.049(4)	0.053(6)	0.024(4)	0.030(4)	0.006(4)
C3	0.049(5)	0.068(7)	0.063(5)	0.011(4)	0.019(4)	-0.005(5)
C4	0.036(4)	0.091(7)	0.053(6)	0.015(4)	0.009(4)	0.003(5)
C5	0.052(5)	0.049(4)	0.031(4)	-0.006(4)	0.005(3)	0.000(3)
C6	0.045(4)	0.034(3)	0.027(4)	0.003(3)	0.004(3)	-0.004(3)
C7	0.041(4)	0.054(4)	0.049(4)	0.012(4)	0.014(3)	0.021(3)
C8	0.054(4)	0.028(3)	0.045(4)	-0.001(3)	0.018(3)	-0.012(2)
C9	0.037(4)	0.047(5)	0.035(3)	-0.001(3)	-0.003(3)	-0.017(3)
C10	0.087(6)	0.040(4)	0.044(4)	0.008(4)	0.028(5)	0.008(3)
C11	0.034(3)	0.029(3)	0.036(3)	-0.009(3)	0.007(2)	-0.010(3)
C12	0.051(4)	0.039(4)	0.034(3)	-0.011(3)	0.015(3)	-0.007(3)
C13	0.057(5)	0.044(4)	0.048(4)	-0.017(4)	0.025(4)	-0.016(4)
C14	0.049(4)	0.035(3)	0.067(6)	-0.003(3)	0.017(4)	-0.012(4)
C15	0.046(4)	0.042(4)	0.048(4)	0.004(3)	0.017(4)	-0.002(3)
C16	0.029(3)	0.036(3)	0.040(3)	0.000(3)	0.004(3)	-0.007(3)
Mo'	0.044(1)	0.041(1)	0.054(2)	-0.0005(8)	0.007(1)	-0.0059(9)
Cl'	0.069(4)	0.101(6)	0.053(3)	0.026(4)	-0.005(3)	-0.029(4)
S1'	0.045(7)	0.059(7)	0.048(4)	0.004(4)	0.005(4)	-0.011(4)
S2'	0.081(9)	0.039(7)	0.12(1)	0.026(6)	0.025(8)	0.005(7)
O'	0.022(7)	0.14(2)	0.08(1)	0.007(9)	0.001(8)	0.04(1)
N1'	0.053(9)					
N2'	0.053(9)					
C1'	0.041(4)					
C2'	0.041(4)					
C3'	0.041(4)					
C4'	0.041(4)					
C5'	0.041(4)					
C6'	0.041(4)					
C7'	0.042(4)					
C8'	0.042(4)					
C9'	0.042(4)					
C10'	0.042(4)					
C11'	0.028(3)					
C12'	0.028(3)					
C13'	0.028(3)					
C14'	0.028(3)					
C15'	0.028(3)					
C16'	0.028(3)					

Table S4. Estimated Hydrogen Atom Coordinates and their Isotropic Displacement Parameters ($Å^2$) for *cis,trans*-MoOClL.

Atoms were positioned at geometrical estimates, but not otherwise included in the refinement..

Atom	x	y	z	Uiso
H2	-0.0234	0.5049	0.1111	0.037
H3	-0.2377	0.4322	0.0931	0.037
H4	-0.2501	0.2564	0.1196	0.037
H5	-0.0461	0.1644	0.1710	0.037
H7a	0.2890	0.1369	0.3463	0.092
H7b	0.1825	0.2225	0.3813	0.092
H7c	0.1177	0.1256	0.2961	0.092
H8a	0.3045	0.1118	0.1549	0.021
H8b	0.1366	0.1207	0.0886	0.021
H9a	0.2585	0.1672	-0.0488	0.043
H9b	0.1907	0.2696	-0.0030	0.043
H10a	0.3336	0.3830	-0.0264	0.075
H10b	0.5044	0.3626	0.0032	0.075
H10c	0.3999	0.3012	-0.1082	0.075
H12	0.4667	0.1710	-0.1207	0.052
H13	0.6458	0.0559	-0.1104	0.052
H14	0.7750	0.0023	0.0758	0.052
H15	0.7098	0.0514	0.2520	0.052

Table S5. Fractional Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for *cis,cis*-MoOClL; e.s.d. values are given in parentheses.

Atom	x	y	z	B_{eq}[a]
Mo	0.20785(4)	0.15669(8)	0.07186(3)	2.681(9)
Cl	0.1861(1)	-0.0164(3)	-0.04124(9)	4.13(4)
S1	0.2542(1)	0.2541(2)	0.19397(9)	3.43(3)
S2	0.3394(1)	0.3470(2)	0.03665(9)	3.39(3)
O	0.1112(3)	0.2959(7)	0.0499(3)	4.4(1)
N1	0.1528(3)	-0.0918(7)	0.1321(3)	2.7(1)
N2	0.3575(3)	-0.0413(7)	0.0928(2)	2.38(9)
C1	0.1856(4)	0.1014(9)	0.2436(3)	3.1(1)
C2	0.1773(5)	0.131(1)	0.3184(3)	4.1(2)
C3	0.1277(5)	0.009(1)	0.3583(4)	4.9(2)
C4	0.0835(5)	-0.145(1)	0.3258(4)	5.2(2)
C5	0.0911(5)	-0.179(1)	0.2523(4)	4.3(2)
C6	0.1414(4)	-0.0554(9)	0.2112(3)	3.1(1)
C7	0.0557(4)	-0.152(1)	0.0946(4)	4.2(2)
C8	0.2253(4)	-0.2469(9)	0.1259(3)	3.3(1)
C9	0.3296(4)	-0.1821(8)	0.1473(3)	2.8(1)
C10	0.3906(4)	-0.1388(9)	0.0276(3)	2.9(1)
C11	0.4413(4)	0.0766(9)	0.1198(3)	2.6(1)
C12	0.5218(5)	0.011(1)	0.1646(3)	3.8(1)
C13	0.6020(5)	0.123(1)	0.1798(4)	4.5(2)
C14	0.6036(5)	0.300(1)	0.1524(4)	4.5(2)
C15	0.5238(4)	0.3698(9)	0.1104(3)	3.6(1)
C16	0.4404(4)	0.2598(9)	0.0934(3)	2.8(1)

[a] $B_{eq} = (4/3)\Sigma\Sigma B_{ij}\ \mathbf{a}_i \cdot \mathbf{a}_j$

Table S6. Interatomic Distances (Å) and Angles (°) for *cis,cis*-MoOClL.

Mo-Cl	2.403(2)	C1-C2	1.394(9)
Mo-S1	2.365(2)	C1-C6	1.382(9)
Mo-S2	2.381(2)	C2-C3	1.35(1)
Mo-O	1.668(4)	C3-C4	1.37(1)
Mo-N1	2.257(5)	C4-C5	1.38(1)
Mo-N2	2.478(5)	C5-C6	1.381(9)
S1-C1	1.743(7)	C8-C9	1.507(8)
S2-C16	1.756(6)	C11-C12	1.386(9)
N1-C6	1.488(8)	C11-C16	1.400(9)
N1-C7	1.492(8)	C12-C13	1.36(1)
N1-C8	1.496(8)	C13-C14	1.36(1)
N2-C9	1.489(7)	C14-C15	1.36(1)
N2-C10	1.485(7)	C15-C16	1.391(9)
N2-C11	1.466(7)		

Cl-Mo-S1	164.34(7)	Mo-N2-C11	108.7(4)
Cl-Mo-S2	95.80(6)	C9-N2-C10	109.2(5)
Cl-Mo-O	94.0(2)	C9-N2-C11	113.8(5)
Cl-Mo-N1	89.4(1)	C10-N2-C11	105.0(4)
Cl-Mo-N2	82.6(1)	S1-C1-C2	120.5(6)
S1-Mo-S2	86.72(6)	S1-C1-C6	121.3(5)
S1-Mo-O	100.7(2)	C2-C1-C6	118.1(7)
S1-Mo-N1	81.2(1)	C1-C2-C3	121.2(8)
S1-Mo-N2	83.1(1)	C2-C3-C4	120.4(7)
S2-Mo-O	100.6(2)	C3-C4-C5	119.8(7)
S2-Mo-N1	150.9(1)	C4-C5-C6	120.0(8)
S2-Mo-N2	75.3(1)	N1-C6-C1	118.7(5)
O-Mo-N1	107.6(2)	N1-C6-C5	120.9(6)
O-Mo-N2	174.4(2)	C1-C6-C5	120.4(6)
N1-Mo-N2	77.0(2)	N1-C8-C9	111.1(5)
Mo-S1-C1	101.2(2)	N2-C9-C8	109.0(5)
Mo-S2-C16	101.6(2)	N2-C11-C12	123.1(6)
Mo-N1-C6	113.7(4)	N2-C11-C16	116.3(5)
Mo-N1-C7	108.9(4)	C12-C11-C16	120.4(6)
Mo-N1-C8	107.5(3)	C11-C12-C13	119.2(7)
C6-N1-C7	109.4(5)	C12-C13-C14	121.1(7)
C6-N1-C8	109.3(5)	C13-C14-C15	120.6(7)
C7-N1-C8	107.9(5)	C14-C15-C16	120.4(7)
Mo-N2-C9	103.7(3)	S2-C16-C11	121.3(5)
Mo-N2-C10	116.7(3)	S2-C16-C15	120.3(5)
		C11-C16-C15	118.3(6)

Table S7. Anisotropic Displacement Parameters ($Å^2$) for *cis,cis*-MoOClL
The anisotropic temperature factor is given by:

$$T = \exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2hka^*b^*U_{12} + 2hla^*c^*U_{13} + 2klb^*c^*U_{23})]$$

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mo	0.0356(2)	0.0293(2)	0.0373(2)	0.0034(3)	0.0047(2)	0.0055(3)
Cl	0.0527(9)	0.063(1)	0.0396(8)	-0.0022(9)	-0.0042(7)	-0.0022(8)
S1	0.0552(9)	0.0317(8)	0.0447(8)	-0.0027(8)	0.0117(7)	-0.0067(8)
S2	0.0477(8)	0.0289(7)	0.0532(9)	-0.0003(8)	0.0104(7)	0.0106(8)
O	0.043(2)	0.057(3)	0.068(3)	0.021(2)	0.005(2)	0.012(2)
N1	0.031(2)	0.035(3)	0.038(2)	-0.005(2)	0.007(2)	0.000(2)
N2	0.039(2)	0.024(2)	0.028(2)	-0.000(2)	0.007(2)	0.004(2)
C1	0.039(3)	0.037(4)	0.041(3)	0.010(3)	0.004(3)	0.002(3)
C2	0.052(3)	0.063(5)	0.043(3)	0.023(3)	0.010(3)	-0.002(3)
C3	0.076(4)	0.071(5)	0.043(3)	0.022(4)	0.024(3)	0.006(4)
C4	0.064(4)	0.084(5)	0.052(4)	0.006(4)	0.026(3)	0.029(4)
C5	0.058(4)	0.051(4)	0.058(4)	-0.011(4)	0.016(3)	0.008(4)
C6	0.038(3)	0.039(3)	0.043(3)	0.008(3)	0.015(3)	0.009(3)
C7	0.037(3)	0.061(4)	0.061(4)	-0.009(4)	0.001(3)	0.010(4)
C8	0.058(4)	0.027(3)	0.042(3)	-0.000(3)	0.013(3)	0.004(3)
C9	0.042(3)	0.028(3)	0.037(3)	0.006(3)	0.007(2)	0.005(3)
C10	0.033(3)	0.036(3)	0.042(3)	0.003(3)	0.007(2)	-0.006(3)
C11	0.031(3)	0.037(3)	0.031(3)	-0.003(3)	0.007(2)	-0.009(3)
C12	0.047(3)	0.053(4)	0.042(3)	0.006(3)	-0.000(3)	-0.003(3)
C13	0.047(4)	0.074(5)	0.047(4)	-0.002(4)	-0.008(3)	-0.003(4)
C14	0.041(3)	0.073(5)	0.058(4)	-0.020(3)	0.003(3)	-0.015(4)
C15	0.051(3)	0.040(4)	0.049(3)	-0.008(3)	0.017(3)	-0.013(3)
C16	0.045(3)	0.032(3)	0.029(3)	-0.005(3)	0.006(3)	-0.002(3)

Table S8. Estimated Hydrogen Atom Coordinates and their Isotropic Displacement Parameters ($Å^2$) for *cis,cis*-MoOClL.

All H-atoms were placed in idealized positions and refined using the riding model with an isotropic temperature factor assigned.

Atom	x	y	z	B_{iso}
H2	0.208	0.237	0.342	5.0
H3	0.123	0.031	0.409	5.0
H4	0.048	-0.228	0.354	5.0
H5	0.062	-0.287	0.229	5.0
H7a	0.060	-0.155	0.043	5.7
H7b	0.006	-0.067	0.105	5.7
H7c	0.039	-0.273	0.111	5.7
H8a	0.221	-0.290	0.076	5.0
H8b	0.210	-0.346	0.157	5.0
H9a	0.333	-0.127	0.195	5.0
H9b	0.374	-0.285	0.148	5.0
H10a	0.455	-0.188	0.039	3.9
H10b	0.392	-0.054	-0.012	3.9
H10c	0.346	-0.237	0.014	3.9
H12	0.521	-0.111	0.185	5.0
H13	0.658	0.076	0.208	5.0
H14	0.659	0.378	0.164	5.0
H15	0.526	0.492	0.091	5.0

Table S9. Final Fractional Atomic Coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for *cis,trans*-MoO(OSiMe3)L; e.s.d. values are given in parentheses.

Atom	x	y	z	B_{eq}[a]
Mo	0.33038(2)	0.26358(2)	0.22730(2)	4.306(6)
O1	0.3553(2)	0.3532(2)	0.1475(2)	5.93(5)
S1	0.42293(7)	0.34495(8)	0.39004(6)	5.12(2)
S2	0.23852(8)	0.13399(9)	0.08747(6)	6.00(2)
N1	0.4589(2)	0.1515(2)	0.2568(2)	4.66(6)
N2	0.3088(2)	0.0862(3)	0.3180(2)	4.81(6)
C1	0.5303(3)	0.2932(3)	0.4009(2)	4.51(7)
C2	0.6071(3)	0.3432(4)	0.4744(3)	5.48(8)
C3	0.6923(3)	0.3061(4)	0.4845(3)	7.2(1)
C4	0.7034(3)	0.2152(4)	0.4237(4)	7.5(1)
C5	0.6260(3)	0.1642(4)	0.3518(4)	6.49(9)
C6	0.5403(3)	0.2026(3)	0.3380(3)	4.82(8)
C7	0.4729(3)	0.1444(4)	0.1573(3)	6.5(1)
C8	0.4419(3)	0.0250(3)	0.2842(3)	5.81(9)
C9	0.3991(3)	0.0304(3)	0.3621(3)	5.93(8)
C10	0.2805(4)	0.1241(4)	0.4032(3)	7.1(1)
C11	0.2415(3)	0.0021(3)	0.2527(3)	5.06(8)
C12	0.2122(3)	-0.0963(4)	0.2929(3)	6.9(1)
C13	0.1451(4)	-0.1719(4)	0.2327(4)	8.2(1)
C14	0.1051(3)	-0.1517(4)	0.1310(4)	7.7(1)
C15	0.1332(3)	-0.0573(4)	0.0868(3)	6.5(1)
C16	0.2026(3)	0.0195(3)	0.1473(3)	5.18(8)
O2	0.2280(2)	0.3277(2)	0.2480(2)	6.19(6)
Si	0.12488(9)	0.3784(1)	0.1921(1)	7.43(3)
C17	0.1019(4)	0.4785(6)	0.2806(6)	14.3(2)
C18	0.1176(5)	0.4595(9)	0.0771(6)	19.7(3)
C19	0.0417(4)	0.2562(5)	0.1556(6)	10.5(2)

[a] $B_{eq} = (8\pi^2/3)\Sigma\Sigma U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$

Table S10. Interatomic Distances (Å) and Angles (deg) for *cis,trans*-MoO(OSiMe3)L.

Distances

Mo-O1	1.668(3)	C2-C3	1.372(7)
Mo-S1	2.388(1)	C3-C4	1.385(7)
Mo-S2	2.434(1)	C4-C5	1.384(6)
Mo-N1	2.294(3)	C5-C6	1.370(7)
Mo-N2	2.453(3)	C8-C9	1.506(7)
Mo-O2	1.903(3)	C11-C12	1.396(6)
S1-C1	1.754(5)	C11-C16	1.394(5)
S2-C16	1.746(4)	C12-C13	1.370(6)
N1-C6	1.477(4)	C13-C14	1.353(7)
N1-C7	1.513(6)	C14-C15	1.384(7)
N1-C8	1.514(4)	C15-C16	1.400(5)
N2-C9	1.467(5)	O2-Si	1.625(3)
N2-C10	1.504(7)	Si-C17	1.819(8)
N2-C11	1.456(5)	Si-C18	1.829(9)
C1-C2	1.382(5)	Si-C19	1.830(6)
C1-C6	1.396(5)		

Angles

O1-Mo-S1	102.1(1)	S1-C1-C2	118.9(3)
O1-Mo-S2	91.6(1)	S1-C1-C6	121.9(3)
O1-Mo-N1	91.2(1)	C2-C1-C6	119.2(3)
O1-Mo-N2	163.0(1)	C1-C2-C3	120.6(3)
O1-Mo-O2	108.8(1)	C2-C3-C4	120.9(3)
S1-Mo-S2	165.1(1)	C3-C4-C5	117.9(4)
S1-Mo-N1	81.7(1)	C4-C5-C6	122.2(4)
S1-Mo-N2	87.6(1)	N1-C6-C1	119.7(3)
S1-Mo-O2	87.4(1)	N1-C6-C5	121.2(3)
S2-Mo-N1	92.3(1)	C1-C6-C5	119.1(3)
S2-Mo-N2	77.8(1)	N1-C8-C9	109.1(3)
S2-Mo-O2	93.8(1)	N2-C9-C8	110.5(3)
N1-Mo-O2	158.9(1)	N2-C11-C12	121.7(3)
N1-Mo-N2	76.2(1)	N2-C11-C16	120.5(3)
N2-Mo-O2	85.4(1)	C12-C11-C16	117.8(3)
Mo-S1-C1	100.3(2)	C11-C12-C13	122.1(3)
Mo-S2-C16	104.1(2)	C12-C13-C14	119.8(4)
Mo-N1-C6	112.7(2)	C13-C14-C15	120.5(4)
Mo-N1-C7	107.4(2)	C14-C15-C16	120.2(4)
Mo-N1-C8	108.6(2)	S2-C16-C11	122.0(3)
C6-N1-C7	110.3(3)	S2-C16-C15	118.5(3)
C6-N1-C8	110.4(3)	C11-C16-C15	119.5(3)
C7-N1-C8	107.2(3)	Mo-O2-Si	145.0(2)
Mo-N2-C9	104.6(3)	O2-Si-C17	108.1(3)
Mo-N2-C10	109.9(3)	O2-Si-C18	108.2(3)
Mo-N2-C11	113.7(3)	O2-Si-C19	111.4(3)
C9-N2-C10	108.9(3)	C17-Si-C18	110.6(4)
C9-N2-C11	111.0(3)	C17-Si-C19	109.6(3)
C10-N2-C11	108.5(3)	C18-Si-C19	109.0(4)

Table S11. Anisotropic Displacement Parameters ($Å^2$) for *cis,trans*-MoO(OSiMe3)L.
The anisotropic temperature factor is given by:

$$T = \exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2hka^*b^*U_{12} + 2hla^*c^*U_{13} + 2klb^*c^*U_{23})]$$

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mo	0.0747(2)	0.0455(2)	0.0413(1)	-0.0023(1)	0.0200(1)	0.0012(1)
O1	0.107(2)	0.061(1)	0.053(1)	-0.015(1)	0.026(1)	0.007(1)
S1	0.0839(7)	0.0617(5)	0.0495(4)	-0.0001(5)	0.0265(5)	-0.0146(4)
S2	0.1052(8)	0.0718(6)	0.0438(4)	-0.0235(6)	0.0207(5)	-0.0040(4)
N1	0.082(2)	0.049(1)	0.054(2)	-0.002(1)	0.035(2)	-0.007(1)
N2	0.079(2)	0.061(2)	0.047(1)	-0.004(2)	0.029(1)	0.005(1)
C1	0.077(2)	0.050(2)	0.044(2)	-0.001(2)	0.023(2)	0.006(1)
C2	0.080(3)	0.067(2)	0.054(2)	-0.008(2)	0.018(2)	0.007(2)
C3	0.086(3)	0.083(3)	0.082(3)	-0.016(3)	0.009(3)	0.013(2)
C4	0.070(3)	0.089(3)	0.120(4)	0.003(3)	0.029(3)	0.010(3)
C5	0.084(3)	0.064(2)	0.104(3)	0.007(2)	0.042(3)	0.002(2)
C6	0.075(3)	0.050(2)	0.060(2)	0.001(2)	0.028(2)	0.005(2)
C7	0.110(4)	0.086(3)	0.071(2)	-0.005(2)	0.059(2)	-0.021(2)
C8	0.088(3)	0.044(2)	0.088(3)	0.008(2)	0.033(2)	-0.001(2)
C9	0.095(3)	0.059(2)	0.062(2)	-0.006(2)	0.020(2)	0.018(2)
C10	0.138(4)	0.092(3)	0.059(2)	-0.020(3)	0.060(3)	-0.007(2)
C11	0.083(3)	0.053(2)	0.065(2)	-0.005(2)	0.038(2)	0.001(2)
C12	0.115(4)	0.073(3)	0.087(3)	-0.016(3)	0.052(3)	0.008(2)
C13	0.121(4)	0.078(3)	0.123(4)	-0.033(3)	0.060(4)	0.003(3)
C14	0.098(4)	0.084(3)	0.118(4)	-0.035(3)	0.048(3)	-0.027(3)
C15	0.085(3)	0.076(3)	0.083(3)	-0.018(2)	0.031(2)	-0.018(2)
C16	0.077(3)	0.056(2)	0.066(2)	-0.005(2)	0.030(2)	-0.006(2)
O2	0.077(2)	0.075(2)	0.081(2)	0.006(1)	0.028(1)	-0.006(1)
Si	0.0710(8)	0.0823(8)	0.120(1)	0.0025(7)	0.0267(8)	0.0081(8)
C17	0.104(5)	0.132(5)	0.283(9)	0.025(4)	0.046(5)	-0.088(6)
C18	0.106(5)	0.34(1)	0.27(1)	0.050(7)	0.038(6)	0.22(1)
C19	0.090(4)	0.134(5)	0.186(6)	-0.030(3)	0.064(4)	-0.046(4)

Table S12. Hydrogen Atom Coordinates and their Isotropic Displacement Parameters (Å^2) for *cis,trans*-MoO(OSiMe3)L.

Atoms were constrained at geometrical estimates, the e.s.d. values are those of the parent carbon atom. A common temperature factor was assigned to the Hydrogen atoms on each methyl carbon and on each aromatic ring.

Atom	x	y	z	Uiso
H2	0.5999(3)	0.4120(4)	0.5244(3)	0.109(7)
H3	0.7515(3)	0.3484(4)	0.5406(3)	0.109(7)
H4	0.7704(3)	0.1852(4)	0.4321(4)	0.109(7)
H5	0.6333(3)	0.0916(4)	0.3051(4)	0.109(7)
H7A	0.4853(3)	0.2333(4)	0.1351(3)	0.092(7)
H7B	0.4128(3)	0.1073(4)	0.0987(3)	0.092(7)
H7C	0.5306(3)	0.0876(4)	0.1672(3)	0.092(7)
H8A	0.5056(3)	-0.0230(3)	0.3158(3)	0.077(7)
H8B	0.3966(3)	-0.0207(3)	0.2166(3)	0.077(7)
H9A	0.4420(3)	0.0826(3)	0.4269(3)	0.078(8)
H9B	0.3924(3)	-0.0596(3)	0.3867(3)	0.078(8)
H10A	0.3298(4)	0.1867(4)	0.4525(3)	0.126(9)
H10B	0.2769(4)	0.0463(4)	0.4469(3)	0.126(9)
H10C	0.2146(4)	0.1667(4)	0.3716(3)	0.126(9)
H12	0.2433(3)	-0.1133(4)	0.3740(3)	0.108(7)
H13	0.1243(4)	-0.2473(4)	0.2664(4)	0.108(7)
H14	0.0508(3)	-0.2097(4)	0.0839(4)	0.108(7)
H15	0.1015(3)	-0.0429(4)	0.0054(3)	0.108(7)
H17A	0.0336(4)	0.5135(6)	0.2451(6)	0.15*
H17B	0.1499(4)	0.5519(6)	0.3004(6)	0.15*
H17C	0.1085(4)	0.4296(6)	0.3488(6)	0.15*
H18A	0.0495(5)	0.4941(9)	0.0387(6)	0.15*
H18B	0.1336(5)	0.3993(9)	0.0267(6)	0.15*
H18C	0.1654(5)	0.5331(9)	0.0981(6)	0.15*
H19A	-0.0259(4)	0.2929(5)	0.1187(6)	0.15*
H19B	0.0461(4)	0.2071(5)	0.2230(6)	0.15*
H19C	0.0558(4)	0.1964(5)	0.1036(6)	0.15*

* Values not refined.

Table S13. Final Fractional Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for *cis,trans*-MoO(NCS)L; e.s.d. values are given in parentheses.

Atom	x	y	z	B_{eq}[a]
Mo	0.13946(3)	0.04039(5)	0.000	2.82(1)
S	0.0204(1)	-0.2523(2)	0.2255(4)	4.29(5)
S1	0.17541(9)	0.2159(2)	-0.0843(4)	3.14(4)
S2	0.2345(1)	-0.0304(2)	-0.0848(4)	3.90(5)
O	0.1015(3)	0.0037(6)	-0.1945(9)	4.4(1)
N	0.1082(3)	-0.0974(6)	0.149(1)	4.1(2)
N1	0.0811(3)	0.1427(5)	0.191(1)	3.1(1)
N2	0.2002(3)	0.0607(5)	0.282(1)	2.9(1)
C	0.0718(4)	-0.1637(6)	0.182(1)	3.1(2)
C1	0.1203(3)	0.3022(6)	0.012(2)	2.8(1)
C2	0.1190(3)	0.4140(7)	-0.037(1)	3.3(2)
C3	0.0777(4)	0.4813(7)	0.047(1)	4.8(3)
C4	0.0391(4)	0.4424(7)	0.181(2)	4.4(2)
C5	0.0394(4)	0.3334(7)	0.227(2)	4.1(2)
C6	0.0803(4)	0.2621(6)	0.139(1)	3.0(2)
C7	0.0179(3)	0.1022(7)	0.179(2)	4.8(2)
C8	0.1032(4)	0.1276(8)	0.387(1)	4.2(2)
C9	0.1689(3)	0.1464(7)	0.398(1)	3.6(2)
C10	0.2076(4)	-0.0420(7)	0.396(1)	3.9(2)
C11	0.2594(3)	0.0949(6)	0.224(1)	2.9(2)
C12	0.2950(4)	0.1649(8)	0.330(2)	4.6(2)
C13	0.3507(4)	0.1931(9)	0.265(2)	5.5(3)
C14	0.3724(4)	0.1497(9)	0.103(2)	5.7(3)
C15	0.3377(3)	0.0812(8)	-0.003(2)	4.6(2)
C16	0.2805(3)	0.0532(7)	0.057(1)	3.3(2)

[a] $B_{eq} = (4/3)\Sigma\Sigma B_{ij}\ \mathbf{a}_i.\mathbf{a}_j$

Table S14. Interatomic Distances (Å) and Angles (°) for *cis,trans*-MoO(NCS)L.

Mo-S1	2.356(2)	N2-C11	1.45(1)
Mo-S2	2.380(3)	C1-C2	1.40(1)
Mo-O	1.691(7)	C1-C6	1.37(1)
Mo-N	2.101(9)	C2-C3	1.38(1)
Mo-N1	2.265(8)	C3-C4	1.38(2)
Mo-N2	2.447(7)	C4-C5	1.36(1)
S-C	1.61(1)	C5-C6	1.41(1)
S1-C1	1.762(9)	C8-C9	1.50(1)
S2-C16	1.768(9)	C11-C12	1.39(1)
N-C	1.17(1)	C11-C16	1.38(1)
N1-C6	1.50(1)	C12-C13	1.38(1)
N1-C7	1.51(1)	C13-C14	1.36(2)
N1-C8	1.50(1)	C14-C15	1.37(2)
N2-C9	1.50(1)	C15-C16	1.40(1)
N2-C10	1.50(1)		

S1-Mo-S2	87.33(9)	Mo-N2-C10	115.1(5)
S1-Mo-O	101.7(3)	Mo-N2-C11	107.8(5)
S1-Mo-N	164.4(3)	C9-N2-C10	109.4(7)
S1-Mo-N1	81.8(2)	C9-N2-C11	112.7(7)
S1-Mo-N2	85.8(2)	C10-N2-C11	106.9(7)
S2-Mo-O	98.6(3)	S-C-N	178.3(9)
S2-Mo-N	98.1(2)	S1-C1-C2	119.4(8)
S2-Mo-N1	150.6(2)	S1-C1-C6	120.7(7)
S2-Mo-N2	75.3(2)	C2-C1-C6	119.9(9)
O-Mo-N	92.0(4)	C1-C2-C3	118.5(9)
O-Mo-N1	110.4(3)	C2-C3-C4	122(1)
O-Mo-N2	170.2(3)	C3-C4-C5	120(1)
N-Mo-N1	86.5(3)	C4-C5-C6	119(1)
N-Mo-N2	81.5(3)	N1-C6-C1	120.1(8)
N1-Mo-N2	76.7(3)	N1-C6-C5	119.4(9)
Mo-S1-C1	101.3(3)	C1-C6-C5	120.4(9)
Mo-S2-C16	99.9(3)	N1-C8-C9	110.8(8)
Mo-N-C	152.0(8)	N2-C9-C8	109.3(8)
Mo-N1-C6	112.8(6)	N2-C11-C12	123.3(9)
Mo-N1-C7	109.3(6)	N2-C11-C16	117.0(8)
Mo-N1-C8	107.8(5)	C12-C11-C16	119.6(9)
C6-N1-C7	106.9(7)	C11-C12-C13	120(1)
C6-N1-C8	110.8(8)	C12-C13-C14	121(1)
C7-N1-C8	109.3(8)	C13-C14-C15	120(1)
Mo-N2-C9	105.1(5)	C14-C15-C16	120(1)
		S2-C16-C11	120.3(7)
		S2-C16-C15	120.3(9)
		C11-C16-C15	119(1)

Table S15. Anisotropic Displacement Parameters ($Å^2$) for *cis,trans*-MoO(NCS)L.
The anisotropic temperature factor is given by:

$$T = \exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2hka^*b^*U_{12} + 2hla^*c^*U_{13} + 2klb^*c^*U_{23})]$$

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mo	0.0336(3)	0.0435(3)	0.0300(3)	-0.0044(3)	-0.0010(5)	-0.0013(5)
S	0.058(1)	0.046(1)	0.058(1)	-0.011(1)	-0.004(1)	0.005(1)
S1	0.0367(9)	0.046(1)	0.036(1)	-0.004(1)	0.010(1)	0.001(1)
S2	0.045(1)	0.063(1)	0.040(1)	0.004(1)	0.003(1)	-0.015(1)
O	0.053(3)	0.069(3)	0.045(4)	-0.014(3)	-0.022(3)	-0.001(4)
N	0.055(4)	0.051(4)	0.050(5)	-0.014(4)	0.007(4)	0.008(4)
N1	0.030(3)	0.048(4)	0.041(4)	0.000(3)	0.009(3)	0.011(4)
N2	0.032(3)	0.048(4)	0.028(3)	0.008(3)	-0.000(3)	-0.002(3)
C	0.055(5)	0.041(4)	0.023(4)	0.012(4)	0.004(4)	-0.003(4)
C1	0.028(3)	0.041(4)	0.036(4)	-0.003(3)	0.003(5)	-0.001(5)
C2	0.048(4)	0.047(4)	0.029(6)	-0.012(4)	0.001(4)	-0.000(4)
C3	0.052(5)	0.044(5)	0.09(1)	-0.005(4)	-0.002(6)	0.004(5)
C4	0.042(5)	0.055(5)	0.070(7)	0.011(4)	0.010(5)	-0.004(6)
C5	0.039(4)	0.054(5)	0.062(6)	0.000(4)	0.013(5)	-0.005(6)
C6	0.038(4)	0.039(4)	0.035(4)	-0.010(4)	-0.004(4)	0.003(4)
C7	0.035(4)	0.058(5)	0.089(7)	-0.006(5)	0.021(5)	0.022(6)
C8	0.054(5)	0.069(5)	0.036(5)	0.014(5)	0.019(4)	0.016(5)
C9	0.048(4)	0.070(5)	0.020(4)	0.011(5)	0.000(4)	-0.004(5)
C10	0.044(4)	0.060(5)	0.045(5)	0.005(5)	-0.011(5)	0.009(6)
C11	0.033(4)	0.047(4)	0.031(4)	0.003(4)	-0.001(4)	0.001(5)
C12	0.050(5)	0.068(6)	0.055(6)	0.001(5)	-0.026(5)	-0.002(5)
C13	0.045(5)	0.065(6)	0.100(9)	-0.008(5)	-0.011(6)	0.005(7)
C14	0.044(5)	0.096(8)	0.078(7)	-0.020(5)	-0.005(6)	0.002(7)
C15	0.039(4)	0.088(6)	0.049(5)	0.011(4)	0.011(7)	0.003(9)
C16	0.035(4)	0.058(5)	0.034(5)	0.006(4)	0.001(4)	0.002(4)

Table S16. Hydrogen Atom Coordinates and their Isotropic Displacement Parameters (Å2) for *cis,trans*-MoO(NCS)L.

All H-atoms were placed in idealized positions and refined using the riding model with an isotropic temperature factor assigned.

Atom	x	y	z	Uiso
H2	0.146	0.442	-0.127	5.0
H3	0.076	0.557	0.012	5.0
H4	0.012	0.490	0.243	5.0
H5	0.012	0.305	0.318	5.0
H7a	0.014	0.038	0.253	6.3
H7b	0.008	0.086	0.052	6.3
H7c	-0.008	0.158	0.224	6.3
H8a	0.095	0.054	0.426	5.0
H8b	0.083	0.178	0.468	5.0
H9a	0.177	0.217	0.348	5.0
H9b	0.182	0.142	0.523	5.0
H10a	0.236	-0.029	0.493	5.1
H10b	0.221	-0.100	0.318	5.1
H10c	0.171	-0.062	0.450	5.1
H12	0.281	0.192	0.446	5.0
H13	0.375	0.242	0.335	5.0
H14	0.411	0.170	0.057	5.0
H15	0.353	0.050	-0.115	5.0

Table S17. Final Fractional Atomic Coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for C_i-(MoOL)$_2$(μ-O).CH_2Cl_2; e.s.d. values are given in parentheses.

Atom	x	y	z	B_{eq}[a]
Mo	0.05784(7)	-0.06958(4)	0.09204(3)	2.61(1)
S1	0.0321(3)	0.0524(1)	0.1794(1)	3.45(4)
S2	0.0096(2)	-0.2072(1)	0.0133(1)	3.79(4)
O1	0.2551(6)	-0.0836(4)	0.1027(3)	3.7(1)
O2	0.000	0.000	0.000	2.8(1)
N1	0.0495(7)	-0.1480(4)	0.2097(3)	2.9(1)
N2	-0.2270(7)	-0.0970(4)	0.0879(3)	2.9(1)
C1	0.0652(9)	-0.0004(5)	0.2743(4)	3.2(2)
C2	0.086(1)	0.0502(5)	0.3434(5)	4.4(2)
C3	0.117(1)	0.0119(6)	0.4192(5)	5.0(2)
C4	0.123(1)	-0.0778(6)	0.4262(5)	4.6(2)
C5	0.0990(9)	-0.1294(5)	0.3585(4)	3.7(2)
C6	0.0735(9)	-0.0920(5)	0.2829(4)	3.2(2)
C7	0.1751(9)	-0.2173(5)	0.2195(5)	4.2(2)
C8	-0.1056(9)	-0.1922(5)	0.2010(4)	3.4(2)
C9	-0.2383(8)	-0.1262(5)	0.1715(4)	3.3(2)
C10	-0.3145(8)	-0.0126(5)	0.0699(5)	3.7(2)
C11	-0.2957(8)	-0.1638(5)	0.0296(4)	3.1(2)
C12	-0.456(1)	-0.1762(6)	0.0128(5)	4.5(2)
C13	-0.523(1)	-0.2376(7)	-0.0425(6)	5.9(3)
C14	-0.426(1)	-0.2888(7)	-0.0818(6)	6.1(2)
C15	-0.268(1)	-0.2776(6)	-0.0646(5)	4.7(2)
C16	-0.1989(9)	-0.2155(5)	-0.0095(4)	3.5(2)
C21	0.465(2)	0.153(1)	0.297(1)	6.0(4)*
C22	0.543(2)	0.122(2)	0.373(1)	6.8(5)*
C23	0.626(3)	0.040(2)	0.360(2)	8.7(7)*
C24	0.547(3)	0.011(2)	0.285(1)	7.9(6)*
C25	0.497(3)	0.087(2)	0.245(2)	7.1(5)*

* Atoms were refined isotropically.

[a] $B_{eq} = (4/3)\Sigma\Sigma B_{ij}\ \mathbf{a}_i.\mathbf{a}_j$

Table S18. Interatomic Distances (Å) and Angles (°) for C_i-(MoOL)$_2$(μ-O).CH_2Cl_2.

Mo-S1	2.398(2)	C2-C3	1.38(1)
Mo-S2	2.469(2)	C3-C4	1.37(1)
Mo-O1	1.685(5)	C4-C5	1.37(1)
Mo-O2	1.8665(6)	C5-C6	1.37(1)
Mo-O2	1.8665(6)	C8-C9	1.53(1)
Mo-N1	2.320(6)	C11-C12	1.37(1)
Mo-N2	2.470(6)	C11-C16	1.39(1)
S1-C1	1.762(7)	C12-C13	1.37(1)
S2-C16	1.768(8)	C13-C14	1.39(1)
N1-C6	1.479(9)	C14-C15	1.35(1)
N1-C7	1.494(9)	C15-C16	1.38(1)
N1-C8	1.48(1)	C21-C22	1.41(3)
N2-C9	1.493(9)	C21-C25	1.38(3)
N2-C10	1.490(9)	C22-C23	1.48(4)
N2-C11	1.460(9)	C23-C24	1.39(3)
C1-C2	1.38(1)	C24-C25	1.37(3)
C1-C6	1.40(1)		

S1-Mo-S2	163.15(8)	Mo-N2-C10	108.8(4)
S1-Mo-O1	103.4(2)	Mo-N2-C11	114.6(4)
S1-Mo-O2	91.75(5)	C9-N2-C10	109.4(6)
S1-Mo-N1	81.6(1)	C9-N2-C11	109.8(6)
S1-Mo-N2	87.1(2)	C10-N2-C11	109.4(6)
S2-Mo-O1	91.2(2)	S1-C1-C2	119.0(6)
S2-Mo-O2	92.29(6)	S1-C1-C6	122.8(6)
S2-Mo-N1	89.7(2)	C2-C1-C6	118.1(7)
S2-Mo-N2	76.7(1)	C1-C2-C3	121.1(8)
O1-Mo-O2	106.0(2)	C2-C3-C4	119.8(9)
O1-Mo-N1	91.5(2)	C3-C4-C5	120.1(8)
O1-Mo-N2	162.5(2)	C4-C5-C6	120.6(8)
O2-Mo-N1	162.4(2)	N1-C6-C1	119.3(6)
O2-Mo-N2	87.4(1)	N1-C6-C5	120.5(7)
N1-Mo-N2	76.0(2)	C1-C6-C5	120.2(7)
Mo-S1-C1	100.7(3)	N1-C8-C9	110.0(6)
Mo-S2-C16	104.1(3)	N2-C9-C8	109.3(6)
Mo-O2-Mo	180	N2-C11-C12	120.4(7)
Mo-N1-C6	113.1(4)	N2-C11-C16	120.3(7)
Mo-N1-C7	108.9(4)	C12-C11-C16	119.3(7)
Mo-N1-C8	108.2(4)	C11-C12-C13	121.3(9)
C6-N1-C7	108.8(6)	C12-C13-C14	119.2(9)
C6-N1-C8	109.5(6)	C13-C14-C15	119.7(9)
C7-N1-C8	108.2(6)	C14-C15-C16	121.7(9)
Mo-N2-C9	104.6(4)	S2-C16-C11	121.6(6)

S2-C16-C15	119.5(7)	C22-C23-C24	103.(2)
C11-C16-C15	118.8(8)	C23-C24-C25	104.(2)
C22-C21-C25	103.(2)	C21-C25-C24	113.(2)
C21-C22-C23	108.(2)		

Table S19. AnisotropicDisplacement Parameters ($Å^2$) for *Ci*-$(MoOL)_2(\mu\text{-}O).CH_2Cl_2$.
The anisotropic temperature factor is given by:

$$T = \exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2hka^*b^*U_{12} + 2hla^*c^*U_{13} + 2klb^*c^*U_{23})]$$

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mo	0.0350(3)	0.0348(3)	0.0299(3)	0.0030(3)	0.0076(2)	0.0031(3)
S1	0.062(1)	0.0316(9)	0.0372(9)	0.0013(8)	0.0078(8)	0.0037(8)
S2	0.049(1)	0.047(1)	0.049(1)	0.0085(9)	0.0104(8)	-0.0115(9)
O1	0.038(3)	0.057(3)	0.046(3)	0.005(2)	0.008(2)	0.004(2)
O2	0.045(4)	0.034(3)	0.028(3)	-0.001(3)	0.008(3)	0.003(3)
N1	0.046(3)	0.029(3)	0.034(3)	0.005(3)	0.008(2)	0.003(3)
N2	0.035(3)	0.037(3)	0.038(3)	0.004(3)	0.008(2)	0.001(3)
C1	0.049(4)	0.037(4)	0.035(3)	-0.002(3)	0.008(3)	0.004(3)
C2	0.085(6)	0.040(4)	0.044(4)	-0.000(4)	0.016(4)	-0.002(4)
C3	0.086(6)	0.067(5)	0.038(4)	-0.011(5)	0.016(4)	-0.009(4)
C4	0.079(6)	0.065(5)	0.032(4)	-0.005(5)	0.011(4)	0.010(4)
C5	0.058(5)	0.046(4)	0.035(4)	0.003(4)	0.006(3)	0.012(3)
C6	0.046(4)	0.040(4)	0.035(3)	0.002(3)	0.007(3)	0.001(3)
C7	0.063(5)	0.045(4)	0.049(4)	0.024(4)	0.010(4)	0.009(4)
C8	0.060(4)	0.033(4)	0.036(3)	-0.002(3)	0.015(3)	0.004(3)
C9	0.045(4)	0.043(4)	0.041(4)	-0.002(3)	0.016(3)	0.002(3)
C10	0.039(4)	0.046(4)	0.056(4)	0.013(3)	0.010(3)	0.006(4)
C11	0.037(4)	0.042(4)	0.040(4)	-0.001(3)	0.004(3)	0.004(3)
C12	0.052(5)	0.056(5)	0.063(5)	-0.004(4)	0.006(4)	-0.003(4)
C13	0.051(5)	0.075(6)	0.088(7)	-0.016(5)	-0.011(5)	-0.004(6)
C14	0.096(7)	0.067(6)	0.063(5)	-0.019(6)	-0.009(5)	-0.019(5)
C15	0.062(5)	0.058(5)	0.053(4)	-0.002(5)	-0.003(4)	-0.017(4)
C16	0.049(4)	0.044(4)	0.039(4)	0.000(4)	0.003(3)	-0.003(3)

Table S20. Hydrogen Atom Coordinates and their Isotropic Displacement Parameters ($Å^2$) for C_i-(MoOL)$_2$(μ-O).CH_2Cl_2.

All H-atoms were placed in idealized positions and refined using the riding model with an isotropic temperature factor assigned.

Atom	x	y	z	Uiso
H2	0.080	0.113	0.339	5.0
H3	0.134	0.048	0.466	5.0
H4	0.141	-0.104	0.478	5.0
H5	0.102	-0.192	0.364	5.0
H7a	0.169	-0.249	0.170	5.0
H7b	0.160	-0.257	0.261	5.0
H7c	0.276	-0.191	0.233	5.0
H8a	-0.120	-0.215	0.252	5.0
H8b	-0.111	-0.239	0.163	5.0
H9a	-0.338	-0.153	0.171	5.0
H9b	-0.227	-0.077	0.207	5.0
H10a	-0.421	-0.021	0.078	5.0
H10b	-0.266	0.032	0.105	5.0
H10c	-0.314	0.004	0.015	5.0
H12	-0.523	-0.142	0.040	5.0
H13	-0.635	-0.245	-0.055	5.0
H14	-0.470	-0.331	-0.121	5.0
H15	-0.202	-0.313	-0.092	5.0

Table S21. Final Fractional Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for C_1-(MoOL)$_2$(μ-O).thf; e.s.d. values are given in parentheses.

Atom	x	y	z	B_{eq}[a]
Mo1	0.10262(3)	0.12905(2)	0.07543(3)	2.629(8)
Mo2	-0.17160(3)	0.16964(2)	0.11792(3)	2.903(8)
S1	0.28479(9)	0.12886(6)	0.0448(1)	3.47(3)
S2	0.1985(1)	0.17227(6)	0.2503(1)	3.84(3)
S3	-0.0905(1)	0.13681(7)	0.3021(1)	4.02(3)
S4	-0.2856(1)	0.18124(6)	-0.0776(1)	3.96(3)
O1	0.0986(3)	0.0622(2)	0.1013(3)	3.79(8)
O2	-0.0416(2)	0.1499(1)	0.0866(2)	2.98(7)
O3	-0.1680(3)	0.2371(2)	0.1336(3)	4.21(8)
N1	0.0436(3)	0.1288(2)	-0.1097(3)	3.10(9)
N2	0.1142(3)	0.2250(2)	0.0275(3)	3.03(8)
N3	-0.3327(3)	0.1655(2)	0.1718(3)	3.59(9)
N4	-0.2472(3)	0.0775(2)	0.0631(3)	3.16(9)
C1	0.2417(4)	0.1081(2)	-0.0936(4)	3.3(1)
C2	0.3218(4)	0.0890(2)	-0.1417(4)	4.3(1)
C3	0.2888(5)	0.0725(3)	-0.2501(5)	5.2(1)
C4	0.1786(5)	0.0744(3)	-0.3139(5)	5.9(2)
C5	0.0986(5)	0.0937(3)	-0.2681(4)	4.8(1)
C6	0.1292(4)	0.1092(2)	-0.1595(4)	3.5(1)
C7	-0.0580(4)	0.0932(2)	-0.1444(4)	3.8(1)
C8	0.0088(4)	0.1856(2)	-0.1486(4)	3.7(1)
C9	0.1005(4)	0.2252(2)	-0.0924(4)	3.6(1)
C10	0.0269(4)	0.2609(2)	0.0474(4)	3.8(1)
C11	0.2209(4)	0.2473(2)	0.0982(4)	3.3(1)
C12	0.2743(4)	0.2898(2)	0.0624(5)	4.0(1)
C13	0.3696(5)	0.3126(3)	0.1358(5)	4.9(1)
C14	0.4090(4)	0.2943(3)	0.2415(5)	5.0(1)
C15	0.3579(4)	0.2513(2)	0.2773(4)	4.1(1)
C16	0.2638(4)	0.2271(2)	0.2046(4)	3.4(1)
C21	-0.2030(4)	0.1453(3)	0.3567(4)	4.0(1)
C22	-0.1848(5)	0.1365(3)	0.4690(5)	5.7(2)
C23	-0.2680(6)	0.1417(4)	0.5156(5)	6.9(2)
C24	-0.3753(5)	0.1539(3)	0.4497(5)	6.5(2)
C25	-0.3968(5)	0.1619(3)	0.3381(5)	5.2(1)
C26	-0.3104(4)	0.1577(2)	0.2904(4)	3.8(1)
C27	-0.3993(4)	0.2168(2)	0.1353(5)	4.5(1)
C28	-0.4023(4)	0.1194(2)	0.1116(5)	4.0(1)
C29	-0.3314(4)	0.0695(2)	0.1240(4)	3.9(1)
C30	-0.1557(4)	0.0367(2)	0.1025(4)	3.7(1)
C31	-0.3036(4)	0.0704(2)	-0.0557(4)	3.4(1)
C32	-0.3378(5)	0.0192(3)	-0.0987(5)	4.7(1)
C33	-0.3904(5)	0.0117(3)	-0.2087(5)	6.1(2)
C34	-0.4070(5)	0.0561(3)	-0.2779(5)	5.8(2)
C35	-0.3752(4)	0.1069(3)	-0.2375(5)	4.8(1)
C36	-0.3234(4)	0.1153(2)	-0.1259(4)	3.8(1)
Cl50	-0.6627(3)	0.0437(2)	-0.5295(3)	19.7(2)
Cl52	-0.8820(4)	0.0029(2)	-0.5957(3)	19.8(2)
C51	-0.7895(9)	0.0409(5)	-0.6209(8)	13.8(4)

[a] $B_{eq} = (4/3)\Sigma\Sigma B_{ij}\ \mathbf{a}_i.\mathbf{a}_j$

Table S22. Interatomic Distances (Å) and Angles (°) for C_1-(MoOL)2(μ-O).thf.

Mo1-S1	2.431(1)	N4-C31	1.467(7)
Mo1-S2	2.423(1)	C1-C2	1.409(7)
Mo1-O1	1.686(4)	C1-C6	1.398(8)
Mo1-O2	1.926(3)	C2-C3	1.373(9)
Mo1-N1	2.240(4)	C3-C4	1.368(9)
Mo2-S3	2.388(2)	C4-C5	1.389(9)
Mo2-S4	2.472(2)	C5-C6	1.369(8)
Mo2-O2	1.857(3)	C8-C9	1.509(8)
Mo2-O3	1.674(4)	C11-C12	1.393(8)
Mo2-N3	2.326(4)	C11-C16	1.384(8)
S1-C1	1.751(6)	C12-C13	1.387(9)
S2-C16	1.771(6)	C13-C14	1.36(1)
S3-C21	1.766(6)	C14-C15	1.387(9)
S4-C36	1.751(6)	C15-C16	1.387(7)
N1-C6	1.486(6)	C21-C22	1.392(8)
N1-C7	1.495(6)	C21-C26	1.382(8)
N1-C8	1.506(7)	C22-C23	1.36(1)
N2-C9	1.480(7)	C23-C24	1.38(1)
N2-C10	1.488(6)	C24-C25	1.37(1)
N2-C11	1.468(7)	C25-C26	1.399(8)
N3-C26	1.460(7)	C28-C29	1.497(8)
N3-C27	1.508(7)	C31-C32	1.390(8)
N3-C28	1.491(7)	C31-C36	1.396(8)
N4-C29	1.502(6)	C32-C33	1.362(9)
N4-C30	1.489(6)	C33-C34	1.38(1)
C34-C35	1.37(1)	C150-C51	1.65(1)
C35-C36	1.381(8)	C152-C51	1.60(1)

S1-Mo1-S2	85.73(5)	Mo1-N1-C6	113.8(3)
S1-Mo1-O1	96.6(1)	Mo1-N1-C7	106.5(3)
S1-Mo1-O2	164.0(1)	Mo1-N1-C8	108.1(3)
S1-Mo1-N1	81.5(1)	C6-N1-C7	110.1(4)
S2-Mo1-O1	106.7(1)	C6-N1-C8	109.7(4)
S2-Mo1-O2	91.4(1)	C7-N1-C8	108.5(4)
S2-Mo1-N1	151.1(1)	C9-N2-C10	108.5(4)
O1-Mo1-O2	99.3(2)	C9-N2-C11	115.0(4)
O1-Mo1-N1	100.5(2)	C10-N2-C11	104.5(4)
O2-Mo1-N1	93.9(1)	Mo2-N3-C26	113.9(3)
S3-Mo2-S4	164.64(6)	Mo2-N3-C27	108.7(3)
S3-Mo2-O2	89.3(1)	Mo2-N3-C28	107.7(3)
S3-Mo2-O3	103.4(2)	C26-N3-C27	109.8(4)
S3-Mo2-N3	80.8(1)	C26-N3-C28	109.0(5)
S4-Mo2-O2	94.9(1)	C27-N3-C28	107.5(4)
S4-Mo2-O3	89.5(1)	C29-N4-C30	109.2(4)
S4-Mo2-N3	91.1(1)	C29-N4-C31	109.0(4)
O2-Mo2-O3	107.1(2)	C30-N4-C31	110.0(4)
O2-Mo2-N3	161.8(2)	S1-C1-C2	119.8(4)
O3-Mo2-N3	90.1(2)	S1-C1-C6	122.5(4)
Mo1-S1-C1	98.6(2)	C2-C1-C6	117.7(5)
Mo1-S2-C16	100.5(2)	C1-C2-C3	120.2(6)
Mo2-S3-C21	101.4(2)	C2-C3-C4	121.3(6)
Mo2-S4-C36	104.7(2)	C3-C4-C5	119.3(6)
Mo1-O2-Mo2	172.3(2)	C4-C5-C6	120.4(6)
N1-C6-C1	118.4(5)	C22-C23-C24	119.4(7)
N1-C6-C5	120.5(5)	C23-C24-C25	120.0(6)

Table S22, contd. Interatomic Distances (Å) and Angles (°) for C_1-(MoOL)$_2$(μ-O).thf.

C1-C6-C5	121.0(5)	C24-C25-C26	120.5(7)
N1-C8-C9	110.3(4)	N3-C26-C21	119.8(5)
N2-C9-C8	108.3(4)	N3-C26-C25	120.9(5)
N2-C11-C12	121.3(5)	C21-C26-C25	119.3(6)
N2-C11-C16	118.0(5)	N3-C28-C29	109.8(4)
C12-C11-C16	120.7(5)	N4-C29-C28	109.1(5)
C11-C12-C13	119.0(6)	N4-C31-C32	120.2(5)
C12-C13-C14	120.3(6)	N4-C31-C36	119.9(5)
C13-C14-C15	121.1(6)	C32-C31-C36	119.8(5)
C14-C15-C16	119.6(6)	C31-C32-C33	121.4(7)
S2-C16-C11	121.1(4)	C32-C33-C34	118.4(7)
S2-C16-C15	119.6(5)	C33-C34-C35	121.3(7)
C11-C16-C15	119.3(5)	C34-C35-C36	120.9(7)
S3-C21-C22	119.3(5)	S4-C36-C31	122.5(4)
S3-C21-C26	122.0(5)	S4-C36-C35	119.3(5)
C22-C21-C26	118.6(6)	C31-C36-C35	118.2(6)
C21-C22-C23	122.1(7)	C150-C51-C152	118.7(8)

Table S23. Anisotropic Displacement Parameters ($Å^2$) for C_1-(MoOL)$_2$(μ-O).thf.
The anisotropic temperature factor is given by:

$$T = \exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2hka^*b^*U_{12} + 2hla^*c^*U_{13} + 2klb^*c^*U_{23})]$$

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mo1	0.0306(2)	0.0341(2)	0.0353(2)	0.0020(2)	0.0103(1)	0.0012(2)
Mo2	0.0327(2)	0.0363(2)	0.0433(2)	0.0014(2)	0.0146(1)	-0.0007(2)
S1	0.0318(5)	0.0500(8)	0.0503(6)	0.0005(5)	0.0130(4)	-0.0064(6)
S2	0.0562(7)	0.0508(8)	0.0378(6)	-0.0087(6)	0.0130(5)	-0.0040(6)
S3	0.0400(6)	0.0668(9)	0.0438(6)	-0.0004(6)	0.0097(5)	0.0015(7)
S4	0.0470(6)	0.0514(8)	0.0494(7)	0.0110(6)	0.0112(5)	0.0101(6)
O1	0.045(2)	0.037(2)	0.061(2)	0.002(2)	0.014(1)	0.006(2)
O2	0.038(1)	0.034(2)	0.044(2)	0.005(1)	0.017(1)	0.008(1)
O3	0.057(2)	0.038(2)	0.071(2)	0.002(2)	0.030(1)	-0.004(2)
N1	0.036(2)	0.045(2)	0.036(2)	-0.001(2)	0.011(1)	0.001(2)
N2	0.034(2)	0.037(2)	0.047(2)	0.002(2)	0.016(1)	0.003(2)
N3	0.034(2)	0.053(3)	0.051(2)	0.009(2)	0.016(1)	0.001(2)
N4	0.031(2)	0.042(2)	0.050(2)	0.001(2)	0.016(1)	0.001(2)
C1	0.043(2)	0.035(3)	0.052(2)	-0.004(2)	0.023(2)	-0.004(2)
C2	0.052(2)	0.053(3)	0.069(3)	-0.008(2)	0.035(2)	-0.005(3)
C3	0.072(3)	0.071(4)	0.074(3)	-0.005(3)	0.048(2)	-0.011(3)
C4	0.092(3)	0.095(5)	0.050(3)	-0.012(4)	0.039(2)	-0.018(3)
C5	0.061(3)	0.077(4)	0.047(3)	-0.002(3)	0.019(2)	-0.003(3)
C6	0.050(2)	0.043(3)	0.043(2)	0.001(2)	0.022(2)	0.002(2)
C7	0.035(2)	0.060(3)	0.045(3)	-0.004(2)	0.006(2)	-0.005(3)
C8	0.049(2)	0.050(3)	0.040(2)	0.008(2)	0.010(2)	0.011(2)
C9	0.047(2)	0.044(3)	0.048(2)	0.004(2)	0.017(2)	0.010(2)
C10	0.046(2)	0.036(3)	0.066(3)	0.005(2)	0.020(2)	0.003(2)
C11	0.039(2)	0.039(3)	0.051(2)	-0.001(2)	0.018(2)	-0.007(2)
C12	0.047(2)	0.039(3)	0.070(3)	-0.001(2)	0.021(2)	0.001(3)
C13	0.053(3)	0.048(3)	0.092(4)	-0.010(3)	0.030(2)	-0.004(3)
C14	0.042(3)	0.059(4)	0.085(4)	-0.014(3)	0.017(2)	-0.028(3)
C15	0.044(2)	0.056(3)	0.053(3)	-0.001(2)	0.012(2)	-0.015(3)
C16	0.041(2)	0.041(3)	0.049(2)	0.001(2)	0.017(2)	-0.009(2)
C21	0.053(3)	0.057(3)	0.043(2)	-0.009(3)	0.015(2)	-0.004(3)
C22	0.069(3)	0.098(5)	0.048(3)	-0.014(3)	0.019(2)	0.011(3)
C23	0.094(4)	0.124(7)	0.052(3)	-0.016(4)	0.034(2)	0.007(4)
C24	0.090(3)	0.106(6)	0.076(3)	-0.005(4)	0.059(2)	-0.003(4)
C25	0.057(3)	0.078(5)	0.076(3)	0.006(3)	0.038(2)	0.003(3)
C26	0.050(2)	0.049(3)	0.050(2)	0.001(2)	0.023(2)	-0.001(2)
C27	0.050(2)	0.055(4)	0.072(3)	0.014(2)	0.027(2)	0.004(3)
C28	0.037(2)	0.056(3)	0.061(3)	-0.002(2)	0.020(2)	-0.005(3)
C29	0.044(2)	0.055(3)	0.054(3)	-0.011(2)	0.021(2)	0.000(3)
C30	0.041(2)	0.036(3)	0.062(3)	0.001(2)	0.013(2)	0.004(3)
C31	0.035(2)	0.049(3)	0.044(2)	-0.001(2)	0.011(2)	-0.009(2)
C32	0.062(3)	0.054(4)	0.063(3)	-0.003(3)	0.019(2)	-0.010(3)
C33	0.074(4)	0.078(4)	0.074(4)	-0.008(3)	0.016(3)	-0.035(3)
C34	0.059(3)	0.103(5)	0.050(3)	0.010(3)	0.004(3)	-0.021(3)
C35	0.049(3)	0.080(4)	0.047(3)	0.016(3)	0.007(2)	-0.004(3)
C36	0.032(2)	0.063(3)	0.048(3)	0.010(2)	0.011(2)	-0.005(3)
Cl50	0.168(3)	0.407(5)	0.130(2)	0.070(3)	-0.018(2)	-0.127(2)
Cl52	0.411(5)	0.180(3)	0.187(3)	-0.133(3)	0.131(3)	-0.071(3)
C51	0.30(1)	0.116(8)	0.090(6)	-0.042(9)	0.042(7)	0.015(6)

Table S24. Hydrogen Atom Coordinates and their Isotropic Displacement Parameters (Å^2) for C_1-(MoOL)$_2$(μ-O).thf.

All H-atoms were placed in idealized positions and refined using the riding model with an isotropic temperature factor assigned.

Atom	x	y	z	Uiso
H2	0.399	0.088	-0.099	5.0
H3	0.343	0.059	-0.281	5.0
H4	0.157	0.063	-0.389	5.0
H5	0.022	0.096	-0.312	5.0
H7a	-0.110	0.104	-0.108	5.0
H7b	-0.036	0.057	-0.125	5.0
H7c	-0.092	0.096	-0.222	5.0
H8a	-0.057	0.195	-0.131	5.0
H8b	-0.006	0.187	-0.226	5.0
H9a	0.169	0.215	-0.104	5.0
H9b	0.080	0.261	-0.121	5.0
H10a	-0.045	0.251	0.001	5.0
H10b	0.041	0.297	0.033	5.0
H10c	0.029	0.257	0.122	5.0
H12	0.245	0.303	-0.011	5.0
H13	0.409	0.341	0.112	5.0
H14	0.473	0.311	0.292	5.0
H15	0.386	0.239	0.351	5.0
H22	-0.112	0.126	0.513	5.0
H23	-0.253	0.139	0.593	5.0
H24	-0.436	0.155	0.480	5.0
H25	-0.470	0.171	0.292	5.0
H27a	-0.471	0.213	0.144	5.0
H27b	-0.407	0.223	0.059	5.0
H27c	-0.361	0.246	0.179	5.0
H28a	-0.430	0.128	0.035	5.0
H28b	-0.463	0.113	0.140	5.0
H29a	-0.293	0.064	0.200	5.0
H29b	-0.377	0.039	0.095	5.0
H30a	-0.107	0.048	0.172	5.0
H30b	-0.115	0.034	0.051	5.0
H30c	-0.187	0.002	0.110	5.0
H32	-0.328	-0.011	-0.049	5.0
H33	-0.412	-0.024	-0.237	5.0
H34	-0.441	0.051	-0.355	5.0
H35	-0.388	0.137	-0.287	5.0
H51A	-0.780	0.029	-0.688	5.0
H51B	-0.818	0.077	-0.630	5.0

Table S25. Electronic Spectra of MoOXL and $(MoOL)_2(m\text{-}O)$

X	isomer	solvent	λ_{max}, nm (log ε)
Cl	*cis,cis*	MeCN	370 (3.46), 425 sh, 570 (3.41), 675 sh,
	cis,trans		373 (3.50), 387sh, 623 (3.60)
Br	*cis,cis*[a]	THF	372 (3.54), 420 sh, 603 (3.42), 665 sh
	cis,trans	CH_2Cl_2	331 (3.58), 378 (3.53), 425 sh, 643 (3.62)
NCS	*cis,cis*	MeCN	370 sh, 417 (3.69), 593 (3.54), 700 sh
	cis.trans		400 (3.68), 455 sh, 660 (3.70)
OMe	*cis,cis*	THF	357 (3.53), 486 (3.35), 575 sh
$OSiMe_3$	*cis,trans*	MeCN	373 (3.55), 387 sh, 509 (3.42)
OPh		CH_2Cl_2	375 (3.70), 5.74 (3.61)
SPh		CH_2Cl_2	365 (3.80), 386 sh, 645 (3.65)
C_i -$(MoOL)_2(\mu\text{-}O)$		MeCN	394 (3.7), 562 (3.8), 750 (3.1)
C_1 -$(MoOL)_2(\mu\text{-}O)$		CH_2Cl_2	391 (3.7), 565 (3.9), 745 (3.0)

[a] Sample is analytically pure but contains ca. 15% of *cis,trans* form

Table S26. EPR data for MoOXL[a]

X	isomer	g	a(Mo)	g_1	g_2	g_3	A_1(Mo)	a(Br)	a(O)
Cl	*cis,cis*	1.971	37.6	2.012	1.961	1.957	59.2		
	cis,trans	1.968	38.0	2.007	1.960	1.949	60.5		
Br	*cis,cis*	1.982	36.4					5.0	
	cis,trans	1.980	37.1					5.2	
NCS	*cis,cis*	1.971	36.4	2.006	1.962	1.956	56.8		
	cis,trans	1.966	36.6	1.996	1.960	1.949	57.5		
OMe	*cis,cis*	1.963	38.5	1.999	1.957	1.947	60.8		
OEt		1.962	38.1	1.998	1.957	1.947	60.5		
$OSiMe_3$	*cis,trans*	1.949	41.1	1.975	1.944	1.938	62.8		
OPh		1.959	39.1	1.988	1.953	1.943	59.5[b]		4.9[c]
SPh		1.979	33.3	2.023	1.966	1.960	53.7		

[a] Isotropic parameters estimated from solutions in THF or CH_2Cl_2. Anisotropic parameters estimated from frozen solutions (77 K) in THF:MeCN (10:1 v:v), 0.01-0.1 Bu_4NBF_4. Hyperfine coupling constants in units of 10^{-4} cm^{-1}. [b.] A_2(Mo), 33.5 x 10^{-4} cm^{-1}. [c] phenolic oxygen.

SUPPLEMENTARY FIGURES

Figure S1. Experimental and simulated mass spectra for $[MoOClL]^+$.

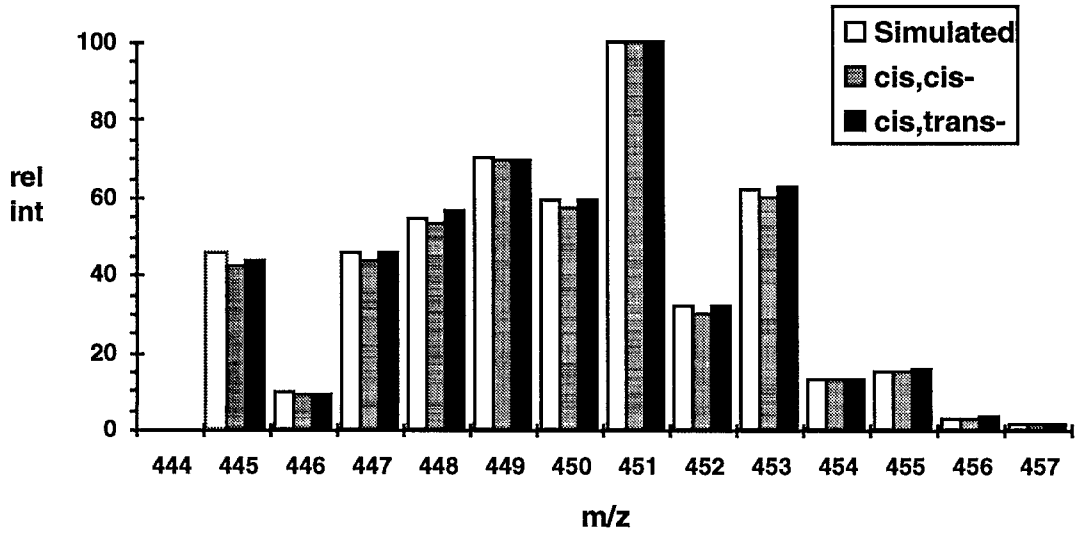

Figure S2. Infrared spectra of MoOClL: (a) *cis,trans*; (b) *cis,cis*.