Supplementary material (ESI) for Dalton Transactions

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S U P P L E M E N T A R Y M A T E R I A L

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O,S-Donor Ligands as Inhibitors of Xantine Oxidase. Synthesis, Molybdenum Complexation and Enzyme Inhibition

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C o n t e n t s

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Table S1 - Global stability constants (log β) for the species formed in the H^+-MoO_4^{2-} system.

Equilibrium	Formed Species	log β
$MoO_4^{2-} + H^+ \rightleftharpoons HMoO_4^-$	$HMoO_4^-$	4.46(2)[a] 4.03 (6)[b] 4.00[c]
$MoO_4^{2-} + 2H^+ \rightleftharpoons H_2MoO_4$	H_2MoO_4	7.20(9)[a] 6.7(4)[b] 7.50[c]
$7MoO_4^{2-} + 8H^+ \rightleftharpoons H_8(MoO_4)_7^{6-}$	$H_8(MoO_4)_7^{6-}$	55.27(3)[a] 53.18(5)[b] 57.699[c]
$7MoO_4^{2-} + 9H^+ \rightleftharpoons H_9(MoO_4)_7^{5-}$	$H_9(MoO_4)_7^{5-}$	60.07(3)[a] 58.10(2)[b] 62.140[c]
$7MoO_4^{2-} + 10H^+ \rightleftharpoons H_{10}(MoO_4)_7^{4-}$	$H_{10}(MoO_4)_7^{4-}$	65.31(3)[a] 62.11(3)[b] 65.595[c]
$7MoO_4^{2-} + 11H^+ \rightleftharpoons H_{11}(MoO_4)_7^{3-}$	$H_{11}(MoO_4)_7^{3-}$	66.78(9)[a] 64.54(7)[b] 68.344[c]

[a] this work (I = 0.1 M KCl, T = 25.0 ± 0.1 °C, in 15% (v/v) CH_3OH/H_2O; [b] ref. 1 (I = 0.2 M KCl, T = 25.0 ± 0.1 °C, in water); [c] ref. 2 (I = 3 M $NaClO_4$)

[1] Farkas E, Csóka H, Micera G, Dessi A, J. Inorg. Biochem. 1997, 65, 281-286.
[2] Petersson L, Andersson I, Őhman L-O, Acta Chem. Scand.A 1985, 39, 53-58.

Figure S2 - Cyclic voltammogram of $MoO_2(thiomaltol)_2$ in 20% (v/v) DMSO (I=0.1 M KNO_3, scan rate = 100 mV s^{-1}, pH = 4.7)

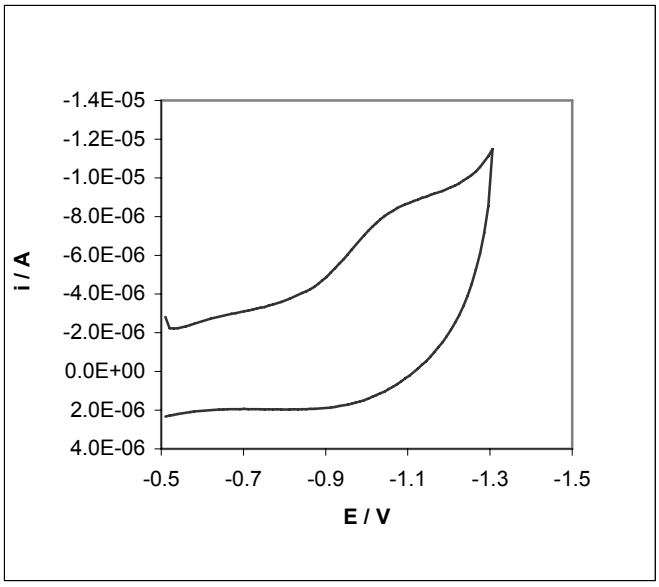

Table S3 - Crystal Data and Details of the Structure Determination for: **Compound *α*-1**

Crystal Data

Formula	C12 H10 Mo2 O9 S2
Formula Weight	554.22
Crystal System	Monoclinic
Space group	C2/c (No. 15)
a, b, c [Angstrom]	31.3625(3) 8.8600(1) 12.3099(1)
alpha, beta, gamma [deg]	90 108.7833(6) 90
V [Ang**3]	3238.40(6)
Z	8
D(calc) [g/cm**3]	2.273
Mu(MoKa) [/mm]	1.853
F(000)	2160
Crystal Size [mm]	0.05 x 0.13 x 0.13

Data Collection

Temperature (K)	173
Radiation [Angstrom]	MoKa 0.71073
Theta Min-Max [Deg]	1.4, 25.3
Dataset	-37: 37 ; -10: 10 ; -14: 14
Tot., Uniq. Data, R(int)	37862, 2966, 0.044
Observed data [I > 2.0 sigma(I)]	2682

Refinement

Nref, Npar	2966, 266
R, wR2, S	0.0204, 0.0476, 1.06
w = 1/[\s^2^(Fo^2^)+(0.0167P)^2^+7.8083P] where P=(Fo^2^+2Fc^2^)/3	
Max. and Av. Shift/Error	0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]	-0.42, 0.35

Table S4 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: **Compound *α*-1**

Atom	x	y	z	U(eq) [Ang^2]
Mo1	0.08994(1)	0.63263(2)	0.09450(2)	0.0173(1)
Mo2	0.16212(1)	0.89080(3)	0.17615(2)	0.0179(1)
S1	0.06601(2)	0.53501(7)	0.25437(6)	0.0205(2)
S2	0.17941(2)	0.94526(7)	0.38286(6)	0.0206(2)
O1	0.03943(6)	0.6439(2)	-0.01127(16)	0.0228(6)
O2	0.10929(6)	0.4571(2)	0.07957(16)	0.0242(6)
O3	0.12756(6)	0.7715(2)	0.04878(14)	0.0201(6)
O4	0.14268(7)	1.0706(2)	0.14749(16)	0.0250(6)
O5	0.21477(6)	0.8975(2)	0.16546(16)	0.0258(6)
O14	0.04148(6)	0.9726(2)	0.40490(15)	0.0212(6)
O18	0.08452(6)	0.83573(19)	0.18546(14)	0.0170(5)
O24	0.19926(6)	0.4754(2)	0.52065(15)	0.0214(6)
O28	0.16385(6)	0.6684(2)	0.24900(15)	0.0192(5)

C11	0.05681(8)	0.7005(3)	0.3150(2)	0.0168(8)
C12	0.03803(9)	0.7067(3)	0.4044(2)	0.0185(8)
C13	0.03155(10)	0.8410(3)	0.4464(2)	0.0230(9)
C15	0.05928(9)	0.9726(3)	0.3175(2)	0.0178(8)
C16	0.06766(8)	0.8382(3)	0.2718(2)	0.0159(8)

Table S4 (cont.) - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: **Compound *α*-1**

Atom	x	y	z	U(eq) [Ang^2]
C17	0.06631(11)	1.1261(3)	0.2795(3)	0.0222(9)
C21	0.18762(9)	0.7655(3)	0.4386(2)	0.0177(8)
C22	0.20387(9)	0.7361(3)	0.5571(2)	0.0211(9)
C23	0.20876(10)	0.5921(3)	0.5932(3)	0.0239(9)
C25	0.18371(9)	0.4970(3)	0.4054(2)	0.0183(8)
C26	0.17773(9)	0.6419(3)	0.3619(2)	0.0170(8)
C27	0.17633(11)	0.3531(3)	0.3417(3)	0.0232(9)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table S5 - Hydrogen Atom Positions and Isotropic Displacement Parameters for: **Compound *α*-1**

Atom	x	y	z	U(iso) [Ang^2]
H121	0.0306(9)	0.624(3)	0.430(2)	0.008(7)
H131	0.0186(10)	0.855(3)	0.504(3)	0.026(8)
H171	0.0834(11)	1.127(3)	0.227(3)	0.039(9)
H172	0.0801(11)	1.179(4)	0.338(3)	0.034(9)
H173	0.0373(12)	1.174(4)	0.241(3)	0.045(10)
H221	0.2108(9)	0.806(3)	0.607(2)	0.012(7)
H231	0.2188(9)	0.563(3)	0.666(3)	0.018(7)
H271	0.1617(10)	0.287(3)	0.376(2)	0.027(8)
H272	0.2063(12)	0.314(4)	0.343(3)	0.041(9)
H273	0.1579(11)	0.370(3)	0.262(3)	0.034(9)

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S6 - (An)isotropic Displacement Parameters for: **Compound *α*-1**

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Mo1	0.0184(1)	0.0173(1)	0.0167(1)	-0.0039(1)	0.0063(1)	-0.0010(1)
Mo2	0.0194(1)	0.0186(1)	0.0167(1)	0.0008(1)	0.0071(1)	-0.0027(1)
S1	0.0250(4)	0.0136(3)	0.0253(4)	0.0001(3)	0.0114(3)	-0.0010(3)
S2	0.0254(4)	0.0169(3)	0.0197(3)	-0.0027(3)	0.0074(3)	-0.0012(3)
O1	0.0203(10)	0.0247(10)	0.0236(10)	-0.0043(8)	0.0072(9)	0.0004(8)
O2	0.0227(10)	0.0222(10)	0.0271(10)	-0.0075(8)	0.0072(9)	0.0006(8)
O3	0.0214(10)	0.0249(10)	0.0151(9)	-0.0009(8)	0.0075(8)	-0.0005(8)
O4	0.0283(11)	0.0199(10)	0.0284(11)	0.0035(8)	0.0113(9)	-0.0027(8)
O5	0.0221(11)	0.0337(12)	0.0221(10)	-0.0004(8)	0.0077(9)	-0.0036(9)
O14	0.0259(11)	0.0203(10)	0.0199(10)	-0.0002(8)	0.0108(8)	0.0012(8)

O18	0.0202(10)	0.0160(9)	0.0170(9)	-0.0019(7)	0.0091(8)	-0.0009(8)
O24	0.0221(10)	0.0220(10)	0.0208(10)	0.0020(8)	0.0079(8)	-0.0009(8)
O28	0.0240(10)	0.0174(9)	0.0157(9)	-0.0002(7)	0.0059(8)	-0.0009(8)
C11	0.0142(14)	0.0179(13)	0.0156(13)	0.0015(10)	0.0011(11)	0.0001(11)

Table S6 (cont.) - (An)isotropic Displacement Parameters for: **Compound *α*-1**

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
C12	0.0169(14)	0.0192(14)	0.0184(14)	0.0068(11)	0.0042(11)	0.0010(11)
C13	0.0234(16)	0.0302(16)	0.0177(14)	0.0027(12)	0.0100(13)	0.0013(12)
C15	0.0168(13)	0.0207(14)	0.0164(13)	-0.0003(11)	0.0059(11)	-0.0005(11)
C16	0.0151(14)	0.0166(13)	0.0142(13)	-0.0004(10)	0.0024(11)	-0.0001(10)
C17	0.0295(18)	0.0146(14)	0.0239(16)	-0.0025(12)	0.0105(14)	-0.0022(13)
C21	0.0152(14)	0.0198(14)	0.0203(13)	-0.0005(11)	0.0090(11)	-0.0008(11)
C22	0.0195(15)	0.0264(16)	0.0186(14)	-0.0059(13)	0.0079(12)	-0.0010(12)
C23	0.0196(15)	0.0351(17)	0.0163(15)	0.0026(13)	0.0049(12)	0.0017(13)
C25	0.0172(14)	0.0214(14)	0.0182(14)	-0.0007(11)	0.0084(11)	-0.0001(11)
C26	0.0133(13)	0.0224(14)	0.0168(14)	-0.0007(11)	0.0069(11)	-0.0016(11)
C27	0.0253(17)	0.0185(14)	0.0274(17)	0.0027(12)	0.0107(14)	-0.0009(12)

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for
Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and
h(i) are the Reflection Indices.

Table S7 - Bond Distances (Angstrom) for: **Compound *α*-1**

Mo1 -S1	2.4770(7)	Mo2 -S2	2.4725(7)
Mo1 -O1	1.6990(19)	Mo2 -O5	1.699(2)
Mo1 -O2	1.7007(18)	Mo2 -O4	1.7016(18)
Mo1 -O3	1.9106(19)	Mo2 -O3	1.9121(17)
Mo1 -O18	2.1548(17)	Mo2 -O18	2.521(2)
Mo1 -O28	2.5003(19)	Mo2 -O28	2.1584(18)
S1 -C11	1.711(3)	S2 -C21	1.720(3)
O14 -C13	1.349(3)	O24 -C23	1.336(4)
O14 -C15	1.362(3)	O24 -C25	1.357(3)
O18 -C16	1.331(3)	O28 -C26	1.337(3)
C11 -C12	1.407(4)	C21 -C22	1.406(3)
C11 -C16	1.416(4)	C21 -C26	1.414(4)
C12 -C13	1.339(4)	C22 -C23	1.344(4)
C15 -C16	1.378(4)	C25 -C26	1.380(4)
C15 -C17	1.478(4)	C25 -C27	1.476(4)
C12 -H121	0.86(3)	C22 -H221	0.85(3)
C13 -H131	0.93(3)	C23 -H231	0.89(3)
C17 -H171	0.96(4)	C27 -H271	0.93(3)
C17 -H172	0.85(4)	C27 -H272	1.00(4)
C17 -H173	0.98(4)	C27 -H273	0.98(3)

Table S8 - Bond Angles (Degrees) for: **Compound *α*-1**

S1 -Mo1 -O1	100.55(7)	S2 -Mo2 -O5	100.16(7)

S1	-Mo1	-O2	88.65(7)	S2	-Mo2	-O4	88.62(7)
S1	-Mo1	-O3	146.38(5)	S2	-Mo2	-O3	146.14(6)
S1	-Mo1	-O18	77.52(5)	S2	-Mo2	-O18	83.45(4)
S1	-Mo1	-O28	83.33(5)	S2	-Mo2	-O28	77.45(5)

Table S8 (cont.) - Bond Angles (Degrees) for: **Compound *α*-1**

O1	-Mo1 -O2	104.36(9)	O4	-Mo2 -O5	104.09(10)
O1	-Mo1 -O3	104.37(8)	O3	-Mo2 -O5	105.32(9)
O1	-Mo1 -O18	97.99(8)	O5	-Mo2 -O28	99.73(8)
O1	-Mo1 -O28	169.35(7)	O5	-Mo2 -O18	170.69(7)
O2	-Mo1 -O3	106.34(9)	O3	-Mo2 -O4	106.07(9)
O2	-Mo1 -O18	155.56(8)	O4	-Mo2 -O28	154.19(9)
O2	-Mo1 -O28	85.55(8)	O4	-Mo2 -O18	84.49(9)
O3	-Mo1 -O18	76.99(7)	O3	-Mo2 -O28	76.57(7)
O3	-Mo1 -O28	68.49(7)	O3	-Mo2 -O18	68.26(7)
O18	-Mo1 -O28	73.01(6)	O18	-Mo2 -O28	72.53(7)
Mo1	-S1 -C11	100.61(9)	Mo2	-S2 -C21	100.65(8)
Mo1	-O3 -Mo2	110.81(8)			
C13	-O14 -C15	120.2(2)	C23	-O24 -C25	121.2(2)
Mo1	-O18 -Mo2	84.21(6)			
Mo1	-O18 -C16	123.14(16)	Mo2	-O18 -C16	132.13(15)
Mo1	-O28 -Mo2	84.64(6)			
Mo1	-O28 -C26	132.88(17)	Mo2	-O28 -C26	123.27(16)
S1	-C11 -C12	123.1(2)	S2	-C21 -C22	122.9(2)
S1	-C11 -C16	118.68(19)	S2	-C21 -C26	118.57(18)
C12	-C11 -C16	118.2(2)	C22	-C21 -C26	118.5(2)
C11	-C12 -C13	119.4(3)	C21	-C22 -C23	118.9(3)
O14	-C13 -C12	122.7(2)	O24	-C23 -C22	122.5(3)
O14	-C15 -C16	120.2(2)	O24	-C25 -C26	119.7(2)
O14	-C15 -C17	113.0(2)	O24	-C25 -C27	112.1(2)
C16	-C15 -C17	126.8(3)	C26	-C25 -C27	128.2(2)
O18	-C16 -C11	119.4(2)	O28	-C26 -C21	119.1(2)
O18	-C16 -C15	121.2(2)	O28	-C26 -C25	121.7(2)
C11	-C16 -C15	119.4(2)	C21	-C26 -C25	119.2(2)
C11	-C12 -H121	119.0(18)	C21	-C22 -H221	122.5(17)
C13	-C12 -H121	121.6(18)	C23	-C22 -H221	118.5(17)
O14	-C13 -H131	112.5(17)	O24	-C23 -H231	112.4(18)
C12	-C13 -H131	124.7(17)	C22	-C23 -H231	125.2(18)
C15	-C17 -H171	113.1(16)	C25	-C27 -H271	108.7(16)
C15	-C17 -H172	109(2)	C25	-C27 -H272	108(2)
C15	-C17 -H173	110(2)	C25	-C27 -H273	110.0(16)
H171	-C17 -H172	109(3)	H271	-C27 -H272	112(3)
H171	-C17 -H173	108(3)	H271	-C27 -H273	110(3)
H172	-C17 -H173	108(3)	H272	-C27 -H273	109(3)

Figure S9 - $[MoO_2(thiomaltol)]_2(\mu\text{-}O)$ (compound ***α*** **-1**)

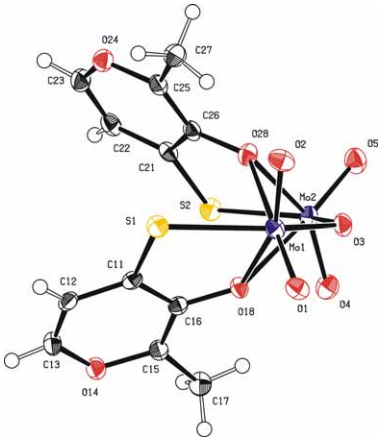

Table S10 - Crystal Data and Details of the Structure Determination for: **Compound *β* -1**

Crystal Data

Formula	C12 H10 Mo2 O9 S2
Formula Weight	554.22
Crystal System	Monoclinic
Space group	P21/n (No. 14)
a, b, c [Angstrom]	8.2509(1) 13.9940(2) 14.6426(2)
alpha, beta, gamma [deg]	90 105.8518(6) 90
V [Ang**3]	1626.39(4)
Z	4
D(calc) [g/cm**3]	2.263
Mu(MoKa) [/mm]	1.845
F(000)	1080
Crystal Size [mm]	0.10 x 0.15 x 0.23

Data Collection

Temperature (K)	173
Radiation [Angstrom]	MoKa 0.71073
Theta Min-Max [Deg]	2.0, 25.3
Dataset	-9: 9 ; -16: 16 ; -17: 17
Tot., Uniq. Data, R(int)	40422, 2963, 0.034
Observed data [I > 2.0 sigma(I)]	2826

Refinement

Nref, Npar	2963, 229
R, wR2, S	0.0164, 0.0407, 1.14
Max. and Av. Shift/Error	0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]	-0.31, 0.30

Table S11 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: **Compound *β* -1**

Atom	x	y	z	U(eq) [Ang^2]
Mo1	0.58082(2)	0.32020(1)	0.29920(1)	0.0164(1)
Mo2	0.25841(2)	0.25148(1)	0.36184(1)	0.0165(1)
S1	0.72983(7)	0.18810(4)	0.24391(4)	0.0212(2)
S2	0.19903(7)	0.07933(4)	0.33218(4)	0.0205(2)
O1	0.5932(2)	0.40730(11)	0.22107(11)	0.0253(5)
O2	0.75375(19)	0.33840(11)	0.39312(11)	0.0227(5)
O3	0.39587(18)	0.35688(10)	0.34687(10)	0.0186(4)
O4	0.06913(19)	0.27569(11)	0.28297(11)	0.0248(5)
O5	0.2246(2)	0.26660(12)	0.46999(11)	0.0262(5)
O14	0.2884(2)	0.01975(11)	0.07784(11)	0.0230(5)
O18	0.37428(18)	0.23756(10)	0.21313(10)	0.0179(5)
O24	0.7244(2)	-0.03367(11)	0.42720(11)	0.0235(5)
O28	0.50561(18)	0.19066(10)	0.40342(10)	0.0179(4)
C11	0.5617(3)	0.12177(15)	0.18137(14)	0.0176(6)

C12	0.5824(3)	0.03204(16)	0.14290(16)	0.0232(7)
C13	0.4452(3)	-0.01644(17)	0.09393(16)	0.0249(7)
C15	0.2626(3)	0.10502(16)	0.11531(15)	0.0199(6)
C16	0.3970(3)	0.15632(15)	0.17044(14)	0.0165(6)

Table S11 (cont.) - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: **Compound *β* -1**

Atom	x	y	z	U(eq) [Ang^2]
C17	0.0834(3)	0.13430(19)	0.08916(17)	0.0298(8)
C21	0.3998(3)	0.03373(15)	0.36681(14)	0.0179(6)
C22	0.4356(3)	-0.06426(16)	0.36036(15)	0.0230(7)
C23	0.5968(3)	-0.09379(17)	0.38902(16)	0.0272(7)
C25	0.6973(3)	0.06145(16)	0.43455(15)	0.0198(6)
C26	0.5353(3)	0.09718(15)	0.40144(14)	0.0164(6)
C27	0.8506(3)	0.11567(18)	0.48184(17)	0.0275(8)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table S12 - Hydrogen Atom Positions and Isotropic Displacement Parameters for: **Compound *β* -1**

Atom	x	y	z	U(iso) [Ang^2]
H121	0.6918	0.0059	0.1513	0.028
H131	0.4593	-0.0781	0.0700	0.030
*H171	0.0179	0.0918	0.0394	0.045
*H172	0.0735	0.2002	0.0657	0.045
*H173	0.0402	0.1302	0.1451	0.045
*H174	0.0698	0.1897	0.1274	0.045
*H175	0.0143	0.0813	0.1011	0.045
*H176	0.0475	0.1513	0.0217	0.045
H221	0.3473	-0.1087	0.3361	0.028
H231	0.6212	-0.1593	0.3821	0.033
H271	0.9362	0.1058	0.4477	0.041
H272	0.8940	0.0934	0.5474	0.041
H273	0.8234	0.1838	0.4817	0.041

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
Starred atoms have an sof of 0.5.

Table S13 - (An)isotropic Displacement Parameters for: **Compound *β* -1**

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Mo1	0.0151(1)	0.0139(1)	0.0198(1)	0.0003(1)	0.0039(1)	-0.0023(1)
Mo2	0.0139(1)	0.0152(1)	0.0202(1)	0.0019(1)	0.0043(1)	0.0008(1)
S1	0.0144(3)	0.0229(3)	0.0261(3)	-0.0020(2)	0.0051(2)	-0.0001(2)
S2	0.0181(3)	0.0186(3)	0.0239(3)	0.0014(2)	0.0043(2)	-0.0044(2)
O1	0.0261(9)	0.0224(9)	0.0276(9)	0.0052(7)	0.0079(7)	-0.0013(7)

O2	0.0203(8)	0.0206(8)	0.0256(8)	-0.0015(7)	0.0034(7)	-0.0054(7)
O3	0.0196(8)	0.0128(7)	0.0241(8)	-0.0017(6)	0.0069(6)	-0.0003(6)
O4	0.0170(8)	0.0234(9)	0.0320(9)	0.0057(7)	0.0034(7)	0.0004(7)
O5	0.0280(9)	0.0266(9)	0.0263(9)	0.0015(7)	0.0113(7)	0.0031(7)

Table S13 (cont.) - (An)isotropic Displacement Parameters for: **Compound *β* -1**

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
O14	0.0291(9)	0.0191(8)	0.0216(8)	-0.0026(6)	0.0085(7)	-0.0059(7)
O18	0.0158(8)	0.0169(8)	0.0199(8)	-0.0017(6)	0.0029(6)	0.0003(6)
O24	0.0273(9)	0.0222(8)	0.0206(8)	0.0027(6)	0.0061(7)	0.0094(7)
O28	0.0164(8)	0.0137(7)	0.0222(8)	0.0005(6)	0.0027(6)	0.0006(6)
C11	0.0200(11)	0.0184(11)	0.0152(10)	0.0027(8)	0.0063(9)	-0.0011(9)
C12	0.0259(13)	0.0202(12)	0.0251(12)	0.0019(9)	0.0097(10)	0.0042(10)
C13	0.0375(14)	0.0168(11)	0.0234(12)	-0.0006(9)	0.0136(10)	-0.0008(10)
C15	0.0230(12)	0.0206(11)	0.0158(10)	0.0016(9)	0.0048(9)	-0.0026(9)
C16	0.0195(11)	0.0157(10)	0.0144(10)	0.0019(8)	0.0049(8)	-0.0001(9)
C17	0.0197(12)	0.0396(15)	0.0260(12)	-0.0041(11)	-0.0008(10)	-0.0035(11)
C21	0.0260(12)	0.0180(11)	0.0111(10)	0.0020(8)	0.0076(9)	0.0005(9)
C22	0.0357(14)	0.0166(11)	0.0175(11)	-0.0005(9)	0.0088(10)	-0.0024(10)
C23	0.0439(15)	0.0164(11)	0.0223(12)	0.0009(9)	0.0109(11)	0.0058(11)
C25	0.0246(12)	0.0200(11)	0.0154(10)	0.0032(9)	0.0067(9)	0.0052(9)
C26	0.0204(11)	0.0170(11)	0.0125(10)	0.0021(8)	0.0058(8)	0.0015(9)
C27	0.0196(12)	0.0313(14)	0.0279(13)	0.0041(10)	0.0002(10)	0.0035(10)

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for
Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and
h(i) are the Reflection Indices.

Table S14 - Bond Distances (Angstrom) for: **Compound *β* -1**

Mo1 -S1	2.4755(6)	Mo2 -S2	2.4731(6)
Mo1 -O1	1.6937(16)	Mo2 -O5	1.6946(16)
Mo1 -O2	1.7088(16)	Mo2 -O4	1.7036(16)
Mo1 -O3	1.9135(15)	Mo2 -O3	1.9094(15)
Mo1 -O18	2.1579(15)	Mo2 -O28	2.1393(15)
S1 -C11	1.712(2)	S2 -C21	1.717(3)
O14 -C13	1.349(3)	O24 -C23	1.344(3)
O14 -C15	1.354(3)	O24 -C25	1.359(3)
O18 -C16	1.335(3)	O28 -C26	1.333(3(
C11 -C12	1.406(3)	C21 -C22	1.411(3)
C11 -C16	1.410(4)	C21 -C26	1.409(3)
C12 -C13	1.346(3)	C22 -C23	1.346(4)
C15 -C16	1.381(3)	C25 -C26	1.385(3)
C15 -C17	1.480(4)	C25 -C27	1.475(3)
C12 -H121	0.95	C22 -H221	0.95
C13 -H131	0.95	C23 -H231	0.95
C17 -H171	0.98	C27 -H271	0.98
C17 -H172	0.98	C27 -H272	0.98
C17 -H173	0.98	C27 -H273	0.98
C17 -H174	0.98		
C17 -H175	0.98		
C17 -H176	0.98		

Table S15 - Bond Angles (Degrees) for: **Compound *β* -1**

S1	-Mo1 -O1	100.93(6)	S2	-Mo2 -O5	102.15(6)
S1	-Mo1 -O2	89.68(5)	S2	-Mo2 -O4	88.49(5)
S1	-Mo1 -O3	146.77(5)	S2	-Mo2 -O3	145.87(5)
S1	-Mo1 -O18	78.01(4)	S2	-Mo2 -O28	77.89(4)
O1	-Mo1 -O2	104.19(8)	O4	-Mo2 -O5	104.73(8)
O1	-Mo1 -O18	100.07(7)	O5	-Mo2 -O28	99.86(7)
O2	-Mo1 -O18	154.49(6)	O4	-Mo2 -O28	153.93(7)
O3	-Mo1 -O1	104.75(7)	O3	-Mo2 -O5	105.39(7)
O3	-Mo1 -O2	103.90(7)	O3	-Mo2 -O4	103.41(7)
O3	-Mo1 -O18	77.03(6)	O3	-Mo2 -O28	77.88(6)
Mo1	-S1 -C11	100.23(8)	Mo2	-S2 -C21	100.44(8)
Mo1	-O3 -Mo2	113.11(7)			
C13	-O14 -C15	120.63(19)	C23	-O24 -C25	121.26(19)
Mo1	-O18 -C16	122.71(14)	Mo2	-O28 -C26	123.43(14)
S1	-C11 -C12	121.96(19)	S2	-C21 -C22	122.95(18)
S1	-C11 -C16	119.34(16)	S2	-C21 -C26	118.59(17)
C12	-C11 -C16	118.7(2)	C22	-C21 -C26	118.4(2)
C11	-C12 -C13	119.1(2)	C21	-C22 -C23	119.0(2)
O14	-C13 -C12	122.1(2)	O24	-C23 -C22	122.2(2)
O14	-C15 -C16	120.3(2)	O24	-C25 -C26	119.3(2)
O14	-C15 -C17	113.3(2)	O24	-C25 -C27	113.7(2)
C16	-C15 -C17	126.4(2)	C26	-C25 -C27	126.9(2)
O18	-C16 -C11	119.6(2)	O28	-C26 -C21	119.6(2)
O18	-C16 -C15	121.6(2)	O28	-C26 -C25	120.8(2)
C11	-C16 -C15	118.9(2)	C21	-C26 -C25	119.6(2)
C11	-C12 -H121	120.47	C21	-C22 -H221	120.53
C13	-C12 -H121	120.38	C23	-C22 -H221	120.49
O14	-C13 -H131	118.99	O24	-C23 -H231	118.92
C12	-C13 -H131	118.95	C22	-C23 -H231	118.90
C15	-C17 -H171	109.46	C25	-C27 -H271	109.45
C15	-C17 -H172	109.45	C25	-C27 -H272	109.48
C15	-C17 -H173	109.46	C25	-C27 -H273	109.46
C15	-C17 -H174	109.46			
C15	-C17 -H175	109.45			
C15	-C17 -H176	109.48			
H171	-C17 -H172	109.52	H271	-C27 -H272	109.49
H171	-C17 -H173	109.45	H271	-C27 -H273	109.44
H172	-C17 -H173	109.49	H272	-C27 -H273	109.52
H174	-C17 -H175	109.49			
H174	-C17 -H176	109.48			
H175	-C17 -H176	109.46			

Figure S16 - $[MoO_2(thiomaltol)]_2(\mu\text{-}O)$ (compound ***β*** **-1**)