Supporting Information For:

Understanding the Origin of Metal-Sulfur Vibrations in an Oxo-Molybdenum Dithiolene Complex: Relevance to Sulfite Oxidase

by

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Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) of (Tp*)MoO(qdt) (**4**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor. Atomic numbering scheme is depicted in Fig. S2.

	x	y	z	U(eq)
Mo(1)	5366(1)	7476(1)	6983(1)	21(1)
S(2)	5190(1)	5431(1)	7539(1)	25(1)
S(1)	7638(1)	7983(1)	8182(1)	27(1)
O(1)	5863(2)	7321(2)	5706(2)	30(1)
C(2)	6988(3)	5416(2)	7914(2)	24(1)
C(1)	8086(3)	6559(2)	8141(2)	25(1)
N(31)	4423(2)	7904(2)	8602(2)	23(1)
N(21)	5371(2)	9407(2)	6836(2)	23(1)
N(22)	4197(2)	9830(2)	6950(2)	22(1)
N(12)	2303(2)	7845(2)	6470(2)	22(1)
N(11)	3119(2)	7051(2)	6262(2)	22(1)
N(32)	3408(2)	8571(2)	8500(2)	25(1)
N(2)	7291(2)	4346(2)	7962(2)	27(1)
N(1)	9438(2)	6583(2)	8345(2)	33(1)
C(23)	4417(3)	11001(2)	6679(2)	25(1)
C(15)	2347(3)	6210(2)	5409(2)	25(1)
C(14)	1045(3)	6469(3)	5072(2)	29(1)
C(27)	3350(3)	11739(3)	6729(2)	33(1)
C(24)	5747(3)	11352(2)	6378(2)	27(1)
C(26)	7719(3)	10232(3)	6241(3)	33(1)
C(35)	4658(3)	7693(3)	9714(2)	29(1)
B(1)	2904(3)	8984(3)	7343(2)	24(1)
C(13)	1043(3)	7491(2)	5758(2)	26(1)
C(36)	5623(3)	6951(3)	10204(2)	36(1)
C(33)	3038(3)	8775(3)	9524(2)	32(1)
C(34)	3831(3)	8240(3)	10304(2)	35(1)
C(3)	8695(3)	4356(2)	8196(2)	28(1)
C(8)	9774(3)	5477(3)	8361(3)	33(1)
C(25)	6314(3)	10339(2)	6482(2)	24(1)
C(16)	2875(3)	5185(3)	4940(3)	35(1)
C(17)	-105(3)	8147(3)	5781(3)	35(1)

C(4)	9096(3)	3229(3)	8239(3)	39(1)
C(37)	1936(4)	9440(3)	9677(3)	43(1)
C(7)	11214(3)	5444(3)	8536(4)	50(1)
C(5)	10498(3)	3230(3)	8422(3)	49(1)
C(6)	11560(4)	4345(3)	8573(4)	57(1)

Table S2. Bond lengths [Å] and angles [°] of **4**.

Mo(1)-O(1)	1.6863(18)
Mo(1)-N(11)	2.171(2)
Mo(1)-N(21)	2.184(2)
Mo(1)-N(31)	2.348(2)
Mo(1)-S(1)	2.3824(7)
Mo(1)-S(2)	2.3938(7)
S(2)-C(2)	1.761(3)
S(1)-C(1)	1.760(3)
C(2)-N(2)	1.309(3)
C(2)-C(1)	1.444(4)
C(1)-N(1)	1.308(3)
N(31)-C(35)	1.354(3)
N(31)-N(32)	1.383(3)
N(21)-C(25)	1.351(3)
N(21)-N(22)	1.375(3)
N(22)-C(23)	1.344(3)
N(22)-B(1)	1.542(4)
N(12)-C(13)	1.348(3)
N(12)-N(11)	1.377(3)
N(12)-B(1)	1.543(4)
N(11)-C(15)	1.350(3)
N(32)-C(33)	1.354(3)
N(32)-B(1)	1.527(4)
N(2)-C(3)	1.364(3)
N(1)-C(8)	1.361(4)
C(23)-C(24)	1.381(4)
C(23)-C(27)	1.495(4)
C(15)-C(14)	1.385(4)
C(15)-C(16)	1.493(4)
C(14)-C(13)	1.379(4)
C(14)-H(14A)	0.9500
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(6)-H(6A)	0.9500
O(1)-Mo(1)-N(11)	93.49(9)
C(27)-H(27C)	0.9800
C(24)-C(25)	1.387(4)
C(24)-H(24A)	0.9500
C(26)-C(25)	1.487(4)
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(35)-C(34)	1.384(4)
C(35)-C(36)	1.484(4)
B(1)-H(9A)	1.0000
C(13)-C(17)	1.496(4)
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(33)-C(34)	1.378(4)
C(33)-C(37)	1.488(4)
C(34)-H(34A)	0.9500
C(3)-C(4)	1.416(4)
C(3)-C(8)	1.417(4)
C(8)-C(7)	1.409(4)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(4)-C(5)	1.363(4)
C(4)-H(4A)	0.9500
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
C(7)-C(6)	1.360(5)
C(7)-H(7A)	0.9500
C(5)-C(6)	1.404(5)
C(5)-H(5A)	0.9500
O(1)-Mo(1)-N(21)	93.00(8)
N(11)-Mo(1)-N(21)	86.30(8)
O(1)-Mo(1)-N(31)	169.85(8)

N(11)-Mo(1)-N(31)	79.68(8)	N(12)-N(11)-Mo(1)	121.13(16)
N(21)-Mo(1)-N(31)	79.16(7)	C(33)-N(32)-N(31)	110.3(2)
O(1)-Mo(1)-S(1)	99.82(7)	C(33)-N(32)-B(1)	130.0(2)
N(11)-Mo(1)-S(1)	166.68(6)	N(31)-N(32)-B(1)	119.7(2)
N(21)-Mo(1)-S(1)	93.06(6)	C(2)-N(2)-C(3)	117.0(2)
N(31)-Mo(1)-S(1)	87.13(6)	C(1)-N(1)-C(8)	117.2(2)
O(1)-Mo(1)-S(2)	99.75(7)	N(22)-C(23)-C(24)	108.3(2)
N(11)-Mo(1)-S(2)	92.55(6)	N(22)-C(23)-C(27)	123.0(2)
N(21)-Mo(1)-S(2)	167.25(6)	C(24)-C(23)-C(27)	128.7(2)
N(31)-Mo(1)-S(2)	88.13(5)	N(11)-C(15)-C(14)	109.1(2)
S(1)-Mo(1)-S(2)	85.14(2)	N(11)-C(15)-C(16)	123.1(2)
C(2)-S(2)-Mo(1)	102.38(9)	C(14)-C(15)-C(16)	127.8(2)
C(1)-S(1)-Mo(1)	101.69(9)	C(13)-C(14)-C(15)	106.5(2)
N(2)-C(2)-C(1)	121.6(2)	C(13)-C(14)-H(14A)	126.8
N(2)-C(2)-S(2)	118.1(2)	C(15)-C(14)-H(14A)	126.8
C(1)-C(2)-S(2)	120.29(19)	C(23)-C(27)-H(27A)	109.5
N(1)-C(1)-C(2)	122.0(2)	C(23)-C(27)-H(27B)	109.5
N(1)-C(1)-S(1)	117.5(2)	H(27A)-C(27)-H(27B)	109.5
C(2)-C(1)-S(1)	120.53(19)	C(23)-C(27)-H(27C)	109.5
C(35)-N(31)-N(32)	105.8(2)	H(27A)-C(27)-H(27C)	109.5
C(35)-N(31)-Mo(1)	135.59(18)	H(27B)-C(27)-H(27C)	109.5
N(32)-N(31)-Mo(1)	118.59(15)	C(23)-C(24)-C(25)	106.1(2)
C(25)-N(21)-N(22)	106.83(19)	C(23)-C(24)-H(24A)	126.9
C(25)-N(21)-Mo(1)	131.00(17)	C(25)-C(24)-H(24A)	126.9
N(22)-N(21)-Mo(1)	121.54(15)	C(25)-C(26)-H(26A)	109.5
C(23)-N(22)-N(21)	109.4(2)	C(25)-C(26)-H(26B)	109.5
C(23)-N(22)-B(1)	130.3(2)	H(26A)-C(26)-H(26B)	109.5
N(21)-N(22)-B(1)	120.30(19)	C(25)-C(26)-H(26C)	109.5
C(13)-N(12)-N(11)	109.0(2)	H(26A)-C(26)-H(26C)	109.5
C(13)-N(12)-B(1)	129.8(2)	H(26B)-C(26)-H(26C)	109.5
N(11)-N(12)-B(1)	121.0(2)	N(31)-C(35)-C(34)	109.7(2)
C(15)-N(11)-N(12)	107.1(2)	N(31)-C(35)-C(36)	124.5(2)
C(15)-N(11)-Mo(1)	130.31(17)	C(34)-C(35)-C(36)	125.7(2)
N(32)-B(1)-N(22)	108.3(2)	N(12)-B(1)-H(9A)	110.2
N(32)-B(1)-N(12)	109.4(2)	N(12)-C(13)-C(14)	108.3(2)
N(22)-B(1)-N(12)	108.7(2)	N(12)-C(13)-C(17)	122.6(2)
N(32)-B(1)-H(9A)	110.2	C(14)-C(13)-C(17)	129.2(3)
N(22)-B(1)-H(9A)	110.2	C(35)-C(36)-H(36A)	109.5

C(35)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(35)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
N(32)-C(33)-C(34)	107.1(2)
N(32)-C(33)-C(37)	122.7(3)
C(34)-C(33)-C(37)	130.1(3)
C(33)-C(34)-C(35)	107.0(2)
C(33)-C(34)-H(34A)	126.5
C(35)-C(34)-H(34A)	126.5
N(2)-C(3)-C(4)	119.8(3)
N(2)-C(3)-C(8)	121.3(2)
C(4)-C(3)-C(8)	118.8(2)
N(1)-C(8)-C(7)	119.7(3)
N(1)-C(8)-C(3)	120.9(2)
C(7)-C(8)-C(3)	119.5(3)
N(21)-C(25)-C(24)	109.4(2)
N(21)-C(25)-C(26)	123.1(2)
C(24)-C(25)-C(26)	127.6(2)
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(13)-C(17)-H(17A)	109.5
C(13)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(13)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(5)-C(4)-C(3)	120.2(3)
C(5)-C(4)-H(4A)	119.9
C(3)-C(4)-H(4A)	119.9
C(33)-C(37)-H(37A)	109.5
C(33)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
C(33)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
C(6)-C(7)-C(8)	120.1(3)
C(6)-C(7)-H(7A)	120.0
C(8)-C(7)-H(7A)	120.0
C(4)-C(5)-C(6)	120.5(3)
C(4)-C(5)-H(5A)	119.7
C(6)-C(5)-H(5A)	119.7
C(7)-C(6)-C(5)	120.8(3)
C(7)-C(6)-H(6A)	119.6
C(5)-C(6)-H(6A)	119.6

Symmetry transformations used to generate equivalent atoms

Table S3. Anisotropic displacement parameters ($Å^2 x\ 10^3$) of **4**. 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(1)	21(1)	19(1)	25(1)	5(1)	6(1)	8(1)
S(2)	20(1)	20(1)	36(1)	8(1)	3(1)	5(1)
S(1)	24(1)	19(1)	36(1)	4(1)	3(1)	5(1)
O(1)	36(1)	29(1)	30(1)	5(1)	11(1)	13(1)
C(2)	22(1)	24(1)	25(1)	6(1)	5(1)	6(1)
C(1)	26(1)	23(1)	27(1)	7(1)	4(1)	7(1)
N(31)	25(1)	24(1)	23(1)	6(1)	6(1)	8(1)
N(21)	25(1)	20(1)	26(1)	6(1)	8(1)	8(1)
N(22)	26(1)	20(1)	25(1)	5(1)	5(1)	11(1)
N(12)	23(1)	21(1)	27(1)	5(1)	6(1)	10(1)
N(11)	24(1)	22(1)	24(1)	4(1)	6(1)	11(1)
N(32)	30(1)	22(1)	27(1)	2(1)	10(1)	8(1)
N(2)	23(1)	23(1)	37(1)	9(1)	5(1)	7(1)
N(1)	23(1)	26(1)	48(1)	8(1)	3(1)	5(1)
C(23)	35(1)	20(1)	21(1)	4(1)	2(1)	10(1)
C(15)	26(1)	23(1)	25(1)	5(1)	3(1)	6(1)
C(14)	25(1)	30(1)	30(1)	5(1)	1(1)	5(1)
C(27)	44(2)	25(1)	34(1)	5(1)	7(1)	17(1)
C(24)	34(1)	20(1)	27(1)	7(1)	5(1)	6(1)
C(26)	33(2)	27(1)	41(2)	10(1)	16(1)	7(1)
C(35)	31(1)	29(1)	24(1)	5(1)	5(1)	2(1)
B(1)	23(1)	23(1)	28(1)	3(1)	6(1)	10(1)
C(13)	23(1)	26(1)	30(1)	10(1)	5(1)	7(1)
C(36)	41(2)	42(2)	25(1)	12(1)	4(1)	12(1)
C(33)	36(2)	28(1)	31(1)	0(1)	15(1)	4(1)
C(34)	39(2)	41(2)	22(1)	3(1)	8(1)	4(1)
C(3)	24(1)	26(1)	35(1)	8(1)	4(1)	9(1)
C(8)	24(1)	29(1)	47(2)	10(1)	5(1)	9(1)
C(25)	28(1)	20(1)	25(1)	6(1)	6(1)	6(1)
C(16)	39(2)	29(2)	35(2)	-5(1)	3(1)	12(1)
C(17)	23(1)	35(2)	51(2)	8(1)	2(1)	14(1)
C(4)	33(2)	29(2)	58(2)	13(1)	10(1)	11(1)

C(37)	56(2)	38(2)	42(2)	-2(1)	24(2)	17(2)
C(7)	23(2)	36(2)	93(3)	18(2)	7(2)	9(1)
C(5)	34(2)	37(2)	84(3)	21(2)	11(2)	22(1)
C(6)	26(2)	47(2)	105(3)	27(2)	13(2)	17(2)

Table S4. Torsion angles [°] of **4**.

O(1)-Mo(1)-S(2)-C(2)	74.61(11)
N(11)-Mo(1)-S(2)-C(2)	168.60(10)
N(21)-Mo(1)-S(2)-C(2)	-106.9(3)
N(31)-Mo(1)-S(2)-C(2)	-111.82(10)
S(1)-Mo(1)-S(2)-C(2)	-24.55(9)
O(1)-Mo(1)-S(1)-C(1)	-72.27(11)
N(11)-Mo(1)-S(1)-C(1)	107.3(3)
N(21)-Mo(1)-S(1)-C(1)	-165.85(10)
N(31)-Mo(1)-S(1)-C(1)	115.17(10)
S(2)-Mo(1)-S(1)-C(1)	26.80(9)
Mo(1)-S(2)-C(2)-N(2)	-161.58(19)
Mo(1)-S(2)-C(2)-C(1)	17.4(2)
N(2)-C(2)-C(1)-N(1)	3.7(4)
S(2)-C(2)-C(1)-N(1)	-175.2(2)
N(2)-C(2)-C(1)-S(1)	-174.9(2)
S(2)-C(2)-C(1)-S(1)	6.2(3)
Mo(1)-S(1)-C(1)-N(1)	155.2(2)
Mo(1)-S(1)-C(1)-C(2)	-26.1(2)
O(1)-Mo(1)-N(31)-C(35)	-173.5(4)
N(11)-Mo(1)-N(31)-C(35)	138.3(3)
N(21)-Mo(1)-N(31)-C(35)	-133.5(3)
S(1)-Mo(1)-N(31)-C(35)	-39.9(2)
S(2)-Mo(1)-N(31)-C(35)	45.3(2)
O(1)-Mo(1)-N(31)-N(32)	3.5(6)
N(11)-Mo(1)-N(31)-N(32)	-44.75(17)
N(21)-Mo(1)-N(31)-N(32)	43.42(17)
S(1)-Mo(1)-N(31)-N(32)	137.09(17)
S(2)-Mo(1)-N(31)-N(32)	-137.68(17)
O(1)-Mo(1)-N(21)-C(25)	-44.0(2)
N(11)-Mo(1)-N(21)-C(25)	-137.3(2)
N(31)-Mo(1)-N(21)-C(25)	142.5(2)
S(1)-Mo(1)-N(21)-C(25)	56.0(2)
S(2)-Mo(1)-N(21)-C(25)	137.5(2)
O(1)-Mo(1)-N(21)-N(22)	125.56(18)
N(12)-N(11)-C(15)-C(16)	-179.8(2)
Mo(1)-N(11)-C(15)-C(16)	13.9(4)
N(11)-Mo(1)-N(21)-N(22)	32.25(18)
N(31)-Mo(1)-N(21)-N(22)	-47.94(17)
S(1)-Mo(1)-N(21)-N(22)	-134.42(17)
S(2)-Mo(1)-N(21)-N(22)	-52.9(4)
C(25)-N(21)-N(22)-C(23)	-0.4(3)
Mo(1)-N(21)-N(22)-C(23)	-172.18(16)
C(25)-N(21)-N(22)-B(1)	179.8(2)
Mo(1)-N(21)-N(22)-B(1)	8.0(3)
C(13)-N(12)-N(11)-C(15)	0.3(3)
B(1)-N(12)-N(11)-C(15)	-175.6(2)
C(13)-N(12)-N(11)-Mo(1)	168.12(16)
B(1)-N(12)-N(11)-Mo(1)	-7.8(3)
O(1)-Mo(1)-N(11)-C(15)	39.6(2)
N(21)-Mo(1)-N(11)-C(15)	132.4(2)
N(31)-Mo(1)-N(11)-C(15)	-148.0(2)
S(1)-Mo(1)-N(11)-C(15)	-140.0(2)
S(2)-Mo(1)-N(11)-C(15)	-60.3(2)
O(1)-Mo(1)-N(11)-N(12)	-125.02(18)
N(21)-Mo(1)-N(11)-N(12)	-32.23(17)
N(31)-Mo(1)-N(11)-N(12)	47.41(17)
S(1)-Mo(1)-N(11)-N(12)	55.4(3)
S(2)-Mo(1)-N(11)-N(12)	135.05(17)
C(35)-N(31)-N(32)-C(33)	0.6(3)
Mo(1)-N(31)-N(32)-C(33)	-177.21(17)
C(35)-N(31)-N(32)-B(1)	179.2(2)
Mo(1)-N(31)-N(32)-B(1)	1.4(3)
C(1)-C(2)-N(2)-C(3)	-2.3(4)
S(2)-C(2)-N(2)-C(3)	176.69(19)
C(2)-C(1)-N(1)-C(8)	-1.5(4)
S(1)-C(1)-N(1)-C(8)	177.2(2)
N(21)-N(22)-C(23)-C(24)	0.2(3)
B(1)-N(22)-C(23)-C(24)	-180.0(2)
N(21)-N(22)-C(23)-C(27)	-179.2(2)
B(1)-N(22)-C(23)-C(27)	0.6(4)
N(12)-N(11)-C(15)-C(14)	0.2(3)
Mo(1)-N(11)-C(15)-C(14)	-166.08(17)
N(11)-C(15)-C(14)-C(13)	-0.6(3)
C(16)-C(15)-C(14)-C(13)	179.4(3)

N(22)-C(23)-C(24)-C(25)	0.0(3)
C(27)-C(23)-C(24)-C(25)	179.4(3)
N(32)-N(31)-C(35)-C(34)	-1.3(3)
Mo(1)-N(31)-C(35)-C(34)	175.93(19)
N(32)-N(31)-C(35)-C(36)	176.8(3)
Mo(1)-N(31)-C(35)-C(36)	-5.9(4)
C(33)-N(32)-B(1)-N(22)	117.6(3)
N(31)-N(32)-B(1)-N(22)	-60.7(3)
C(33)-N(32)-B(1)-N(12)	-124.2(3)
N(31)-N(32)-B(1)-N(12)	57.6(3)
C(23)-N(22)-B(1)-N(32)	-121.9(3)
N(21)-N(22)-B(1)-N(32)	57.8(3)
C(23)-N(22)-B(1)-N(12)	119.4(3)
N(21)-N(22)-B(1)-N(12)	-60.9(3)
C(13)-N(12)-B(1)-N(32)	128.1(3)
N(11)-N(12)-B(1)-N(32)	-56.9(3)
C(13)-N(12)-B(1)-N(22)	-113.8(3)
N(11)-N(12)-B(1)-N(22)	61.1(3)
N(11)-N(12)-C(13)-C(14)	-0.7(3)
B(1)-N(12)-C(13)-C(14)	174.7(2)
N(11)-N(12)-C(13)-C(17)	178.7(2)
B(1)-N(12)-C(13)-C(17)	-5.9(4)
C(15)-C(14)-C(13)-N(12)	0.8(3)
C(15)-C(14)-C(13)-C(17)	-178.5(3)
N(31)-N(32)-C(33)-C(34)	0.4(3)
B(1)-N(32)-C(33)-C(34)	-178.0(3)
N(31)-N(32)-C(33)-C(37)	-178.2(3)
B(1)-N(32)-C(33)-C(37)	3.4(5)
N(32)-C(33)-C(34)-C(35)	-1.1(3)
C(37)-C(33)-C(34)-C(35)	177.3(3)
N(31)-C(35)-C(34)-C(33)	1.6(3)
C(36)-C(35)-C(34)-C(33)	-176.6(3)
C(2)-N(2)-C(3)-C(4)	-178.8(3)
C(2)-N(2)-C(3)-C(8)	-1.0(4)
C(1)-N(1)-C(8)-C(7)	177.7(3)
C(1)-N(1)-C(8)-C(3)	-1.8(4)
N(2)-C(3)-C(8)-N(1)	3.2(4)
C(4)-C(3)-C(8)-N(1)	-179.0(3)
N(2)-C(3)-C(8)-C(7)	-176.3(3)
C(4)-C(3)-C(8)-C(7)	1.5(5)
N(22)-N(21)-C(25)-C(24)	0.4(3)
Mo(1)-N(21)-C(25)-C(24)	171.11(17)
N(22)-N(21)-C(25)-C(26)	-178.9(2)
Mo(1)-N(21)-C(25)-C(26)	-8.2(4)
C(23)-C(24)-C(25)-N(21)	-0.2(3)
C(23)-C(24)-C(25)-C(26)	179.0(3)
N(2)-C(3)-C(4)-C(5)	177.0(3)
C(8)-C(3)-C(4)-C(5)	-0.8(5)
N(1)-C(8)-C(7)-C(6)	178.9(4)
C(3)-C(8)-C(7)-C(6)	-1.5(6)
C(3)-C(4)-C(5)-C(6)	0.2(6)
C(8)-C(7)-C(6)-C(5)	0.9(7)
C(4)-C(5)-C(6)-C(7)	-0.2(7)
Mo(1)-S(1)-S(2)-C(2)	151.91(10)

Symmetry transformations used to generate equivalent atoms:

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) of **4**.

	x	y	z	U(eq)
H(14A)	301	6028	4485	35
H(27A)	3076	11726	7484	49
H(27B)	2507	11384	6149	49
H(27C)	3767	12592	6586	49
H(24A)	6186	12131	6147	33
H(26A)	7583	9506	5706	49
H(26B)	8322	10145	6951	49
H(26C)	8178	10973	5907	49
H(9A)	2159	9438	7403	29
H(36A)	5449	6183	9717	54
H(36B)	5444	6759	10968	54
H(36C)	6613	7421	10250	54
H(34A)	3815	8245	11098	42
H(16A)	3752	5529	4648	52
H(16B)	2152	4696	4321	52
H(16C)	3066	4657	5544	52
H(17A)	258	9013	5649	53
H(17B)	-409	8100	6524	53
H(17C)	-917	7758	5183	53
H(4A)	8386	2470	8140	47
H(37A)	2190	10255	9393	64
H(37B)	1879	9535	10487	64
H(37C)	1011	8967	9253	64
H(7A)	11943	6191	8628	60
H(5A)	10759	2470	8447	59
H(6A)	12533	4331	8702	69

Figure S1. Projection view of (Tp*)MoO(qdt) (**4**) along *a* showing the solid-state packing in the triclinic unit cell.

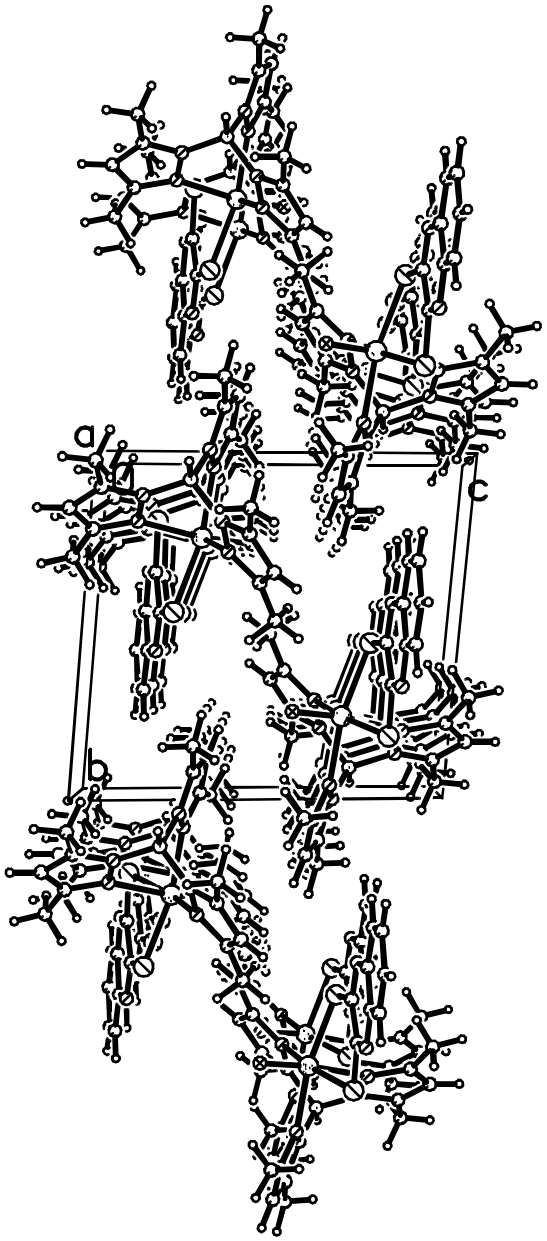
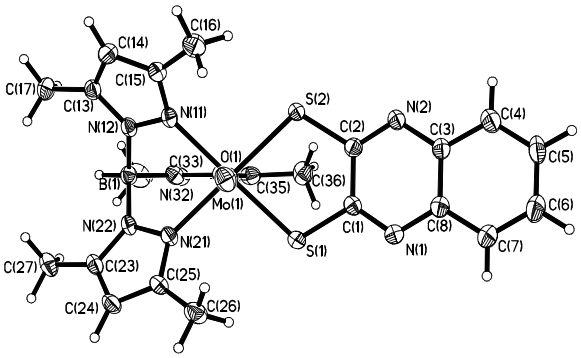
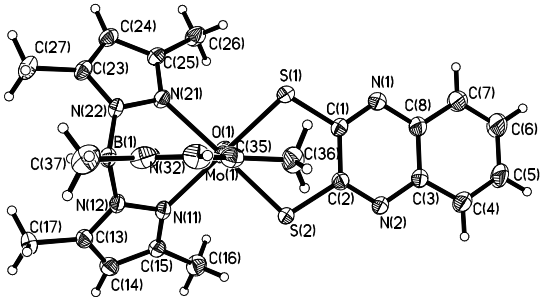


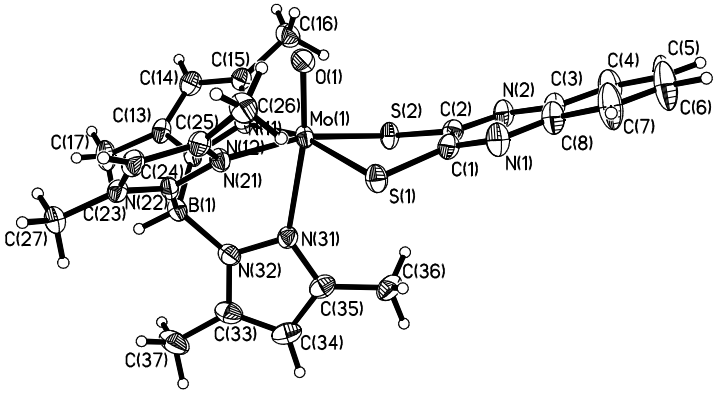
Figure S2. ORTEP views of (Tp*)MoO(qdt) (**4**) with 50% probability displacement ellipsoids. H-atoms arbitrarily drawn small for clarity. (a-e) show different orientations.



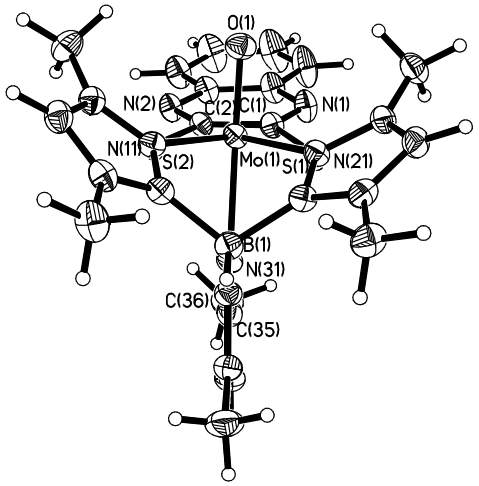
(a). Top View along O≡Mo bond.



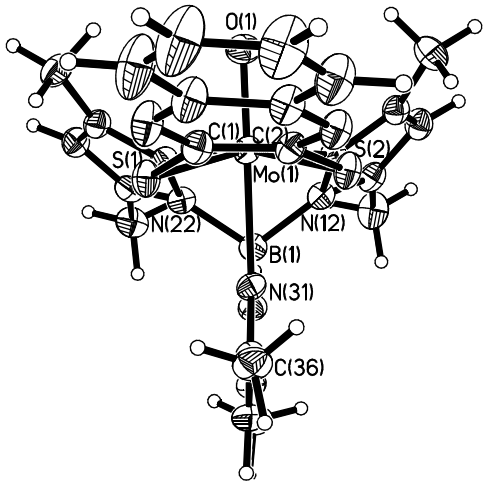
(b). Bottom View along N31-Mo bond.



(c). Side View.



(d). Front View along HB-Mo bond.



(e). Rear View along qdt plane.