Table S1. Crystal data and structure refinement for $(Et_4N)[MoOCl_2(S_2C_2Me_2)]$.

Identification code	bsl77a
Empirical formula	C12 H26 Cl2 Mo N O S2
Formula weight	431.30
Temperature	213(2) K
Wavelength	0.71073 Å
Crystal system, space group	monoclinic, C2/c
Unit cell dimensions	a = 9.2689(7) Å alpha = 90 deg.
	b = 14.383(2) Å beta = 94.046(7) deg.
	c = 27.723(3) Å gamma = 90 deg.
Volume	3686.6(7) $Å^3$
Z, Calculated density	8, 1.554 Mg/m^3
Absorption coefficient	1.221 mm^{-1}
F(000)	1768
Crystal size	0.02 x 0.40 x 0.29 mm
Theta range for data collection	1.47 to 28.29 deg.
Limiting indices	-12<=h<=11, -8<=k<=18, -36<=l<=36
Reflections collected / unique	11838 / 4459 [R(int) = 0.0306]
Completeness to theta = 28.29	97.0 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4459 / 0 / 193
Goodness-of-fit on F^2	1.070
Final R indices [I>2sigma(I)]	R1 = 0.0319, wR2 = 0.0785
R indices (all data)	R1 = 0.0396, wR2 = 0.0820
Largest diff. peak and hole	0.505 and -0.535 $e.Å^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $(Et_4N)[MoOCl_2(S_2C_2Me_2)]$.

	x	y	z	U(eq)
Mo(1)	2671(1)	3829(1)	1151(1)	28(1)
S(1)	688(1)	3133(1)	1502(1)	33(1)
S(2)	2800(1)	2363(1)	782(1)	41(1)
Cl(1)	1251(1)	5202(1)	1174(1)	39(1)
Cl(2)	3601(1)	4377(1)	433(1)	49(1)
O(1)	4014(2)	3872(1)	1590(1)	42(1)
N(1)	0	6381(2)	2500	30(1)
N(2)	-2500	7500	5000	27(1)
C(1)	1768(3)	1589(2)	1110(1)	34(1)
C(2)	862(3)	1919(2)	1421(1)	33(1)
C(3)	-133(4)	1339(2)	1706(1)	51(1)
C(4)	1974(4)	579(2)	985(1)	49(1)
C(5)	-747(3)	6980(2)	2862(1)	35(1)
C(6)	1078(3)	5783(2)	2801(1)	36(1)
C(7)	1946(4)	5109(2)	2519(1)	48(1)
C(8)	-1840(4)	7657(2)	2644(1)	55(1)
C(9)	-2848(5)	7219(3)	4465(2)	28(1)
C(10)	-2573(6)	8509(3)	5064(2)	30(1)
C(9A)	-1588(5)	8073(4)	4711(2)	30(1)
C(10A)	-4159(5)	7754(3)	4878(2)	29(1)
C(11)	-1915(4)	7809(3)	4128(1)	57(1)
C(12)	-4314(5)	8841(2)	4919(1)	69(1)

Table S3. Bond lengths [Å] and angles [°] for $(Et_4N)[MoOCl_2(S_2C_2Me_2)]$.

Mo(1)-O(1)	1.6794(19)	C(2)-S(1)-Mo(1)	106.60(9)
Mo(1)-S(2)	2.3500(8)	C(1)-S(2)-Mo(1)	107.27(9)
Mo(1)-Cl(2)	2.3597(8)	C(6)-N(1)-C(6)#1	111.2(3)
Mo(1)-S(1)	2.3620(7)	C(6)-N(1)-C(5)	105.67(15)
Mo(1)-Cl(1)	2.3770(7)	C(6)#1-N(1)-C(5)	111.63(16)
S(1)-C(2)	1.769(3)	C(6)-N(1)-C(5)#1	111.63(16)
S(2)-C(1)	1.760(3)	C(6)#1-N(1)-C(5)#1	105.67(15)
N(1)-C(6)	1.522(3)	C(5)-N(1)-C(5)#1	111.1(3)
N(1)-C(6)#1	1.522(3)	C(9A)#2-N(2)-C(9A)	180.0(5)
N(1)-C(5)	1.525(3)	C(9A)#2-N(2)-C(10)	117.3(3)
N(1)-C(5)#1	1.525(3)	C(9A)-N(2)-C(10)	62.7(3)
N(2)-C(9A)#2	1.460(5)	C(9A)#2-N(2)-C(10)#2	62.7(3)
N(2)-C(9A)	1.460(5)	C(9A)-N(2)-C(10)#2	117.3(3)
N(2)-C(10)	1.464(5)	C(10)-N(2)-C(10)#2	180.000(2)
N(2)-C(10)#2	1.464(5)	C(9A)#2-N(2)-C(9)#2	73.2(3)
N(2)-C(9)#2	1.549(5)	C(9A)-N(2)-C(9)#2	106.8(3)
N(2)-C(9)	1.549(5)	C(10)-N(2)-C(9)#2	68.5(3)
N(2)-C(10A)#2	1.594(4)	C(10)#2-N(2)-C(9)#2	111.5(3)
N(2)-C(10A)	1.594(4)	C(9A)#2-N(2)-C(9)	106.8(3)
C(1)-C(2)	1.333(4)	C(9A)-N(2)-C(9)	73.2(3)
C(1)-C(4)	1.509(4)	C(10)-N(2)-C(9)	111.5(3)
C(2)-C(3)	1.509(4)	C(10)#2-N(2)-C(9)	68.5(3)
C(5)-C(8)	1.501(4)	C(9)#2-N(2)-C(9)	180.000(2)
C(6)-C(7)	1.513(4)	C(9A)#2-N(2)-C(10A)#2	110.0(3)
C(9)-C(11)	1.567(6)	C(9A)-N(2)-C(10A)#2	70.0(3)
C(9)-C(10)#2	1.697(7)	C(10)-N(2)-C(10A)#2	104.7(3)
C(10)-C(9)#2	1.697(7)	C(10)#2-N(2)-C(10A)#2	75.3(3)
C(10)-C(12)	1.704(7)	C(9)#2-N(2)-C(10A)#2	73.9(3)
C(9A)-C(11)	1.667(6)	C(9)-N(2)-C(10A)#2	106.1(3)
C(9A)-C(10A)#2	1.756(7)	C(9A)#2-N(2)-C(10A)	70.0(3)
C(10A)-C(12)	1.574(6)	C(9A)-N(2)-C(10A)	110.0(3)
C(10A)-C(9A)#2	1.756(7)	C(10)-N(2)-C(10A)	75.3(3)
		C(10)#2-N(2)-C(10A)	104.7(3)
O(1)-Mo(1)-S(2)	106.89(8)	C(9)#2-N(2)-C(10A)	106.1(3)
O(1)-Mo(1)-Cl(2)	107.64(8)	C(9)-N(2)-C(10A)	73.9(3)
S(2)-Mo(1)-Cl(2)	84.27(3)	C(10A)#2-N(2)-C(10A)	180.000(1)
O(1)-Mo(1)-S(1)	106.01(7)	C(2)-C(1)-C(4)	125.9(3)
S(2)-Mo(1)-S(1)	82.15(3)	C(2)-C(1)-S(2)	119.9(2)
Cl(2)-Mo(1)-S(1)	146.10(3)	C(4)-C(1)-S(2)	114.1(2)
O(1)-Mo(1)-Cl(1)	109.47(8)	C(1)-C(2)-C(3)	125.4(3)
S(2)-Mo(1)-Cl(1)	143.37(3)	C(1)-C(2)-S(1)	120.0(2)
Cl(2)-Mo(1)-Cl(1)	88.92(3)	C(3)-C(2)-S(1)	114.5(2)
S(1)-Mo(1)-Cl(1)	83.83(3)	C(8)-C(5)-N(1)	115.3(2)

C(7)-C(6)-N(1)	115.5(2)	N(2)-C(9A)-C(10A)#2	58.5(2)
N(2)-C(9)-C(11)	110.1(3)	C(11)-C(9A)-C(10A)#2	120.8(4)
N(2)-C(9)-C(10)#2	53.4(2)	C(12)-C(10A)-N(2)	107.7(3)
C(11)-C(9)-C(10)#2	133.3(4)	C(12)-C(10A)-C(9A)#2	131.2(4)
N(2)-C(10)-C(9)#2	58.1(2)	N(2)-C(10A)-C(9A)#2	51.4(2)
N(2)-C(10)-C(12)	107.5(3)	C(9)-C(11)-C(9A)	67.3(3)
C(9)#2-C(10)-C(12)	121.1(4)	C(10A)-C(12)-C(10)	69.5(3)
N(2)-C(9A)-C(11)	109.4(3)		

Table S4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $(Et_4N)[MoOCl_2(S_2C_2Me_2)]$. The anisotropic displacement factor exponent takes the form: $-2\,pi^2\,[\,h^2\,a^{*2}\,U11 + ... + 2\,h\,k\,a^*\,b^*\,U12\,]$

	U11	U22	U33	U23	U13	U12
Mo(1)	29(1)	28(1)	27(1)	2(1)	2(1)	-3(1)
S(1)	31(1)	33(1)	34(1)	-1(1)	7(1)	-3(1)
S(2)	46(1)	35(1)	44(1)	-7(1)	16(1)	-1(1)
Cl(1)	50(1)	30(1)	38(1)	1(1)	4(1)	5(1)
Cl(2)	55(1)	54(1)	41(1)	9(1)	17(1)	-7(1)
O(1)	39(1)	44(1)	42(1)	8(1)	-7(1)	-7(1)
N(1)	37(2)	24(1)	27(1)	0	1(1)	0
N(2)	29(1)	24(1)	27(1)	1(1)	-4(1)	-2(1)
C(1)	35(1)	29(1)	38(1)	-3(1)	-5(1)	-3(1)
C(2)	31(1)	31(1)	36(1)	1(1)	-4(1)	-6(1)
C(3)	45(2)	46(2)	62(2)	9(2)	10(2)	-12(1)
C(4)	58(2)	33(2)	54(2)	-8(1)	-5(2)	-1(1)
C(5)	49(2)	28(1)	29(1)	-3(1)	7(1)	1(1)
C(6)	44(1)	32(1)	33(1)	1(1)	-5(1)	3(1)
C(7)	56(2)	41(2)	47(2)	-1(1)	-1(1)	16(1)
C(8)	69(2)	44(2)	53(2)	10(2)	20(2)	22(2)
C(9)	28(2)	25(2)	29(2)	-6(2)	-1(2)	0(2)
C(10)	39(3)	20(2)	30(3)	-3(2)	1(2)	0(2)
C(9A)	28(2)	29(2)	35(3)	1(2)	5(2)	-5(2)
C(10A)	23(2)	31(2)	32(3)	-2(2)	-1(2)	1(2)
C(11)	46(2)	83(3)	42(2)	22(2)	14(1)	9(2)
C(12)	111(3)	44(2)	50(2)	-2(2)	-1(2)	43(2)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for $(Et_4N)[MoOCl_2(S_2C_2Me_2)]$.

	x	y	z	U(eq)
H(3A)	-675	1738	1904	76
H(3B)	428	911	1908	76
H(3C)	-787	999	1488	76
H(4A)	2688	527	752	73
H(4B)	1074	325	852	73
H(4C)	2292	241	1272	73
H(5A)	-1226	6573	3079	42
H(5B)	-13	7325	3054	42
H(6A)	1746	6191	2984	44
H(6B)	555	5432	3031	44
H(7A)	2592	4765	2738	72
H(7B)	2495	5448	2296	72
H(7C)	1301	4687	2343	72
H(8A)	-2252	8002	2897	82
H(8B)	-2591	7325	2460	82
H(8C)	-1376	8078	2435	82
H(9A)	-3862	7306	4381	33
H(9B)	-2637	6571	4428	33
H(10A)	-1923	8826	4865	36
H(10B)	-2319	8664	5396	36
H(9AA)	-584	7972	4806	37
H(9AB)	-1807	8716	4760	37
H(10A)	-4765	7443	5094	34
H(10A)	-4441	7564	4553	34
H(11A)	-2144	7627	3798	85
H(11B)	-2121	8458	4164	85
H(11C)	-907	7698	4212	85
H(11D)	-1320	8187	3937	85
H(11E)	-1693	7165	4080	85
H(11F)	-2915	7919	4031	85
H(12A)	-4398	9502	4957	103
H(12B)	-4584	8674	4590	103
H(12C)	-4942	8533	5129	103
H(12D)	-5308	9010	4847	103
H(12E)	-4011	9037	5241	103
H(12F)	-3724	9138	4693	103

Table S6. Crystal data and structure refinement for $(Et_4N)[MoOCl_2(bdt)]$.

Identification code	mm50
Empirical formula	C14 H24 Cl2 Mo N O S2
Formula weight	453.30
Temperature	213(2) K
Wavelength	0.71073 Å
Crystal system, space group	monoclinic, P2(1)
Unit cell dimensions	a = 7.924(4) Å alpha = 90 deg. b = 14.434(7) Å beta = 94.285(5) deg. c = 8.619(4) Å gamma = 90 deg.
Volume	983.0(9) $Å^3$
Z, Calculated density	2, 1.531 Mg/m^3
Absorption coefficient	1.149 mm^{-1}
F(000)	462
Crystal size	0.5 x 0.38 x 0.04 mm
Theta range for data collection	2.37 to 28.30 deg.
Limiting indices	-9<=h<=10, -19<=k<=17, -11<=l<=11
Reflections collected / unique	6274 / 3873 [R(int) = 0.0192]
Completeness to theta = 28.30	95.3 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3873 / 1 / 190
Goodness-of-fit on F^2	1.071
Final R indices [I>2sigma(I)]	R1 = 0.0208, wR2 = 0.0543
R indices (all data)	R1 = 0.0211, wR2 = 0.0544
Absolute structure parameter	-0.08(3)
Largest diff. peak and hole	0.569 and -0.610 e. $Å^{-3}$

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for (Et_4N)[$MoOCl_2$(bdt)].

	x	y	z	U(eq)
Mo(1)	-4283(1)	9500(1)	-1116(1)	25(1)
S(1)	-1433(1)	9084(1)	-1319(1)	31(1)
S(2)	-4543(1)	7959(1)	-233(1)	31(1)
Cl(1)	-7074(1)	9257(1)	-2166(1)	45(1)
Cl(2)	-3863(1)	10454(1)	-3300(1)	36(1)
O(1)	-4329(3)	10182(1)	456(2)	43(1)
N(1)	823(3)	10401(2)	3493(2)	33(1)
C(1)	556(3)	7791(2)	276(3)	31(1)
C(2)	830(3)	6989(2)	1149(3)	35(1)
C(3)	-2468(3)	7588(2)	328(3)	26(1)
C(4)	-544(4)	6480(2)	1590(3)	37(1)
C(5)	-1088(3)	8091(2)	-153(3)	26(1)
C(6)	-2190(3)	6775(2)	1191(3)	33(1)
C(7)	-375(4)	10982(3)	2421(3)	47(1)
C(8)	-1536(5)	11619(3)	3248(5)	69(1)
C(9)	1963(4)	11013(2)	4551(3)	38(1)
C(10)	3098(5)	11662(3)	3735(4)	56(1)
C(11)	1855(4)	9820(2)	2435(3)	44(1)
C(12)	3120(4)	9179(3)	3254(4)	55(1)
C(13)	-153(3)	9789(2)	4545(3)	36(1)
C(14)	-1365(4)	9106(3)	3733(4)	53(1)

Table S8. Bond lengths [Å] and angles [°] for $(Et_4N)[MoOCl_2(bdt)]$.

Mo(1)-O(1)	1.677(2)	C(3)-S(2)-Mo(1)	105.81(8)
Mo(1)-Cl(1)	2.3523(12)	C(9)-N(1)-C(13)	106.62(19)
Mo(1)-S(1)	2.3558(12)	C(9)-N(1)-C(11)	111.0(2)
Mo(1)-S(2)	2.3648(12)	O(1)-Mo(1)-S(2)	106.51(8)
Mo(1)-Cl(2)	2.3760(11)	Cl(1)-Mo(1)-S(2)	83.21(2)
S(1)-C(5)	1.759(2)	S(1)-Mo(1)-S(2)	83.73(3)
S(2)-C(3)	1.762(2)	O(1)-Mo(1)-Cl(2)	108.24(8)
N(1)-C(9)	1.518(3)	Cl(1)-Mo(1)-Cl(2)	87.98(3)
N(1)-C(13)	1.518(3)	S(1)-Mo(1)-Cl(2)	84.10(2)
N(1)-C(11)	1.521(4)	C(13)-N(1)-C(11)	111.0(2)
N(1)-C(7)	1.526(3)	C(9)-N(1)-C(7)	111.0(2)
C(1)-C(2)	1.389(4)	C(13)-N(1)-C(7)	111.1(2)
C(1)-C(5)	1.396(3)	C(11)-N(1)-C(7)	106.2(2)
C(2)-C(4)	1.390(4)	C(2)-C(1)-C(5)	120.5(2)
C(3)-C(6)	1.398(3)	C(1)-C(2)-C(4)	119.7(2)
C(3)-C(5)	1.401(3)	C(6)-C(3)-C(5)	119.8(2)
C(4)-C(6)	1.391(4)	C(6)-C(3)-S(2)	120.54(18)
C(7)-C(8)	1.515(5)	C(5)-C(3)-S(2)	119.61(17)
C(9)-C(10)	1.509(4)	C(2)-C(4)-C(6)	120.7(3)
C(11)-C(12)	1.501(5)	C(1)-C(5)-C(3)	119.6(2)
C(13)-C(14)	1.511(4)	C(1)-C(5)-S(1)	120.43(18)
		C(3)-C(5)-S(1)	119.96(17)
O(1)-Mo(1)-Cl(1)	108.78(8)	C(4)-C(6)-C(3)	119.8(2)
O(1)-Mo(1)-S(1)	106.78(7)	C(8)-C(7)-N(1)	114.9(2)
Cl(1)-Mo(1)-S(1)	144.29(3)	C(10)-C(9)-N(1)	115.5(2)
S(2)-Mo(1)-Cl(2)	145.16(3)	C(12)-C(11)-N(1)	115.3(2)
C(5)-S(1)-Mo(1)	105.93(8)	C(14)-C(13)-N(1)	115.9(2)

Table S9. Anisotropic displacement parameters ($Å^2$ x 10^3) for $(Et_4N)[MoOCl_2(bdt)]$. The anisotropic displacement factor exponent takes the form: $-2\ pi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
Mo(1)	21(1)	26(1)	29(1)	2(1)	2(1)	2(1)
S(1)	21(1)	30(1)	42(1)	11(1)	5(1)	1(1)
S(2)	22(1)	31(1)	42(1)	6(1)	6(1)	-1(1)
Cl(1)	22(1)	55(1)	57(1)	22(1)	-3(1)	-4(1)
Cl(2)	29(1)	39(1)	40(1)	13(1)	1(1)	-3(1)
O(1)	50(1)	38(1)	40(1)	-8(1)	5(1)	7(1)
N(1)	32(1)	43(1)	24(1)	2(1)	2(1)	1(1)
C(1)	27(1)	32(1)	33(1)	-1(1)	2(1)	3(1)
C(2)	35(1)	37(2)	33(1)	0(1)	-1(1)	12(1)
C(3)	25(1)	26(1)	28(1)	1(1)	5(1)	1(1)
C(4)	51(2)	30(1)	32(1)	5(1)	5(1)	10(1)
C(5)	26(1)	24(1)	28(1)	2(1)	4(1)	2(1)
C(6)	39(1)	28(1)	32(1)	3(1)	8(1)	0(1)
C(7)	39(1)	67(2)	34(1)	16(1)	-3(1)	2(1)
C(8)	57(2)	86(3)	66(2)	30(2)	13(2)	29(2)
C(9)	40(1)	43(2)	30(1)	2(1)	-1(1)	-5(1)
C(10)	55(2)	58(2)	53(2)	10(2)	0(2)	-17(2)
C(11)	40(1)	58(2)	34(1)	-9(1)	11(1)	-2(1)
C(12)	49(2)	64(2)	52(2)	-10(2)	10(1)	12(1)
C(13)	36(1)	46(2)	27(1)	1(1)	6(1)	-3(1)
C(14)	48(2)	64(2)	48(2)	-5(2)	5(1)	-16(2)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $(Et_4N)[MoOCl_2(bdt)]$.

	x	y	z	U(eq)
H(1B)	1474	8130	-26	37
H(2A)	1927	6794	1438	42
H(4A)	-360	5937	2158	45
H(6A)	-3102	6432	1497	39
H(7A)	294	11354	1759	56
H(7B)	-1066	10567	1754	56
H(8A)	-2230	11964	2493	104
H(8B)	-869	12039	3904	104
H(8C)	-2244	11257	3871	104
H(9A)	1257	11378	5190	46
H(9B)	2666	10618	5242	46
H(10A)	3742	12032	4492	84
H(10B)	2420	12059	3047	84
H(10C)	3854	11309	3147	84
H(11A)	1081	9453	1760	52
H(11B)	2451	10234	1779	52
H(12A)	3719	8850	2499	82
H(12B)	2543	8746	3872	82
H(12C)	3908	9533	3915	82
H(13A)	655	9446	5223	43
H(13B)	-789	10185	5199	43
H(14A)	-1910	8752	4495	80
H(14B)	-752	8697	3100	80
H(14C)	-2203	9436	3088	80

Table S11. Crystal data and structure refinement for $(Et_4N)[MoO(2\text{-}AdS)_2(S_2C_2Me_2)]$.

Identification code	bsl80a
Empirical formula	C32 H56 Cl0 Mo N O S4
Formula weight	694.96
Temperature	213(2) K
Wavelength	0.71073 A
Crystal system, space group	monoclinic, P2(1)/c
Unit cell dimensions	a = 12.178(6) Å alpha = 90 deg. b = 17.812(9) Å beta = 109.132(7) deg. c = 17.054(9) Å gamma = 90 deg.
Volume	3495(3) $Å^3$
Z, Calculated density	4, 1.321 Mg/m^3
Absorption coefficient	0.639 mm^{-1}
F(000)	1476
Crystal size	0.40 x 0.26 x 0.26 mm
Theta range for data collection	1.70 to 22.50 deg.
Limiting indices	-12<=h<=13, -12<=k<=19, -18<=l<=17
Reflections collected / unique	14609 / 4573 [R(int) = 0.0505]
Completeness to theta = 22.50	100.0 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4573 / 0 / 453
Goodness-of-fit on F^2	1.054
Final R indices [I>2sigma(I)]	R1 = 0.0347, wR2 = 0.0874
R indices (all data)	R1 = 0.0402, wR2 = 0.0930
Largest diff. peak and hole	0.768 and -0.366 e. $Å^{-3}$

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $(Et_4N)[MoO(2\text{-}AdS)_2(S_2C_2Me_2)]$.

	x	y	z	U(eq)
Mo(1)	1487(1)	6042(1)	3430(1)	42(1)
S(1)	-142(1)	5836(1)	2205(1)	49(1)
S(2)	62(1)	6746(1)	3809(1)	53(1)
S(3)	2659(1)	6148(1)	2568(1)	62(1)
S(4)	2642(1)	7024(1)	4260(1)	50(1)
O(1)	1765(2)	5218(1)	3952(2)	60(1)
N(1)	1126(2)	8545(2)	1722(2)	50(1)
C(1)	-1402(3)	6154(2)	2400(2)	48(1)
C(2)	-1310(3)	6557(2)	3074(2)	51(1)
C(3)	-2521(3)	5941(2)	1747(3)	68(1)
C(4)	-2321(3)	6905(3)	3276(3)	76(1)
C(5)	2356(8)	5315(6)	1862(7)	44(2)
C(7)	3113(9)	4126(4)	1477(6)	80(3)
C(8)	1971(6)	5581(4)	969(7)	58(2)
C(9)	1630(8)	4872(6)	411(6)	74(3)
C(10)	2683(15)	4379(9)	560(9)	62(4)
C(12)	4395(6)	5227(6)	1821(7)	72(3)
C(14)	3640(16)	4801(7)	359(11)	73(4)
C(5T)	2408(11)	4807(10)	1755(7)	71(4)
C(6T)	1843(14)	4345(8)	947(10)	102(6)
C(7T)	2080(10)	5443(10)	110(6)	95(5)
C(8T)	4185(8)	4972(7)	1305(9)	66(3)
C(9T)	2117(11)	5629(9)	1570(10)	49(3)
C(10T)	3640(20)	4491(10)	563(14)	73(5)
C(11T)	2290(20)	4595(15)	267(17)	85(8)
C(6)	3548(6)	4763(3)	2031(3)	90(2)
C(11)	3950(5)	5617(5)	1049(5)	129(3)
C(13)	2813(6)	5958(3)	848(3)	92(2)
C(15)	4188(3)	6857(2)	4370(2)	45(1)
C(16)	4732(3)	6055(2)	5658(2)	51(1)
C(17)	4660(3)	6095(2)	4752(2)	45(1)
C(18)	5893(3)	6010(2)	4694(2)	52(1)
C(19)	4935(3)	7490(2)	4886(2)	50(1)
C(20)	5505(3)	6676(2)	6157(2)	54(1)
C(21)	6668(3)	6638(2)	5188(2)	53(1)
C(22)	6169(3)	7401(2)	4835(3)	58(1)
C(23)	4997(3)	7433(2)	5796(2)	54(1)
C(24)	6734(3)	6592(2)	6094(2)	61(1)
C(25)	46(6)	8361(4)	978(5)	69(2)
C(27)	916(6)	8329(4)	2512(4)	67(2)

C(29)	2152(6)	8159(4)	1632(5)	74(2)
C(31)	1232(7)	9415(4)	1673(5)	73(2)
C(25A)	919(9)	7687(5)	1529(8)	76(3)
C(27A)	156(10)	8904(6)	1882(9)	85(4)
C(29A)	2247(10)	8594(7)	2490(8)	85(4)
C(31A)	1343(10)	8874(5)	985(7)	70(3)
C(26)	-221(4)	7517(3)	890(3)	92(2)
C(28)	-137(5)	8628(3)	2656(3)	97(2)
C(30)	3313(4)	8319(3)	2367(4)	103(2)
C(32)	1607(6)	9706(3)	989(4)	111(2)

Table S13. Bond lengths [Å] and angles [°] for $(Et_4N)[MoO(2\text{-}AdS)_2(S_2C_2Me_2)]$.

Mo(1)-O(1)	1.692(2)	C(11)-C(13)	1.447(8)
Mo(1)-S(3)	2.3687(13)	C(15)-C(19)	1.532(5)
Mo(1)-S(1)	2.3906(13)	C(15)-C(17)	1.535(5)
Mo(1)-S(4)	2.3951(12)	C(16)-C(17)	1.520(5)
Mo(1)-S(2)	2.3953(12)	C(16)-C(20)	1.520(5)
S(1)-C(1)	1.767(3)	C(17)-C(18)	1.544(5)
S(2)-C(2)	1.762(4)	C(18)-C(21)	1.527(5)
S(3)-C(9T)	1.857(15)	C(19)-C(23)	1.532(5)
S(3)-C(5)	1.870(11)	C(19)-C(22)	1.542(5)
S(4)-C(15)	1.854(3)	C(20)-C(23)	1.527(5)
N(1)-C(27A)	1.447(11)	C(20)-C(24)	1.543(5)
N(1)-C(29)	1.477(7)	C(21)-C(24)	1.522(5)
N(1)-C(31A)	1.488(11)	C(21)-C(22)	1.530(5)
N(1)-C(27)	1.502(7)	C(25)-C(26)	1.535(8)
N(1)-C(25)	1.534(7)	C(27)-C(28)	1.481(7)
N(1)-C(29A)	1.554(12)	C(29)-C(30)	1.578(9)
N(1)-C(31)	1.561(8)	C(31)-C(32)	1.478(8)
N(1)-C(25A)	1.565(10)	C(25A)-C(26)	1.489(11)
C(1)-C(2)	1.327(5)	C(27A)-C(28)	1.555(13)
C(1)-C(3)	1.499(5)	C(29A)-C(30)	1.465(12)
C(2)-C(4)	1.515(5)	C(31A)-C(32)	1.515(10)
C(5)-C(8)	1.515(13)		
C(5)-C(6)	1.697(10)	O(1)-Mo(1)-S(3)	109.80(9)
C(7)-C(6)	1.460(9)	O(1)-Mo(1)-S(1)	107.00(9)
C(7)-C(10)	1.543(18)	S(3)-Mo(1)-S(1)	88.05(6)
C(8)-C(13)	1.297(9)	O(1)-Mo(1)-S(4)	110.14(10)
C(8)-C(9)	1.553(12)	S(3)-Mo(1)-S(4)	87.27(4)
C(9)-C(10)	1.505(19)	S(1)-Mo(1)-S(4)	141.90(4)
C(10)-C(14)	1.52(3)	O(1)-Mo(1)-S(2)	110.43(9)
C(12)-C(11)	1.430(11)	S(3)-Mo(1)-S(2)	139.76(4)
C(12)-C(6)	1.455(9)	S(1)-Mo(1)-S(2)	81.34(5)
C(14)-C(11)	1.830(17)	S(4)-Mo(1)-S(2)	78.18(5)
C(5T)-C(6)	1.313(12)	C(1)-S(1)-Mo(1)	108.00(13)
C(5T)-C(9T)	1.515(18)	C(2)-S(2)-Mo(1)	108.04(12)
C(5T)-C(6T)	1.557(18)	C(9T)-S(3)-C(5)	22.9(3)
C(6T)-C(11T)	1.50(3)	C(9T)-S(3)-Mo(1)	115.0(4)
C(7T)-C(11T)	1.54(3)	C(5)-S(3)-Mo(1)	107.7(3)
C(7T)-C(13)	1.578(13)	C(15)-S(4)-Mo(1)	108.84(11)
C(8T)-C(11)	1.230(12)	C(27A)-N(1)-C(29)	175.2(7)
C(8T)-C(10T)	1.49(3)	C(27A)-N(1)-C(31A)	111.6(7)
C(8T)-C(6)	1.703(14)	C(29)-N(1)-C(31A)	72.8(5)
C(9T)-C(13)	1.807(15)	C(27A)-N(1)-C(27)	63.5(6)
C(10T)-C(11T)	1.57(4)	C(29)-N(1)-C(27)	112.0(4)

C(31A)-N(1)-C(27)	171.5(5)	C(11T)-C(7T)-C(13)	114.3(11)
C(27A)-N(1)-C(25)	73.7(6)	C(11)-C(8T)-C(10T)	104.4(13)
C(29)-N(1)-C(25)	109.9(5)	C(11)-C(8T)-C(6)	110.8(8)
C(31A)-N(1)-C(25)	74.1(5)	C(10T)-C(8T)-C(6)	108.1(10)
C(27)-N(1)-C(25)	109.6(4)	C(5T)-C(9T)-C(13)	108.9(9)
C(27A)-N(1)-C(29A)	111.3(7)	C(5T)-C(9T)-S(3)	107.6(11)
C(29)-N(1)-C(29A)	64.8(5)	C(13)-C(9T)-S(3)1T)	109.4(17)
C(31A)-N(1)-C(29A)	109.8(7)	C(6T)-C(11T)-C(7T)	110(2)
C(27)-N(1)-C(29A)	67.6(5)	C(6T)-C(11T)-C(10T)	109(2)
C(25)-N(1)-C(29A)	170.9(6)	C(7T)-C(11T)-C(10T)	105.7(17)
C(27A)-N(1)-C(31)	70.0(5)	C(5T)-C(6)-C(12)	129.0(7)
C(29)-N(1)-C(31)	111.6(4)	C(5T)-C(6)-C(7)	72.4(9)
C(31A)-N(1)-C(31)	61.5(5)	C(12)-C(6)-C(7)	114.7(7)
C(27)-N(1)-C(31)	110.1(4)	C(5T)-C(6)-C(5)	32.9(7)
C(25)-N(1)-C(31)	103.4(4)	C(12)-C(6)-C(5)	105.3(6)
C(29A)-N(1)-C(31)	85.6(6)	C(7)-C(6)-C(5)	103.4(6)
C(27A)-N(1)-C(25A)	112.7(7)	C(5T)-C(6)-C(8T)	113.9(7)
C(29)-N(1)-C(25A)	67.0(5)	C(12)-C(6)-C(8T)	33.7(5)
C(31A)-N(1)-C(25A)	105.6(6)	C(7)-C(6)-C(8T)	81.6(6)
C(27)-N(1)-C(25A)	82.9(6)	C(5)-C(6)-C(8T)	108.5(6)
C(25)-N(1)-C(25A)	65.3(5)	C(8T)-C(11)-C(12)	40.8(5)
C(29A)-N(1)-C(25A)	105.6(6)	C(8T)-C(11)-C(13)	124.6(6)
C(31)-N(1)-C(25A)	165.7(6)	C(12)-C(11)-C(13)	117.7(6)
C(2)-C(1)-C(3)	125.3(3)	C(8T)-C(11)-C(14)	57.4(10)
C(2)-C(1)-S(1)	120.3(3)	C(12)-C(11)-C(14)	98.1(9)
C(3)-C(1)-S(1)	114.4(3)	C(13)-C(11)-C(14)	101.6(7)
C(1)-C(2)-C(4)	125.0(3)	C(8)-C(13)-C(11)	119.4(5)
C(1)-C(2)-S(2)	120.7(3)	C(8)-C(13)-C(7T)	63.6(8)
C(4)-C(2)-S(2)	114.3(3)	C(11)-C(13)-C(7T)	101.1(6)
C(8)-C(5)-C(6)	108.6(6)	C(8)-C(13)-C(9T)	32.0(6)
C(8)-C(5)-S(3)	109.2(8)	C(11)-C(13)-C(9T)	109.3(6)
C(6)-C(5)-S(3)	111.9(6)	C(7T)-C(13)-C(9T)	95.0(8)
C(6)-C(7)-C(10)	111.1(8)	C(19)-C(15)-C(17)	109.7(3)
C(13)-C(8)-C(5)	108.7(8)	C(19)-C(15)-S(4)	109.4(2)
C(13)-C(8)-C(9)	113.0(9)	C(17)-C(15)-S(4)	114.3(2)
C(5)-C(8)-C(9)	107.1(7)	C(17)-C(16)-C(20)	110.7(3)
C(10)-C(9)-C(8)	109.2(8)	C(16)-C(17)-C(15)	111.2(3)
C(9)-C(10)-C(14)	110.3(13)	C(16)-C(17)-C(18)	109.1(3)
C(9)-C(10)-C(7)	109.2(11)	C(15)-C(17)-C(18)	107.2(3)
C(14)-C(10)-C(7)	110.0(13)	C(21)-C(18)-C(17)	109.3(3)
C(11)-C(12)-C(6)	114.7(7)	C(15)-C(19)-C(23)	110.9(3)
C(10)-C(14)-C(11)	105.1(10)	C(15)-C(19)-C(22)	107.4(3)
C(6)-C(5T)-C(9T)	106.3(10)	C(23)-C(19)-C(22)	109.0(3)
C(6)-C(5T)-C(6T)	113.2(13)	C(16)-C(20)-C(23)	108.8(3)
C(9T)-C(5T)-C(6T)	108.7(11)	C(16)-C(20)-C(24)	109.1(3)
C(11T)-C(6T)-C(5T)	111.0(12)	C(23)-C(20)-C(24)	109.4(3)

C(24)-C(21)-C(18)	109.8(3)	C(32)-C(31)-N(1)	116.2(5)
C(24)-C(21)-C(22)	109.2(3)	C(26)-C(25A)-N(1)	113.6(6)
C(18)-C(21)-C(22)	109.9(3)	N(1)-C(27A)-C(28)	116.7(8)
C(21)-C(22)-C(19)	109.7(3)	C(30)-C(29A)-N(1)	115.9(8)
C(20)-C(23)-C(19)	110.2(3)	N(1)-C(31A)-C(32)	118.5(7)
C(21)-C(24)-C(20)	109.6(3)	C(25A)-C(26)-C(25)	67.2(5)
N(1)-C(25)-C(26)	112.7(5)	C(27)-C(28)-C(27A)	61.4(5)
C(28)-C(27)-N(1)	117.9(5)	C(29A)-C(30)-C(29)	64.4(6)
N(1)-C(29)-C(30)	113.7(5)	C(31)-C(32)-C(31A)	62.8(5)

Table S14. Anisotropic displacement parameters ($Å^2$ x 10^3) for $(Et_4N)[MoO(2\text{-}AdS)_2(S_2C_2Me_2)]$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
Mo(1)	42(1)	40(1)	48(1)	-2(1)	19(1)	3(1)
S(1)	48(1)	57(1)	45(1)	-3(1)	21(1)	4(1)
S(2)	52(1)	60(1)	52(1)	-7(1)	25(1)	8(1)
S(3)	57(1)	72(1)	68(1)	-27(1)	36(1)	-16(1)
S(4)	48(1)	46(1)	56(1)	-8(1)	16(1)	6(1)
O(1)	60(2)	48(1)	68(2)	7(1)	17(1)	6(1)
N(1)	55(2)	49(2)	51(2)	1(1)	24(2)	5(1)
C(1)	44(2)	53(2)	51(2)	16(2)	21(2)	9(2)
C(2)	47(2)	60(2)	53(2)	11(2)	25(2)	12(2)
C(3)	51(2)	87(3)	61(3)	5(2)	12(2)	6(2)
C(4)	58(2)	95(3)	82(3)	2(2)	34(2)	24(2)
C(5)	45(5)	33(7)	63(7)	-3(5)	28(5)	0(4)
C(7)	105(7)	51(5)	94(7)	-5(4)	46(6)	17(4)
C(8)	57(5)	49(5)	62(7)	-5(4)	10(4)	18(3)
C(9)	55(5)	89(8)	75(6)	-38(6)	16(5)	-7(5)
C(10)	57(10)	64(7)	71(11)	-38(6)	30(7)	-15(6)
C(12)	40(4)	93(7)	89(7)	-17(6)	29(4)	5(4)
C(14)	83(7)	65(9)	92(9)	-28(7)	56(7)	-15(8)
C(5T)	74(8)	77(10)	72(7)	6(7)	36(6)	-27(7)
C(6T)	132(13)	84(10)	119(12)	-56(10)	80(11)	-66(10)
C(7T)	61(7)	178(16)	48(6)	-13(7)	19(5)	5(8)
C(8T)	36(5)	92(8)	71(8)	-35(7)	17(5)	13(5)
C(9T)	39(6)	62(10)	49(11)	-5(7)	17(6)	6(6)
C(10T)	93(11)	54(11)	91(12)	-14(8)	54(9)	-7(11)
C(11T)	59(16)	130(20)	68(15)	-45(13)	24(10)	-27(12)
C(6)	134(5)	62(3)	68(3)	8(2)	24(3)	2(3)
C(11)	68(4)	156(7)	167(7)	64(5)	45(4)	-27(4)
C(13)	37(5)	65(3)	66(3)	-4(2)	21(3)	19(3)
C(15)	47(2)	39(2)	50(2)	-1(2)	18(2)	0(2)
C(16)	51(2)	41(2)	64(2)	7(2)	25(2)	3(2)
C(17)	44(2)	32(2)	60(2)	-6(2)	18(2)	-2(1)
C(18)	48(2)	44(2)	67(2)	-2(2)	23(2)	5(2)
C(19)	57(2)	32(2)	64(2)	1(2)	21(2)	0(2)
C(20)	59(2)	55(2)	48(2)	3(2)	16(2)	0(2)
C(21)	42(2)	50(2)	69(2)	-3(2)	20(2)	-2(2)
C(22)	56(2)	47(2)	75(3)	-7(2)	26(2)	-15(2)

C(23)	53(2)	47(2)	62(2)	-14(2)	17(2)	-1(2)
C(24)	51(2)	55(2)	70(3)	-3(2)	10(2)	0(2)
C(25)	61(4)	69(5)	71(5)	6(4)	13(4)	2(3)
C(27)	62(4)	89(5)	55(4)	20(4)	28(3)	25(4)
C(29)	75(5)	67(5)	93(6)	10(4)	45(4)	17(4)
C(31)	91(5)	61(4)	82(5)	-4(4)	50(4)	6(4)
C(25A)	59(6)	50(6)	109(9)	-12(6)	12(6)	15(5)
C(27A)	79(8)	73(8)	117(10)	-2(6)	48(7)	18(6)
C(29A)	85(8)	73(8)	94(9)	-8(6)	24(7)	2(6)
C(31A)	85(7)	58(6)	74(7)	-5(5)	35(6)	3(5)
C(26)	86(3)	60(3)	109(4)	8(3)	2(3)	-10(2)
C(28)	108(4)	100(4)	113(4)	23(3)	76(4)	21(3)
C(30)	48(3)	121(5)	134(5)	-9(4)	22(3)	-4(3)
C(32)	177(6)	57(3)	135(5)	-2(3)	102(5)	-6(3)

Table S15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $(Et_4N)[MoO(2\text{-}AdS)_2(S_2C_2Me_2)]$.

	x	y	z	U(eq)
H(3A)	-3162	6133	1896	102
H(3B)	-2576	5404	1704	102
H(3C)	-2542	6149	1223	102
H(4A)	-3035	6776	2851	113
H(4B)	-2233	7440	3305	113
H(4C)	-2334	6717	3800	113
H(5A)	1731	5018	1952	53
H(7A)	2479	3890	1611	96
H(7B)	3728	3758	1559	96
H(8A)	1290	5907	865	70
H(9A)	1023	4599	541	89
H(9B)	1337	5019	-168	89
H(10A)	2468	3935	203	74
H(12A)	4705	5592	2260	87
H(12B)	5034	4910	1802	87
H(14A)	3382	4957	-218	88
H(14B)	4326	4489	463	88
H(5TA)	2098	4636	2187	85
H(6TA)	2015	3817	1061	122
H(6TB)	1006	4407	768	122
H(7TA)	1261	5546	1	114
H(7TB)	2263	5577	-385	114
H(8TA)	5027	4894	1525	80
H(9TA)	1273	5691	1329	59
H(10B)	3836	3969	702	88
H(10C)	3939	4631	120	88
H(11A)	1922	4310	-242	102
H(6A)	3848	4606	2600	108
H(6C)	3773	4261	2223	108
H(6D)	3840	5097	2495	108
H(11A)	4522	5946	957	155
H(11B)	4186	5672	567	155
H(11C)	4462	5929	1472	155
H(13A)	2889	6409	1170	111
H(13B)	2582	6105	276	111
H(13C)	2772	6489	746	111
H(15A)	4258	6878	3814	54
H(16A)	5044	5571	5886	61
H(16B)	3959	6102	5699	61
H(17A)	4159	5691	4439	54

H(18A)	6214	5526	4915	62
H(18B)	5857	6035	4118	62
H(19A)	4613	7978	4659	60
H(20A)	5544	6644	6739	65
H(21A)	7450	6584	5151	64
H(22A)	6142	7439	4262	69
H(22B)	6666	7799	5148	69
H(23A)	5479	7835	6113	65
H(23B)	4224	7489	5835	65
H(24A)	7234	6987	6409	73
H(24B)	7063	6113	6326	73
H(25A)	163	8542	474	83
H(25B)	-618	8624	1040	83
H(27A)	883	7786	2532	80
H(27D)	1586	8487	2972	80
H(29A)	2252	8318	1115	89
H(29B)	2009	7623	1597	89
H(31A)	483	9634	1622	87
H(31B)	1780	9589	2194	87
H(25C)	1535	7496	1341	92
H(25D)	964	7425	2037	92
H(27B)	-529	8835	1398	103
H(27C)	311	9438	1943	103
H(29C)	2366	9114	2665	103
H(29D)	2123	8310	2939	103
H(31A)	666	8774	504	84
H(31B)	1990	8605	903	84
H(26A)	-900	7433	416	138
H(26B)	425	7250	819	138
H(26C)	-360	7341	1381	138
H(26D)	-295	6984	803	138
H(26E)	-838	7695	1075	138
H(26F)	-265	7760	378	138
H(28A)	-172	8445	3177	146
H(28B)	-101	9166	2669	146
H(28C)	-818	8469	2217	146
H(28D)	-796	8900	2699	146
H(28E)	-313	8101	2604	146
H(28F)	521	8714	3144	146
H(30A)	3941	8054	2268	155
H(30B)	3477	8847	2404	155
H(30C)	3229	8148	2878	155
H(30D)	3948	8375	2877	155
H(30E)	3223	7798	2213	155
H(30F)	3470	8603	1938	155
H(32A)	1646	10244	1014	166

H(32B)	2361	9506	1044	166
H(32C)	1062	9552	467	166
H(32D)	1732	9848	482	166
H(32E)	964	9985	1048	166
H(32F)	2293	9811	1450	166

Table S16. Crystal data and structure refinement for $(Et_4N)[MoOCl(SC_6H_2\text{-}2,4,6\text{-}Pr^i_3)(bdt)]$.

Identification code	bsl93
Empirical formula	C29 H47 Cl Mo N O S3
Formula weight	653.25
Temperature	213(2) K
Wavelength	0.71073 Å
Crystal system	triclinic
Space group	P(-1)
Unit cell dimensions	a = 9.9320(4) Å alpha = 85.9670(10) deg. b = 10.1206(4) Å beta = 80.1480(10) deg. c = 19.0606(8) Å gamma = 60.8600(10) deg.
Volume, Z	1648.57(12) $Å^3$, 2
Density (calculated)	1.316 Mg/m^3
Absorption coefficient	0.690 mm^{-1}
F(000)	686
Crystal size	0.4 x 0.1 x 0.08 mm
Theta range for data collection	1.08 to 27.71 deg.
Limiting indices	-12<=h<=6, -12<=k<=8, -22<=l<=23
Reflections collected	10330
Independent reflections	6628 [R(int) = 0.0143]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6626 / 1 / 341
Goodness-of-fit on F^2	1.024
Final R indices [I>2sigma(I)]	R1 = 0.0269, wR2 = 0.0739
R indices (all data)	R1 = 0.0304, wR2 = 0.0824
Largest diff. peak and hole	0.462 and -0.265 e. $Å^{-3}$

Table S17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $(Et_4N)[MoOCl(SC_6H_2\text{-}2,4,6\text{-}Pr^i_3)(bdt)]$.

	x	y	z	U(eq)
Mo(1)	7964(1)	8560(1)	8431(1)	33(1)
S(1)	7066(1)	10503(1)	7593(1)	40(1)
S(2)	6248(1)	10549(1)	9269(1)	40(1)
S(3)	7942(1)	6976(1)	7563(1)	37(1)
Cl(1)	7284(1)	7045(1)	9263(1)	47(1)
O(1)	9807(2)	8136(2)	8475(1)	50(1)
N(1)	1103(2)	11831(2)	8720(1)	40(1)
C(1)	6375(2)	12188(2)	8081(1)	35(1)
C(2)	5993(2)	12208(2)	8820(1)	35(1)
C(3)	5384(3)	13568(2)	9197(1)	46(1)
C(4)	5221(3)	14857(2)	8841(1)	54(1)
C(5)	5624(3)	14833(2)	8113(1)	52(1)
C(6)	6180(3)	13515(2)	7731(1)	45(1)
C(7)	8619(2)	7345(2)	6674(1)	37(1)
C(8)	7548(2)	8121(2)	6204(1)	44(1)
C(9)	8132(3)	8197(3)	5491(1)	52(1)
C(10)	9694(3)	7564(3)	5232(1)	55(1)
C(11)	10718(3)	6857(3)	5715(1)	54(1)
C(12)	10231(2)	6723(2)	6433(1)	44(1)
C(13)	5801(3)	8839(3)	6430(1)	58(1)
C(14)	5184(4)	7861(4)	6212(2)	99(1)
C(15)	4916(3)	10430(3)	6151(2)	73(1)
C(16)	10278(4)	7593(3)	4441(1)	72(1)
C(17)	11018(6)	6080(4)	4112(2)	105(1)
C(18)	11258(8)	8336(6)	4287(2)	164(3)
C(19)	11445(3)	5908(3)	6918(1)	55(1)
C(20)	12518(4)	4260(3)	6687(2)	89(1)
C(21)	12347(4)	6727(5)	6955(2)	95(1)
C(22)	2836(3)	10772(3)	8482(2)	61(1)
C(23)	3351(3)	9104(3)	8582(2)	77(1)
C(24)	741(3)	11709(3)	9518(1)	56(1)
C(25)	-938(3)	12726(3)	9845(1)	71(1)
C(26)	115(3)	11409(3)	8360(1)	51(1)
C(27)	500(3)	11275(4)	7561(1)	70(1)
C(28)	740(3)	13429(2)	8513(1)	49(1)
C(29)	1605(3)	14042(3)	8840(2)	65(1)
Mo(1B)	6623(6)	8638(6)	8303(3)	33(1)
S(1B)	7544(33)	10476(34)	7621(15)	40(1)
S(2B)	6474(34)	10089(28)	9153(14)	40(1)
S(3B)	8512(27)	6577(26)	7490(13)	37(1)

O(1B)	4789(59)	8979(61)	8191(32)	50(1)

Table S18. Bond lengths [Å] and angles [°] for $(Et_4N)[MoOCl(SC_6H_2\text{-}2,4,6\text{-}Pr^i_3)(bdt)]$.

Mo(1)-O(1)	1.6808(14)	Mo(1B)-S(3B)	2.43(2)
Mo(1)-S(1)	2.3560(7)	Mo(1B)-S(1B)	2.63(3)
Mo(1)-Cl(1)	2.3716(5)		
Mo(1)-S(2)	2.3849(6)	O(1)-Mo(1)-S(1)	106.47(6)
Mo(1)-S(3)	2.3928(6)	O(1)-Mo(1)-Cl(1)	108.16(6)
S(1)-C(1)	1.763(2)	S(1)-Mo(1)-Cl(1)	145.30(2)
S(2)-C(2)	1.753(2)	O(1)-Mo(1)-S(2)	108.30(6)
S(3)-C(7)	1.797(2)	S(1)-Mo(1)-S(2)	83.46(2)
Cl(1)-Mo(1B)	2.313(6)	Cl(1)-Mo(1)-S(2)	83.77(2)
N(1)-C(24)	1.512(3)	O(1)-Mo(1)-S(3)	110.29(6)
N(1)-C(26)	1.515(3)	S(1)-Mo(1)-S(3)	86.00(2)
N(1)-C(28)	1.515(2)	Cl(1)-Mo(1)-S(3)	84.16(2)
N(1)-C(22)	1.524(3)	S(2)-Mo(1)-S(3)	141.41(2)
C(1)-C(2)	1.394(3)	C(1)-S(1)-Mo(1)	104.90(6)
C(1)-C(6)	1.397(3)	C(2)-S(2)-Mo(1)	104.57(7)
C(1)-S(1B)	1.74(3)	C(7)-S(3)-Mo(1)	112.22(6)
C(2)-C(3)	1.397(3)	C(24)-N(1)-C(26)	109.3(2)
C(2)-S(2B)	2.04(3)	C(24)-N(1)-C(28)	111.1(2)
C(3)-C(4)	1.377(3)	C(26)-N(1)-C(28)	108.3(2)
C(4)-C(5)	1.375(3)	C(24)-N(1)-C(22)	108.4(2)
C(5)-C(6)	1.378(3)	C(26)-N(1)-C(22)	111.1(2)
C(7)-C(8)	1.402(3)	C(28)-N(1)-C(22)	108.7(2)
C(7)-C(12)	1.407(3)	C(2)-C(1)-C(6)	119.6(2)
C(7)-S(3B)	1.70(2)	C(2)-C(1)-S(1B)	120.1(10)
C(8)-C(9)	1.397(3)	C(6)-C(1)-S(1B)	118.2(10)
C(8)-C(13)	1.511(3)	C(2)-C(1)-S(1)	119.97(14)
C(9)-C(10)	1.370(3)	C(6)-C(1)-S(1)	120.4(2)
C(10)-C(11)	1.382(4)	C(1)-C(2)-C(3)	119.3(2)
C(10)-C(16)	1.523(3)	C(1)-C(2)-S(2)	120.15(14)
C(11)-C(12)	1.392(3)	C(3)-C(2)-S(2)	120.5(2)
C(12)-C(19)	1.515(3)	C(1)-C(2)-S(2B)	109.2(7)
C(13)-C(14)	1.505(4)	C(3)-C(2)-S(2B)	131.6(7)
C(13)-C(15)	1.519(4)	C(4)-C(3)-C(2)	120.1(2)
C(16)-C(17)	1.471(4)	C(5)-C(4)-C(3)	120.7(2)
C(16)-C(18)	1.477(5)	C(4)-C(5)-C(6)	120.0(2)
C(19)-C(21)	1.499(4)	C(5)-C(6)-C(1)	120.3(2)
C(19)-C(20)	1.524(4)	C(8)-C(7)-C(12)	120.3(2)
C(22)-C(23)	1.516(3)	C(8)-C(7)-S(3B)	134.2(8)
C(24)-C(25)	1.515(4)	C(12)-C(7)-S(3B)	104.0(8)
C(26)-C(27)	1.504(3)	C(8)-C(7)-S(3)	119.7(2)
C(28)-C(29)	1.506(3)	C(12)-C(7)-S(3)	119.7(2)
Mo(1B)-O(1B)	1.73(5)	C(9)-C(8)-C(7)	118.1(2)
Mo(1B)-S(2B)	2.20(3)	C(9)-C(8)-C(13)	118.8(2)

C(7)-C(8)-C(13)	123.1(2)	C(12)-C(19)-C(20)	111.4(2)
C(10)-C(9)-C(8)	123.2(2)	C(23)-C(22)-N(1)	115.0(2)
C(9)-C(10)-C(11)	117.3(2)	N(1)-C(24)-C(25)	115.2(2)
C(9)-C(10)-C(16)	121.2(2)	C(27)-C(26)-N(1)	115.3(2)
C(11)-C(10)-C(16)	121.4(2)	C(29)-C(28)-N(1)	115.2(2)
C(10)-C(11)-C(12)	123.1(2)	O(1B)-Mo(1B)-S(2B)	111(2)
C(11)-C(12)-C(7)	118.0(2)	O(1B)-Mo(1B)-Cl(1)	106(2)
C(11)-C(12)-C(19)	119.1(2)	S(2B)-Mo(1B)-Cl(1)	76.0(7)
C(7)-C(12)-C(19)	122.8(2)	O(1B)-Mo(1B)-S(3B)	107(2)
C(14)-C(13)-C(8)	110.9(2)	S(2B)-Mo(1B)-S(3B)	141.6(10)
C(14)-C(13)-C(15)	110.0(2)	Cl(1)-Mo(1B)-S(3B)	90.6(6)
C(8)-C(13)-C(15)	113.4(2)	O(1B)-Mo(1B)-S(1B)	115(2)
C(17)-C(16)-C(18)	113.1(3)	S(2B)-Mo(1B)-S(1B)	76.2(10)
C(17)-C(16)-C(10)	111.3(2)	Cl(1)-Mo(1B)-S(1B)	136.1(6)
C(18)-C(16)-C(10)	113.4(3)	S(3B)-Mo(1B)-S(1B)	90.5(9)
C(21)-C(19)-C(12)	110.5(2)	C(1)-S(1B)-Mo(1B)	103.9(12)
C(21)-C(19)-C(20)	111.7(3)	C(2)-S(2B)-Mo(1B)	113.1(12)
		C(7)-S(3B)-Mo(1B)	106.9(11)

Table S19. Anisotropic displacement parameters ($Å^2$ x 10^3) for $(Et_4N)[MoOCl(SC_6H_2$-2,4,6-$Pr^i_3)(bdt)]$. The anisotropic displacement factor exponent takes the form: $-2\ pi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
Mo(1)	33(1)	30(1)	34(1)	1(1)	-7(1)	-14(1)
S(1)	52(1)	35(1)	30(1)	1(1)	-6(1)	-21(1)
S(2)	49(1)	35(1)	30(1)	0(1)	-5(1)	-17(1)
S(3)	42(1)	35(1)	35(1)	-1(1)	-1(1)	-21(1)
Cl(1)	60(1)	41(1)	39(1)	7(1)	-7(1)	-25(1)
O(1)	37(1)	44(1)	68(1)	1(1)	-16(1)	-17(1)
N(1)	39(1)	33(1)	53(1)	5(1)	-18(1)	-18(1)
C(1)	34(1)	34(1)	38(1)	2(1)	-11(1)	-16(1)
C(2)	34(1)	36(1)	39(1)	2(1)	-11(1)	-18(1)
C(3)	52(1)	43(1)	42(1)	-7(1)	-11(1)	-19(1)
C(4)	67(1)	37(1)	61(1)	-7(1)	-17(1)	-23(1)
C(5)	63(1)	37(1)	63(1)	7(1)	-18(1)	-27(1)
C(6)	52(1)	40(1)	45(1)	7(1)	-12(1)	-23(1)
C(7)	45(1)	31(1)	37(1)	-4(1)	-1(1)	-20(1)
C(8)	51(1)	42(1)	40(1)	-2(1)	-5(1)	-23(1)
C(9)	65(1)	48(1)	41(1)	3(1)	-8(1)	-26(1)
C(10)	73(2)	42(1)	44(1)	-1(1)	6(1)	-28(1)
C(11)	52(1)	46(1)	56(1)	-7(1)	14(1)	-23(1)
C(12)	45(1)	34(1)	49(1)	-4(1)	2(1)	-18(1)
C(13)	52(1)	67(2)	51(1)	3(1)	-11(1)	-26(1)
C(14)	71(2)	90(2)	150(4)	-3(2)	-15(2)	-50(2)
C(15)	59(2)	71(2)	72(2)	-1(1)	-21(1)	-14(1)
C(16)	96(2)	61(2)	47(1)	0(1)	14(1)	-36(2)
C(17)	191(4)	89(2)	48(2)	-17(2)	15(2)	-86(3)
C(18)	317(7)	175(4)	71(2)	-47(3)	79(3)	-202(5)
C(19)	41(1)	52(1)	63(1)	-1(1)	-2(1)	-17(1)
C(20)	74(2)	59(2)	91(2)	5(2)	-3(2)	-2(2)
C(21)	72(2)	107(3)	122(3)	14(2)	-33(2)	-53(2)
C(22)	38(1)	47(1)	95(2)	-5(1)	-15(1)	-16(1)
C(23)	53(1)	40(1)	124(3)	-6(1)	-18(2)	-10(1)
C(24)	63(1)	55(1)	58(1)	15(1)	-28(1)	-31(1)
C(25)	77(2)	78(2)	48(1)	-4(1)	-10(1)	-30(2)
C(26)	46(1)	53(1)	62(1)	-2(1)	-14(1)	-28(1)
C(27)	71(2)	94(2)	60(2)	-13(1)	-12(1)	-50(2)
C(28)	51(1)	38(1)	58(1)	9(1)	-18(1)	-21(1)
C(29)	75(2)	45(1)	89(2)	9(1)	-34(1)	-35(1)

Mo(1B)	33(1)	30(1)	34(1)	1(1)	-7(1)	-14(1)
S(1B)	52(1)	35(1)	30(1)	1(1)	-6(1)	-21(1)
S(2B)	49(1)	35(1)	30(1)	0(1)	-5(1)	-17(1)
S(3B)	42(1)	35(1)	35(1)	-1(1)	-1(1)	-21(1)
O(1B)	37(1)	44(1)	68(1)	1(1)	-16(1)	-17(1)

Table S20. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $(Et_4N)[MoOCl(SC_6H_2\text{-}2,4,6\text{-}Pr^i_3)(bdt)]$.

	x	y	z	U(eq)
H(3A)	5088(3)	13601(2)	9688(1)	56
H(4A)	4833(3)	15753(2)	9096(1)	65
H(5A)	5522(3)	15707(2)	7879(1)	63
H(6A)	6426(3)	13508(2)	7237(1)	54
H(9A)	7426(3)	8702(3)	5176(1)	62
H(11A)	11782(3)	6451(3)	5552(1)	65
H(13A)	5596(3)	8909(3)	6951(1)	69
H(14A)	4075(4)	8338(4)	6360(2)	148
H(14B)	5669(4)	6892(4)	6433(2)	148
H(14C)	5415(4)	7728(4)	5703(2)	148
H(15A)	5317(3)	11045(3)	6293(2)	110
H(15B)	3828(3)	10856(3)	6344(2)	110
H(15C)	5045(3)	10392(3)	5641(2)	110
H(16A)	9347(4)	8216(3)	4219(1)	86
H(17A)	10332(6)	5653(4)	4229(2)	157
H(17B)	11981(6)	5440(4)	4287(2)	157
H(17C)	11223(6)	6157(4)	3604(2)	157
H(18A)	10719(8)	9316(6)	4515(2)	246
H(18B)	11467(8)	8446(6)	3782(2)	246
H(18C)	12225(8)	7729(6)	4465(2)	246
H(19A)	10893(3)	5920(3)	7398(1)	66
H(20A)	11903(4)	3771(3)	6669(2)	133
H(20B)	13224(4)	3755(3)	7023(2)	133
H(20C)	13102(4)	4215(3)	6225(2)	133
H(21A)	13110(4)	6197(5)	7264(2)	142
H(21B)	11645(4)	7735(5)	7138(2)	142
H(21C)	12863(4)	6774(5)	6488(2)	142
H(22A)	3098(3)	10941(3)	7982(2)	73
H(22B)	3427(3)	11038(3)	8745(2)	73
H(23A)	4452(3)	8522(3)	8419(2)	115
H(23B)	2798(3)	8817(3)	8312(2)	115
H(23C)	3128(3)	8914(3)	9077(2)	115
H(24A)	1409(3)	11944(3)	9741(1)	67
H(24B)	1004(3)	10668(3)	9628(1)	67
H(25A)	-1061(3)	12575(3)	10350(1)	106
H(25B)	-1612(3)	12485(3)	9640(1)	106
H(25C)	-1207(3)	13763(3)	9753(1)	106
H(26A)	226(3)	10451(3)	8547(1)	61
H(26B)	-971(3)	12165(3)	8488(1)	61
H(27A)	-181(3)	11006(4)	7381(1)	105

H(27B)	1564(3)	10508(4)	7426(1)	105
H(27C)	364(3)	12226(4)	7367(1)	105
H(28A)	980(3)	13460(2)	7999(1)	58
H(28B)	-371(3)	14093(2)	8648(1)	58
H(29A)	1304(3)	15055(3)	8680(2)	97
H(29B)	2708(3)	13414(3)	8699(2)	97
H(29C)	1355(3)	14049(3)	9349(2)	97

Table S21. Crystal data and structure refinement for $(Et_4N)_2[Mo_2O_2(\mu\text{-}O)_2(bdt)_2]$.

Identification code	bsl101
Empirical formula	C28 H48 Mo2 N2 O4 S4
Formula weight	796.80
Temperature	213(2) K
Wavelength	0.71073 Å
Crystal system, space group	orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 8.504(3) Å alpha = 90 deg. b = 15.536(5) Å beta = 90 deg. c = 27.298(9) Å gamma = 90 deg.
Volume	3607(2) $Å^3$
Z, Calculated density	4, 1.467 Mg/m^3
Absorption coefficient	0.959 mm^{-1}
F(000)	1640
Crystal size	0.5 x 0.4 x 0.32 mm
Theta range for data collection	1.49 to 28.12 deg.
Limiting indices	-10<=h<=8, -20<=k<=17, -36<=l<=33
Reflections collected / unique	23092 / 8499 [R(int) = 0.0260]
Completeness to theta = 28.12	98.1 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8499 / 0 / 361
Goodness-of-fit on F^2	1.106
Final R indices [I>2sigma(I)]	R1 = 0.0237, wR2 = 0.0632
R indices (all data)	R1 = 0.0242, wR2 = 0.0636
Absolute structure parameter	-0.02(3)
Largest diff. peak and hole	0.819 and -0.324 e. $Å^{-3}$

Table S22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $(Et_4N)_2[Mo_2O_2(\mu\text{-}O)_2(bdt)_2]$.

	x	y	z	U(eq)
Mo(2)	6575(1)	6938(1)	1856(1)	25(1)
Mo(1)	6507(1)	6175(1)	1003(1)	26(1)
S(1)	4190(1)	5555(1)	620(1)	35(1)
S(2)	7641(1)	4792(1)	794(1)	37(1)
S(3)	7742(1)	6427(1)	2617(1)	36(1)
S(4)	4296(1)	7143(1)	2378(1)	33(1)
O(1)	7240(3)	6898(1)	595(1)	40(1)
O(2)	7370(3)	7929(1)	1754(1)	39(1)
O(3)	4847(2)	6699(1)	1402(1)	31(1)
O(4)	7866(2)	6018(1)	1580(1)	30(1)
N(1)	1608(3)	4431(1)	2072(1)	29(1)
N(2)	7239(3)	6402(2)	-934(1)	37(1)
C(1)	6469(4)	6738(2)	3094(1)	34(1)
C(2)	6936(5)	6664(2)	3589(1)	49(1)
C(3)	5911(5)	6891(3)	3961(1)	64(1)
C(4)	4433(5)	7201(3)	3857(1)	65(1)
C(5)	3934(4)	7281(2)	3377(1)	49(1)
C(6)	4938(3)	7051(2)	2989(1)	34(1)
C(7)	6349(4)	4306(2)	371(1)	36(1)
C(8)	4823(4)	4626(2)	304(1)	35(1)
C(9)	3792(4)	4195(2)	-14(1)	49(1)
C(10)	4292(6)	3460(2)	-267(1)	63(1)
C(11)	5791(6)	3150(2)	-201(1)	63(1)
C(12)	6821(5)	3559(2)	115(1)	48(1)
C(13)	3234(3)	4032(2)	2151(1)	39(1)
C(14)	4604(3)	4586(2)	1991(1)	52(1)
C(15)	1318(3)	4622(2)	1529(1)	38(1)
C(16)	1425(5)	3860(3)	1188(1)	60(1)
C(17)	436(3)	3770(2)	2266(1)	38(1)
C(18)	-1274(3)	4040(2)	2230(1)	47(1)
C(19)	1454(4)	5290(2)	2336(1)	38(1)
C(20)	1675(5)	5255(3)	2886(1)	64(1)
C(21)	5965(4)	6188(3)	-562(1)	57(1)
C(22)	4355(4)	5972(3)	-784(1)	61(1)
C(23)	7671(5)	5587(3)	-1210(2)	63(1)
C(24)	9017(5)	5651(3)	-1562(2)	65(1)
C(25)	8679(5)	6745(3)	-660(1)	60(1)
C(26)	9507(5)	6103(3)	-333(1)	63(1)
C(27)	6700(5)	7074(2)	-1299(1)	61(1)
C(28)	6059(4)	7905(2)	-1084(2)	64(1)

Table S23. Bond lengths [Å] and angles [°] for $(Et_4N)_2[Mo_2O_2(\mu\text{-}O)_2(bdt)_2]$.

Mo(2)-O(2)	1.7043(19)	O(2)-Mo(2)-O(4)	112.02(9)
Mo(2)-O(4)	1.9532(17)	O(2)-Mo(2)-O(3)	111.47(9)
Mo(2)-O(3)	1.9579(19)	O(4)-Mo(2)-O(3)	92.19(7)
Mo(2)-S(4)	2.4264(9)	O(2)-Mo(2)-S(4)	107.12(7)
Mo(2)-S(3)	2.4350(9)	O(4)-Mo(2)-S(4)	140.48(6)
Mo(2)-Mo(1)	2.6141(7)	O(3)-Mo(2)-S(4)	78.31(6)
Mo(1)-O(1)	1.7014(19)	O(2)-Mo(2)-S(3)	105.80(7)
Mo(1)-O(3)	1.9601(18)	O(4)-Mo(2)-S(3)	82.07(6)
Mo(1)-O(4)	1.9682(18)	O(3)-Mo(2)-S(3)	141.61(6)
Mo(1)-S(2)	2.4234(9)	S(4)-Mo(2)-S(3)	82.36(3)
Mo(1)-S(1)	2.4306(9)	O(2)-Mo(2)-Mo(1)	105.84(7)
S(1)-C(8)	1.765(3)	O(4)-Mo(2)-Mo(1)	48.44(5)
S(2)-C(7)	1.764(3)	O(3)-Mo(2)-Mo(1)	48.18(5)
S(3)-C(1)	1.760(3)	S(4)-Mo(2)-Mo(1)	124.41(2)
S(4)-C(6)	1.759(3)	S(3)-Mo(2)-Mo(1)	128.40(3)
N(1)-C(19)	1.522(3)	O(1)-Mo(1)-O(3)	110.74(9)
N(1)-C(17)	1.525(3)	O(1)-Mo(1)-O(4)	113.05(9)
N(1)-C(13)	1.531(3)	O(3)-Mo(1)-O(4)	91.67(7)
N(1)-C(15)	1.532(3)	O(1)-Mo(1)-S(2)	106.56(8)
N(2)-C(27)	1.515(4)	O(3)-Mo(1)-S(2)	141.78(6)
N(2)-C(23)	1.518(4)	O(4)-Mo(1)-S(2)	81.14(5)
N(2)-C(21)	1.522(4)	O(1)-Mo(1)-S(1)	106.01(8)
N(2)-C(25)	1.530(4)	O(3)-Mo(1)-S(1)	79.61(6)
C(1)-C(2)	1.414(4)	O(4)-Mo(1)-S(1)	140.51(6)
C(1)-C(6)	1.419(4)	S(2)-Mo(1)-S(1)	82.52(3)
C(2)-C(3)	1.384(5)	O(1)-Mo(1)-Mo(2)	106.06(7)
C(3)-C(4)	1.376(6)	O(3)-Mo(1)-Mo(2)	48.11(5)
C(4)-C(5)	1.384(5)	O(4)-Mo(1)-Mo(2)	47.95(5)
C(5)-C(6)	1.407(4)	S(2)-Mo(1)-Mo(2)	127.135(19)
C(7)-C(8)	1.402(4)	S(1)-Mo(1)-Mo(2)	125.54(2)
C(7)-C(12)	1.413(4)	C(8)-S(1)-Mo(1)	106.67(10)
C(8)-C(9)	1.404(4)	C(7)-S(2)-Mo(1)	106.65(10)
C(9)-C(10)	1.400(5)	C(1)-S(3)-Mo(2)	106.89(10)
C(10)-C(11)	1.375(7)	C(6)-S(4)-Mo(2)	107.33(10)
C(11)-C(12)	1.382(5)	Mo(2)-O(3)-Mo(1)	83.70(7)
C(13)-C(14)	1.513(4)	Mo(2)-O(4)-Mo(1)	83.61(7)
C(15)-C(16)	1.510(4)	C(19)-N(1)-C(17)	111.7(2)
C(17)-C(18)	1.517(4)	C(19)-N(1)-C(13)	111.5(2)
C(19)-C(20)	1.515(5)	C(17)-N(1)-C(13)	105.63(18)
C(21)-C(22)	1.535(5)	C(19)-N(1)-C(15)	105.78(19)
C(23)-C(24)	1.498(5)	C(17)-N(1)-C(15)	111.2(2)
C(25)-C(26)	1.512(5)	C(13)-N(1)-C(15)	111.1(2)
C(27)-C(28)	1.520(6)	C(27)-N(2)-C(23)	108.7(3)

C(27)-N(2)-C(21)	112.0(3)	C(12)-C(7)-S(2)	119.9(3)
C(23)-N(2)-C(21)	108.8(3)	C(7)-C(8)-C(9)	119.3(3)
C(27)-N(2)-C(25)	108.9(3)	C(7)-C(8)-S(1)	120.6(2)
C(23)-N(2)-C(25)	109.8(3)	C(9)-C(8)-S(1)	120.1(3)
C(21)-N(2)-C(25)	108.7(3)	C(10)-C(9)-C(8)	120.3(4)
C(2)-C(1)-C(6)	118.6(3)	C(11)-C(10)-C(9)	120.2(3)
C(2)-C(1)-S(3)	120.8(3)	C(10)-C(11)-C(12)	120.5(3)
C(6)-C(1)-S(3)	120.57(19)	C(11)-C(12)-C(7)	120.4(4)
C(3)-C(2)-C(1)	120.2(4)	C(14)-C(13)-N(1)	115.1(2)
C(4)-C(3)-C(2)	120.9(3)	C(16)-C(15)-N(1)	115.8(2)
C(3)-C(4)-C(5)	120.5(3)	C(18)-C(17)-N(1)	114.7(2)
C(4)-C(5)-C(6)	120.3(4)	C(20)-C(19)-N(1)	115.2(2)
C(5)-C(6)-C(1)	119.4(3)	N(2)-C(21)-C(22)	114.7(3)
C(5)-C(6)-S(4)	120.3(2)	C(24)-C(23)-N(2)	116.7(3)
C(1)-C(6)-S(4)	120.28(19)	C(26)-C(25)-N(2)	115.5(3)
C(8)-C(7)-C(12)	119.3(3)	N(2)-C(27)-C(28)	116.0(3)
C(8)-C(7)-S(2)	120.66(19)		

Table S24. Anisotropic displacement parameters ($Å^2$ x 10^3) for $(Et_4N)_2[Mo_2O_2(\mu\text{-}O)_2(bdt)_2]$. The anisotropic displacement factor exponent takes the form: $-2\,pi^2\,[\,h^2\,a^{*2}\,U11 + ... + 2\,h\,k\,a^*\,b^*\,U12\,]$

	U11	U22	U33	U23	U13	U12
Mo(2)	27(1)	24(1)	23(1)	-2(1)	0(1)	1(1)
Mo(1)	28(1)	28(1)	22(1)	-2(1)	1(1)	1(1)
S(1)	32(1)	41(1)	33(1)	-5(1)	-2(1)	-2(1)
S(2)	41(1)	38(1)	33(1)	-8(1)	-4(1)	10(1)
S(3)	39(1)	38(1)	31(1)	-2(1)	-5(1)	10(1)
S(4)	31(1)	39(1)	29(1)	-3(1)	3(1)	5(1)
O(1)	49(1)	41(1)	30(1)	4(1)	6(1)	-7(1)
O(2)	52(1)	29(1)	35(1)	-2(1)	6(1)	-6(1)
O(3)	29(1)	38(1)	27(1)	-4(1)	-2(1)	8(1)
O(4)	26(1)	37(1)	27(1)	-7(1)	-3(1)	6(1)
N(1)	22(1)	28(1)	38(1)	9(1)	1(1)	1(1)
N(2)	41(1)	36(1)	34(1)	5(1)	3(1)	-6(1)
C(1)	50(2)	27(1)	26(1)	-1(1)	-3(1)	-3(1)
C(2)	70(2)	48(2)	30(1)	3(1)	-11(1)	-8(2)
C(3)	88(3)	78(2)	25(1)	-1(2)	0(2)	-20(2)
C(4)	80(3)	79(3)	35(2)	-13(2)	21(2)	-15(2)
C(5)	55(2)	55(2)	36(2)	-6(1)	14(1)	-5(2)
C(6)	42(1)	30(1)	28(1)	-4(1)	6(1)	-8(1)
C(7)	56(2)	29(1)	23(1)	-2(1)	4(1)	-5(1)
C(8)	48(2)	32(1)	26(1)	1(1)	1(1)	-10(1)
C(9)	58(2)	50(2)	39(2)	-2(1)	-5(1)	-19(2)
C(10)	90(3)	54(2)	45(2)	-15(2)	-4(2)	-28(2)
C(11)	106(3)	43(2)	41(2)	-16(1)	7(2)	-11(2)
C(12)	73(2)	36(1)	35(1)	-7(1)	7(1)	1(1)
C(13)	27(1)	36(1)	55(2)	15(1)	-3(1)	6(1)
C(14)	23(1)	60(2)	72(2)	20(2)	2(1)	2(1)
C(15)	32(1)	41(1)	40(1)	12(1)	3(1)	5(1)
C(16)	58(2)	70(2)	52(2)	-9(2)	4(2)	12(2)
C(17)	32(1)	32(1)	50(2)	13(1)	2(1)	-5(1)
C(18)	30(1)	47(2)	64(2)	11(1)	2(1)	-7(1)
C(19)	33(1)	32(1)	50(2)	-1(1)	3(1)	0(1)
C(20)	63(2)	73(2)	55(2)	-14(2)	-6(2)	-1(2)
C(21)	56(2)	71(2)	45(2)	11(2)	8(2)	-6(2)
C(22)	52(2)	77(3)	55(2)	20(2)	1(2)	-23(2)
C(23)	74(3)	56(2)	60(2)	-4(2)	10(2)	-5(2)
C(24)	77(3)	61(2)	55(2)	-12(2)	18(2)	-2(2)
C(25)	58(2)	66(2)	56(2)	-7(2)	-3(2)	-7(2)
C(26)	52(2)	92(3)	46(2)	15(2)	-3(2)	8(2)

C(27)	54(2)	68(2)	60(2)	24(2)	-1(2)	-10(2)
C(28)	41(2)	45(2)	106(3)	9(2)	-2(2)	1(1)

Table S25. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $(Et_4N)_2[Mo_2O_2(\mu\text{-}O)_2(bdt)_2]$.

	x	y	z	U(eq)
H(2B)	7936	6461	3665	59
H(3A)	6225	6832	4286	76
H(4A)	3764	7358	4111	78
H(5A)	2930	7487	3310	58
H(9A)	2773	4398	-57	59
H(10A)	3607	3180	-480	76
H(11A)	6115	2661	-369	76
H(12A)	7830	3341	158	58
H(13A)	3356	3902	2497	47
H(13B)	3281	3491	1974	47
H(14A)	5571	4287	2053	78
H(14B)	4593	5117	2171	78
H(14C)	4516	4706	1647	78
H(15A)	280	4875	1497	45
H(15B)	2075	5051	1424	45
H(16A)	1230	4046	858	90
H(16B)	656	3438	1280	90
H(16C)	2457	3612	1208	90
H(17A)	574	3237	2086	45
H(17B)	679	3654	2607	45
H(18A)	-1932	3592	2359	70
H(18B)	-1539	4142	1893	70
H(18C)	-1434	4558	2415	70
H(19A)	2224	5685	2200	46
H(19B)	420	5525	2267	46
H(20A)	1559	5823	3020	95
H(20B)	2706	5040	2960	95
H(20C)	898	4881	3027	95
H(21A)	5842	6675	-342	69
H(21B)	6312	5702	-367	69
H(22A)	3625	5839	-527	92
H(22B)	4457	5485	-998	92
H(22C)	3977	6458	-967	92
H(23A)	7920	5144	-972	76
H(23B)	6752	5396	-1390	76
H(24A)	9188	5101	-1714	97
H(24B)	9948	5823	-1390	97
H(24C)	8775	6070	-1810	97
H(25A)	9427	6958	-899	72
H(25B)	8352	7231	-461	72

H(26A)	10388	6376	-178	95
H(26B)	9870	5627	-527	95
H(26C)	8790	5899	-88	95
H(27A)	5890	6820	-1504	73
H(27B)	7580	7215	-1510	73
H(28A)	5754	8285	-1344	96
H(28B)	6857	8175	-888	96
H(28C)	5162	7779	-883	96

Table S26. Crystal data and structure refinement for $(Ph_4P)[MoO_2(OSiPh_3)(bdt)]$.

Identification code	asadb
Empirical formula	C48 H39 Mo O3 P S2 Si
Formula weight	882.91
Temperature	213(2) K
Wavelength	0.71073 Å
Crystal system, space group	monoclinic, P2(1)/n
Unit cell dimensions	a = 10.09(2) Å alpha = 90 deg. b = 27.51(7) Å beta = 92.70(3) deg. c = 15.45(4) Å gamma = 90 deg.
Volume	4284(18) $Å^3$
Z, Calculated density	4, 1.369 Mg/m^3
Absorption coefficient	0.510 mm^{-1}
F(000)	1816
Crystal size	0.15 x 0.15 x 0.15 mm
Theta range for data collection	1.48 to 28.25 deg.
Limiting indices	-12<=h<=13, -23<=k<=36, -18<=l<=20
Reflections collected / unique	26458 / 10304 [R(int) = 0.0410]
Completeness to theta = 28.25	97.1 %
Max. and min. transmission	0.9275 and 0.9275
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10304 / 0 / 573
Goodness-of-fit on F^2	1.002
Final R indices [I>2sigma(I)]	R1 = 0.0449, wR2 = 0.0951
R indices (all data)	R1 = 0.0799, wR2 = 0.1088
Largest diff. peak and hole	0.577 and -0.424 e. $Å^{-3}$