JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
J. Am. Chem. Soc., 1998, 120(49), 12869-12881, DOI:10.1021/ja982914f

Table II. Selected bond lengths (Å) for $[Et_4N][Mo^{IV}(bdt)_2(OSiBu^tPh_2)]$
Symmetry transformations used to generate equivalent atoms:

Mo(1)-O(1)	1.840(2)
Mo(1)-S(2)	2.3361(6)
Mo(1)-S(3)	2.3376(7)
Mo(1)-S(1)	2.3385(6)
Mo(1)-S(4)	2.3402(6)
S(1)-C(1)	1.777(3)
S(2)-C(2)	1.779(3)
S(3)-C(7)	1.773(2)
S(4)-C(8)	1.773(3)
Si(1)-O(1)	1.649(2)
Si(1)-C(17)	1.877(3)
Si(1)-C(23)	1.884(2)
Si(1)-C(13)	1.890(3)
N(1)-C(29)	1.494(5)
N(1)-C(33)	1.500(4)
N(1)-C(31)	1.534(4)
N(1)-C(35)	1.537(4)
C(1)-C(2)	1.391(4)
C(1)-C(6)	1.408(4)
C(2)-C(3)	1.392(3)
C(3)-C(4)	1.381(4)
C(4)-C(5)	1.391(5)
C(5)-C(6)	1.383(4)
C(7)-C(12)	1.395(4)
C(7)-C(8)	1.401(4)
C(8)-C(9)	1.399(4)
C(9)-C(10)	1.390(5)
C(10)-C(11)	1.383(5)
C(11)-C(12)	1.379(4)
C(13)-C(15)	1.531(4)
C(13)-C(14)	1.540(4)
C(13)-C(16)	1.541(4)
C(17)-C(22)	1.397(3)
C(17)-C(18)	1.400(4)
C(18)-C(19)	1.391(4)
C(19)-C(20)	1.377(5)
C(20)-C(21)	1.375(5)
C(21)-C(22)	1.380(4)
C(23)-C(28)	1.390(4)
C(23)-C(24)	1.403(4)
C(24)-C(25)	1.401(4)
C(25)-C(26)	1.374(5)
C(26)-C(27)	1.365(5)
C(27)-C(28)	1.401(4)
C(29)-C(30)	1.564(7)
C(31)-C(32)	1.514(7)
C(33)-C(34)	1.540(6)
C(35)-C(36)	1.529(6)

Table III. Selected bond angles (deg.) for $[Et_4N][Mo^{IV}(bdt)_2(OSiBu^tPh_2)]$
Symmetry transformations used to generate equivalent atoms:

O(1)-Mo(1)-S(2)	109.35(6)	C(15)-C(13)-Si(1)	112.5(2)
O(1)-Mo(1)-S(3)	108.14(6)	C(14)-C(13)-Si(1)	108.3(2)
S(2)-Mo(1)-S(3)	84.24(2)	C(16)-C(13)-Si(1)	108.0(2)
O(1)-Mo(1)-S(1)	108.47(6)	C(22)-C(17)-C(18)	116.8(2)
S(2)-Mo(1)-S(1)	83.81(2)	C(22)-C(17)-Si(1)	124.8(2)
S(3)-Mo(1)-S(1)	143.39(3)	C(18)-C(17)-Si(1)	118.4(2)
O(1)-Mo(1)-S(4)	108.48(6)	C(19)-C(18)-C(17)	121.1(3)
S(2)-Mo(1)-S(4)	142.17(2)	C(20)-C(19)-C(18)	120.3(3)
S(3)-Mo(1)-S(4)	83.85(2)	C(21)-C(20)-C(19)	119.8(3)
S(1)-Mo(1)-S(4)	84.73(2)	C(20)-C(21)-C(22)	120.0(3)
C(1)-S(1)-Mo(1)	106.62(9)	C(21)-C(22)-C(17)	122.1(3)
C(2)-S(2)-Mo(1)	107.21(9)	C(28)-C(23)-C(24)	117.8(2)
C(7)-S(3)-Mo(1)	106.85(9)	C(28)-C(23)-Si(1)	123.2(2)
C(8)-S(4)-Mo(1)	106.69(8)	C(24)-C(23)-Si(1)	119.0(2)
O(1)-Si(1)-C(17)	105.35(10)	C(25)-C(24)-C(23)	120.6(3)
O(1)-Si(1)-C(23)	106.56(10)	C(26)-C(25)-C(24)	119.8(3)
C(17)-Si(1)-C(23)	112.13(11)	C(27)-C(26)-C(25)	120.7(3)
O(1)-Si(1)-C(13)	106.81(11)	C(26)-C(27)-C(28)	119.9(3)
C(17)-Si(1)-C(13)	113.86(12)	C(23)-C(28)-C(27)	121.1(3)
C(23)-Si(1)-C(13)	111.51(12)	N(1)-C(29)-C(30)	114.2(3)
Si(1)-O(1)-Mo(1)	175.18(12)	C(32)-C(31)-N(1)	113.8(3)
C(29)-N(1)-C(33)	111.9(3)	N(1)-C(33)-C(34)	113.6(3)
C(29)-N(1)-C(31)	110.9(3)	C(36)-C(35)-N(1)	114.1(3)
C(33)-N(1)-C(31)	105.6(3)		
C(29)-N(1)-C(35)	106.7(3)		
C(33)-N(1)-C(35)	111.1(3)		
C(31)-N(1)-C(35)	110.6(3)		
C(2)-C(1)-C(6)	119.4(2)		
C(2)-C(1)-S(1)	119.6(2)		
C(6)-C(1)-S(1)	121.0(2)		
C(1)-C(2)-C(3)	120.0(2)		
C(1)-C(2)-S(2)	118.6(2)		
C(3)-C(2)-S(2)	121.3(2)		
C(4)-C(3)-C(2)	120.2(3)		
C(3)-C(4)-C(5)	120.3(3)		
C(6)-C(5)-C(4)	120.1(3)		
C(5)-C(6)-C(1)	119.9(3)		
C(12)-C(7)-C(8)	119.5(2)		
C(12)-C(7)-S(3)	121.5(2)		
C(8)-C(7)-S(3)	119.0(2)		
C(9)-C(8)-C(7)	119.7(2)		
C(9)-C(8)-S(4)	121.1(2)		
C(7)-C(8)-S(4)	119.2(2)		
C(10)-C(9)-C(8)	119.6(3)		
C(11)-C(10)-C(9)	120.6(3)		
C(12)-C(11)-C(10)	120.1(3)		
C(11)-C(12)-C(7)	120.5(3)		
C(15)-C(13)-C(14)	109.2(2)		
C(15)-C(13)-C(16)	110.3(3)		
C(14)-C(13)-C(16)	108.5(3)		

Table IV. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $[Et_4N][Mo^{IV}(bdt)_2(OSiBu^tPh_2)]$
The anisotropic displacement factor exponent takes the form:
$-2\pi^2[(ha^*)^2U_{11} + ... + 2hka^*b^*U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mo(1)	19(1)	25(1)	18(1)	0(1)	4(1)	-2(1)
S(1)	30(1)	33(1)	28(1)	0(1)	-5(1)	-4(1)
S(2)	38(1)	34(1)	24(1)	-1(1)	7(1)	9(1)
S(3)	41(1)	30(1)	20(1)	0(1)	4(1)	-1(1)
S(4)	34(1)	26(1)	26(1)	-2(1)	2(1)	-2(1)
Si(1)	20(1)	27(1)	24(1)	4(1)	4(1)	-1(1)
O(1)	23(1)	32(1)	26(1)	2(1)	5(1)	-1(1)
N(1)	37(1)	62(2)	33(1)	-15(1)	8(1)	-2(1)
C(1)	21(1)	36(1)	33(1)	8(1)	1(1)	-2(1)
C(2)	24(1)	39(1)	32(1)	7(1)	8(1)	2(1)
C(3)	33(1)	41(1)	48(2)	7(1)	12(1)	9(1)
C(4)	39(2)	44(2)	62(2)	15(2)	3(2)	11(1)
C(5)	38(2)	52(2)	58(2)	22(2)	-12(1)	1(1)
C(6)	40(2)	46(2)	40(2)	9(1)	-10(1)	-6(1)
C(7)	26(1)	32(1)	29(1)	3(1)	6(1)	1(1)
C(8)	27(1)	30(1)	32(1)	5(1)	5(1)	0(1)
C(9)	44(2)	29(1)	46(2)	1(1)	5(1)	4(1)
C(10)	57(2)	35(1)	58(2)	16(1)	7(2)	11(1)
C(11)	49(2)	54(2)	43(2)	20(1)	2(1)	12(1)
C(12)	42(2)	46(2)	31(2)	7(1)	3(1)	0(1)
C(13)	33(1)	38(1)	36(2)	-2(1)	3(1)	-11(1)
C(14)	62(2)	35(2)	75(3)	-16(2)	10(2)	-4(1)
C(15)	37(2)	61(2)	63(3)	-10(2)	4(2)	-19(2)
C(16)	72(2)	72(2)	32(2)	-4(2)	-4(2)	-27(2)
C(17)	31(1)	31(1)	26(1)	4(1)	8(1)	0(1)
C(18)	30(1)	66(2)	32(2)	13(1)	6(1)	-4(1)
C(19)	44(2)	87(2)	31(2)	14(2)	-1(1)	0(2)
C(20)	70(2)	64(2)	24(2)	11(1)	11(2)	2(2)
C(21)	50(2)	62(2)	41(2)	13(2)	21(1)	3(1)
C(22)	35(1)	57(2)	40(2)	14(1)	13(1)	1(1)
C(23)	24(1)	33(1)	32(1)	2(1)	1(1)	2(1)
C(24)	35(1)	31(1)	42(2)	4(1)	3(1)	1(1)
C(25)	53(2)	31(1)	56(2)	5(1)	-3(2)	1(1)
C(26)	54(2)	38(2)	65(2)	-6(2)	-4(2)	21(1)
C(27)	33(2)	54(2)	75(2)	-2(2)	12(2)	13(1)
C(28)	35(1)	43(2)	62(2)	9(1)	14(1)	7(1)
C(29)	68(3)	90(3)	97(4)	-54(3)	29(2)	-28(2)
C(30)	85(3)	84(3)	110(5)	-10(3)	52(3)	-24(2)
C(31)	78(3)	85(3)	55(2)	-14(2)	25(2)	18(2)
C(32)	73(3)	268(9)	84(4)	-35(5)	4(3)	93(4)
C(33)	58(2)	85(3)	42(2)	-10(2)	0(2)	-16(2)
C(34)	55(2)	112(3)	60(3)	19(2)	-1(2)	12(2)
C(35)	50(2)	107(3)	43(2)	-4(2)	10(2)	19(2)
C(36)	67(3)	117(4)	103(4)	51(3)	30(3)	14(3)

Table V. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $[Et_4N][Mo^{IV}(bdt)_2(OSiBu^tPh_2)]$

H atom	x	y	z	U(eq)
H(3A)	4462(2)	-2083(3)	1867(2)	48
H(4A)	5482(3)	-2908(3)	2980(2)	58
H(5A)	5779(3)	-1554(3)	4041(2)	61
H(6A)	5045(3)	628(3)	3991(2)	52
H(9A)	2088(3)	7373(3)	1281(2)	48
H(10A)	1388(3)	8244(3)	104(2)	60
H(11A)	1012(3)	6848(3)	-929(2)	59
H(12A)	1334(3)	4572(3)	-797(2)	48
H(14A)	461(3)	-609(3)	1513(2)	86
H(14B)	-632(3)	-1572(3)	1196(2)	86
H(14C)	-412(3)	-1264(3)	2063(2)	86
H(15A)	-3195(3)	584(3)	1471(2)	81
H(15B)	-2655(3)	-530(3)	2037(2)	81
H(15C)	-2875(3)	-837(3)	1170(2)	81
H(16A)	-372(4)	1168(4)	610(2)	89
H(16B)	-1782(4)	1626(4)	576(2)	89
H(16C)	-1454(4)	197(4)	289(2)	89
H(18A)	1327(3)	1186(3)	3322(2)	51
H(19A)	1591(3)	560(4)	4578(2)	65
H(20A)	-126(4)	-49(3)	5181(2)	63
H(21A)	-2123(3)	44(3)	4541(2)	60
H(22A)	-2404(3)	732(3)	3305(2)	52
H(24A)	-369(3)	4274(2)	1521(2)	43
H(25A)	-1521(3)	6248(3)	1324(2)	57
H(26A)	-3513(3)	6393(3)	1693(2)	64
H(27A)	-4402(3)	4589(3)	2227(2)	64
H(28A)	-3262(3)	2618(3)	2445(2)	55
H(29A)	2270(4)	6999(5)	4498(3)	100
H(29B)	975(4)	7717(5)	4286(3)	100
H(30A)	2386(5)	8338(4)	3411(4)	134
H(30B)	1255(5)	7551(4)	2981(4)	134
H(30C)	2551(5)	6831(4)	3193(4)	134
H(31A)	1316(4)	3743(4)	3899(2)	86
H(31B)	2010(4)	4741(4)	3408(2)	86
H(32A)	3461(5)	3746(8)	4306(3)	213
H(32B)	2723(5)	4291(8)	4955(3)	213
H(32C)	3418(5)	5290(8)	4463(3)	213
H(33A)	-637(4)	4811(4)	3527(2)	74
H(33B)	97(4)	5725(4)	3010(2)	74
H(34A)	-1856(4)	6711(5)	3165(2)	114
H(34B)	-776(4)	7650(5)	3526(2)	114
H(34C)	-1510(4)	6734(5)	4043(2)	114
H(35A)	1173(3)	5620(4)	5264(2)	80
H(35B)	-164(3)	6175(4)	4973(2)	80
H(36A)	-360(5)	4051(5)	5499(3)	141
H(36B)	497(5)	3435(5)	4928(3)	141
H(36C)	-842(5)	3991(5)	4637(3)	141

Structure Determination Summary

Crystal Data and Structure Refinement for $[Et_4N][Mo^{VI}O(bdt)_2(OSiBu^tPh_2)]$

Identification code	jpd91m
Empirical formula	$C_{36}H_{47}MoNO_2S_4Si$
Formula weight	778.02
Temperature	213(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	*Pbca*
Unit cell dimensions	a = 10.6275(4) Å α = 90°
	b = 22.7953(9) Å β = 90°
	c = 31.4287(12) Å γ = 90°
Volume, Z	7613.8(5) $Å^3$, 8
Density (calculated)	1.357 mg/m^3
Absorption coefficient	0.627 mm^{-1}
F(000)	3248
Crystal size	0.07 x 0.09 x 0.18 mm
θ range for data collection	1.30 to 28.33°
Limiting indices	$-13 < h < 14$, $-29 < k < 30$, $-23 < l < 41$
Reflections collected	48564
Independent reflections	9405 (R_{int} = 0.1430)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9405 / 0 / 356
Goodness-of-fit on F^2	1.164
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.0559, wR_2 = 0.0777
R indices (all data)	R_1 = 0.1609, wR_2 = 0.0926
Largest diff. peak and hole	0.617 and -0.683 e $Å^{-3}$

Table I. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $[Et_4N][Mo^{VI}O(bdt)_2(OSiBu^tPh_2)]$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U(eq)
Mo(1)	7030(1)	375(1)	1261(1)	29(1)
S(1)	8393(1)	267(1)	620(1)	36(1)
S(2)	6114(1)	1084(1)	768(1)	41(1)
S(3)	8284(1)	114(1)	1870(1)	37(1)
S(4)	7804(1)	1335(1)	1468(1)	33(1)
Si(1)	6983(1)	-1159(1)	1272(1)	32(1)
O(1)	5502(2)	363(1)	1436(1)	37(1)
O(2)	7205(2)	-464(1)	1197(1)	33(1)
N(1)	2117(3)	828(1)	1173(1)	35(1)
C(1)	8313(4)	920(2)	336(1)	32(1)
C(2)	7302(4)	1311(2)	421(1)	36(1)
C(3)	7252(4)	1847(2)	216(1)	49(1)
C(4)	8151(5)	1997(2)	-76(2)	58(1)
C(5)	9119(5)	1614(2)	-173(1)	54(1)
C(6)	9192(4)	1080(2)	29(1)	44(1)
C(7)	8894(3)	739(2)	2120(1)	33(1)
C(8)	8694(3)	1284(2)	1937(1)	32(1)
C(9)	9204(4)	1787(2)	2126(1)	39(1)
C(10)	9945(4)	1740(2)	2483(1)	47(1)
C(11)	10159(4)	1197(2)	2662(1)	47(1)
C(12)	9657(4)	693(2)	2488(1)	43(1)
C(13)	5921(4)	-1422(2)	829(1)	44(1)
C(14)	6649(4)	-1378(2)	405(1)	67(2)
C(15)	4743(4)	-1019(2)	795(2)	79(2)
C(16)	5473(4)	-2053(2)	892(2)	76(2)
C(17)	8567(3)	-1530(2)	1256(1)	33(1)
C(18)	9647(4)	-1191(2)	1229(1)	40(1)
C(19)	10850(4)	-1444(2)	1240(1)	50(1)
C(20)	10953(4)	-2041(2)	1278(1)	55(1)
C(21)	9908(5)	-2387(2)	1304(2)	61(1)
C(22)	8734(4)	-2132(2)	1291(1)	50(1)
C(23)	6272(4)	-1281(2)	1809(1)	39(1)
C(24)	6778(4)	-1633(2)	2114(2)	51(1)
C(25)	6268(5)	-1706(2)	2516(2)	73(2)
C(27)	4637(5)	-1048(2)	2335(2)	73(2)
C(28)	5184(4)	-978(2)	1929(2)	61(1)
C(29)	3016(4)	1207(2)	1423(1)	39(1)
C(30)	2401(4)	1592(2)	1761(1)	57(1)

Table I. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $[Et_4N][Mo^{VI}O(bdt)_2(OSiBu^tPh_2)]$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U(eq)
C(31)	1377(4)	424(2)	1456(1)	50(1)
C(32)	2142(4)	15(2)	1733(2)	71(2)
C(33)	1151(4)	1206(2)	946(1)	46(1)
C(34)	1681(4)	1666(2)	648(1)	63(1)
C(35)	2914(4)	486(2)	858(1)	42(1)
C(36)	2216(4)	71(2)	563(1)	58(1)
C(26)	5202(5)	-1410(2)	2619(2)	72(2)

Table II. Selected bond lengths (Å) and angles (deg.) for $[Et_4N][Mo^{VI}O(bdt)_2(OSiBu^tPh_2)]$
Symmetry transformations used to generate equivalent atoms:

Mo(1)-O(1)	1.715(2)	C(25)-C(26)	1.358(6)
Mo(1)-O(2)	1.932(2)	C(27)-C(26)	1.358(6)
Mo(1)-S(3)	2.4073(11)	C(27)-C(28)	1.411(6)
Mo(1)-S(4)	2.4274(10)	C(29)-C(30)	1.523(5)
Mo(1)-S(2)	2.4425(11)	C(31)-C(32)	1.512(5)
Mo(1)-S(1)	2.4922(11)	C(33)-C(34)	1.514(5)
S(1)-C(1)	1.738(4)	C(35)-C(36)	1.517(5)
S(2)-C(2)	1.745(4)		
S(3)-C(7)	1.750(4)		
S(4)-C(8)	1.755(4)		
Si(1)-O(2)	1.618(2)		
Si(1)-C(23)	1.869(4)		
Si(1)-C(13)	1.890(4)		
Si(1)-C(17)	1.884(4)		
N(1)-C(31)	1.503(5)		
N(1)-C(29)	1.509(4)		
N(1)-C(35)	1.518(4)		
N(1)-C(33)	1.518(5)		
C(1)-C(6)	1.392(5)		
C(1)-C(2)	1.422(5)		
C(2)-C(3)	1.383(5)		
C(3)-C(4)	1.369(6)		
C(4)-C(5)	1.384(6)		
C(5)-C(6)	1.375(5)		
C(7)-C(8)	1.385(5)		
C(7)-C(12)	1.418(5)		
C(8)-C(9)	1.401(5)		
C(9)-C(10)	1.376(5)		
C(10)-C(11)	1.378(5)		
C(11)-C(12)	1.380(5)		
C(13)-C(16)	1.527(5)		
C(13)-C(14)	1.545(5)		
C(13)-C(15)	1.557(5)		
C(17)-C(22)	1.388(5)		
C(17)-C(18)	1.387(5)		
C(18)-C(19)	1.404(5)		
C(19)-C(20)	1.369(5)		
C(20)-C(21)	1.365(6)		
C(21)-C(22)	1.378(5)		
C(23)-C(24)	1.361(5)		
C(23)-C(28)	1.398(6)		
C(24)-C(25)	1.385(6)		

Table III. Selected bond angles (deg.) for $[Et_4N][Mo^{VI}O(bdt)_2(OSiBu^tPh_2)]$
Symmetry transformations used to generate equivalent atoms:

O(1)-Mo(1)-O(2)	96.26(11)	C(8)-C(7)-C(12)	119.5(4)
O(1)-Mo(1)-S(3)	105.33(9)	C(8)-C(7)-S(3)	119.2(3)
O(2)-Mo(1)-S(3)	77.57(7)	C(12)-C(7)-S(3)	121.2(3)
O(1)-Mo(1)-S(4)	104.40(9)	C(7)-C(8)-C(9)	120.0(4)
O(2)-Mo(1)-S(4)	152.63(8)	C(7)-C(8)-S(4)	119.4(3)
S(3)-Mo(1)-S(4)	79.76(3)	C(9)-C(8)-S(4)	120.6(3)
O(1)-Mo(1)-S(2)	80.60(9)	C(10)-C(9)-C(8)	120.2(4)
O(2)-Mo(1)-S(2)	128.90(7)	C(9)-C(10)-C(11)	119.8(4)
S(3)-Mo(1)-S(2)	152.75(4)	C(10)-C(11)-C(12)	121.6(4)
S(4)-Mo(1)-S(2)	73.02(3)	C(11)-C(12)-C(7)	118.9(4)
O(1)-Mo(1)-S(1)	143.93(9)	C(16)-C(13)-C(14)	109.2(4)
O(2)-Mo(1)-S(1)	76.26(7)	C(16)-C(13)-C(15)	108.3(4)
S(3)-Mo(1)-S(1)	107.25(3)	C(14)-C(13)-C(15)	107.8(4)
S(4)-Mo(1)-S(1)	96.24(3)	C(16)-C(13)-Si(1)	113.0(3)
S(2)-Mo(1)-S(1)	77.55(4)	C(14)-C(13)-Si(1)	108.4(3)
C(1)-S(1)-Mo(1)	107.57(14)	C(15)-C(13)-Si(1)	110.1(3)
C(2)-S(2)-Mo(1)	107.67(13)	C(22)-C(17)-C(18)	116.8(4)
C(7)-S(3)-Mo(1)	111.11(14)	C(22)-C(17)-Si(1)	123.7(3)
C(8)-S(4)-Mo(1)	110.31(14)	C(18)-C(17)-Si(1)	119.4(3)
O(2)-Si(1)-C(23)	109.6(2)	C(17)-C(18)-C(19)	121.5(4)
O(2)-Si(1)-C(13)	106.9(2)	C(20)-C(19)-C(18)	118.9(4)
C(23)-Si(1)-C(13)	112.1(2)	C(21)-C(20)-C(19)	120.9(4)
O(2)-Si(1)-C(17)	107.8(2)	C(22)-C(21)-C(20)	119.5(4)
C(23)-Si(1)-C(17)	108.6(2)	C(21)-C(22)-C(17)	122.3(4)
C(13)-Si(1)-C(17)	111.8(2)	C(24)-C(23)-C(28)	115.3(4)
Si(1)-O(2)-Mo(1)	160.0(2)	C(24)-C(23)-Si(1)	124.4(3)
C(31)-N(1)-C(29)	112.0(3)	C(28)-C(23)-Si(1)	120.2(3)
C(31)-N(1)-C(35)	111.2(3)	C(23)-C(24)-C(25)	124.1(5)
C(29)-N(1)-C(35)	106.3(3)	C(26)-C(25)-C(24)	118.9(5)
C(31)-N(1)-C(33)	105.8(3)	C(26)-C(27)-C(28)	118.8(5)
C(29)-N(1)-C(33)	110.5(3)	C(23)-C(28)-C(27)	121.9(5)
C(35)-N(1)-C(33)	111.2(3)	C(30)-C(29)-N(1)	114.9(3)
C(6)-C(1)-C(2)	118.2(4)	C(32)-C(31)-N(1)	115.9(3)
C(6)-C(1)-S(1)	123.3(3)	C(34)-C(33)-N(1)	115.6(3)
C(2)-C(1)-S(1)	118.5(3)	C(36)-C(35)-N(1)	116.5(3)
C(3)-C(2)-C(1)	119.7(4)	C(27)-C(26)-C(25)	121.0(5)
C(3)-C(2)-S(2)	121.7(3)		
C(1)-C(2)-S(2)	118.6(3)		
C(4)-C(3)-C(2)	120.6(4)		
C(3)-C(4)-C(5)	120.5(4)		
C(6)-C(5)-C(4)	119.9(4)		
C(5)-C(6)-C(1)	121.0(4)		

Table IV. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $[Et_4N][Mo^{VI}O(bdt)_2(OSiBu^tPh_2)]$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[(ha^*)_2U_{11} + ... + 2hka^*b^*U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mo(1)	22(1)	28(1)	36(1)	0(1)	1(1)	1(1)
S(1)	33(1)	37(1)	38(1)	1(1)	5(1)	1(1)
S(2)	29(1)	43(1)	49(1)	4(1)	-6(1)	6(1)
S(3)	37(1)	33(1)	41(1)	6(1)	-4(1)	1(1)
S(4)	32(1)	29(1)	38(1)	1(1)	-2(1)	1(1)
Si(1)	32(1)	26(1)	37(1)	-1(1)	5(1)	0(1)
O(1)	20(1)	43(2)	50(2)	3(2)	6(1)	-1(1)
O(2)	36(2)	28(2)	37(2)	2(1)	3(1)	-1(1)
N(1)	19(2)	41(2)	44(2)	-6(2)	3(2)	-7(2)
C(1)	35(2)	33(2)	29(3)	5(2)	-5(2)	-8(2)
C(2)	39(3)	37(2)	34(3)	2(2)	-9(2)	-4(2)
C(3)	59(3)	45(3)	42(3)	3(2)	-6(3)	5(2)
C(4)	77(4)	43(3)	54(3)	21(2)	-7(3)	-7(3)
C(5)	64(4)	59(3)	40(3)	11(3)	-3(3)	-23(3)
C(6)	41(3)	53(3)	38(3)	0(2)	0(2)	-12(2)
C(7)	27(2)	37(3)	35(3)	-2(2)	9(2)	-4(2)
C(8)	29(2)	38(3)	30(3)	-3(2)	6(2)	0(2)
C(9)	44(3)	39(3)	34(3)	-4(2)	1(2)	-4(2)
C(10)	45(3)	56(3)	39(3)	-10(2)	1(2)	-13(2)
C(11)	38(3)	66(3)	38(3)	-1(3)	-2(2)	-7(2)
C(12)	43(3)	51(3)	35(3)	8(3)	2(2)	-2(2)
C(13)	39(3)	43(3)	48(3)	-10(2)	1(2)	-4(2)
C(14)	75(4)	77(4)	48(3)	-12(3)	-14(3)	1(3)
C(15)	48(3)	87(4)	103(5)	-35(3)	-29(3)	17(3)
C(16)	70(4)	60(4)	96(5)	-17(3)	-6(3)	-23(3)
C(17)	33(2)	31(2)	35(2)	-5(2)	0(2)	1(2)
C(18)	45(3)	35(2)	41(3)	7(2)	4(2)	3(2)
C(19)	34(3)	56(3)	59(3)	-10(3)	-3(2)	4(2)
C(20)	44(3)	62(3)	58(3)	-14(3)	0(3)	21(3)
C(21)	67(3)	37(3)	78(4)	-6(3)	-8(3)	13(3)
C(22)	43(3)	36(3)	71(3)	0(3)	0(3)	3(2)
C(23)	45(3)	30(2)	42(3)	2(2)	4(2)	-7(2)
C(24)	40(3)	68(3)	45(3)	0(3)	7(2)	-5(2)
C(25)	74(4)	91(4)	54(4)	19(3)	-12(3)	-8(3)
C(27)	71(4)	66(4)	83(4)	-9(3)	49(3)	3(3)

Table V. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $[Et_4N][Mo^{VI}O(bdt)_2(OSiBu^tPh_2)]$.

H atom	x	y	z	U(eq)
H(3A)	6603(4)	2107(2)	277(1)	58
H(4A)	8111(5)	2360(2)	-211(2)	70
H(5A)	9720(5)	1717(2)	-375(1)	65
H(6A)	9839(4)	823(2)	-40(1)	53
H(9A)	9041(4)	2155(2)	2009(1)	47
H(10A)	10300(4)	2074(2)	2604(1)	56
H(11A)	10654(4)	1170(2)	2905(1)	57
H(12A)	9815(4)	329(2)	2611(1)	51
H(14A)	6933(4)	-982(2)	365(1)	100
H(14B)	6106(4)	-1488(2)	174(1)	100
H(14C)	7361(4)	-1637(2)	413(1)	100
H(15A)	5007(4)	-620(2)	755(2)	119
H(15B)	4257(4)	-1048(2)	1052(2)	119
H(15C)	4238(4)	-1140(2)	557(2)	119
H(16A)	5021(4)	-2083(2)	1155(2)	113
H(16B)	6187(4)	-2311(2)	898(2)	113
H(16C)	4930(4)	-2162(2)	661(2)	113
H(18A)	9573(4)	-786(2)	1203(1)	48
H(19A)	11566(4)	-1211(2)	1222(1)	60
H(20A)	11747(4)	-2212(2)	1286(1)	65
H(21A)	9989(5)	-2792(2)	1330(2)	73
H(22A)	8027(4)	-2372(2)	1307(1)	60
H(24A)	7512(4)	-1836(2)	2049(2)	61
H(25A)	6651(5)	-1954(2)	2713(2)	88
H(26A)	4853(5)	-1457(2)	2888(2)	86
H(27A)	3902(5)	-849(2)	2406(2)	88
H(28A)	4811(4)	-724(2)	1735(2)	73
H(29A)	3628(4)	954(2)	1561(1)	47
H(29B)	3470(4)	1457(2)	1226(1)	47
H(30A)	3037(4)	1815(2)	1905(1)	85
H(30B)	1965(4)	1349(2)	1962(1)	85
H(30C)	1815(4)	1854(2)	1627(1)	85
H(31A)	845(4)	660(2)	1639(1)	59
H(31B)	828(4)	188(2)	1278(1)	59
H(32A)	1586(4)	-223(2)	1900(2)	106
H(32B)	2672(4)	242(2)	1917(2)	106
H(32C)	2653(4)	-232(2)	1556(2)	106
H(33A)	600(4)	951(2)	784(1)	55
H(33B)	641(4)	1402(2)	1158(1)	55
H(34A)	1003(4)	1882(2)	521(1)	94

Table V. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $[Et_4N][Mo^{VI}O(bdt)_2(OSiBu^tPh_2)]$.

H atom	x	y	z	U(eq)
H(34B)	2165(4)	1477(2)	429(1)	94
H(34C)	2212(4)	1929(2)	805(1)	94
H(35A)	3375(4)	765(2)	685(1)	50
H(35B)	3526(4)	260(2)	1017(1)	50
H(36A)	2807(4)	-122(2)	380(1)	87
H(36B)	1626(4)	290(2)	395(1)	87
H(36C)	1773(4)	-216(2)	729(1)	87