SUPPORTING INFORMATION

Modeling Aspects of Hydrodesulfurization at Molybdenum: Carbon–Sulfur Bond Cleavage of Thiophenes by *Ansa* Molybdenocene Complexes

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Experimental details, spectroscopic data and crystallographic data.

Synthesis of $[Me_2Si(C_5Me_4)_2]Mo(SC_4H_4)$

A solution of $[Me_2Si(C_5Me_4)_2]MoH_2$ (40 mg, 0.10 mmol) and thiophene (0.1 mL) in C_6H_{12} (*ca.* 1 mL) was photolyzed with uv light for 1 day, thereby depositing dark red crystals which were isolated by filtration, washed with pentane, and dried *in vacuo* giving $[Me_2Si(C_5Me_4)_2]Mo(SC_4H_4)$ (15 mg, 31%). Analysis calculated for $C_{24}H_{34}SSiMo$: C, 60.2 %; H, 7.2 %. Found: C, 59.5 %; H, 6.8 %. IR Data (KBr pellet, cm^{-1}): 2985 (vs), 2905 (vs), 1563 (w), 1544 (w), 1510 (w), 1459 (w), 1362 (s), 1305 (m), 1254 (m), 1190 (w), 1129 (w), 1020 (m), 841 (m), 815 (m), 769 (w), 660 (m).

NMR Data

Compound/Assignment	**δ (ppm)**	**Coupling (Hz)**
$[Me_2Si(C_5Me_4)_2]Mo(SC_4H_4)$		
^1H NMR (C_6D_6)		
$[Me_2Si(C_5Me_4)_2]$		
$(C\underline{H}_3)_2Si\{C_5(CH_3)_4\}_2$		
1 (CH_3)	0.18	s
1 (CH_3)	0.20	s
$(CH_3)_2Si\{C_5(C\underline{H}_3)_4\}_2$		
2 (CH_3)	1.44	s
2 (CH_3)	1.49	s
2 (CH_3)	1.67	s
2 (CH_3)	1.77	s
$Mo(SC_4\underline{H}_4)$		
1H	6.41	dd, $^3J_{H-H} = 10$ $^3J_{H-H} = 7$
1H	6.54	d, $^3J_{H-H} = 10$
1H	7.19	dd, $^3J_{H-H} = 11$ $^3J_{H-H} = 7$
1H	7.28	d, $^3J_{H-H} = 11$

^{13}C NMR (C_6D_6)

$[Me_2Si(C_5Me_4)_2]$

$(\underline{C}H_3)_2Si\{C_5(CH_3)_4\}_2$		
1 (CH_3)	2.2	q, $^1J_{C-H}$ = 121
1(CH_3)	2.5	q, $^1J_{C-H}$ = 121
$(CH_3)_2Si\{\underline{C}_5(CH_3)_4\}_2$		
2 C	59.1	s
2 C	93.4	s
2 C	94.8	s
2 C	119.7	s
2 C	126.2	s
$(CH_3)_2Si\{C_5(\underline{C}H_3)_4\}_2$		
2 (CH_3)	10.2	q, $^1J_{C-H}$ = 131
2 (CH_3)	11.2	q, $^1J_{C-H}$ = 127
2 (CH_3)	12.3	q, $^1J_{C-H}$ = 128
2 (CH_3)	13.0	q, $^1J_{C-H}$ = 127
$Mo(S\underline{C}_4H_4)$		
1 C	123.2	d, $^1J_{C-H}$ = 171
1 C	126.6	d, $^1J_{C-H}$ = 176
1 C	131.8	d, $^1J_{C-H}$ = 147
1 C	162.6	d, $^1J_{C-H}$ = 140

Synthesis of $[Me_2Si(C_5Me_4)_2]Mo(SC_8H_6)$

A solution of $[Me_2Si(C_5Me_4)_2]MoH_2$ (40 mg, 0.10 mmol) and benzothiophene (0.1 mL) in C_6H_{12} (*ca.* 1 mL) was photolyzed with uv light for 1 day, thereby depositing dark red crystals formed which were isolated by filteration, washed with pentane, and dried *in vacuo* giving $[Me_2Si(C_5Me_4)_2]Mo(SC_8H_6)$ (25 mg, 47%). Analysis calculated for $C_{28}H_{36}SSiMo$: C, 63.6 %; H, 6.9 %. Found: C, 63.2 %; H, 6.7 %. IR Data (KBr pellet, cm^{-1}): 3032 (m), 2990 (m), 2898 (s), 1578 (m), 1561 (w), 1543 (w), 1509 (w), 1459 (vs), 1410 (m), 1376 (s), 1335 (s), 1310 (s), 1254 (s), 1210 (w), 1152 (w), 1129 (m), 1064 (m), 1032 (m), 841 (vs), 811 (s), 770 (s), 736 (vs), 674 (vs), 680 (vs), 494 (w), 459 (w).

NMR Data

Compound/Assignment	**δ (ppm)**	**Coupling (Hz)**
$[Me_2Si(C_5Me_4)_2]Mo(SC_8H_6)$		
^1H NMR (C_6D_6)		
$[Me_2Si(C_5Me_4)_2]$		
$(C\underline{H}_3)_2Si\{C_5(CH_3)_4\}_2$		
1 (CH_3)	0.17	s
1 (CH_3)	0.20	s
$(CH_3)_2Si\{C_5(C\underline{H}_3)_4\}_2$		
2 (CH_3)	1.35	s
2 (CH_3)	1.46	s
2 (CH_3)	1.64	s
2 (CH_3)	1.64	s
$Mo(SC_8\underline{H}_6)$		
1H	6.92	t, $^3J_{H-H} = 7$ d, $^4J_{H-H} = 2$
1H	6.96	t, $^3J_{H-H} = 7$ d, $^4J_{H-H} = 2$
1H	7.08	d, $^3J_{H-H} = 7$ d, $^4J_{H-H} = 2$
1H	7.34	d, $^3J_{H-H} = 12$
1H	7.71	d, $^3J_{H-H} = 12$
1H	7.98	d, $^3J_{H-H} = 7$

^{13}C NMR (C_6D_6)

$[Me_2Si(C_5Me_4)_2]$

$(\underline{C}H_3)_2Si\{C_5(CH_3)_4\}_2$		
1 (CH_3)	2.2	q, $^1J_{C-H}$ = 120
1(CH_3)	2.4	q, $^1J_{C-H}$ = 120
$(CH_3)_2Si\{\underline{C}_5(CH_3)_4\}_2$		
2 C	58.9	s
2 C	92.9	s
2 C	95.3	s
2 C	119.0	s
2 C	127.2	s
$(CH_3)_2Si\{C_5(\underline{C}H_3)_4\}_2$		
2 (CH_3)	10.1	q, $^1J_{C-H}$ = 127
2 (CH_3)	11.2	q, $^1J_{C-H}$ = 127
2 (CH_3)	12.4	q, $^1J_{C-H}$ = 127
2 (CH_3)	13.2	q, $^1J_{C-H}$ = 127
$Mo(\underline{C}_8H_6)$		
1 C	121.6	d, $^1J_{C-H}$ = 153
1 C	125.7	d, $^1J_{C-H}$ = 165
1 C	131.5	d, $^1J_{C-H}$ = 157
1 C	132.4	d, $^1J_{C-H}$ = 151
1 C	136.5	s
1 C	138.9	d, $^1J_{C-H}$ = 146
1 C	141.9	s
1 C	164.7	d, $^1J_{C-H}$ = 138

Synthesis of $[Me_2Si(C_5Me_4)_2]Mo(SC_{12}H_8)$

A solution of $[Me_2Si(C_5Me_4)_2]MoH_2$ (30 mg, 0.076 mmol) and dibenzothiophene (0.1 mL) in C_6H_{12} (*ca.* 1 mL) was photolyzed with uv light for 1 day, thereby depositing dark red crystals which were isolated by filtration, washed with cyclohexane, and dried *in vacuo* giving $[Me_2Si(C_5Me_4)_2]Mo(SC_{12}H_8)$ (17 mg, 39%). IR Data (KBr pellet, cm^{-1}): 2900 (s), 1594 (w), 1442 (s), 1377 (s), 1315 (m), 1252 (s), 1125 (m), 1022 (s), 903 (s), 879 (s), 838 (s), 742 (vs), 665 (s), 513 (m), 404 (w).

NMR Data

Compound/Assignment	**δ (ppm)**	**Coupling (Hz)**
$[Me_2Si(C_5Me_4)_2]Mo(SC_{12}H_8)$		
^1H NMR (C_6D_{12})		
$[Me_2Si(C_5Me_4)_2]$		
$(C\underline{H}_3)_2Si\{C_5(CH_3)_4\}_2$		
1 (CH_3)	0.51	s
$(CH_3)_2Si\{C_5(C\underline{H}_3)_4\}_2$		
4 (CH_3)	1.34	s
4 (CH_3)	2.16	s
$Mo(SC_{12}\underline{H}_8)$		
4H	7.27	m
2H	7.49	m
2H	7.98	m

^{13}C NMR (C_6D_{12})

$[Me_2Si(C_5Me_4)_2]$

$(\underline{C}H_3)_2Si\{C_5(CH_3)_4\}_2$	
2 (CH_3)	3.6
$(CH_3)_2Si\{\underline{C}_5(CH_3)_4\}_2$	
4 C	91.9
4 C	102.6
2 C	not located
$(CH_3)_2Si\{C_5(\underline{C}H_3)_4\}_2$	
4 (CH_3)	12.9
4 (CH_3)	14.6
$Mo(S\underline{C}_{12}H_8)$	
2 C	123.4
2 C	125.0
2 C	126.0
2 C	136.5
2 C	140.6
2 C	not located

Table 1. Crystal data and structure refinement for [Me2Si(C5Me4)2]Mo(SC4H4).

Identification code	this10
Empirical formula	$C_{24}H_{34}MoSSi$
Formula weight	478.60
Temperature	233(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 9.8588(9) Å alpha = 90° b = 24.716(2) Å beta = 112.7420(10)° c = 9.8994(9) Å gamma = 90°
Volume, Z	2224.7(3) $Å^3$, 4
Density (calculated)	1.429 Mg/m^3
Absorption coefficient	0.744 mm^{-1}
F(000)	1000
Crystal size	0.30 x 0.20 x 0.20 mm
θ range for data collection	1.65 to 28.15°
Limiting indices	$-12 \le h \le 11$, $-32 \le k \le 22$, $-13 \le l \le 13$
Reflections collected	15039
Independent reflections	5000 (R_{int} = 0.0170)
Completeness to θ = 28.15°	92.0 %
Absorption correction	SADABS
Max. and min. transmission	0.8654 and 0.8076
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5000 / 8 / 300
Goodness-of-fit on F^2	1.175
Final R indices [I>2σ(I)]	R1 = 0.0297, wR2 = 0.0699
R indices (all data)	R1 = 0.0317, wR2 = 0.0708
Extinction coefficient	0.00033(13)

Largest diff. peak and hole	**0.403 and -0.405 eÅ**

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for [Me2Si(C5Me4)2]Mo(SC4H4). U(eq one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Mo	7023(1)	8779(1)	2404(1)	29(1)
Si	9747(1)	8480(1)	1650(1)	41(1)
C(11)	7800(2)	8237(1)	996(2)	33(1)
C(12)	7253(2)	7883(1)	1839(2)	35(1)
C(13)	5694(3)	7944(1)	1286(3)	37(1)
C(14)	5270(2)	8336(1)	178(3)	37(1)
C(15)	6538(2)	8536(1)	-7(2)	34(1)
C(21)	9424(2)	8983(1)	2911(2)	35(1)
C(22)	9298(3)	8848(1)	4294(3)	41(1)
C(23)	8506(3)	9270(1)	4624(3)	46(1)
C(24)	8084(3)	9653(1)	3496(3)	44(1)
C(25)	8600(3)	9482(1)	2407(3)	40(1)
C(32)	8037(3)	7428(1)	2849(3)	50(1)
C(33)	4662(3)	7602(1)	1705(4)	57(1)
C(34)	3712(3)	8474(1)	-781(3)	56(1)
C(35)	6431(3)	8891(1)	-1275(3)	48(1)
C(42)	10129(3)	8419(1)	5386(3)	61(1)
C(43)	8272(4)	9339(2)	6027(3)	73(1)
C(44)	7359(4)	10185(1)	3525(4)	69(1)
C(45)	8525(4)	9841(1)	1150(3)	57(1)
C(51)	10311(4)	8769(2)	202(4)	66(1)
C(52)	11181(3)	7959(1)	2556(4)	67(1)
S	5004(2)	9397(1)	1532(3)	46(1)
C(1)	3960(20)	9409(9)	2580(20)	87(7)
C(2)	4050(20)	9101(11)	3700(20)	77(8)
C(3)	5017(15)	8663(5)	4289(15)	61(4)
C(4)	6110(20)	8509(8)	3990(20)	57(5)
SA	6086(5)	8452(2)	4231(5)	42(1)
C(1A)	4618(15)	8810(5)	4295(14)	47(2)
C(2A)	3840(20)	9201(11)	3430(20)	50(2)
C(3A)	4080(20)	9443(7)	2250(18)	44(2)
C(4A)	5080(20)	9340(6)	1769(18)	127(7)

Table 3. Bond lengths [Å] and angles [°] for [Me2Si(C5Me4)2]Mo(SC4H4). C

Mo-C(4)	2.194(16)	Mo-C(4A)	2.248(17)
Mo-C(11)	2.269(2)	Mo-C(21)	2.278(2)
Mo-C(22)	2.305(2)	Mo-C(12)	2.317(2)
Mo-C(15)	2.324(2)	Mo-C(25)	2.332(2)
Mo-S	2.390(2)	Mo-C(23)	2.440(2)
Mo-C(24)	2.462(2)	Mo-SA	2.463(4)
Mo-C(13)	2.466(2)	Mo-C(14)	2.470(2)
Si-C(52)	1.866(3)	Si-C(51)	1.868(3)
Si-C(11)	1.872(2)	Si-C(21)	1.873(2)
C(11)-C(12)	1.450(3)	C(11)-C(15)	1.457(3)
C(12)-C(13)	1.426(3)	C(12)-C(32)	1.504(3)
C(13)-C(14)	1.401(3)	C(13)-C(33)	1.499(3)
C(14)-C(15)	1.421(3)	C(14)-C(34)	1.500(3)
C(15)-C(35)	1.501(3)	C(21)-C(25)	1.457(3)
C(21)-C(22)	1.460(3)	C(22)-C(23)	1.414(4)
C(22)-C(42)	1.511(4)	C(23)-C(24)	1.400(4)
C(23)-C(43)	1.502(4)	C(24)-C(25)	1.423(4)
C(24)-C(44)	1.500(4)	C(25)-C(45)	1.506(3)
S-C(1)	1.719(12)	C(1)-C(2)	1.32(2)
C(2)-C(3)	1.41(2)	C(3)-C(4)	1.279(18)
SA-C(1A)	1.718(12)	C(1A)-C(2A)	1.32(2)
C(2A)-C(3A)	1.41(2)	C(3A)-C(4A)	1.280(18)

C(4)-Mo-C(4A)	81.2(9)	C(4)-Mo-C(11)	126.1(6)
C(4A)-Mo-C(11)	130.2(4)	C(4)-Mo-C(21)	126.1(6)
C(4A)-Mo-C(21)	128.7(5)	C(11)-Mo-C(21)	72.38(8)
C(4)-Mo-C(22)	89.0(6)	C(4A)-Mo-C(22)	129.6(4)
C(11)-Mo-C(22)	95.13(9)	C(21)-Mo-C(22)	37.14(8)
C(4)-Mo-C(12)	89.3(6)	C(4A)-Mo-C(12)	132.4(4)
C(11)-Mo-C(12)	36.86(8)	C(21)-Mo-C(12)	94.28(8)
C(22)-Mo-C(12)	96.45(9)	C(4)-Mo-C(15)	132.7(6)
C(4A)-Mo-C(15)	93.2(4)	C(11)-Mo-C(15)	36.98(8)
C(21)-Mo-C(15)	93.85(8)	C(22)-Mo-C(15)	127.02(9)
C(12)-Mo-C(15)	60.40(8)	C(4)-Mo-C(25)	133.2(6)
C(4A)-Mo-C(25)	92.0(5)	C(11)-Mo-C(25)	93.30(8)
C(21)-Mo-C(25)	36.83(8)	C(22)-Mo-C(25)	60.31(8)
C(12)-Mo-C(25)	125.88(9)	C(15)-Mo-C(25)	93.77(8)
C(4)-Mo-S	86.4(4)	C(4A)-Mo-S	5.3(5)
C(11)-Mo-S	125.93(8)	C(21)-Mo-S	125.98(9)
C(22)-Mo-S	131.18(9)	C(12)-Mo-S	132.00(9)
C(15)-Mo-S	88.95(8)	C(25)-Mo-S	89.16(9)
C(4)-Mo-C(23)	77.1(6)	C(4A)-Mo-C(23)	95.4(4)
C(11)-Mo-C(23)	128.33(9)	C(21)-Mo-C(23)	58.81(9)
C(22)-Mo-C(23)	34.52(9)	C(12)-Mo-C(23)	127.79(9)
C(15)-Mo-C(23)	150.10(8)	C(25)-Mo-C(23)	57.41(8)
S-Mo-C(23)	97.61(9)	C(4)-Mo-C(24)	100.1(6)
C(4A)-Mo-C(24)	75.7(4)	C(11)-Mo-C(24)	126.94(8)
C(21)-Mo-C(24)	58.69(9)	C(22)-Mo-C(24)	57.54(9)
C(12)-Mo-C(24)	151.76(8)	C(15)-Mo-C(24)	124.13(8)
C(25)-Mo-C(24)	34.40(9)	S-Mo-C(24)	75.55(9)
C(23)-Mo-C(24)	33.18(9)	C(4)-Mo-SA	2.4(5)
C(4A)-Mo-SA	83.5(4)	C(11)-Mo-SA	124.72(13)
C(21)-Mo-SA	124.29(13)	C(22)-Mo-SA	87.25(13)
C(12)-Mo-SA	87.92(14)	C(15)-Mo-SA	133.06(15)
C(25)-Mo-SA	133.06(15)	S-Mo-SA	88.74(13)
C(23)-Mo-SA	76.46(15)	C(24)-Mo-SA	100.46(15)

C(4)-Mo-C(13)	76.8(6)	C(4A)-Mo-C(13)	98.3(4)
C(11)-Mo-C(13)	58.49(7)	C(21)-Mo-C(13)	127.63(8)
C(22)-Mo-C(13)	127.46(9)	C(12)-Mo-C(13)	34.50(8)
C(15)-Mo-C(13)	57.35(8)	C(25)-Mo-C(13)	149.65(8)
S-Mo-C(13)	98.57(9)	C(23)-Mo-C(13)	148.20(9)
C(24)-Mo-C(13)	173.63(8)	SA-Mo-C(13)	76.72(15)
C(4)-Mo-C(14)	99.4(6)	C(4A)-Mo-C(14)	78.3(4)
C(11)-Mo-C(14)	58.39(8)	C(21)-Mo-C(14)	127.15(8)
C(22)-Mo-C(14)	152.00(8)	C(12)-Mo-C(14)	57.34(8)
C(15)-Mo-C(14)	34.31(8)	C(25)-Mo-C(14)	124.60(8)
S-Mo-C(14)	76.31(8)	C(23)-Mo-C(14)	173.26(8)
C(24)-Mo-C(14)	144.41(8)	SA-Mo-C(14)	100.25(15)
C(13)-Mo-C(14)	32.97(8)	C(52)-Si-C(51)	103.74(17)
C(52)-Si-C(11)	115.47(13)	C(51)-Si-C(11)	115.25(13)
C(52)-Si-C(21)	115.46(14)	C(51)-Si-C(21)	115.83(13)
C(11)-Si-C(21)	91.57(10)	C(12)-C(11)-C(15)	106.80(18)
C(12)-C(11)-Si	123.66(16)	C(15)-C(11)-Si	124.35(16)
C(12)-C(11)-Mo	73.37(12)	C(15)-C(11)-Mo	73.59(12)
Si-C(11)-Mo	98.20(9)	C(13)-C(12)-C(11)	107.49(19)
C(13)-C(12)-C(32)	122.3(2)	C(11)-C(12)-C(32)	128.6(2)
C(13)-C(12)-Mo	78.48(13)	C(11)-C(12)-Mo	69.76(12)
C(32)-C(12)-Mo	128.75(17)	C(14)-C(13)-C(12)	109.0(2)
C(14)-C(13)-C(33)	125.2(2)	C(12)-C(13)-C(33)	125.5(2)
C(14)-C(13)-Mo	73.67(13)	C(12)-C(13)-Mo	67.01(12)
C(33)-C(13)-Mo	130.30(17)	C(13)-C(14)-C(15)	109.3(2)
C(13)-C(14)-C(34)	125.2(2)	C(15)-C(14)-C(34)	125.1(2)
C(13)-C(14)-Mo	73.36(13)	C(15)-C(14)-Mo	67.22(12)
C(34)-C(14)-Mo	130.99(17)	C(14)-C(15)-C(11)	107.27(19)
C(14)-C(15)-C(35)	122.1(2)	C(11)-C(15)-C(35)	129.2(2)
C(14)-C(15)-Mo	78.46(13)	C(11)-C(15)-Mo	69.43(12)
C(35)-C(15)-Mo	128.90(17)	C(25)-C(21)-C(22)	106.0(2)
C(25)-C(21)-Si	123.33(17)	C(22)-C(21)-Si	124.91(18)
C(25)-C(21)-Mo	73.60(13)	C(22)-C(21)-Mo	72.44(13)
Si-C(21)-Mo	97.84(9)	C(23)-C(22)-C(21)	107.7(2)
C(23)-C(22)-C(42)	123.2(2)	C(21)-C(22)-C(42)	127.7(2)
C(23)-C(22)-Mo	77.98(14)	C(21)-C(22)-Mo	70.43(12)
C(42)-C(22)-Mo	128.08(19)	C(24)-C(23)-C(22)	109.6(2)
C(24)-C(23)-C(43)	123.8(3)	C(22)-C(23)-C(43)	126.4(3)
C(24)-C(23)-Mo	74.26(14)	C(22)-C(23)-Mo	67.50(13)
C(43)-C(23)-Mo	129.53(19)	C(23)-C(24)-C(25)	108.7(2)
C(23)-C(24)-C(44)	125.1(3)	C(25)-C(24)-C(44)	125.9(3)
C(23)-C(24)-Mo	72.56(14)	C(25)-C(24)-Mo	67.79(13)
C(44)-C(24)-Mo	130.7(2)	C(24)-C(25)-C(21)	107.9(2)
C(24)-C(25)-C(45)	122.2(2)	C(21)-C(25)-C(45)	128.7(2)
C(24)-C(25)-Mo	77.81(14)	C(21)-C(25)-Mo	69.58(12)
C(45)-C(25)-Mo	128.23(17)	C(1)-S-Mo	113.7(6)
C(2)-C(1)-S	129.4(11)	C(1)-C(2)-C(3)	127.2(6)
C(4)-C(3)-C(2)	128.8(11)	C(3)-C(4)-Mo	133.7(10)
C(1A)-SA-Mo	114.8(4)	C(2A)-C(1A)-SA	129.7(11)
C(1A)-C(2A)-C(3A)	127.3(6)	C(4A)-C(3A)-C(2A)	128.6(11)
C(3A)-C(4A)-Mo	135.7(10)		

Symmetry transformations used to generate equivalent atoms:

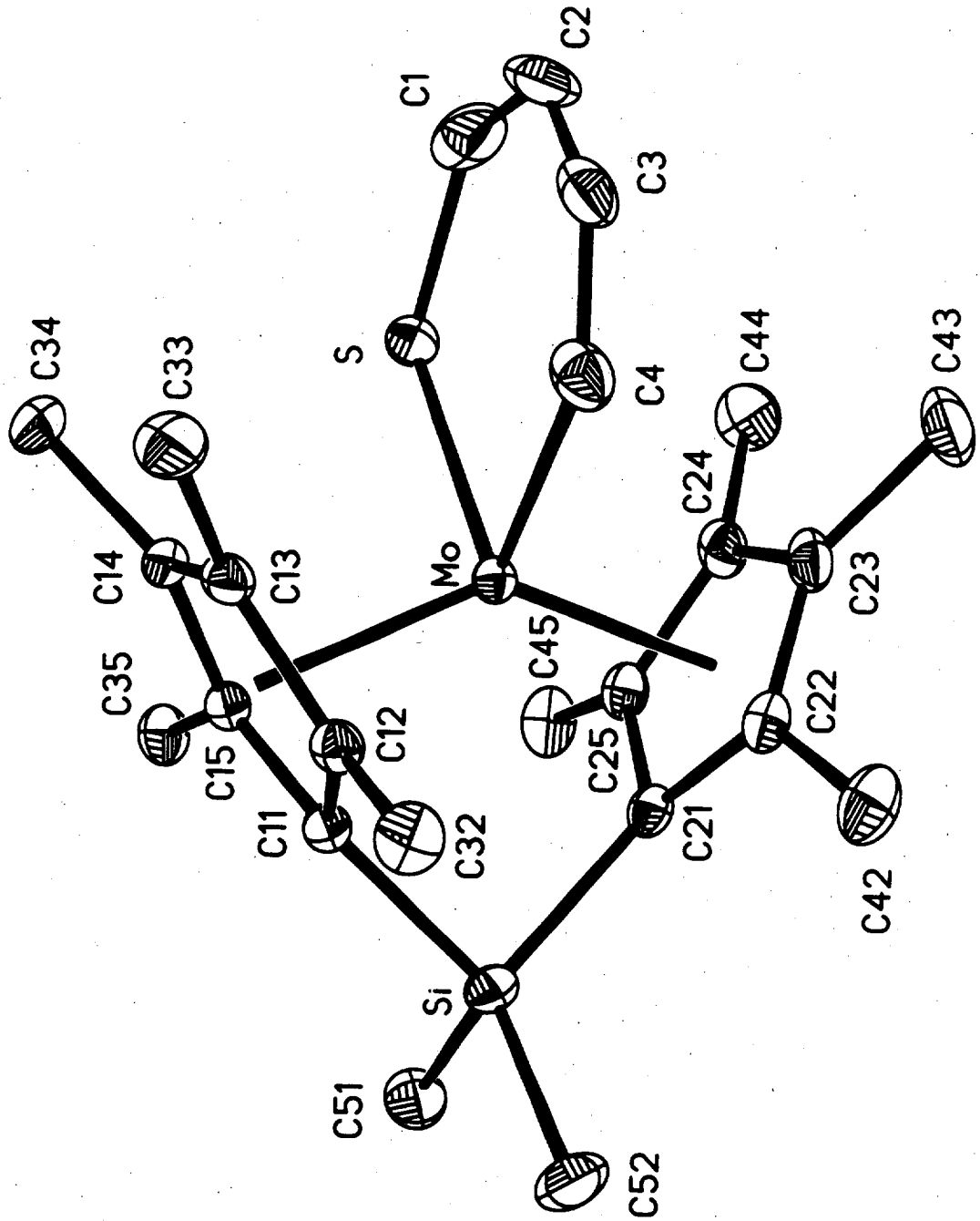
Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for [Me2Si(C5Me4)2]Mo(SC4H4).

The anisotropic displacement factor exponent take $-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
Mo	30(1)	29(1)	29(1)	-1(1)	10(1)	-2(1)
Si	28(1)	49(1)	48(1)	-5(1)	16(1)	-3(1)
C(11)	30(1)	36(1)	33(1)	-2(1)	13(1)	-2(1)
C(12)	37(1)	29(1)	39(1)	-2(1)	16(1)	-1(1)
C(13)	38(1)	35(1)	45(1)	-11(1)	21(1)	-8(1)
C(14)	29(1)	41(1)	40(1)	-11(1)	11(1)	-3(1)
C(15)	34(1)	37(1)	31(1)	-3(1)	12(1)	-2(1)
C(21)	30(1)	36(1)	36(1)	0(1)	9(1)	-9(1)
C(22)	38(1)	45(1)	33(1)	4(1)	5(1)	-7(1)
C(23)	47(1)	52(1)	35(1)	-11(1)	11(1)	-15(1)
C(24)	48(1)	35(1)	46(1)	-11(1)	14(1)	-9(1)
C(25)	41(1)	36(1)	37(1)	1(1)	10(1)	-8(1)
C(32)	55(2)	37(1)	54(2)	7(1)	18(1)	1(1)
C(33)	55(2)	54(2)	75(2)	-12(1)	38(2)	-22(1)
C(34)	32(1)	67(2)	59(2)	-13(1)	6(1)	4(1)
C(35)	54(2)	54(2)	33(1)	4(1)	12(1)	-1(1)
C(42)	56(2)	68(2)	46(2)	18(1)	4(1)	4(1)
C(43)	82(2)	95(3)	41(2)	-25(2)	25(2)	-25(2)
C(44)	74(2)	41(2)	88(2)	-21(2)	28(2)	-4(1)
C(45)	70(2)	45(1)	50(2)	10(1)	16(1)	-15(1)
C(51)	52(2)	92(2)	68(2)	-17(2)	39(2)	-22(2)
C(52)	34(1)	64(2)	92(2)	-10(2)	13(2)	8(1)
S	42(1)	45(1)	50(1)	-10(1)	17(1)	6(1)
C(1)	49(6)	66(12)	130(20)	-40(11)	23(11)	9(7)
C(2)	75(13)	92(18)	94(19)	-42(13)	65(15)	-22(9)
C(3)	73(10)	73(8)	49(4)	-22(5)	38(6)	-30(6)
C(4)	68(7)	54(8)	56(9)	-14(5)	31(6)	-17(5)
SA	48(1)	41(1)	38(1)	6(1)	20(1)	0(1)
C(1A)	51(7)	52(6)	40(4)	-4(4)	20(4)	-2(4)
C(2A)	46(5)	57(6)	44(4)	-3(4)	14(4)	6(4)
C(3A)	40(6)	39(5)	43(3)	3(3)	3(3)	7(4)
C(4A)	169(15)	89(10)	79(9)	-2(7)	0(9)	-51(9)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for [Me2Si(C5Me4)2]Mo(SC4H4).

	x	y	z	U(eq)
H(32A)	7738	7419	3675	75
H(32B)	9091	7486	3201	75
H(32C)	7788	7088	2325	75
H(33A)	4281	7312	1001	86
H(33B)	3854	7824	1715	86
H(33C)	5184	7450	2672	86
H(34A)	3671	8840	-1146	85
H(34B)	3099	8446	-219	85
H(34C)	3359	8224	-1600	85
H(35A)	5909	8700	-2185	73
H(35B)	7411	8983	-1208	73
H(35C)	5902	9220	-1250	73
H(42A)	10854	8590	6244	92
H(42B)	10620	8179	4945	92
H(42C)	9446	8212	5672	92
H(43A)	8943	9612	6627	109
H(43B)	8456	8998	6552	109
H(43C)	7267	9452	5806	109
H(44A)	6633	10134	3953	103
H(44B)	6880	10321	2533	103
H(44C)	8095	10442	4107	103
H(45A)	7512	9947	601	86
H(45B)	8895	9646	513	86
H(45C)	9119	10162	1528	86
H(51A)	10339	8483	-458	99
H(51B)	11279	8931	657	99
H(51C)	9608	9043	-343	99
H(52A)	11011	7802	3375	100
H(52B)	12146	8126	2906	100
H(52C)	11132	7677	1857	100
H(1A)	3220	9674	2316	104
H(2A)	3401	9183	4160	93
H(3A)	4834	8456	4997	73
H(4A)	6629	8218	4572	69
H(1AA)	4325	8714	5061	57
H(2AA)	3037	9332	3624	60
H(3AA)	3407	9716	1749	53
H(4AA)	4984	9552	947	152



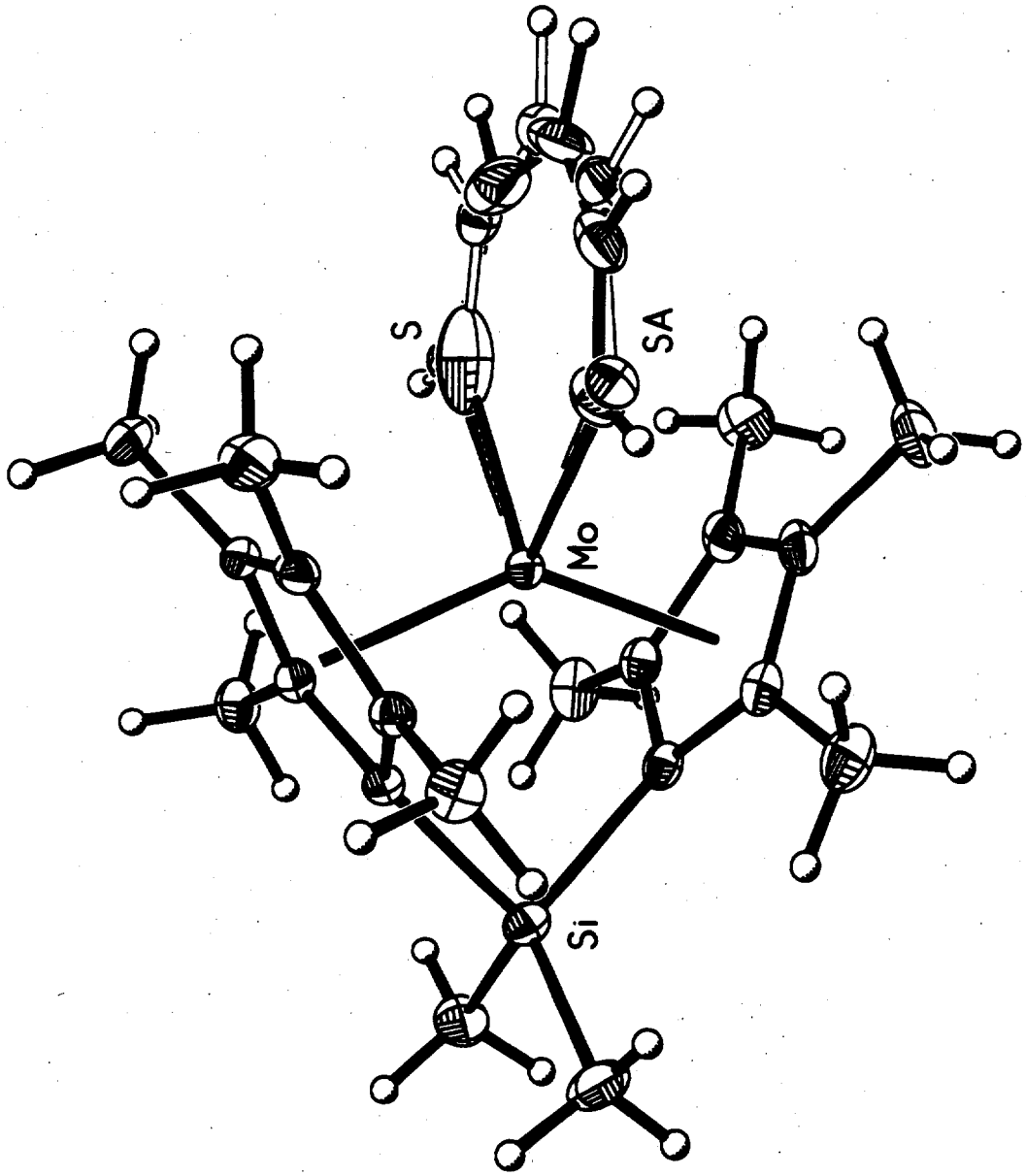


Table 1. Crystal data and structure refinement for [Me2Si(C5Me4)]Mo(SC8H6).

Identification code	bts10
Empirical formula	$C_{28}H_{36}MoSSi$
Formula weight	528.66
Temperature	233(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 10.0056(6) Å alpha = 90° b = 27.4494(15) Å beta = 114.1420(10)° c = 9.9254(6) Å gamma = 90°
Volume, Z	2487.6(3) $Å^3$, 4
Density (calculated)	1.412 Mg/m^3
Absorption coefficient	0.673 mm^{-1}
F(000)	1104
Crystal size	0.20 x 0.20 x 0.10 mm
θ range for data collection	1.48 to 28.28°
Limiting indices	$-13 \le h \le 12$, $-22 \le k \le 36$, $-10 \le l \le 13$
Reflections collected	17512
Independent reflections	5674 (R_{int} = 0.0173)
Completeness to θ = 28.28°	91.9 %
Absorption correction	SADABS
Max. and min. transmission	0.9357 and 0.8771
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5674 / 23 / 349
Goodness-of-fit on F^2	1.039
Final R indices [$I>2\sigma(I)$]	R1 = 0.0257, wR2 = 0.0598
R indices (all data)	R1 = 0.0284, wR2 = 0.0609
Extinction coefficient	0.00005(7)
Largest diff. peak and hole	0.310 and -0.274 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for [Me2Si(C5Me4)]Mo(SC8H6). U(eq) one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Mo	9730(1)	1347(1)	2956(1)	29(1)
S	11731(2)	789(1)	3803(2)	43(1)
C(1)	12639(6)	692(2)	2678(6)	53(2)
C(2)	13508(3)	268(1)	2960(4)	88(2)
C(3)	14333(3)	163(1)	2159(4)	99(3)
C(4)	14299(3)	476(1)	1044(4)	87(3)
C(5)	13440(3)	894(1)	731(4)	75(2)
C(6)	12616(3)	999(1)	1532(4)	58(2)
C(7)	11696(5)	1446(2)	1041(4)	56(1)
C(8)	10636(6)	1608(2)	1456(6)	41(1)
SA	11198(2)	1514(1)	1530(3)	44(1)
C(1A)	12403(7)	1069(2)	1497(6)	31(2)
C(2A)	12955(3)	1107(1)	402(4)	47(2)
C(3A)	13948(3)	770(1)	305(4)	58(2)
C(4A)	14421(3)	386(1)	1304(4)	69(3)
C(5A)	13901(3)	340(1)	2399(4)	54(2)
C(6A)	12908(3)	677(1)	2496(4)	41(2)
C(7A)	12487(5)	594(2)	3754(5)	44(1)
C(8A)	11396(9)	804(3)	4026(10)	33(2)
C(11)	7324(2)	1186(1)	2308(2)	33(1)
C(12)	7466(2)	1330(1)	963(2)	36(1)
C(13)	8237(2)	954(1)	604(2)	38(1)
C(14)	8614(2)	589(1)	1695(2)	37(1)
C(15)	8090(2)	727(1)	2771(2)	35(1)
C(21)	8918(2)	1836(1)	4315(2)	34(1)
C(22)	9500(2)	2158(1)	3526(2)	37(1)
C(23)	11049(2)	2093(1)	4133(2)	41(1)
C(24)	11439(2)	1735(1)	5237(2)	40(1)
C(25)	10150(2)	1559(1)	5354(2)	36(1)
C(32)	6679(3)	1732(1)	-101(2)	53(1)
C(33)	8461(3)	919(1)	-800(2)	55(1)
C(34)	9296(3)	109(1)	1621(3)	53(1)
C(35)	8099(3)	386(1)	3957(2)	47(1)
C(42)	8752(3)	2575(1)	2519(3)	53(1)
C(43)	12107(3)	2397(1)	3774(3)	60(1)
C(44)	12983(2)	1604(1)	6253(3)	59(1)
C(45)	10196(3)	1232(1)	6582(2)	50(1)
C(51)	6355(3)	1348(1)	4950(3)	61(1)
C(52)	5530(3)	2098(1)	2652(3)	60(1)
Si	6961(1)	1622(1)	3571(1)	39(1)

Table 3. Bond lengths [Å] and angles [°] for [Me2Si(C5Me4)]Mo(SC8H6).

Mo-C(8)	2.158(6)	Mo-C(8A)	2.162(6)
Mo-C(11)	2.2667(19)	Mo-C(21)	2.2753(18)
Mo-C(25)	2.3156(18)	Mo-C(12)	2.3194(19)
Mo-C(15)	2.3190(19)	Mo-C(22)	2.3317(19)
Mo-S	2.3837(16)	Mo-C(13)	2.4481(19)
Mo-C(14)	2.4490(19)	Mo-C(24)	2.453(2)
Mo-C(23)	2.4568(19)	Mo-SA	2.464(2)
S-C(1)	1.724(6)	C(1)-C(6)	1.409(5)
C(1)-C(2)	1.409(5)	C(2)-C(3)	1.3900
C(3)-C(4)	1.3900	C(4)-C(5)	1.3900
C(5)-C(6)	1.3900	C(6)-C(7)	1.490(5)
C(7)-C(8)	1.360(5)	SA-C(1A)	1.726(6)
C(1A)-C(6A)	1.409(5)	C(1A)-C(2A)	1.410(5)
C(2A)-C(3A)	1.3900	C(3A)-C(4A)	1.3900
C(4A)-C(5A)	1.3900	C(5A)-C(6A)	1.3900
C(6A)-C(7A)	1.490(5)	C(7A)-C(8A)	1.357(5)
C(11)-C(15)	1.450(3)	C(11)-C(12)	1.454(3)
C(11)-Si	1.873(2)	C(12)-C(13)	1.419(3)
C(12)-C(32)	1.506(3)	C(13)-C(14)	1.408(3)
C(13)-C(33)	1.502(3)	C(14)-C(15)	1.420(3)
C(14)-C(34)	1.500(3)	C(15)-C(35)	1.500(3)
C(21)-C(22)	1.452(3)	C(21)-C(25)	1.457(3)
C(21)-Si	1.881(2)	C(22)-C(23)	1.426(3)
C(22)-C(42)	1.501(3)	C(23)-C(24)	1.403(3)
C(23)-C(43)	1.501(3)	C(24)-C(25)	1.425(3)
C(24)-C(44)	1.503(3)	C(25)-C(45)	1.499(3)
C(51)-Si	1.867(3)	C(52)-Si	1.876(2)

C(8)-Mo-C(8A)	96.3(2)	C(8)-Mo-C(11)	124.49(15)
C(8A)-Mo-C(11)	121.4(2)	C(8)-Mo-C(21)	124.49(16)
C(8A)-Mo-C(21)	120.3(2)	C(11)-Mo-C(21)	71.77(7)
C(8)-Mo-C(25)	132.45(17)	C(8A)-Mo-C(25)	83.6(2)
C(11)-Mo-C(25)	93.76(7)	C(21)-Mo-C(25)	36.98(7)
C(8)-Mo-C(12)	87.57(15)	C(8A)-Mo-C(12)	133.9(3)
C(11)-Mo-C(12)	36.95(7)	C(21)-Mo-C(12)	93.23(7)
C(25)-Mo-C(12)	125.81(7)	C(8)-Mo-C(15)	132.26(17)
C(8A)-Mo-C(15)	84.9(3)	C(11)-Mo-C(15)	36.85(7)
C(21)-Mo-C(15)	93.84(7)	C(25)-Mo-C(15)	95.21(7)
C(12)-Mo-C(15)	60.36(7)	C(8)-Mo-C(22)	87.80(16)
C(8A)-Mo-C(22)	132.2(3)	C(11)-Mo-C(22)	93.18(7)
C(21)-Mo-C(22)	36.73(7)	C(25)-Mo-C(22)	60.35(7)
C(12)-Mo-C(22)	93.83(7)	C(15)-Mo-C(22)	125.68(7)
C(8)-Mo-S	85.82(13)	C(8A)-Mo-S	10.58(14)
C(11)-Mo-S	128.06(7)	C(21)-Mo-S	128.45(7)
C(25)-Mo-S	91.48(7)	C(12)-Mo-S	132.39(7)
C(15)-Mo-S	91.22(7)	C(22)-Mo-S	132.84(8)
C(8)-Mo-C(13)	75.71(17)	C(8A)-Mo-C(13)	102.2(3)
C(11)-Mo-C(13)	58.72(7)	C(21)-Mo-C(13)	126.77(7)
C(25)-Mo-C(13)	150.96(7)	C(12)-Mo-C(13)	34.50(7)
C(15)-Mo-C(13)	57.64(7)	C(22)-Mo-C(13)	124.75(7)
S-Mo-C(13)	98.62(7)	C(8)-Mo-C(14)	99.31(17)
C(8A)-Mo-C(14)	76.4(3)	C(11)-Mo-C(14)	58.71(7)
C(21)-Mo-C(14)	127.23(7)	C(25)-Mo-C(14)	126.28(7)
C(12)-Mo-C(14)	57.68(7)	C(15)-Mo-C(14)	34.52(7)
C(22)-Mo-C(14)	149.94(7)	S-Mo-C(14)	77.06(7)

C(13)-Mo-C(14)	33.42(7)
C(8A)-Mo-C(24)	74.9(3)
C(21)-Mo-C(24)	58.67(7)
C(12)-Mo-C(24)	149.85(7)
C(22)-Mo-C(24)	57.49(7)
C(13)-Mo-C(24)	174.08(7)
C(8)-Mo-C(23)	75.89(17)
C(11)-Mo-C(23)	126.75(7)
C(25)-Mo-C(23)	57.68(7)
C(15)-Mo-C(23)	150.96(7)
S-Mo-C(23)	99.06(8)
C(14)-Mo-C(23)	174.14(7)
C(8)-Mo-SA	12.69(13)
C(11)-Mo-SA	133.39(7)
C(25)-Mo-SA	130.04(8)
C(15)-Mo-SA	131.30(7)
S-Mo-SA	73.15(7)
C(14)-Mo-SA	96.84(7)
C(23)-Mo-SA	77.74(7)
C(6)-C(1)-C(2)	117.3(5)
C(2)-C(1)-S	116.5(3)
C(4)-C(3)-C(2)	120.0
C(4)-C(5)-C(6)	120.0
C(5)-C(6)-C(7)	114.5(2)
C(8)-C(7)-C(6)	128.6(4)
C(1A)-SA-Mo	117.66(19)
C(6A)-C(1A)-SA	125.4(4)
C(3A)-C(2A)-C(1A)	121.3(3)
C(5A)-C(4A)-C(3A)	120.0
C(5A)-C(6A)-C(1A)	121.4(3)
C(1A)-C(6A)-C(7A)	124.3(4)
C(7A)-C(8A)-Mo	135.8(4)
C(15)-C(11)-Si	124.48(14)
C(15)-C(11)-Mo	73.54(11)
Si-C(11)-Mo	99.22(8)
C(13)-C(12)-C(32)	122.61(19)
C(13)-C(12)-Mo	77.72(11)
C(32)-C(12)-Mo	129.18(15)
C(14)-C(13)-C(33)	125.0(2)
C(14)-C(13)-Mo	73.33(11)
C(33)-C(13)-Mo	130.39(15)
C(13)-C(14)-C(34)	124.86(19)
C(13)-C(14)-Mo	73.25(11)
C(34)-C(14)-Mo	130.58(15)
C(14)-C(15)-C(35)	122.56(18)
C(14)-C(15)-Mo	77.76(11)
C(35)-C(15)-Mo	128.19(14)
C(22)-C(21)-Si	124.09(15)
C(22)-C(21)-Mo	73.75(10)
Si-C(21)-Mo	98.66(8)
C(23)-C(22)-C(42)	122.47(19)
C(23)-C(22)-Mo	77.54(11)
C(42)-C(22)-Mo	129.62(15)
C(24)-C(23)-C(43)	125.2(2)
C(24)-C(23)-Mo	73.23(11)
C(43)-C(23)-Mo	130.08(15)
C(23)-C(24)-C(44)	124.9(2)
C(23)-C(24)-Mo	73.54(11)
C(44)-C(24)-Mo	130.73(15)
C(8)-Mo-C(24)	99.33(17)
C(11)-Mo-C(24)	127.20(7)
C(25)-Mo-C(24)	34.62(7)
C(15)-Mo-C(24)	126.51(7)
S-Mo-C(24)	77.61(7)
C(14)-Mo-C(24)	147.16(7)
C(8A)-Mo-C(23)	100.6(3)
C(21)-Mo-C(23)	58.62(7)
C(12)-Mo-C(23)	124.70(7)
C(22)-Mo-C(23)	34.52(7)
C(13)-Mo-C(23)	145.14(7)
C(24)-Mo-C(23)	33.22(7)
C(8A)-Mo-SA	83.66(14)
C(21)-Mo-SA	132.23(7)
C(12)-Mo-SA	96.75(7)
C(22)-Mo-SA	95.90(7)
C(13)-Mo-SA	79.00(8)
C(24)-Mo-SA	95.46(8)
C(1)-S-Mo	117.43(19)
C(6)-C(1)-S	126.2(4)
C(3)-C(2)-C(1)	121.3(3)
C(5)-C(4)-C(3)	120.0
C(5)-C(6)-C(1)	121.3(3)
C(1)-C(6)-C(7)	124.1(4)
C(7)-C(8)-Mo	134.5(4)
C(6A)-C(1A)-C(2A)	117.3(5)
C(2A)-C(1A)-SA	117.3(3)
C(2A)-C(3A)-C(4A)	120.0
C(6A)-C(5A)-C(4A)	120.0
C(5A)-C(6A)-C(7A)	114.3(2)
C(8A)-C(7A)-C(6A)	128.9(4)
C(15)-C(11)-C(12)	106.81(16)
C(12)-C(11)-Si	124.05(14)
C(12)-C(11)-Mo	73.49(11)
C(13)-C(12)-C(11)	107.47(16)
C(11)-C(12)-C(32)	128.49(19)
C(11)-C(12)-Mo	69.55(10)
C(14)-C(13)-C(12)	109.09(17)
C(12)-C(13)-C(33)	125.59(19)
C(12)-C(13)-Mo	67.78(10)
C(13)-C(14)-C(15)	108.89(17)
C(15)-C(14)-C(34)	125.87(19)
C(15)-C(14)-Mo	67.72(10)
C(14)-C(15)-C(11)	107.67(16)
C(11)-C(15)-C(35)	128.59(18)
C(11)-C(15)-Mo	69.61(10)
C(22)-C(21)-C(25)	106.84(16)
C(25)-C(21)-Si	124.02(15)
C(25)-C(21)-Mo	73.01(10)
C(23)-C(22)-C(21)	107.54(17)
C(21)-C(22)-C(42)	128.50(19)
C(21)-C(22)-Mo	69.52(10)
C(24)-C(23)-C(22)	108.99(18)
C(22)-C(23)-C(43)	125.5(2)
C(22)-C(23)-Mo	67.94(11)
C(23)-C(24)-C(25)	109.19(18)
C(25)-C(24)-C(44)	125.5(2)
C(25)-C(24)-Mo	67.42(10)
C(24)-C(25)-C(21)	107.34(18)

C(24)-C(25)-C(45)	122.73(19)	C(21)-C(25)-C(45)	128.60(18)
C(24)-C(25)-Mo	77.96(11)	C(21)-C(25)-Mo	70.00(10)
C(45)-C(25)-Mo	128.11(15)	C(51)-Si-C(11)	116.29(11)
C(51)-Si-C(52)	103.00(13)	C(11)-Si-C(52)	115.95(11)
C(51)-Si-C(21)	115.83(11)	C(11)-Si-C(21)	90.35(8)
C(52)-Si-C(21)	116.05(11)		

Symmetry transformations used to generate equivalent atoms:

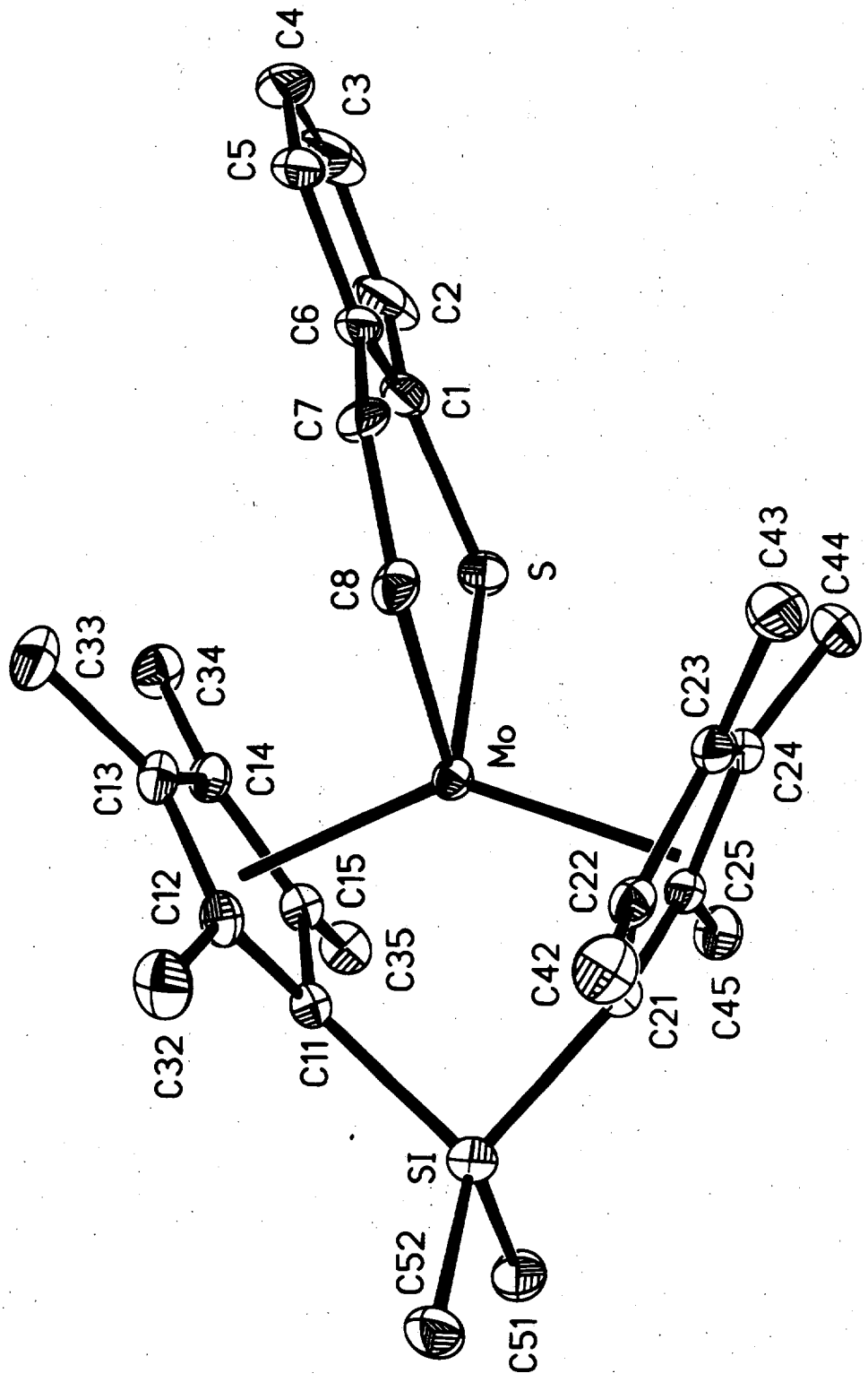
Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for [Me2Si(C5Me4)]Mo(SC8H6).

The anisotropic displacement factor exponent takes $-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
Mo	33(1)	27(1)	28(1)	0(1)	14(1)	-1(1)
S	37(1)	42(1)	47(1)	1(1)	14(1)	12(1)
C(1)	33(2)	49(3)	74(4)	-26(3)	21(3)	-8(2)
C(2)	36(3)	64(4)	155(7)	-42(4)	33(3)	-7(2)
C(3)	48(3)	75(5)	173(8)	-56(5)	44(4)	-9(3)
C(4)	53(5)	111(6)	117(6)	-71(5)	55(5)	-18(4)
C(5)	46(3)	101(5)	92(5)	-56(4)	44(3)	-31(3)
C(6)	35(3)	70(4)	75(5)	-41(4)	28(3)	-12(3)
C(7)	55(3)	85(4)	46(2)	-23(2)	40(2)	-23(2)
C(8)	50(4)	45(3)	30(2)	0(2)	19(3)	-7(2)
SA	54(1)	37(1)	50(1)	5(1)	29(1)	1(1)
C(1A)	23(3)	35(3)	39(4)	-10(2)	16(2)	-3(2)
C(2A)	42(3)	57(4)	42(3)	-12(3)	19(3)	-12(3)
C(3A)	40(3)	90(5)	53(4)	-30(3)	29(3)	-20(3)
C(4A)	37(5)	67(5)	87(7)	-22(5)	10(5)	3(4)
C(5A)	35(3)	45(4)	66(4)	-10(3)	4(3)	4(3)
C(6A)	37(4)	51(4)	36(3)	-10(3)	15(3)	-12(3)
C(7A)	43(3)	46(3)	42(3)	5(2)	17(2)	5(3)
C(8A)	30(4)	39(3)	42(3)	7(2)	26(2)	5(2)
C(11)	31(1)	35(1)	30(1)	0(1)	9(1)	-2(1)
C(12)	38(1)	35(1)	29(1)	2(1)	8(1)	-2(1)
C(13)	44(1)	38(1)	30(1)	-5(1)	13(1)	-7(1)
C(14)	43(1)	31(1)	38(1)	-4(1)	16(1)	-3(1)
C(15)	37(1)	31(1)	35(1)	3(1)	13(1)	-2(1)
C(21)	33(1)	36(1)	32(1)	-6(1)	15(1)	0(1)
C(22)	44(1)	31(1)	39(1)	-5(1)	20(1)	-1(1)
C(23)	43(1)	38(1)	47(1)	-14(1)	24(1)	-10(1)
C(24)	33(1)	47(1)	39(1)	-13(1)	12(1)	-3(1)
C(25)	35(1)	42(1)	29(1)	-5(1)	12(1)	0(1)
C(32)	60(1)	49(1)	39(1)	13(1)	9(1)	7(1)
C(33)	72(2)	58(1)	37(1)	-10(1)	25(1)	-9(1)
C(34)	62(2)	34(1)	61(1)	-8(1)	24(1)	2(1)
C(35)	51(1)	43(1)	48(1)	13(1)	20(1)	-2(1)
C(42)	66(2)	32(1)	62(1)	5(1)	26(1)	3(1)
C(43)	60(2)	52(1)	83(2)	-16(1)	43(1)	-21(1)
C(44)	35(1)	75(2)	57(1)	-15(1)	8(1)	-1(1)
C(45)	53(1)	63(2)	31(1)	4(1)	15(1)	3(1)
C(51)	51(1)	85(2)	61(2)	-16(1)	37(1)	-16(1)
C(52)	38(1)	55(1)	77(2)	-15(1)	14(1)	8(1)
Si	31(1)	44(1)	42(1)	-6(1)	16(1)	1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for [Me2Si(C5Me4)]Mo(SC8H6).

	x	y	z	U(eq)
H(2A)	13531	53	3705	105
H(3A)	14913	-119	2371	119
H(4A)	14856	405	503	104
H(5A)	13417	1106	-23	90
H(7A)	11873	1642	354	67
H(8A)	10200	1899	982	49
H(2AA)	12646	1366	-276	56
H(3AA)	14300	801	-436	69
H(4AA)	15093	158	1238	82
H(5AA)	14221	80	3074	65
H(7AA)	13056	364	4456	53
H(8AA)	11353	685	4895	40
H(32A)	5997	1590	-1022	79
H(32B)	7386	1931	-285	79
H(32C)	6146	1931	320	79
H(33A)	7664	735	-1526	82
H(33B)	9382	755	-603	82
H(33C)	8483	1243	-1176	82
H(34A)	8546	-111	981	79
H(34B)	9752	-31	2603	79
H(34C)	10031	157	1231	79
H(35A)	7661	78	3517	71
H(35B)	7542	528	4461	71
H(35C)	9101	332	4660	71
H(42A)	9029	2878	3063	80
H(42B)	7699	2533	2144	80
H(42C)	9045	2582	1701	80
H(43A)	12480	2658	4491	91
H(43B)	11611	2534	2794	91
H(43C)	12915	2194	3806	91
H(44A)	13344	1833	7066	89
H(44B)	13600	1616	5712	89
H(44C)	13002	1277	6635	89
H(45A)	10521	1416	7494	75
H(45B)	10873	966	6695	75
H(45C)	9226	1101	6351	75
H(51A)	7058	1104	5523	92
H(51B)	5402	1197	4439	92
H(51C)	6289	1601	5603	92
H(52A)	4576	1944	2198	90
H(52B)	5746	2263	1901	90
H(52C)	5527	2333	3382	90



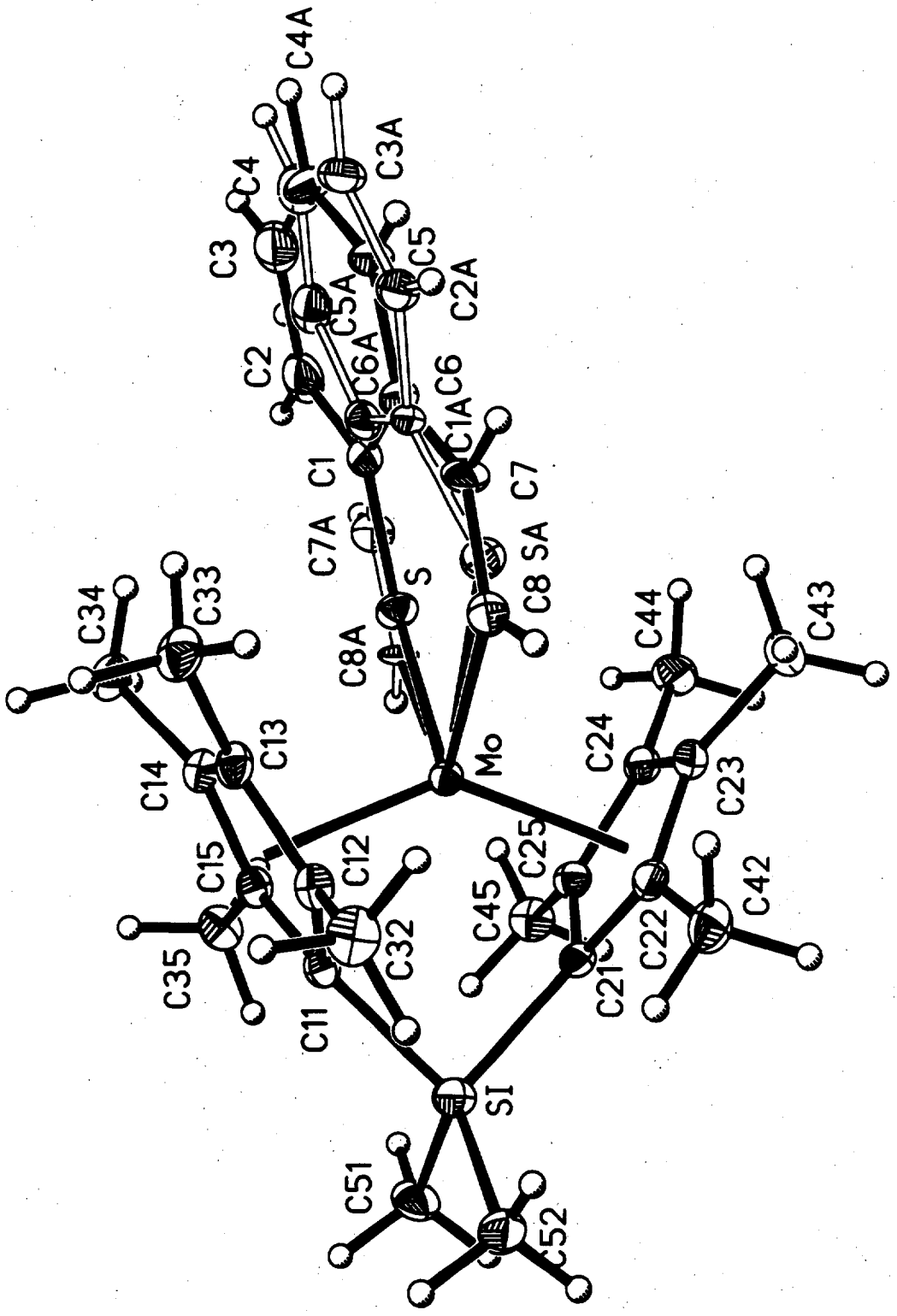


Table 1. Crystal data and structure refinement for [Me2Si(C5Me4)2]Mo(SC12H8).

Identification code	dbts10
Empirical formula	$C_{32}H_{38}MoSSi$
Formula weight	578.71
Temperature	233(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 9.9465(15) Å alpha = 84.812(3)° b = 10.2512(15) Å beta = 87.780(3)° c = 13.4669(18) Å gamma = 87.801(2)°
Volume, Z	1365.6(3) $Å^3$, 2
Density (calculated)	1.407 Mg/m^3
Absorption coefficient	0.620 mm^{-1}
F(000)	604
Crystal size	0.10 x 0.10 x 0.05 mm
θ range for data collection	1.52 to 28.25°
Limiting indices	$-12 \le h \le 11$, $-12 \le k \le 13$, $-8 \le l \le 17$
Reflections collected	9448
Independent reflections	6016 (R_{int} = 0.0309)
Completeness to θ = 28.25°	88.8 %
Absorption correction	SADABS
Max. and min. transmission	0.9697 and 0.9406
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6016 / 0 / 326
Goodness-of-fit on F^2	1.018
Final R indices [I>2σ(I)]	R1 = 0.0464, wR2 = 0.0843
R indices (all data)	R1 = 0.0910, wR2 = 0.0955
Largest diff. peak and hole	0.746 and -0.412 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for [Me2Si(C5Me4)2]Mo(SC12H8). U(e one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Mo	2846(1)	1178(1)	7425(1)	30(1)
S	2445(1)	3388(1)	7725(1)	42(1)
Si	3322(1)	-1620(1)	6812(1)	41(1)
C(11)	2116(4)	-871(4)	7723(3)	35(1)
C(12)	2526(4)	-461(4)	8674(3)	35(1)
C(13)	1641(4)	575(4)	8927(3)	37(1)
C(14)	690(4)	838(4)	8161(3)	37(1)
C(15)	973(4)	-36(4)	7413(3)	36(1)
C(21)	4161(3)	-41(4)	6435(2)	34(1)
C(22)	3539(4)	1021(4)	5802(3)	37(1)
C(23)	4040(4)	2212(4)	6047(3)	39(1)
C(24)	4949(4)	1943(4)	6843(3)	38(1)
C(25)	5033(4)	576(4)	7091(3)	38(1)
C(32)	3507(4)	-1136(4)	9387(3)	47(1)
C(33)	1575(4)	1180(4)	9898(3)	48(1)
C(34)	-514(4)	1763(4)	8213(3)	50(1)
C(35)	31(4)	-197(4)	6583(3)	47(1)
C(42)	2724(4)	896(5)	4899(3)	50(1)
C(43)	3807(4)	3524(4)	5487(3)	55(1)
C(44)	5809(4)	2938(4)	7243(3)	55(1)
C(45)	6078(4)	-74(5)	7761(3)	49(1)
C(51)	2523(5)	-2373(5)	5762(3)	62(1)
C(52)	4448(5)	-2968(4)	7361(3)	59(1)
C(61)	1036(4)	4407(4)	7365(3)	41(1)
C(62)	718(4)	5342(4)	8025(3)	43(1)
C(63)	-361(5)	6228(5)	7827(3)	61(1)
C(64)	-1088(5)	6132(5)	6989(4)	67(2)
C(65)	-752(5)	5183(5)	6346(3)	66(2)
C(66)	319(4)	4305(5)	6516(3)	53(1)
C(71)	2529(4)	4185(4)	8826(3)	36(1)
C(72)	1576(4)	5210(4)	8885(3)	41(1)
C(73)	1522(5)	5928(5)	9709(3)	56(1)
C(74)	2424(5)	5603(5)	10459(3)	59(1)
C(75)	3369(5)	4610(5)	10381(3)	56(1)
C(76)	3448(4)	3881(4)	9568(3)	48(1)

Table 3. Bond lengths [Å] and angles [°] for [Me2Si(C5Me4)2]Mo(SC12H8).

Mo-C(11)	2.246(4)	Mo-C(21)	2.256(3)
Mo-C(25)	2.277(4)	Mo-C(15)	2.281(4)
Mo-C(22)	2.284(3)	Mo-C(12)	2.289(4)
Mo-C(24)	2.343(4)	Mo-C(14)	2.352(4)
Mo-S	2.3531(12)	Mo-C(23)	2.355(4)
Mo-C(13)	2.356(4)	S-C(71)	1.763(4)
S-C(61)	1.771(4)	Si-C(52)	1.864(4)
Si-C(21)	1.870(4)	Si-C(11)	1.875(4)
Si-C(51)	1.887(4)	C(11)-C(15)	1.448(5)
C(11)-C(12)	1.461(5)	C(12)-C(13)	1.410(5)
C(12)-C(32)	1.502(5)	C(13)-C(14)	1.427(5)
C(13)-C(33)	1.496(5)	C(14)-C(15)	1.422(5)
C(14)-C(34)	1.502(5)	C(15)-C(35)	1.510(5)
C(21)-C(22)	1.455(5)	C(21)-C(25)	1.462(5)
C(22)-C(23)	1.407(5)	C(22)-C(42)	1.505(5)
C(23)-C(24)	1.430(5)	C(23)-C(43)	1.496(5)
C(24)-C(25)	1.411(5)	C(24)-C(44)	1.505(5)
C(25)-C(45)	1.499(5)	C(61)-C(66)	1.385(5)
C(61)-C(62)	1.384(5)	C(62)-C(63)	1.397(6)
C(62)-C(72)	1.459(5)	C(63)-C(64)	1.377(6)
C(64)-C(65)	1.382(6)	C(65)-C(66)	1.381(6)
C(71)-C(76)	1.386(5)	C(71)-C(72)	1.394(5)
C(72)-C(73)	1.385(5)	C(73)-C(74)	1.386(6)
C(74)-C(75)	1.367(6)	C(75)-C(76)	1.379(6)

C(11)-Mo-C(21)	74.69(13)	C(11)-Mo-C(25)	95.73(14)
C(21)-Mo-C(25)	37.61(12)	C(11)-Mo-C(15)	37.30(13)
C(21)-Mo-C(15)	96.50(14)	C(25)-Mo-C(15)	128.77(15)
C(11)-Mo-C(22)	96.80(14)	C(21)-Mo-C(22)	37.38(13)
C(25)-Mo-C(22)	61.48(13)	C(15)-Mo-C(22)	97.32(14)
C(11)-Mo-C(12)	37.58(12)	C(21)-Mo-C(12)	95.71(14)
C(25)-Mo-C(12)	94.65(14)	C(15)-Mo-C(12)	61.61(13)
C(22)-Mo-C(12)	128.97(15)	C(11)-Mo-C(24)	130.80(14)
C(21)-Mo-C(24)	60.73(14)	C(25)-Mo-C(24)	35.53(13)
C(15)-Mo-C(24)	155.71(13)	C(22)-Mo-C(24)	59.77(13)
C(12)-Mo-C(24)	124.80(14)	C(11)-Mo-C(14)	60.43(13)
C(21)-Mo-C(14)	131.45(14)	C(25)-Mo-C(14)	153.50(15)
C(15)-Mo-C(14)	35.69(13)	C(22)-Mo-C(14)	128.18(13)
C(12)-Mo-C(14)	59.64(13)	C(24)-Mo-C(14)	167.80(14)
C(11)-Mo-S	145.40(10)	C(21)-Mo-S	139.50(11)
C(25)-Mo-S	115.71(11)	C(15)-Mo-S	115.40(10)
C(22)-Mo-S	110.34(11)	C(12)-Mo-S	120.69(10)
C(24)-Mo-S	82.64(11)	C(14)-Mo-S	85.57(10)
C(11)-Mo-C(23)	131.36(13)	C(21)-Mo-C(23)	60.39(14)
C(25)-Mo-C(23)	59.69(14)	C(15)-Mo-C(23)	127.77(13)
C(22)-Mo-C(23)	35.26(14)	C(12)-Mo-C(23)	153.51(14)
C(24)-Mo-C(23)	35.44(13)	C(14)-Mo-C(23)	144.40(14)
S-Mo-C(23)	79.92(11)	C(11)-Mo-C(13)	60.43(13)
C(21)-Mo-C(13)	130.52(14)	C(25)-Mo-C(13)	124.71(14)
C(15)-Mo-C(13)	59.86(13)	C(22)-Mo-C(13)	155.76(14)
C(12)-Mo-C(13)	35.31(13)	C(24)-Mo-C(13)	140.76(13)
C(14)-Mo-C(13)	35.28(13)	S-Mo-C(13)	88.54(10)
C(23)-Mo-C(13)	168.18(14)	C(71)-S-C(61)	90.01(19)
C(71)-S-Mo	131.04(14)	C(61)-S-Mo	127.16(15)
C(52)-Si-C(21)	115.11(19)	C(52)-Si-C(11)	115.15(19)
C(21)-Si-C(11)	93.68(16)	C(52)-Si-C(51)	103.4(2)

C(21)-Si-C(51)	114.63(19)	C(11)-Si-C(51)	115.40(19)
C(15)-C(11)-C(12)	107.1(3)	C(15)-C(11)-Si	122.7(3)
C(12)-C(11)-Si	123.0(3)	C(15)-C(11)-Mo	72.7(2)
C(12)-C(11)-Mo	72.8(2)	Si-C(11)-Mo	95.90(16)
C(13)-C(12)-C(11)	107.6(3)	C(13)-C(12)-C(32)	123.0(3)
C(11)-C(12)-C(32)	128.3(4)	C(13)-C(12)-Mo	75.0(2)
C(11)-C(12)-Mo	69.6(2)	C(32)-C(12)-Mo	130.1(3)
C(12)-C(13)-C(14)	108.9(3)	C(12)-C(13)-C(33)	125.9(3)
C(14)-C(13)-C(33)	124.6(4)	C(12)-C(13)-Mo	69.7(2)
C(14)-C(13)-Mo	72.2(2)	C(33)-C(13)-Mo	130.5(3)
C(15)-C(14)-C(13)	108.7(3)	C(15)-C(14)-C(34)	125.8(4)
C(13)-C(14)-C(34)	125.0(3)	C(15)-C(14)-Mo	69.4(2)
C(13)-C(14)-Mo	72.5(2)	C(34)-C(14)-Mo	130.1(3)
C(14)-C(15)-C(11)	107.6(3)	C(14)-C(15)-C(35)	123.1(4)
C(11)-C(15)-C(35)	128.2(3)	C(14)-C(15)-Mo	74.9(2)
C(11)-C(15)-Mo	70.0(2)	C(35)-C(15)-Mo	130.4(3)
C(22)-C(21)-C(25)	106.1(3)	C(22)-C(21)-Si	123.1(3)
C(25)-C(21)-Si	122.9(3)	C(22)-C(21)-Mo	72.3(2)
C(25)-C(21)-Mo	72.0(2)	Si-C(21)-Mo	95.70(15)
C(23)-C(22)-C(21)	108.4(3)	C(23)-C(22)-C(42)	123.7(4)
C(21)-C(22)-C(42)	126.8(4)	C(23)-C(22)-Mo	75.1(2)
C(21)-C(22)-Mo	70.28(19)	C(42)-C(22)-Mo	129.8(3)
C(22)-C(23)-C(24)	108.8(4)	C(22)-C(23)-C(43)	125.8(4)
C(24)-C(23)-C(43)	125.0(4)	C(22)-C(23)-Mo	69.6(2)
C(24)-C(23)-Mo	71.8(2)	C(43)-C(23)-Mo	130.4(3)
C(25)-C(24)-C(23)	108.5(4)	C(25)-C(24)-C(44)	125.9(4)
C(23)-C(24)-C(44)	125.0(4)	C(25)-C(24)-Mo	69.7(2)
C(23)-C(24)-Mo	72.7(2)	C(44)-C(24)-Mo	129.8(3)
C(24)-C(25)-C(21)	108.1(3)	C(24)-C(25)-C(45)	122.8(4)
C(21)-C(25)-C(45)	127.8(4)	C(24)-C(25)-Mo	74.8(2)
C(21)-C(25)-Mo	70.4(2)	C(45)-C(25)-Mo	130.6(3)
C(66)-C(61)-C(62)	122.6(4)	C(66)-C(61)-S	124.6(3)
C(62)-C(61)-S	112.8(3)	C(61)-C(62)-C(63)	119.1(4)
C(61)-C(62)-C(72)	112.3(4)	C(63)-C(62)-C(72)	128.6(4)
C(64)-C(63)-C(62)	118.9(4)	C(63)-C(64)-C(65)	120.8(4)
C(66)-C(65)-C(64)	121.6(4)	C(65)-C(66)-C(61)	117.0(4)
C(76)-C(71)-C(72)	121.5(4)	C(76)-C(71)-S	125.5(3)
C(72)-C(71)-S	113.1(3)	C(73)-C(72)-C(71)	119.6(4)
C(73)-C(72)-C(62)	128.7(4)	C(71)-C(72)-C(62)	111.7(3)
C(72)-C(73)-C(74)	118.8(4)	C(75)-C(74)-C(73)	120.9(4)
C(74)-C(75)-C(76)	121.6(4)	C(75)-C(76)-C(71)	117.7(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for [Me2Si(C5Me4)2]Mo(SC12H8).

The anisotropic displacement factor exponent tak $-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
Mo	24(1)	41(1)	25(1)	-5(1)	-3(1)	-2(1)
S	42(1)	45(1)	39(1)	-7(1)	-5(1)	4(1)
Si	38(1)	45(1)	42(1)	-13(1)	-4(1)	2(1)
C(11)	33(2)	33(2)	38(2)	-6(2)	-1(2)	-8(2)
C(12)	33(2)	44(3)	29(2)	0(2)	-4(2)	-4(2)
C(13)	36(2)	47(3)	28(2)	-1(2)	3(2)	-10(2)
C(14)	28(2)	44(3)	40(2)	-3(2)	7(2)	-4(2)
C(15)	30(2)	44(3)	35(2)	-4(2)	-4(2)	-7(2)
C(21)	26(2)	49(3)	27(2)	-10(2)	1(2)	2(2)
C(22)	26(2)	57(3)	29(2)	-10(2)	-2(2)	3(2)
C(23)	33(2)	51(3)	31(2)	1(2)	6(2)	-1(2)
C(24)	24(2)	54(3)	36(2)	-11(2)	4(2)	-7(2)
C(25)	28(2)	50(3)	36(2)	-10(2)	-1(2)	0(2)
C(32)	50(3)	53(3)	38(2)	2(2)	-10(2)	-2(2)
C(33)	53(3)	55(3)	38(2)	-6(2)	7(2)	-10(2)
C(34)	35(2)	58(3)	55(3)	-4(2)	5(2)	-1(2)
C(35)	31(2)	63(3)	50(2)	-14(2)	-13(2)	-1(2)
C(42)	42(3)	75(3)	31(2)	-4(2)	-7(2)	3(2)
C(43)	52(3)	57(3)	51(3)	9(2)	9(2)	-3(2)
C(44)	40(3)	64(3)	62(3)	-8(2)	-1(2)	-18(2)
C(45)	28(2)	76(3)	45(2)	-8(2)	-9(2)	4(2)
C(51)	66(3)	66(3)	58(3)	-29(3)	-6(2)	-6(3)
C(52)	61(3)	48(3)	66(3)	-4(2)	5(2)	11(2)
C(61)	37(2)	45(3)	39(2)	8(2)	-5(2)	-1(2)
C(62)	41(3)	41(3)	46(2)	1(2)	6(2)	1(2)
C(63)	60(3)	62(3)	59(3)	-2(3)	1(2)	18(3)
C(64)	56(3)	76(4)	62(3)	14(3)	-9(3)	25(3)
C(65)	57(3)	90(4)	47(3)	14(3)	-14(2)	4(3)
C(66)	54(3)	59(3)	43(2)	5(2)	-6(2)	-1(2)
C(71)	38(2)	38(2)	34(2)	-4(2)	3(2)	-6(2)
C(72)	39(2)	41(3)	44(2)	-7(2)	2(2)	-3(2)
C(73)	60(3)	52(3)	56(3)	-15(2)	6(2)	5(2)
C(74)	71(3)	58(3)	51(3)	-14(2)	-5(2)	-8(3)
C(75)	59(3)	60(3)	49(3)	-5(2)	-14(2)	-9(3)
C(76)	43(3)	48(3)	53(3)	-5(2)	-3(2)	-1(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for [Me2Si(C5Me4)2]Mo(SC12H8).

	x	Y	z	U(eq)
H(32A)	4018	-486	9675	70
H(32B)	4117	-1709	9033	70
H(32C)	3020	-1650	9914	70
H(33A)	859	794	10324	72
H(33B)	1395	2116	9777	72
H(33C)	2426	1022	10223	72
H(34A)	-1241	1326	8593	74
H(34B)	-801	2035	7543	74
H(34C)	-277	2527	8536	74
H(35A)	-635	-832	6813	71
H(35B)	541	-500	6014	71
H(35C)	-417	639	6388	71
H(42A)	2004	1562	4868	74
H(42B)	2343	35	4946	74
H(42C)	3300	1010	4302	74
H(43A)	4511	3668	4974	82
H(43B)	3818	4202	5944	82
H(43C)	2939	3552	5179	82
H(44A)	6059	2634	7916	82
H(44B)	5307	3767	7250	82
H(44C)	6615	3054	6820	82
H(45A)	6934	-123	7394	74
H(45B)	5807	-952	7993	74
H(45C)	6167	431	8328	74
H(51A)	1894	-1742	5437	92
H(51B)	2047	-3144	6028	92
H(51C)	3217	-2621	5282	92
H(52A)	5019	-3309	6837	88
H(52B)	3908	-3664	7682	88
H(52C)	5005	-2634	7850	88
H(63A)	-586	6880	8259	73
H(64A)	-1821	6718	6852	80
H(65A)	-1266	5134	5780	79
H(66A)	552	3666	6075	63
H(73A)	886	6623	9760	67
H(74A)	2385	6072	11028	71
H(75A)	3979	4420	10894	67
H(76A)	4102	3201	9518	57