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A Bimetallic *bis*-Pentalene Sandwich Complex: Synthesis and Structure of $\text{Mo}_2[\text{C}_8\text{H}_4(1,4\text{-SiPr}^i_3)_2]_2$

Supporting Information

Experimental Details

General Comments:

All manipulations were carried out using a combination of standard Schlenk, high vacuum and glovebox techniques. All solvents were distilled from appropriate drying agents and degassed prior to use. $\text{K}_2[\text{C}_8\text{H}_4(1,4\text{-SiPr}^i_3)_2]$ ¹ and $\text{Mo}_2(\text{OAc})_4$ ² were prepared according to literature methods. The heteronuclear nOe experiments were recorded on a Bruker AMX 500 Spectrometer operating at 125.76 MHz for ¹³C. The UV-Vis spectrum was recorded on a Unicam UV2 Spectrometer as a solution in pentane and is presented as $\lambda(\text{nm})$ and $\epsilon(\text{M}^{-1} \text{cm}^{-1})$. Carbon and hydrogen elemental analyses were performed by *Canadian Microanalytical Service Ltd.*. The X-ray data were recorded on an Enraf-Nonius CAD4 diffractometer at 173 K using monochromated Mo-K α radiation (0.71073 Å).

Synthesis of $\text{Mo}_2[\text{C}_8\text{H}_4(1,4\text{-SiPr}^i_3)_2]_2$

THF (*ca.* 30 mL) was added to a stirred mixture of $\text{K}_2[\text{C}_8\text{H}_4(1,4\text{-SiPr}^i_3)_2]$ (2.00 g, 4.06 mmol) and $\text{Mo}_2(\text{OAc})_4$ (0.87 g, 2.03 mmol) at room temperature and the resulting brown mixture was stirred overnight at room temperature. The solvent was removed under reduced pressure, the residue extracted into petroleum ether (B. P. = 40-60°C) (*ca.* 200 mL) and filtered through a bed of celite supported on a glass frit producing a clear green filtrate. The solvent was removed from the filtrate under reduced pressure giving a green solid (*ca.* 0.90 g) composed of $\text{Mo}_2[\text{C}_8\text{H}_4(1,4\text{-SiPr}^i_3)_2]_2$ and an unidentified compound in an approximately 4:3 ratio as determined by ¹H NMR spectroscopy. Degassed water (*ca.* 0.6 mL) was added to a benzene solution (*ca.* 35 mL) of the green mixture and

the resulting mixture was stirred overnight at room temperature during which time a gradual color change from green to brown was observed. The solvent was removed under reduced pressure, the residue extracted into petroleum ether (*ca.* 60 mL), filtered and the solvent removed from the filtrate under reduced pressure. The residue was redissolved in petroleum ether, concentrated to *ca.* 5 mL and stored at *ca.* -50°C overnight giving green crystals which were washed with cold (*ca.* -78°C) petroleum ether (2 x 2 mL). ¹H NMR spectroscopy indicated a small impurity in the resulting green crystals which were ground into a powder in a glove-box and washed a second time with cold (*ca.* -78°C) petroleum ether (2 x 2 mL) giving Mo₂[C₈H₄(1,4-SiPrⁱ₃)₂]₂ as a green solid (0.45 g, 22%). Analysis calculated for C₅₂H₉₂Si₄Mo₂: C, 61.14 %; H, 9.08 %. Found: C, 60.97 %; H, 9.27 %. Mass spectrum: m/z = 1021 (M⁺).

NMR Data for Mo₂[C₈H₄(1,4-SiPrⁱ₃)₂]₂³

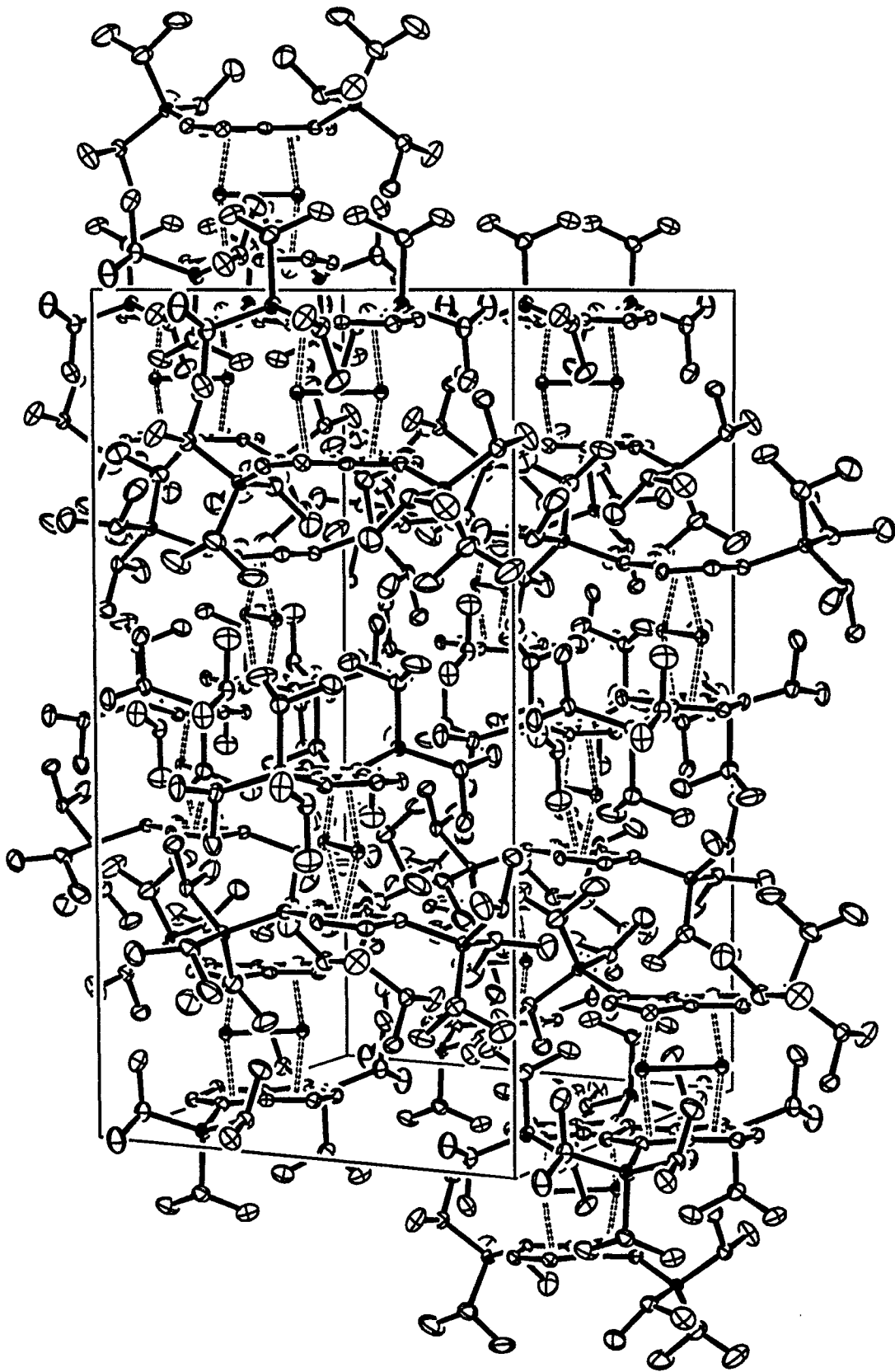
Assignment	δ (ppm)	Coupling (Hz)
¹H (300.132 MHz, C₆D₆)		
CH(CH ₃) ₂ , 36H	1.14	d, J _{H-H} = 7.4
CH(CH ₃) ₂ , 36H	1.33	d, J _{H-H} = 7.4
CH(CH ₃) ₂ , 12H	1.59	sept, J _{H-H} = 7.4
CH, 4H	2.67	d, J _{H-H} = 2.5
CH, 4H	7.14	d, J _{H-H} = 2.5
¹H (300.132 MHz, C₇D₈)		
CH(CH ₃) ₂ , 36H	1.12	d, J _{H-H} = 7.4
CH(CH ₃) ₂ , 36H	1.32	d, J _{H-H} = 7.4
CH(CH ₃) ₂ , 12H	1.57	sept, J _{H-H} = 7.4
CH, 4H	2.64	d, J _{H-H} = 2.4
CH, 4H	7.13	d, J _{H-H} = 2.4
¹³C (75.475 MHz, C₆D₆)		
CH(CH ₃) ₂	13.2	d, J _{C-H} = 114

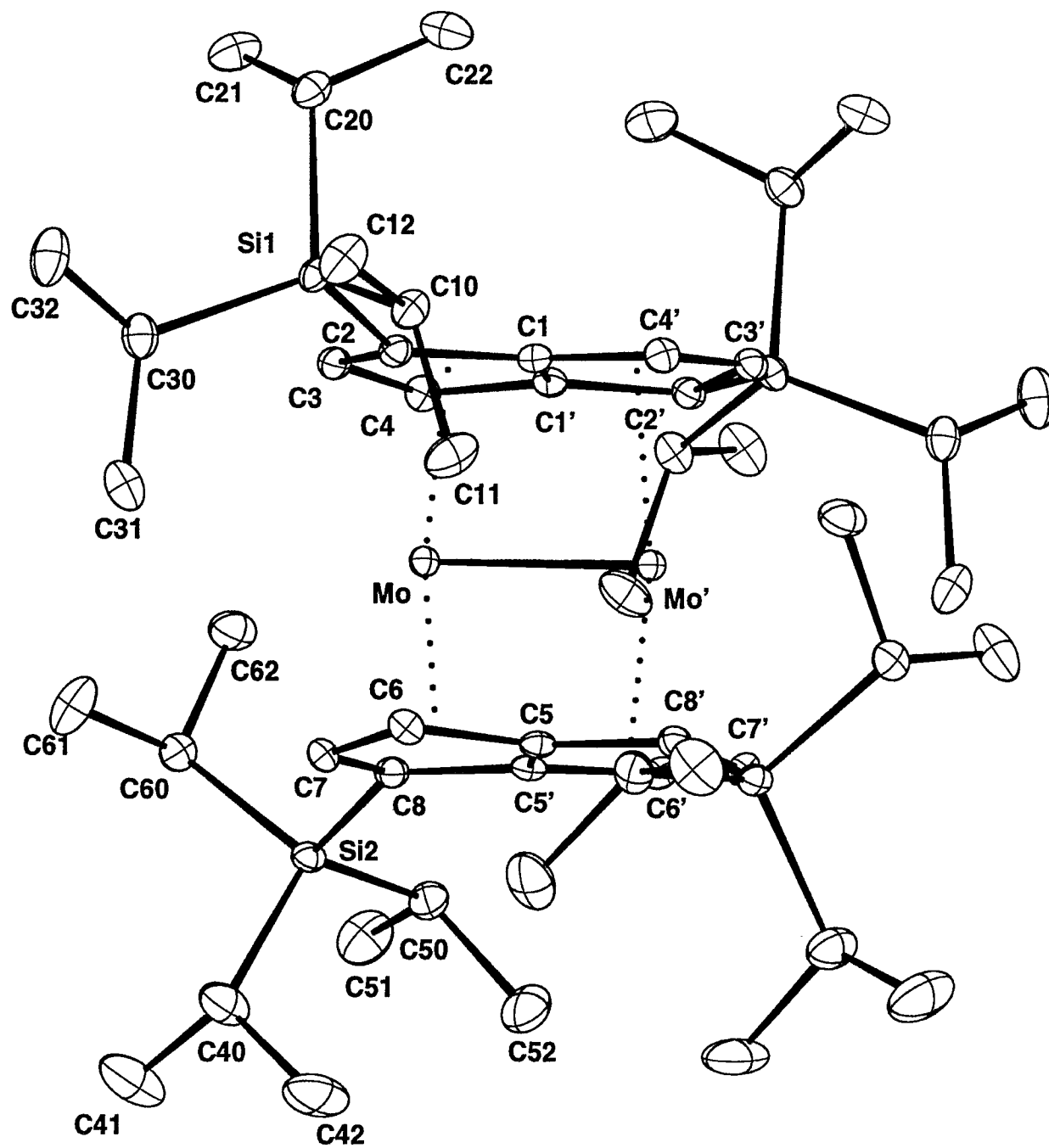
CH(CH ₃) ₂	19.7	q, J _{C-H} = 124
CH(CH ₃) ₂	19.8	q, J _{C-H} = 124
C	73.2	s
CH	82.7	d, J _{C-H} = 180
CH	101.0	d, J _{C-H} = 164
C	108.8	s

UV-Vis Data for Mo₂[C₈H₄(1,4-SiPr₃)₂]₂

λ(nm)	ε(M ⁻¹ cm ⁻¹)
209	22279
218	24279
227	23023
276	9628
327	5116
383	3814
426	605
706	465

- (1) See the supplementary information of Cloke, F. G. N.; Hitchcock, P. B. *J. Am. Chem. Soc.* **1997**, *119*, 7899-7900.
- (2) Brignole, A. B.; Cotton, F. A. *Inorg. Synth.* **1972**, *13*, 87-89.
- (3) ¹H NMR data are reported in two solvents because in *d*₆-benzene the downfield [CH] resonance is partially obscured by the solvent peak and thus *d*₈-toluene was used to verify its existence.





Identification code	NOV697
Empirical formula	C ₅₂ H ₉₂ Mo ₂ Si ₄
Formula weight	1021.5
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Pccn (No.56)
Unit cell dimensions	a = 13.7859(11) Å alpha = 90 deg. b = 15.3758(12) Å beta = 90 deg. c = 25.442(3) Å gamma = 90 deg.
Volume	5392.8(8) Å ³
Z	4
Density (calculated)	1.26 Mg/m ³
Absorption coefficient	0.59 mm ⁻¹
F(000)	2176
Crystal size	0.4 x 0.4 x 0.1 mm
Theta range for data collection	2.08 to 24.97 deg.
Index ranges	0 ≤ h ≤ 16, 0 ≤ k ≤ 18, 0 ≤ l ≤ 30
Reflections collected	4741
Independent reflections	4741 [R(int) = 0.0000]
Reflections with I > 2σ(I)	3689
Structure solution	Direct methods
Refinement method	Full-matrix least-squares on all F ²
Data / restraints / parameters	4741 / 0 / 278
Goodness-of-fit on F ²	1.043
Final R indices [I > 2σ(I)]	R1 = 0.036, wR2 = 0.077
R indices (all data)	R1 = 0.054, wR2 = 0.086
Largest diff. peak and hole	0.53 and -0.53 e.Å ⁻³
Abs.correction from psi scans	Tmax=1.00 , Tmin=0.97
Maximum shift/e.s.d.	0.001

All non-H atoms were anisotropic. H's were included in riding mode with Uiso(H) equal to 1.2Ueq(C) or 1.5Ueq(C) for methyl

groups.

Programs used were :

Data collection - Enraf-Nonius CAD4 software
Structure solution - SHELXS-86
Structure refinement - SHELXL-93
Interactive graphics and final drawings - CAMERON

References :

Enraf-Nonius (1989) CAD4 Software. Version 5.0. Enraf-Nonius,
The Netherlands.
Sheldrick, G.M. (1985) SHELXS-86. Program for the Solution of
Crystal Structures. Univ. of Gottingen, Germany.
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Refinement. Univ. of Gottingen, Germany.
Watkin, D.J. and Pearce, L.J. (1993) CAMERON. An Interactive
Graphics Editor. Univ. of Oxford, England.

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
Mo	1832.7 (2)	7030.0 (2)	3879.1 (1)	15 (1)
Si (1)	2443.9 (7)	5190.0 (5)	4834.2 (4)	18 (1)
Si (2)	-36.3 (6)	7865.6 (6)	2854.5 (3)	19 (1)
C (1)	2795 (2)	7111 (2)	4650 (1)	18 (1)
C (2)	2165 (2)	6335 (2)	4642 (1)	19 (1)
C (3)	1200 (2)	6710 (2)	4675 (1)	19 (1)
C (4)	1199 (2)	7626 (2)	4633 (1)	19 (1)
C (5)	2867 (2)	7159 (2)	3109 (1)	16 (1)
C (6)	2361 (2)	6333 (2)	3133 (1)	18 (1)
C (7)	1365 (2)	6527 (2)	3084 (1)	20 (1)
C (8)	1156 (2)	7452 (2)	3104 (1)	19 (1)
C (10)	3702 (2)	4870 (2)	4607 (1)	24 (1)
C (11)	3928 (3)	5096 (3)	4035 (1)	36 (1)
C (12)	3938 (3)	3918 (2)	4713 (2)	34 (1)
C (20)	2412 (3)	5145 (2)	5576 (1)	25 (1)
C (21)	1420 (3)	5380 (3)	5800 (1)	37 (1)
C (22)	3180 (3)	5723 (3)	5830 (2)	50 (1)
C (30)	1424 (2)	4480 (2)	4579 (1)	26 (1)
C (31)	1361 (3)	4426 (3)	3982 (2)	43 (1)
C (32)	1395 (3)	3564 (2)	4818 (2)	39 (1)
C (40)	-223 (3)	7231 (3)	2220 (1)	37 (1)
C (41)	-1207 (3)	7331 (4)	1970 (2)	60 (1)
C (42)	602 (3)	7333 (3)	1820 (2)	55 (1)
C (50)	-15 (3)	9083 (2)	2783 (1)	28 (1)
C (51)	-1025 (3)	9496 (3)	2720 (2)	44 (1)
C (52)	653 (3)	9418 (3)	2347 (2)	47 (1)
C (60)	-1074 (2)	7576 (2)	3308 (1)	22 (1)
C (61)	-1173 (3)	6600 (2)	3416 (2)	43 (1)
C (62)	-1036 (3)	8068 (3)	3834 (1)	35 (1)

Table 3. Bond lengths [Å] and angles [deg] for 1.

Mo-M(1)	1.971(3)	Mo-M(2)	1.973(3)
Mo-C(1)	2.370(3)	Mo-C(1)'	2.419(3)
Mo-C(2)	2.263(3)	Mo-C(3)	2.258(3)
Mo-C(4)	2.298(3)	Mo-C(5)	2.432(3)
Mo-C(5)'	2.360(3)	Mo-C(6)	2.297(3)
Mo-C(7)	2.260(3)	Mo-C(8)	2.276(3)
Mo-Mo'	2.340(1)	Si(1)-C(2)	1.867(3)
Si(1)-C(20)	1.889(3)	Si(1)-C(10)	1.893(3)
Si(1)-C(30)	1.895(3)	Si(2)-C(8)	1.873(3)
Si(2)-C(50)	1.880(3)	Si(2)-C(60)	1.890(3)
Si(2)-C(40)	1.905(4)	C(1)-C(4)'	1.445(4)
C(1)-C(1)'	1.447(6)	C(1)-C(2)	1.476(4)
C(2)-C(3)	1.452(4)	C(3)-C(4)	1.412(5)
C(4)-C(1)'	1.445(4)	C(5)-C(6)	1.450(4)
C(5)-C(5)'	1.458(6)	C(5)-C(8)'	1.473(4)
C(6)-C(7)	1.410(4)	C(7)-C(8)	1.453(5)
C(8)-C(5)'	1.473(4)	C(10)-C(12)	1.523(5)
C(10)-C(11)	1.528(5)	C(20)-C(21)	1.525(5)
C(20)-C(22)	1.526(5)	C(30)-C(31)	1.524(5)
C(30)-C(32)	1.534(5)	C(40)-C(41)	1.507(5)
C(40)-C(42)	1.533(5)	C(50)-C(52)	1.531(5)
C(50)-C(51)	1.540(5)	C(60)-C(61)	1.531(5)
C(60)-C(62)	1.540(5)		
M(1)-Mo-M(2)	169.1(1)	M(1)-Mo-Mo'	84.6(1)
M(2)-Mo-Mo'	84.5(1)	C(2)-Si(1)-C(20)	106.9(2)
C(2)-Si(1)-C(10)	110.7(2)	C(20)-Si(1)-C(10)	108.5(2)
C(2)-Si(1)-C(30)	107.5(2)	C(20)-Si(1)-C(30)	107.7(2)
C(10)-Si(1)-C(30)	115.1(2)	C(8)-Si(2)-C(50)	110.9(2)
C(8)-Si(2)-C(60)	112.14(14)	C(50)-Si(2)-C(60)	107.8(2)
C(8)-Si(2)-C(40)	103.4(2)	C(50)-Si(2)-C(40)	115.5(2)
C(60)-Si(2)-C(40)	107.1(2)	C(4)'-C(1)-C(1)'	107.9(3)
C(4)'-C(1)-C(2)	142.3(3)	C(1)'-C(1)-C(2)	109.7(3)
C(3)-C(2)-C(1)	102.5(3)	C(3)-C(2)-Si(1)	123.3(2)
C(1)-C(2)-Si(1)	129.6(2)	C(4)-C(3)-C(2)	113.2(3)
C(3)-C(4)-C(1)'	106.0(3)	C(6)-C(5)-C(5)'	107.2(3)
C(6)-C(5)-C(8)'	142.7(3)	C(5)'-C(5)-C(8)'	110.1(3)
C(7)-C(6)-C(5)	106.2(3)	C(6)-C(7)-C(8)	113.4(3)
C(7)-C(8)-C(5)'	102.5(3)	C(7)-C(8)-Si(2)	119.6(2)
C(5)'-C(8)-Si(2)	131.8(2)	C(12)-C(10)-C(11)	110.1(3)
C(12)-C(10)-Si(1)	113.1(2)	C(11)-C(10)-Si(1)	114.7(2)
C(21)-C(20)-C(22)	109.0(3)	C(21)-C(20)-Si(1)	112.7(2)
C(22)-C(20)-Si(1)	112.7(2)	C(31)-C(30)-C(32)	110.0(3)
C(31)-C(30)-Si(1)	114.5(3)	C(32)-C(30)-Si(1)	114.4(3)
C(41)-C(40)-C(42)	112.2(3)	C(41)-C(40)-Si(2)	115.3(3)
C(42)-C(40)-Si(2)	114.2(3)	C(52)-C(50)-C(51)	109.2(3)
C(52)-C(50)-Si(2)	114.5(3)	C(51)-C(50)-Si(2)	114.0(3)
C(61)-C(60)-C(62)	109.2(3)	C(61)-C(60)-Si(2)	114.1(2)
C(62)-C(60)-Si(2)	112.9(2)		

M(1) is the centroid of the C(1),C(2),C(3),C(4),C(1)' ring
M(2) is the centroid of the C(5),C(6),C(7),C(8),C(5)' ring
Symmetry transformations used to generate equivalent atoms:
' -x+1/2,-y+3/2,z

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1.
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Mo	14(1)	16(1)	15(1)	0(1)	0(1)	1(1)
Si(1)	17(1)	17(1)	20(1)	4(1)	1(1)	1(1)
Si(2)	16(1)	24(1)	16(1)	1(1)	-2(1)	2(1)
C(1)	21(2)	19(2)	14(2)	2(1)	0(1)	1(1)
C(2)	18(2)	22(2)	16(2)	0(1)	2(1)	0(1)
C(3)	16(2)	24(2)	17(2)	1(1)	0(1)	0(2)
C(4)	15(2)	21(2)	21(2)	-2(1)	2(1)	5(2)
C(5)	17(2)	21(2)	12(2)	-1(1)	2(1)	4(1)
C(6)	17(2)	17(2)	20(2)	-5(1)	0(1)	6(1)
C(7)	22(2)	19(2)	18(2)	-3(1)	-2(1)	-3(2)
C(8)	19(2)	22(2)	16(2)	1(1)	-1(1)	0(2)
C(10)	20(2)	24(2)	27(2)	6(2)	1(2)	3(2)
C(11)	29(2)	44(2)	34(2)	10(2)	12(2)	12(2)
C(12)	26(2)	31(2)	45(2)	12(2)	6(2)	10(2)
C(20)	26(2)	25(2)	25(2)	6(2)	2(2)	1(2)
C(21)	41(2)	45(2)	26(2)	6(2)	9(2)	6(2)
C(22)	53(3)	72(3)	24(2)	1(2)	-8(2)	-14(3)
C(30)	20(2)	24(2)	33(2)	-1(2)	0(2)	0(2)
C(31)	45(2)	45(2)	39(2)	-7(2)	-8(2)	-18(2)
C(32)	33(2)	25(2)	60(3)	6(2)	1(2)	-4(2)
C(40)	29(2)	53(3)	29(2)	-8(2)	-5(2)	4(2)
C(41)	51(3)	86(4)	44(3)	-19(3)	-19(2)	8(3)
C(42)	52(3)	86(4)	25(2)	-15(2)	5(2)	10(3)
C(50)	31(2)	25(2)	28(2)	9(2)	-5(2)	-2(2)
C(51)	46(3)	33(2)	52(3)	13(2)	2(2)	13(2)
C(52)	42(2)	52(3)	46(3)	25(2)	-6(2)	-5(2)
C(60)	15(2)	25(2)	26(2)	2(2)	-1(1)	5(1)
C(61)	40(2)	34(2)	56(3)	8(2)	21(2)	-1(2)
C(62)	23(2)	59(3)	24(2)	-2(2)	3(2)	1(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1.

	x	y	z	U(eq)
H(3)	684(22)	6348(19)	4667(11)	10(8)
H(4)	703(21)	8014(18)	4639(11)	5(7)
H(6)	2609(23)	5827(20)	3124(12)	13(8)
H(7)	890(22)	6064(20)	3079(11)	10(8)
H(10)	4165(2)	5216(2)	4825(1)	28
H(11C)	3811(3)	5718(3)	3976(1)	43
H(11B)	3508(3)	4755(3)	3802(1)	43
H(11A)	4608(3)	4962(3)	3959(1)	43
H(12C)	3783(3)	3778(2)	5079(2)	41
H(12B)	4630(3)	3816(2)	4649(2)	41
H(12A)	3554(3)	3548(2)	4478(2)	41
H(20)	2554(3)	4532(2)	5682(1)	30
H(21C)	930(3)	4979(3)	5661(1)	44
H(21B)	1253(3)	5977(3)	5699(1)	44
H(21A)	1438(3)	5336(3)	6184(1)	44
H(22C)	3088(3)	6325(3)	5714(2)	60
H(22B)	3827(3)	5522(3)	5726(2)	60
H(22A)	3118(3)	5693(3)	6213(2)	60
H(30)	810(2)	4769(2)	4695(1)	31
H(31C)	1300(3)	5013(3)	3835(2)	52
H(31B)	793(3)	4080(3)	3882(2)	52
H(31A)	1949(3)	4150(3)	3844(2)	52
H(32C)	1416(3)	3606(2)	5202(2)	47
H(32B)	1954(3)	3230(2)	4693(2)	47
H(32A)	795(3)	3272(2)	4710(2)	47
H(40)	-193(3)	6607(3)	2329(1)	45
H(41C)	-1315(3)	7942(4)	1879(2)	72
H(41B)	-1708(3)	7139(4)	2217(2)	72
H(41A)	-1239(3)	6975(4)	1650(2)	72
H(42C)	1226(3)	7248(3)	1997(2)	66
H(42B)	579(3)	7918(3)	1667(2)	66
H(42A)	528(3)	6899(3)	1541(2)	66
H(50)	255(3)	9315(2)	3120(1)	34
H(51C)	-1428(3)	9348(3)	3024(2)	52
H(51B)	-1331(3)	9274(3)	2399(2)	52
H(51A)	-960(3)	10130(3)	2695(2)	52
H(52C)	1257(3)	9083(3)	2347(2)	56
H(52B)	798(3)	10033(3)	2408(2)	56
H(52A)	329(3)	9351(3)	2006(2)	56
H(60)	-1683(2)	7762(2)	3127(1)	27
H(61C)	-1231(3)	6287(2)	3082(2)	52
H(61B)	-1754(3)	6496(2)	3629(2)	52
H(61A)	-600(3)	6394(2)	3606(2)	52
H(62C)	-1031(3)	8696(3)	3767(1)	42
H(62B)	-447(3)	7905(3)	4026(1)	42
H(62A)	-1607(3)	7918(3)	4045(1)	42

Selected torsion angles

-9.79 (0.36) C1 - C1_\$1 - C5_\$1 - C5

Least-squares planes (x,y,z in crystal coordinates) and deviations from them
(* indicates atom used to define plane)

0.108 (0.025) x + 0.209 (0.025) y + 25.438 (0.003) z = 11.998 (0.019)

* 0.008 (0.001) C1
* -0.033 (0.002) C2
* 0.047 (0.002) C3
* -0.041 (0.002) C4
* 0.018 (0.001) C1_\$1
-1.963 (0.002) Mo

Rms deviation of fitted atoms = 0.033

- 0.108 (0.025) x - 0.209 (0.025) y + 25.438 (0.003) z = 11.631 (0.024)

Angle to previous plane (with approximate esd) = 1.79 (0.01)

* 0.018 (0.001) C1
* 0.008 (0.001) C1_\$1
* -0.033 (0.002) C2_\$1
* 0.047 (0.002) C3_\$1
* -0.041 (0.002) C4_\$1

Rms deviation of fitted atoms = 0.033

- 0.355 (0.023) x + 0.092 (0.026) y + 25.433 (0.003) z = 7.899 (0.020)

Angle to previous plane (with approximate esd) = 1.52 (0.01)

* -0.029 (0.001) C5
* 0.045 (0.002) C6
* -0.044 (0.002) C7
* 0.024 (0.002) C8
* 0.004 (0.001) C5_\$1
1.967 (0.002) Mo

Rms deviation of fitted atoms = 0.033

0.355 (0.023) x - 0.092 (0.026) y + 25.433 (0.003) z = 7.938 (0.024)

Angle to previous plane (with approximate esd) = 3.03 (0.01)

* 0.004 (0.001) C5
* -0.029 (0.001) C5_\$1
* 0.045 (0.002) C6_\$1
* -0.044 (0.002) C7_\$1
* 0.024 (0.002) C8_\$1

Rms deviation of fitted atoms = 0.033

$$0.108 (0.023) x + 0.209 (0.023) y + 25.438 (0.003) z = 11.998 (0.019)$$

Angle to previous plane (with approximate esd) = 1.52 (0.01)

* 0.008 (0.001) C1
* -0.033 (0.002) C2
* 0.047 (0.002) C3
* -0.041 (0.002) C4
* 0.018 (0.001) C1_\$1
-1.963 (0.002) Mo

Rms deviation of fitted atoms = 0.033

$$- 0.355 (0.023) x + 0.092 (0.026) y + 25.433 (0.003) z = 7.899 (0.020)$$

Angle to previous plane (with approximate esd) = 1.97 (0.01)

* -0.029 (0.001) C5
* 0.045 (0.002) C6
* -0.044 (0.002) C7
* 0.024 (0.002) C8
* 0.004 (0.001) C5_\$1
1.967 (0.002) Mo

Rms deviation of fitted atoms = 0.033