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EXPERIMENTAL DETAILS FOR THE SYNTHESIS OF 1

Synthesis of $K_2[C_8H_4(Si^iPr_3\text{-}1,5)_2]$[1]

(a) Cyclooctatetraene (11.3 gm, 0.108 mol) in a slow stream (1.5 cm^3 min^{-1} at STP) of dinitrogen was passed through a quartz tube at 615 ± 1°C under a controlled dynamic vacuum of 1.0 ± 0.05 mbar over a period of 24 hours in a FVP apparatus; the resultant mixture of dihydropentalenes was collected in a trap at -78°C.[2] The latter was then dissolved in precooled (-78°C) hexane (100 cm^3) and DME (23 cm^3, 0.22 mol) added, followed by $LiBu^n$ (2.5M in hexanes, 88 cm^3, 0.22 mol) dropwise with stirring, which resulted in the precipitation of white $[Li(DME)]_2[C_8H_6]$.[3] After warm up to room temperature, the latter was isolated by filtration on a frit, washed with hexane (3 x 50 cm^3), and dried under vacuum. Yield 27.8 gm, 87% based on cyclooctatetraene.

NMR data (THF-d_8, 295K, Bruker DMX300): ^1H: δ 5.76 (t, 2H, ring C<u>H</u>, J_{HH} 3.0), 5.00 (d, 4H, ring C<u>H</u>, J_{HH} 3.0), 3.42 (s, 8H, DME C<u>H</u>$_2$), 3.27 (s, 12H, DME C<u>H</u>$_3$); $^7Li\{^1H\}$: δ -8.57 (s).

(b) To a stirred solution of $[Li(DME)]_2[C_8H_6]$ (2.95 gm, 10 mmol) in THF (100 cm^3) at -78°C was added tri(isopropylsilyl) triflate (6.12 gm, 20 mmol) dropwise; the mixture was the allowed to warm to 0°C and the solvent removed *in vacuo* at this temperature. The resultant white solids were extracted with pentane (3 x 100 cm^3), filtered and the pale yellow filtrates concentrated and cooled to -40°C to afford white crystals of $[C_8H_6(Si^iPr_3\text{-}1,5)_2]$. These were collected and washed with pentane (2 x 10 cm^3) at -78°C. Total yield (two crops) 3.2 gm, 77%.

HRMS (EI): 416.330456 (calculated 416.329459)

NMR data (benzene-d_6) , 295K, Bruker DMX300): ^1H: δ 6.82 (d, 2H, ring C<u>H</u>, J_{HH} 4.8), 6.65 (d, 2H, ring C<u>H</u>, J_{HH} 4.8), 3.56 (s, 2H, ring C<u>H</u>), 1.12 (m, 6H, ^iPr-C<u>H</u>), 1.08 (d, 18H, ^iPr-C<u>H</u>$_3$, J_{HH} 6.4, 1.01 (d, 18H, ^iPr-C<u>H</u>$_3$, J_{HH} 6.4); $^{13}C\{^1H\}$: δ 153.0 (ring-<u>C</u>), 134.3 (ring-<u>C</u>H), 127.9 (ring-<u>C</u>H), 39.7 (ring-<u>C</u>HSi$^iPr_3$), 19.3 (^iPr-<u>C</u>H$_3$), 19.1 (^iPr-<u>C</u>H$_3$), 12.7 (^iPr-<u>C</u>H).

(c) To a stirred, solid mixture of $[C_8H_6(Si^iPr_3\text{-}1,5)_2]$ (2.08 gm, 5mmol) and [KMe] (0.54 gm, 10 mmol) in a -78°C bath was added diethyl ether, precooled to -78°C, and the mixture allowed to warm to room temperature overnight. The orange solution was then filtered from small amounts of insoluble material and evaporated to dryness *in vacuo* to afford off-white $K_2[C_8H_4(Si^iPr_3\text{-}1,5)_2]$ in essentially quantitative yield.

NMR data (benzene-d_6) , 295K, Bruker DMX300): ^1H: δ 6.41 (d, 2H, ring C<u>H</u>, J_{HH} 3.2), 5.80 (d, 2H, ring C<u>H</u>, J_{HH} 3.2), 1.45 (m, 6H, ^iPr-C<u>H</u>, J_{HH} 7.1), 1.28 (d, 36H, ^iPr-C<u>H</u>$_3$, J_{HH} 7.1) $^{13}C\{^1H\}$: δ 139.2 (ring-<u>C</u>), 121.6 (ring-<u>C</u>H), 94.1 (ring-<u>C</u>H), 79.5 (ring-<u>C</u>Si$^iPr_3$), 20.5 (^iPr-<u>C</u>H$_3$), 13.6 (^iPr-<u>C</u>H); $^{29}Si\{^1H\}$: δ 4.19 (<u>Si</u>$^iPr_3$).

Synthesis of $[Th\{C_8H_4(Si^iPr_3\text{-}1,5)_2\}_2]$, **1**

To mixture of solid $[ThCl_4]$ (0.373 gm., 1 mmol) and solid $K_2[C_8H_4(Si^iPr_3\text{-}1,5)_2]$ (0.984 gm, 2 mmol) was added THF (75 cm^3) and the resultant suspension stirred overnight at room temperature. The solvent was then removed *in vacuo* and the residue extracted with pentane (150 cm^3) and filtered through Celite on a frit. Concentration of the orange filtrate and slow cooling to -50°C afforded deep orange crystals of **1**, which were washed with cold (-78°C) pentane and dried under vacuum. Yield 0.74 gm, 70%.

MS (EI): *m/z* 1061 (100%) ($[M+H]^+$).

Elemental analysis: Found C 59.22%; H 9.04%. Calculated for $[C_{52}H_{92}Si_4Th]$: C 58.83%; H 8.73%.

λ_{max} (pentane): 435 nm

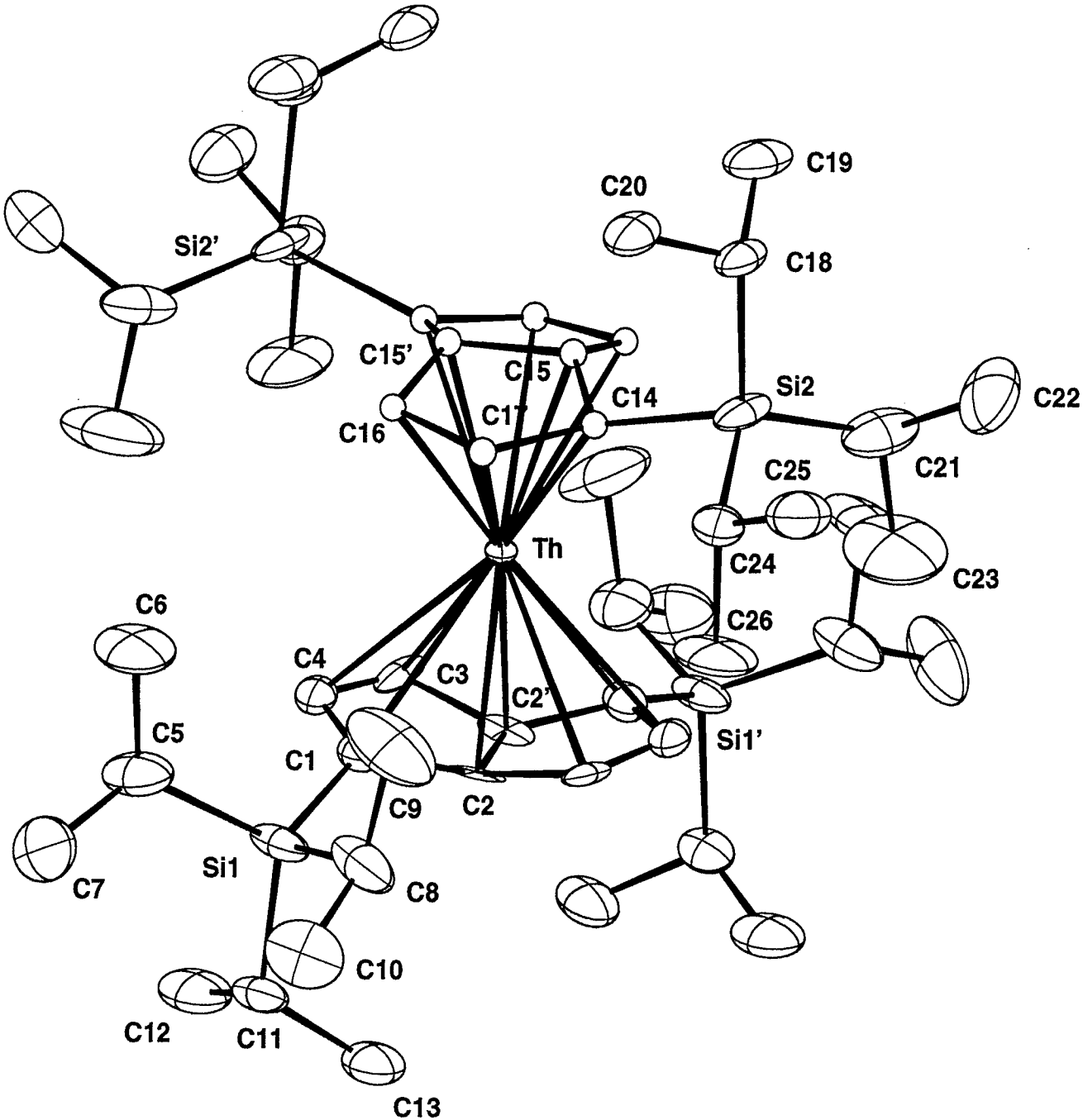
NMR data (toluene-d_8, 295K, Bruker DMX300): ^1H: δ 6.69 (d, 2H, ring C<u>H</u>, J_{HH} 3.1), 6.67 (d, 2H, ring C<u>H</u>, J_{HH} 3.0), 5.65 (d, 2H, ring C<u>H</u>, J_{HH} 3.0), 5.51 (d, 2H, ring C<u>H</u>, J_{HH} 3.1), 1.23 (m, 12H, ^{i}Pr-C<u>H</u>), 1.11 (d, 18H, ^{i}Pr-C<u>H</u>$_3$, J_{HH} 7.4), 1.10 (d, 18H, ^{i}Pr-C<u>H</u>$_3$, J_{HH} 7.4), 1.09 (d, 18H, ^{i}Pr-C<u>H</u>$_3$, J_{HH} 7.3), 1.06 (d, 18H, ^{i}Pr-C<u>H</u>$_3$, J_{HH} 7.3); $^{13}C\{^1H\}$: δ 156.9 (ring-<u>C</u>), 155.9 (ring-<u>C</u>), 137.4 (ring-<u>C</u>H), 134.3 (ring-<u>C</u>H), 111.6 (ring-<u>C</u>Si^{i}Pr$_3$), 111.2 (ring-<u>C</u>H), 109.5 (ring-<u>C</u>Si^{i}Pr$_3$), 106.9 (ring-<u>C</u>H), 20.2 (^{i}Pr-<u>C</u>H$_3$), 20.1 (^{i}Pr-<u>C</u>H$_3$), 19.9 (^{i}Pr-<u>C</u>H$_3$), 19.7 (^{i}Pr-<u>C</u>H$_3$), 13.1 (^{i}Pr-<u>C</u>H), 13.0 (^{i}Pr-<u>C</u>H); $^{29}Si\{^1H\}$: δ 2.37 (<u>Si</u>^{i}Pr$_3$), 1.83 (<u>Si</u>^{i}Pr$_3$).

References

[1] Cloke, F.G.N., to be submitted.

[2] Meier, H.; Pauli, A.; Kochhan, P. *Synthesis* **1987**, 573.

[3] Stezowski, J.J.; Hoier, H.; Wilhelm, D.; Clark, T.; Schleyer, P. von R. *J.Chem.Soc., Chem.Commun.* **1985**, 1263.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C26
Th
C6
C4
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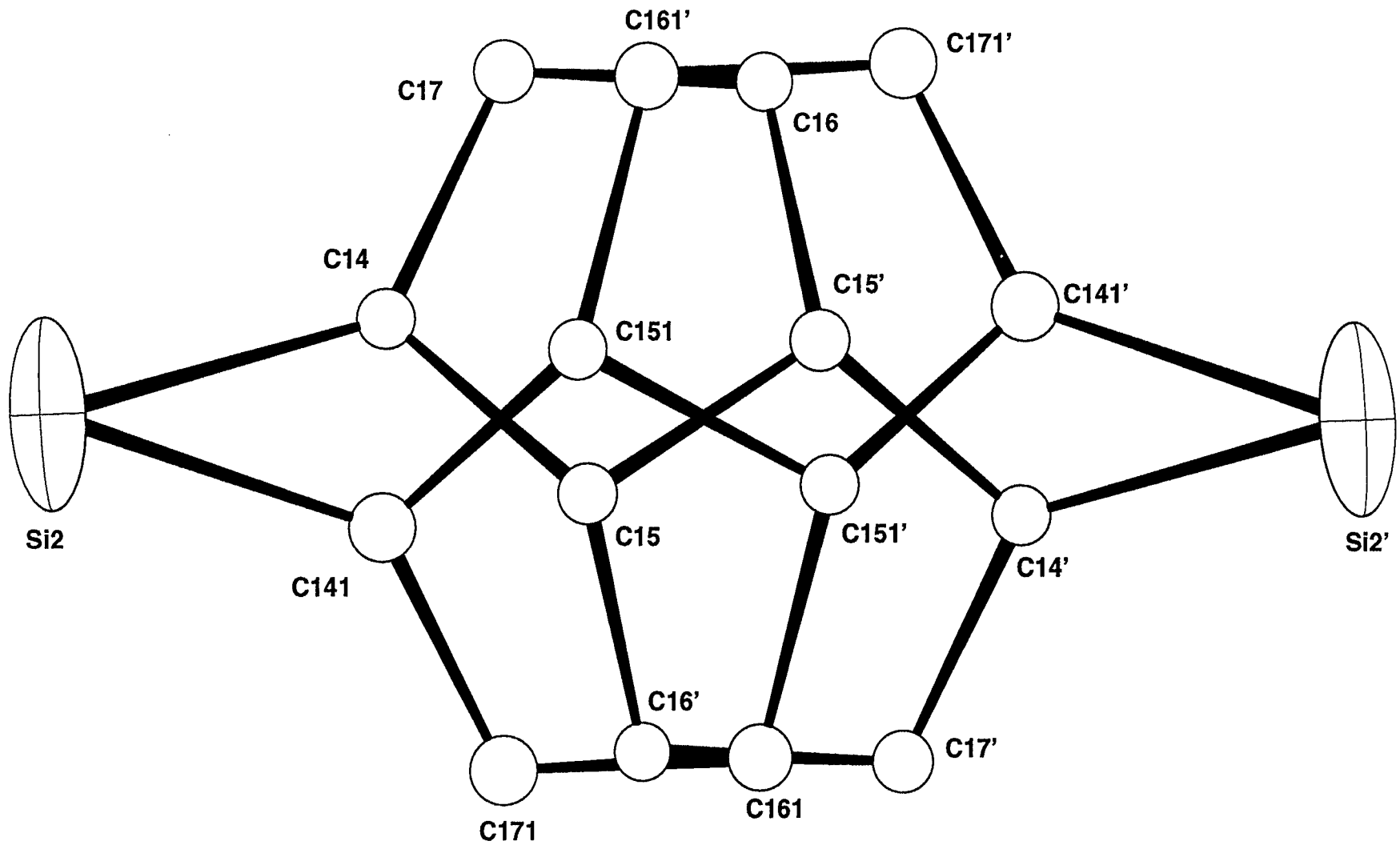
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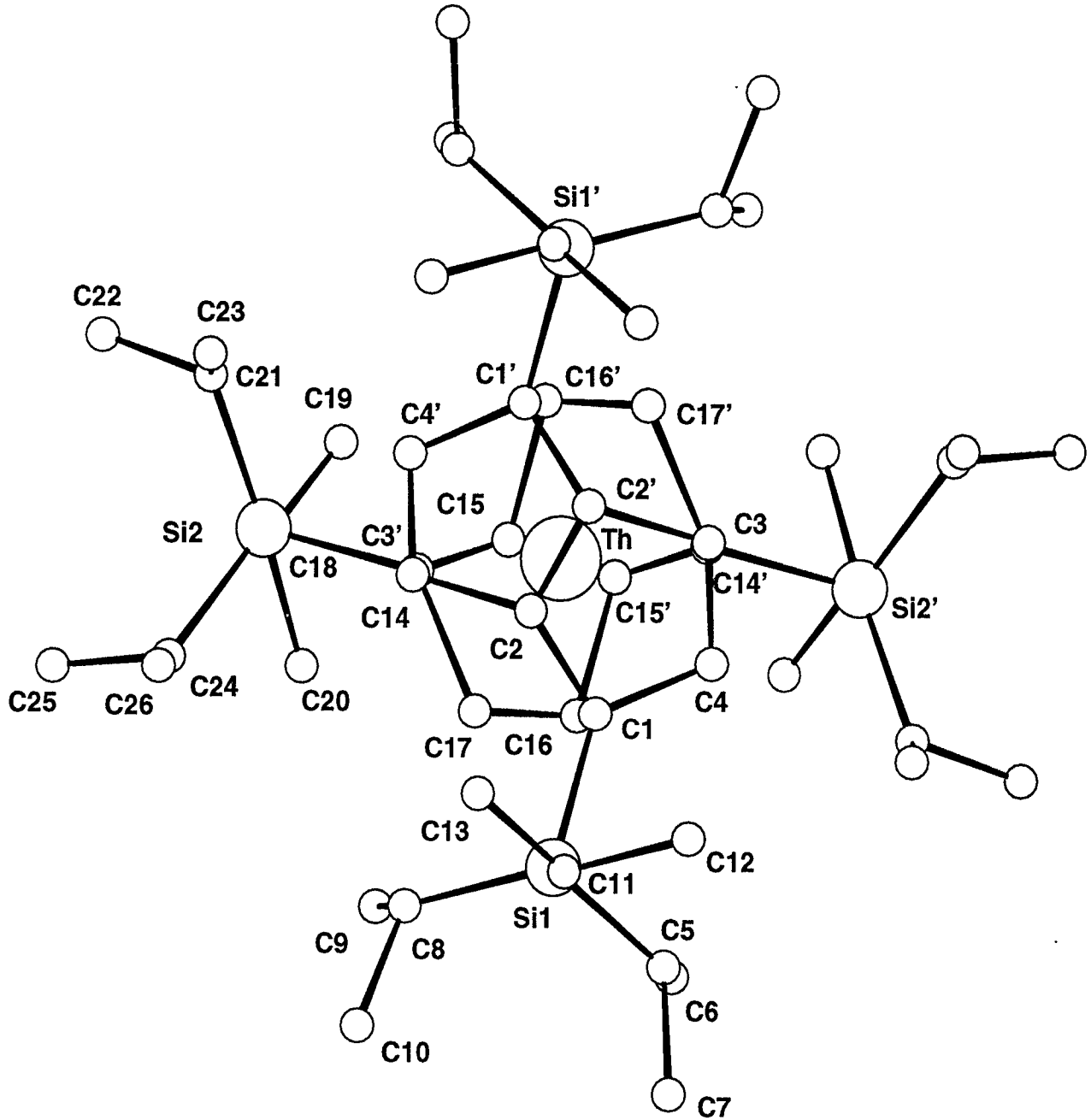
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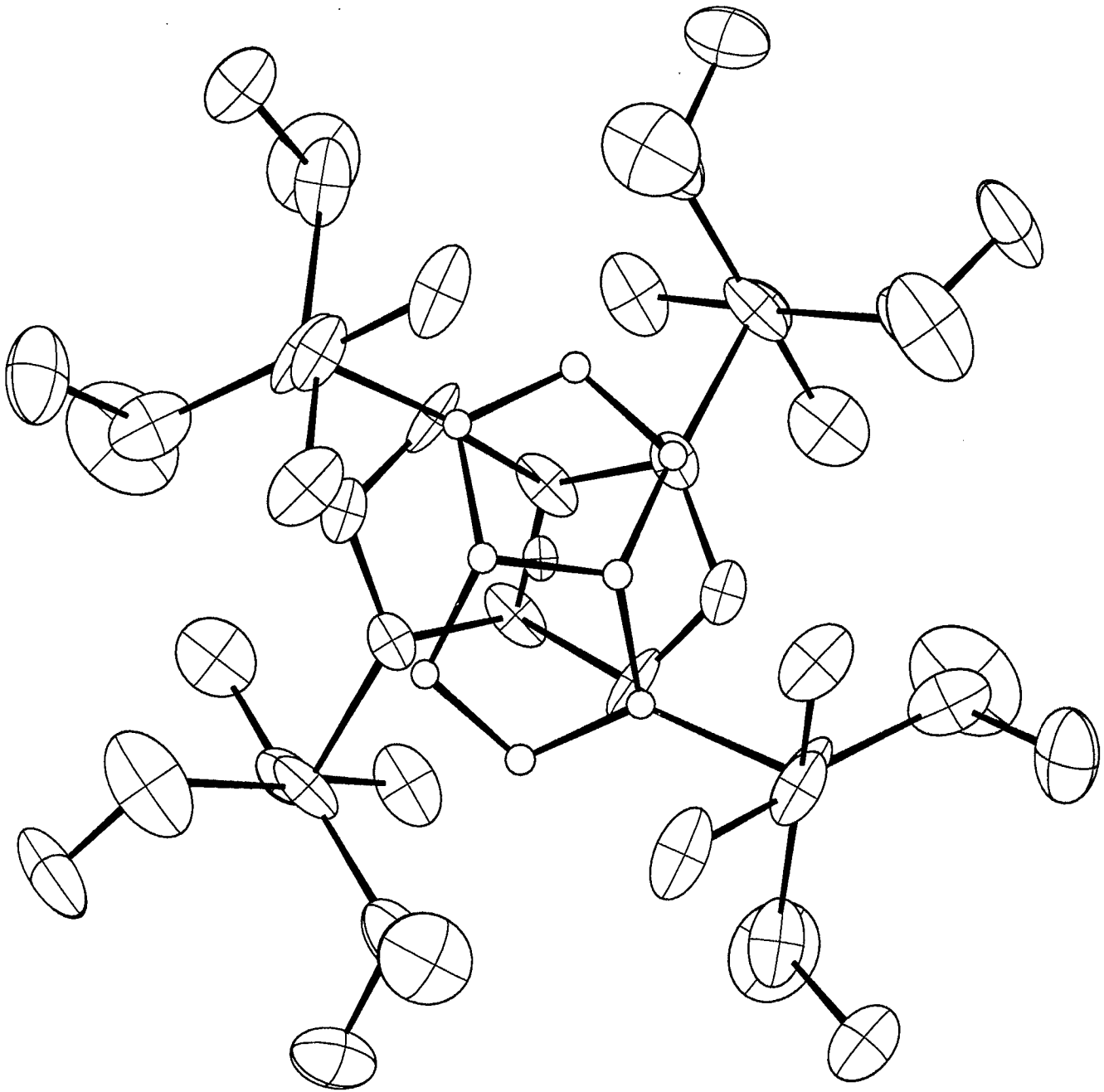

Table 1. Crystal data and structure refinement for [Th{pentalene(SiiPr3)2}2]

Identification code	APR997
Empirical formula	C52 H92 Si4 Th
Formula weight	1061.7
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c (No.15)
Unit cell dimensions	a = 21.296(4) Å alpha = 90 deg. b = 13.357(2) Å beta = 95.26(3) deg. c = 21.095(13) Å gamma = 90 deg.
Volume	5975(4) $Å^3$
Z	4
Density (calculated)	1.18 Mg/m^3
Absorption coefficient	2.60 mm^{-1}
F(000)	2200
Crystal size	0.20 x 0.20 x 0.15 mm
Theta range for data collection	2 to 23 deg.
Index ranges	0<=h<=23, 0<=k<=14, -23<=l<=23
Reflections collected	4257
Independent reflections	4138 [R(int) = 0.0521]
Reflections with I>2sigma(I)	3690
Structure solution	Heavy atom methods
Refinement method	Full-matrix least-squares on all F^2
Data / restraints / parameters	4138 / 6 / 255
Goodness-of-fit on F^2	1.215
Final R indices [I>2sigma(I)]	R1 = 0.059, wR2 = 0.163
R indices (all data)	R1 = 0.068, wR2 = 0.169
Largest diff. peak and hole	4.5 and -1.65 $e.Å^{-3}$ (near Th)
Abs.correction from psi scans	Tmax=1.00 ,Tmin=0.67
Maximum shift/e.s.d.	0.009

The molecule lies on crystallographic 2-fold rotation axis which passes through the mid points of the two pentalene ligands.

The pentalene group attached to Si(2) was disordered 0.52:0.48 over two orientations related by an approximate mirror reflection across the plane joining Th,Si(2) and SI(2)'. the two orientaions were loosely constrained to a similar geometry (SAME in SHELXL-93).

All non-H atoms were anisotropic, except for the disordered pentalene C atoms which were left isotropic. 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.
Sheldrick,G.M.(1993) SHELXL-93. Program for Crystal Structure 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 (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)	
Th	0	817.2(3)	2500	23(1)	
Si(1)	1635(2)	-1166(2)	2469(2)	57(1)	
Si(2)	-312(2)	2818(2)	846(2)	68(1)	
C(1)	838(5)	-789(8)	2698(6)	44(3)	
C(2)	264(5)	-1014(7)	2329(7)	49(3)	
C(3)	-20(8)	-760(7)	3334(5)	51(4)	
C(4)	619(7)	-692(8)	3332(6)	46(3)	
C(5)	2217(7)	-626(11)	3068(10)	81(5)	
C(6)	2250(10)	499(12)	3108(14)	128(9)	
C(7)	2896(7)	-1045(16)	3086(12)	117(8)	
C(8)	1759(8)	-854(11)	1621(10)	83(5)	
C(9)	1715(12)	266(16)	1478(12)	139(10)	
C(10)	2377(9)	-1306(15)	1406(10)	99(6)	
C(11)	1669(5)	-2565(9)	2535(6)	53(3)	
C(12)	1561(9)	-2933(11)	3207(9)	88(5)	
C(13)	1217(7)	-3103(10)	2044(9)	81(5)	
C(18)	-257(8)	4224(8)	858(6)	60(4)	
C(19)	-725(9)	4706(10)	1263(7)	81(5)	
C(20)	409(9)	4597(10)	1064(7)	84(5)	
C(21)	-1135(9)	2451(11)	563(7)	83(5)	
C(22)	-1420(10)	2988(15)	-41(10)	113(7)	
C(23)	-1272(13)	1353(15)	542(16)	171(13)	
C(24)	306(8)	2327(10)	330(7)	76(5)	
C(25)	287(9)	2763(11)	-329(7)	83(5)	
C(26)	337(12)	1185(11)	268(11)	121(8)	
C(14)	78(7)	2418(14)	1671(7)	24(5)	a
C(15)	-239(7)	2642(14)	2225(7)	25(5)	a
C(16)	828(7)	2400(14)	2567(9)	23(5)	a
C(17)	725(7)	2306(13)	1905(9)	26(5)	a
C(141)	-419(8)	2429(17)	1716(8)	32(6)	b
C(151)	98(7)	2646(15)	2163(8)	24(5)	b
C(161)	-784(9)	2406(17)	2733(10)	30(6)	b
C(171)	-940(9)	2323(16)	2087(11)	33(6)	b

a occupancy 0.52
b occupancy 0.48

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

Th-C(1)	2.797(11)	Th-C(2)	2.543(10)
Th-C(3)	2.748(10)	Th-C(4)	2.908(11)
Th-C(14)	2.78(2)	Th-C(15)	2.55(2)
Th-C(16)	2.75(2)	Th-C(17)	2.88(2)
Th-C(141)	2.81(2)	Th-C(151)	2.56(2)
Th-C(161)	2.77(2)	Th-C(171)	2.91(2)
Si(1)-C(5)	1.83(2)	Si(1)-C(11)	1.875(12)
Si(1)-C(1)	1.876(12)	Si(1)-C(8)	1.88(2)
Si(2)-C(21)	1.87(2)	Si(2)-C(18)	1.882(11)
Si(2)-C(24)	1.90(2)	Si(2)-C(14)	1.93(2)
Si(2)-C(141)	1.94(2)	C(1)-C(2)	1.42(2)
C(1)-C(4)	1.46(2)	C(2)-C(2)'	1.39(2)
C(2)-C(3)'	1.49(2)	C(3)-C(4)	1.36(2)
C(5)-C(6)	1.51(2)	C(5)-C(7)	1.55(2)
C(8)-C(9)	1.53(2)	C(8)-C(10)	1.55(2)
C(11)-C(13)	1.53(2)	C(11)-C(12)	1.54(2)
C(18)-C(19)	1.51(2)	C(18)-C(20)	1.53(2)
C(21)-C(23)	1.50(2)	C(21)-C(22)	1.54(2)
C(24)-C(25)	1.51(2)	C(24)-C(26)	1.53(2)
C(14)-C(17)	1.43(2)	C(14)-C(15)	1.43(2)
C(15)-C(16)'	1.41(2)	C(15)-C(15)'	1.47(3)
C(16)-C(17)	1.40(3)	C(141)-C(151)	1.41(2)
C(141)-C(171)	1.42(2)	C(151)-C(161)'	1.49(3)
C(151)-C(151)'	1.52(3)	C(161)-C(171)	1.38(3)

C(5)-Si(1)-C(11)	108.8(7)	C(5)-Si(1)-C(1)	106.7(6)
C(11)-Si(1)-C(1)	106.1(5)	C(5)-Si(1)-C(8)	115.1(8)
C(11)-Si(1)-C(8)	106.4(6)	C(1)-Si(1)-C(8)	113.3(6)
C(21)-Si(2)-C(18)	108.8(7)	C(21)-Si(2)-C(24)	113.9(7)
C(18)-Si(2)-C(24)	107.9(7)	C(21)-Si(2)-C(14)	121.9(7)
C(18)-Si(2)-C(14)	104.0(7)	C(24)-Si(2)-C(14)	99.1(7)
C(21)-Si(2)-C(141)	92.5(7)	C(18)-Si(2)-C(141)	105.5(8)
C(24)-Si(2)-C(141)	126.7(8)	C(2)-C(1)-C(4)	100.9(10)
C(2)-C(1)-Si(1)	123.8(9)	C(4)-C(1)-Si(1)	129.2(9)
C(2)'-C(2)-C(1)	114(2)	C(2)'-C(2)-C(3)'	105.1(14)
C(1)-C(2)-C(3)'	132.6(12)	C(4)-C(3)-C(2)'	106.0(11)
C(3)-C(4)-C(1)	113.5(11)	C(6)-C(5)-C(7)	109(2)
C(6)-C(5)-Si(1)	117(2)	C(7)-C(5)-Si(1)	116.4(12)
C(9)-C(8)-C(10)	111(2)	C(9)-C(8)-Si(1)	113(2)
C(10)-C(8)-Si(1)	113.0(12)	C(13)-C(11)-C(12)	109.7(12)
C(13)-C(11)-Si(1)	113.7(9)	C(12)-C(11)-Si(1)	112.2(9)
C(19)-C(18)-C(20)	110.1(12)	C(19)-C(18)-Si(2)	112.8(10)
C(20)-C(18)-Si(2)	112.6(10)	C(23)-C(21)-C(22)	112(2)
C(23)-C(21)-Si(2)	116(2)	C(22)-C(21)-Si(2)	115.5(11)
C(25)-C(24)-C(26)	107.7(14)	C(25)-C(24)-Si(2)	115.8(10)
C(26)-C(24)-Si(2)	115.5(14)	C(17)-C(14)-C(15)	104.5(13)
C(17)-C(14)-Si(2)	131.3(12)	C(15)-C(14)-Si(2)	118.8(11)
C(16)'-C(15)-C(14)	135(2)	C(16)'-C(15)-C(15)'	109(2)
C(14)-C(15)-C(15)'	108(2)	C(17)-C(16)-C(15)'	105.6(14)
C(16)-C(17)-C(14)	113.2(13)	C(151)-C(141)-C(171)	104.6(14)
C(151)-C(141)-Si(2)	115.2(12)	C(171)-C(141)-Si(2)	135(2)
C(141)-C(151)-C(161)	138(2)	C(141)-C(151)-C(151)	111(2)
C(161)'-C(151)-C(151	102(2)	C(171)-C(161)-C(151)	108(2)

Symmetry transformations used to generate equivalent atoms:
' -x,y,-z+1/2

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for 1.
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
Th	28(1)	10(1)	30(1)	0	-3(1)	0
Si(1)	28(2)	22(2)	122(3)	0(2)	12(2)	1(1)
Si(2)	153(4)	16(2)	29(2)	4(1)	-18(2)	0(2)
C(1)	38(7)	28(6)	64(8)	-3(5)	-1(5)	1(5)
C(2)	37(6)	2(5)	108(11)	-8(5)	10(6)	6(4)
C(3)	118(13)	13(5)	20(5)	5(4)	-15(6)	-15(6)
C(4)	64(9)	25(6)	45(7)	1(5)	-13(6)	1(6)
C(5)	59(9)	42(8)	146(16)	-25(9)	24(10)	-11(7)
C(6)	98(15)	30(8)	251(29)	-20(13)	-8(16)	-16(9)
C(7)	41(9)	122(17)	183(22)	-59(16)	-11(11)	9(10)
C(8)	56(9)	53(10)	141(16)	22(9)	4(10)	14(7)
C(9)	154(21)	85(15)	181(23)	80(16)	29(18)	29(15)
C(10)	92(13)	88(13)	122(15)	17(12)	45(12)	-3(11)
C(11)	41(6)	30(6)	88(9)	-7(7)	13(6)	9(6)
C(12)	100(13)	30(7)	136(16)	1(9)	17(11)	1(8)
C(13)	69(10)	32(8)	140(15)	-11(8)	-5(10)	2(7)
C(18)	113(12)	22(6)	42(7)	-2(5)	-17(7)	1(7)
C(19)	149(16)	27(7)	67(9)	-4(7)	4(10)	6(9)
C(20)	150(16)	25(7)	68(9)	3(7)	-35(10)	5(9)
C(21)	138(15)	35(7)	80(10)	0(8)	30(10)	-20(9)
C(22)	119(16)	88(14)	122(16)	4(12)	-36(13)	-44(12)
C(23)	170(25)	50(13)	294(39)	18(18)	32(25)	-34(15)
C(24)	103(12)	27(7)	90(10)	-3(7)	-33(9)	11(7)
C(25)	133(15)	50(10)	65(9)	-5(7)	1(9)	18(9)
C(26)	192(24)	24(8)	143(18)	6(10)	2(16)	31(12)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(3)	-260(8)	-665(7)	3687(5)	62
H(4)	895(7)	-590(8)	3706(6)	55
H(5)	2069(7)	-836(11)	3485(10)	98
H(6C)	1822(10)	773(12)	3097(14)	192
H(6B)	2457(10)	759(12)	2746(14)	192
H(6A)	2492(10)	696(12)	3506(14)	192
H(7C)	2881(7)	-1777(16)	3060(12)	175
H(7B)	3135(7)	-843(16)	3484(12)	175
H(7A)	3101(7)	-779(16)	2724(12)	175
H(8)	1405(8)	-1178(11)	1352(10)	100
H(9C)	1321(12)	531(16)	1619(12)	208
H(9B)	1720(12)	374(16)	1019(12)	208
H(9A)	2074(12)	611(16)	1705(12)	208
H(10C)	2393(9)	-2024(15)	1503(10)	148
H(10B)	2741(9)	-971(15)	1632(10)	148
H(10A)	2387(9)	-1208(15)	946(10)	148
H(11)	2106(5)	-2771(9)	2452(6)	63
H(12C)	1852(9)	-2586(11)	3520(9)	132
H(12B)	1638(9)	-3656(11)	3235(9)	132
H(12A)	1126(9)	-2791(11)	3293(9)	132
H(13C)	1287(7)	-2867(10)	1616(9)	122
H(13B)	781(7)	-2961(10)	2129(9)	122
H(13A)	1293(7)	-3826(10)	2071(9)	122
H(18)	-364(8)	4459(8)	412(6)	73
H(19C)	-1150(9)	4462(10)	1128(7)	122
H(19B)	-712(9)	5434(10)	1213(7)	122
H(19A)	-616(9)	4532(10)	1711(7)	122
H(20C)	709(9)	4282(10)	800(7)	125
H(20B)	521(9)	4423(10)	1512(7)	125
H(20A)	425(9)	5326(10)	1013(7)	125
H(21)	-1391(9)	2706(11)	903(7)	99
H(22C)	-1320(10)	3704(15)	-10(10)	169
H(22B)	-1879(10)	2898(15)	-84(10)	169
H(22A)	-1242(10)	2705(15)	-415(10)	169
H(23C)	-1084(13)	1037(15)	933(16)	256
H(23B)	-1093(13)	1054(15)	174(16)	256
H(23A)	-1730(13)	1248(15)	504(16)	256
H(24)	722(8)	2532(10)	550(7)	91
H(25C)	267(9)	3495(11)	-303(7)	125
H(25B)	-86(9)	2513(11)	-587(7)	125
H(25A)	668(9)	2566(11)	-525(7)	125
H(26C)	349(12)	880(11)	691(11)	181
H(26B)	717(12)	999(11)	68(11)	181
H(26A)	-36(12)	946(11)	5(11)	181
H(16)	1216(7)	2317(14)	2822(9)	28
H(17)	1052(7)	2181(13)	1638(9)	31
H(161)	-1064(9)	2324(17)	3055(10)	36
H(171)	-1358(9)	2206(16)	1906(11)	39

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

2.283 (0.112) x + 13.055 (0.020) y - 3.620 (0.117) z = 2.220 (0.035)

*	-0.022	(0.006)	C1
*	0.007	(0.005)	C2
*	-0.025	(0.006)	C3
*	0.030	(0.007)	C4
*	0.010	(0.004)	C2_$1
	-2.382	(0.007)	Th

Rms deviation of fitted atoms = 0.021

- 2.283 (0.112) x + 13.055 (0.020) y + 3.620 (0.117) z = 0.410 (0.025)

Angle to previous plane (with approximate esd) = 24.41 (0.26)

*	-0.022	(0.006)	C1_$1
*	0.007	(0.005)	C2_$1
*	-0.025	(0.006)	C3_$1
*	0.030	(0.007)	C4_$1
*	0.010	(0.004)	C2
	-2.382	(0.007)	Th

Rms deviation of fitted atoms = 0.021

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

2.283 (0.112) x + 13.055 (0.020) y - 3.620 (0.117) z = 2.220 (0.035)

*	-0.022	(0.006)	C1
*	0.007	(0.005)	C2
*	-0.025	(0.006)	C3
*	0.030	(0.007)	C4
*	0.010	(0.004)	C2_$1
	-2.382	(0.007)	Th
	0.569	(0.016)	Si1

Rms deviation of fitted atoms = 0.021