JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
J. Am. Chem. Soc., 1998, 120(3), 599-600, DOI:10.1021/ja972093z

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SUPPORTING INFORMATION

Table 1. Crystal data and structure refinement for [(C5Me4SiMe2tBu)HgCl]

Identification code	APR597
Empirical formula	C15 H27 Cl Hg Si
Formula weight	471.5
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P $\bar{1}$ (No.2)
Unit cell dimensions	a = 8.940(10) Å alpha = 92.01(12) deg. b = 14.02(2) Å beta = 95.91(11) deg. c = 14.04(2) Å gamma = 98.50(11) deg.
Volume	1730(4) $Å^3$
Z	4
Density (calculated)	1.81 Mg/m^3
Absorption coefficient	9.11 mm^{-1}
F(000)	912
Crystal size	0.3x0.2x0.1 mm (cut from large crystal)
Theta range for data collection	2 to 25 deg.
Index ranges	-10<=h<=10, -16<=k<=16, 0<=l<=16
Reflections collected	6077
Independent reflections	6077 [R(int) = 0.0000]
Reflections with I>2sigma(I)	3978
Structure solution	Direct methods
Refinement method	Full-matrix least-squares on all F^2
Data / restraints / parameters	6077 / 0 / 343
Goodness-of-fit on F^2	1.006
Final R indices [I>2sigma(I)]	R1 = 0.081, wR2 = 0.196
R indices (all data)	R1 = 0.128, wR2 = 0.231
Largest diff. peak and hole	3.96 and -3.24 $e.Å^{-3}$
Abs.correction from DIFABS	Tmax=1.00 ,Tmin=0.28
Maximum shift/e.s.d.	0.002

All non-H atoms were anisotropic.
Methyl H atoms were fixed at idealised geometry but with the torsion angle defining the H atom positions refined

and Uiso(H) equal to 1.5Ueq(C).

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)
Hg(1)	646.1(8)	1035.6(6)	-1220.6(5)	27(1)
Hg(2)	812.7(9)	-1671.8(6)	-1984.2(5)	27(1)
Cl(1)	-1229(6)	-52(4)	-2132(4)	39(1)
Cl(2)	1436(6)	-1008(4)	-420(4)	37(1)
Si(1)	3749(6)	2338(4)	-1606(4)	27(1)
Si(2)	2321(6)	-1497(4)	-3936(4)	24(1)
C(1)	2358(21)	2201(16)	-665(13)	27(4)
C(2)	2942(24)	2046(16)	299(13)	32(5)
C(3)	2509(20)	2660(12)	919(14)	20(4)
C(4)	1563(21)	3280(15)	389(14)	27(5)
C(5)	1439(23)	3040(15)	-545(14)	30(5)
C(6)	3918(25)	1289(17)	589(16)	38(5)
C(7)	2963(25)	2819(15)	1968(14)	34(5)
C(8)	774(25)	4038(15)	856(16)	34(5)
C(9)	552(21)	3468(17)	-1329(16)	35(5)
C(10)	4685(26)	1243(17)	-1706(13)	36(5)
C(11)	2778(24)	2453(15)	-2812(14)	30(5)
C(12)	5274(24)	3463(14)	-1325(15)	31(5)
C(13)	6346(28)	3496(22)	-2102(19)	61(9)
C(14)	4570(24)	4395(15)	-1310(18)	39(5)
C(15)	6195(26)	3382(16)	-339(17)	42(6)
C(16)	900(23)	-2335(14)	-3329(14)	27(5)
C(17)	1202(21)	-3336(14)	-3128(15)	28(5)
C(18)	-59(27)	-4021(15)	-3568(14)	32(5)
C(19)	-1155(24)	-3538(16)	-4025(13)	30(5)
C(20)	-690(21)	-2561(15)	-3883(13)	26(4)
C(21)	2628(27)	-3546(16)	-2608(16)	40(6)
C(22)	-143(37)	-5094(17)	-3547(17)	58(8)
C(23)	-2599(27)	-4037(18)	-4553(18)	48(6)
C(24)	-1665(24)	-1808(16)	-4243(15)	33(5)
C(25)	4202(25)	-1292(18)	-3172(16)	42(6)
C(26)	1716(22)	-288(14)	-4054(16)	30(5)
C(27)	2626(22)	-1981(17)	-5181(14)	30(5)
C(28)	3844(26)	-1283(18)	-5543(17)	44(7)
C(29)	1176(22)	-2157(17)	-5848(14)	33(5)
C(30)	3247(30)	-2972(18)	-5056(16)	46(6)

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

Hg(1)-C(1)	2.13(2)	Hg(1)-Cl(1)	2.333(7)
Hg(1)-Cl(2)'	3.105(6)	Hg(2)-C(16)	2.09(2)
Hg(2)-Cl(2)	2.336(6)	Hg(2)-Cl(1)	3.117(7)
Si(1)-C(11)	1.84(2)	Si(1)-C(10)	1.86(2)
Si(1)-C(1)	1.90(2)	Si(1)-C(12)	1.93(2)
Si(2)-C(26)	1.86(2)	Si(2)-C(25)	1.88(2)
Si(2)-C(16)	1.89(2)	Si(2)-C(27)	1.91(2)
C(1)-C(2)	1.44(3)	C(1)-C(5)	1.54(3)
C(2)-C(3)	1.33(3)	C(2)-C(6)	1.51(3)
C(3)-C(4)	1.47(3)	C(3)-C(7)	1.49(3)
C(4)-C(5)	1.33(3)	C(4)-C(8)	1.53(3)
C(5)-C(9)	1.49(3)	C(12)-C(13)	1.52(3)
C(12)-C(14)	1.53(3)	C(12)-C(15)	1.55(3)
C(16)-C(17)	1.50(3)	C(16)-C(20)	1.53(3)
C(17)-C(18)	1.44(3)	C(17)-C(21)	1.48(3)
C(18)-C(19)	1.39(3)	C(18)-C(22)	1.50(3)
C(19)-C(20)	1.37(3)	C(19)-C(23)	1.48(3)
C(20)-C(24)	1.53(3)	C(27)-C(28)	1.50(3)
C(27)-C(29)	1.50(3)	C(27)-C(30)	1.58(3)

C(1)-Hg(1)-Cl(1)	167.5(5)	C(1)-Hg(1)-Cl(2)'	98.7(5)
Cl(1)-Hg(1)-Cl(2)'	89.4(2)	C(16)-Hg(2)-Cl(2)	163.6(6)
C(16)-Hg(2)-Cl(1)	111.1(5)	Cl(2)-Hg(2)-Cl(1)	82.4(2)
Hg(1)-Cl(1)-Hg(2)	91.4(2)	Hg(2)-Cl(2)-Hg(1)'	128.0(2)
C(11)-Si(1)-C(10)	105.4(9)	C(11)-Si(1)-C(1)	111.8(9)
C(10)-Si(1)-C(1)	110.7(10)	C(11)-Si(1)-C(12)	107.4(10)
C(10)-Si(1)-C(12)	109.7(10)	C(1)-Si(1)-C(12)	111.7(9)
C(26)-Si(2)-C(25)	106.1(10)	C(26)-Si(2)-C(16)	110.9(8)
C(25)-Si(2)-C(16)	109.5(10)	C(26)-Si(2)-C(27)	108.4(10)
C(25)-Si(2)-C(27)	108.5(9)	C(16)-Si(2)-C(27)	113.2(9)
C(2)-C(1)-C(5)	104(2)	C(2)-C(1)-Si(1)	117.9(14)
C(5)-C(1)-Si(1)	116.1(14)	C(2)-C(1)-Hg(1)	111(2)
C(5)-C(1)-Hg(1)	102.7(12)	Si(1)-C(1)-Hg(1)	104.6(9)
C(3)-C(2)-C(1)	111(2)	C(3)-C(2)-C(6)	124(2)
C(1)-C(2)-C(6)	126(2)	C(2)-C(3)-C(4)	109(2)
C(2)-C(3)-C(7)	129(2)	C(4)-C(3)-C(7)	122(2)
C(5)-C(4)-C(3)	110(2)	C(5)-C(4)-C(8)	126(2)
C(3)-C(4)-C(8)	124(2)	C(4)-C(5)-C(9)	127(2)
C(4)-C(5)-C(1)	107(2)	C(9)-C(5)-C(1)	126(2)
C(13)-C(12)-C(14)	109(2)	C(13)-C(12)-C(15)	109(2)
C(14)-C(12)-C(15)	109(2)	C(13)-C(12)-Si(1)	107.7(14)
C(14)-C(12)-Si(1)	112(2)	C(15)-C(12)-Si(1)	109.9(14)
C(17)-C(16)-C(20)	100(2)	C(17)-C(16)-Si(2)	119.5(13)
C(20)-C(16)-Si(2)	114.7(14)	C(17)-C(16)-Hg(2)	105.1(13)
C(20)-C(16)-Hg(2)	111.0(11)	Si(2)-C(16)-Hg(2)	105.9(10)
C(18)-C(17)-C(21)	127(2)	C(18)-C(17)-C(16)	109(2)
C(21)-C(17)-C(16)	124(2)	C(19)-C(18)-C(17)	110(2)
C(19)-C(18)-C(22)	126(2)	C(17)-C(18)-C(22)	124(2)
C(20)-C(19)-C(18)	109(2)	C(20)-C(19)-C(23)	128(2)
C(18)-C(19)-C(23)	124(2)	C(19)-C(20)-C(16)	112(2)
C(19)-C(20)-C(24)	123(2)	C(16)-C(20)-C(24)	125(2)
C(28)-C(27)-C(29)	113(2)	C(28)-C(27)-C(30)	108(2)
C(29)-C(27)-C(30)	109(2)	C(28)-C(27)-Si(2)	107.3(14)
C(29)-C(27)-Si(2)	112.2(13)	C(30)-C(27)-Si(2)	107.6(14)

Symmetry transformations used to generate equivalent atoms:
' -x,-y,-z

Table 4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for 1. The anisotropic displacement factor exponent takes the form: $-2\,pi^2\,[\,h^2 a^{*2} U11 + \ldots + 2\,h\,k\,a^*\,b^*\,U12\,]$

	U11	U22	U33	U23	U13	U12
Hg(1)	24(1)	28(1)	30(1)	0(1)	4(1)	4(1)
Hg(2)	31(1)	27(1)	24(1)	2(1)	4(1)	4(1)
Cl(1)	34(3)	43(3)	38(3)	-6(2)	2(2)	4(2)
Cl(2)	40(3)	46(3)	26(3)	-2(2)	7(2)	2(3)
Si(1)	27(3)	31(3)	24(3)	1(2)	3(2)	9(2)
Si(2)	23(3)	23(3)	24(3)	0(2)	2(2)	1(2)
C(1)	19(10)	43(13)	19(10)	16(9)	-6(8)	9(9)
C(2)	36(12)	44(13)	17(10)	2(9)	8(9)	8(10)
C(3)	20(10)	7(8)	33(10)	7(8)	6(8)	1(7)
C(4)	18(10)	31(12)	29(11)	-8(9)	-9(8)	0(9)
C(5)	32(12)	26(11)	29(11)	2(9)	-15(9)	12(9)
C(6)	35(13)	43(14)	39(13)	9(11)	4(10)	12(11)
C(7)	41(13)	26(11)	32(12)	1(9)	3(10)	-4(10)
C(8)	42(13)	22(11)	44(13)	6(9)	21(11)	8(10)
C(9)	10(10)	50(14)	44(13)	0(11)	-5(9)	8(9)
C(10)	55(15)	49(14)	9(9)	10(9)	-3(9)	27(12)
C(11)	36(12)	28(11)	23(10)	-8(9)	-3(9)	3(9)
C(12)	33(12)	24(11)	32(11)	-4(9)	10(9)	-14(9)
C(13)	35(14)	79(21)	62(18)	-31(16)	23(13)	-20(14)
C(14)	26(12)	27(12)	62(16)	9(11)	8(11)	-1(9)
C(15)	37(13)	28(12)	57(15)	12(11)	1(11)	-7(10)
C(16)	38(12)	20(10)	32(11)	8(8)	17(9)	24(9)
C(17)	15(10)	25(11)	42(12)	-11(9)	3(9)	0(8)
C(18)	56(15)	24(11)	18(10)	13(8)	10(10)	4(10)
C(19)	33(12)	37(12)	16(10)	-5(9)	3(8)	-6(10)
C(20)	17(10)	39(12)	21(10)	0(9)	3(8)	3(9)
C(21)	57(16)	32(13)	41(13)	13(10)	13(11)	29(12)
C(22)	110(25)	27(13)	34(14)	-2(11)	14(14)	2(14)
C(23)	38(14)	42(15)	53(15)	-6(12)	-8(11)	-16(11)
C(24)	36(12)	40(13)	24(11)	-2(9)	0(9)	12(10)
C(25)	35(13)	50(15)	40(13)	-1(11)	9(10)	5(11)
C(26)	16(10)	17(10)	58(14)	6(9)	4(10)	1(8)
C(27)	17(10)	49(14)	20(10)	2(9)	2(8)	-8(9)
C(28)	33(13)	48(15)	47(14)	-16(12)	20(11)	-11(11)
C(29)	22(11)	56(15)	21(10)	11(10)	9(8)	-3(10)
C(30)	61(17)	52(16)	28(12)	16(11)	14(11)	14(13)

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

	x	y	z	U(eq)
H(6A)	4032(140)	889(69)	23(23)	58
H(6B)	3432(84)	881(67)	1058(79)	58
H(6C)	4922(59)	1606(17)	876(96)	58
H(7A)	2209(90)	3141(94)	2260(21)	51
H(7B)	3961(78)	3225(87)	2080(14)	51
H(7C)	3017(160)	2196(17)	2254(22)	51
H(8A)	1456(68)	4658(30)	930(99)	52
H(8B)	519(155)	3835(54)	1488(48)	52
H(8C)	-160(91)	4110(78)	452(55)	52
H(9A)	556(137)	3096(63)	-1933(25)	52
H(9B)	1012(94)	4138(36)	-1391(68)	52
H(9C)	-499(44)	3450(93)	-1180(51)	52
H(10A)	3927(40)	664(17)	-1688(105)	54
H(10B)	5483(113)	1257(54)	-1169(60)	54
H(10C)	5138(147)	1232(58)	-2312(50)	54
H(11A)	2383(134)	3069(45)	-2833(31)	45
H(11B)	1934(94)	1920(55)	-2954(40)	45
H(11C)	3502(43)	2432(97)	-3288(17)	45
H(13A)	6696(178)	2870(52)	-2171(99)	92
H(13B)	7224(117)	4000(102)	-1924(72)	92
H(13C)	5809(74)	3641(141)	-2712(38)	92
H(14A)	3861(133)	4370(49)	-821(76)	58
H(14B)	4022(146)	4461(57)	-1940(37)	58
H(14C)	5377(29)	4949(18)	-1161(109)	58
H(15A)	6690(143)	2804(61)	-357(39)	63
H(15B)	5507(36)	3335(111)	163(23)	63
H(15C)	6970(114)	3955(53)	-201(52)	63
H(21A)	3034(92)	-3019(53)	-2133(76)	60
H(21B)	3373(63)	-3607(108)	-3064(22)	60
H(21C)	2424(42)	-4151(57)	-2284(87)	60
H(22A)	-790(178)	-5338(24)	-3059(96)	86
H(22B)	882(45)	-5255(18)	-3392(133)	86
H(22C)	-575(200)	-5392(20)	-4177(44)	86
H(23A)	-3284(81)	-4305(107)	-4095(19)	71
H(23B)	-2382(35)	-4560(80)	-4975(93)	71
H(23C)	-3083(99)	-3574(33)	-4939(94)	71
H(24A)	-1372(112)	-1594(76)	-4864(50)	50
H(24B)	-1506(122)	-1254(46)	-3780(51)	50
H(24C)	-2741(27)	-2096(33)	-4316(95)	50
H(25A)	4754(80)	-1833(55)	-3283(85)	62
H(25B)	4033(25)	-1245(114)	-2495(17)	62
H(25C)	4803(73)	-691(59)	-3340(77)	62
H(26A)	656(52)	-365(15)	-4341(89)	45
H(26B)	2367(99)	97(37)	-4464(79)	45
H(26C)	1806(144)	41(41)	-3419(19)	45
H(28A)	4803(48)	-1273(85)	-5134(70)	66
H(28B)	3553(86)	-636(29)	-5532(109)	66
H(28C)	3974(130)	-1483(68)	-6202(43)	66
H(29A)	434(59)	-2632(74)	-5583(51)	50
H(29B)	1385(37)	-2402(97)	-6475(33)	50
H(29C)	764(85)	-1550(25)	-5921(78)	50
H(30A)	3465(176)	-3222(61)	-5679(25)	68
H(30B)	2479(75)	-3438(39)	-4800(108)	68
H(30C)	4181(100)	-2872(27)	-4610(90)	68

[Hg{C5Me4SiMe2tBu}2]

Identification code	APR1497
Empirical formula	C30 H54 Hg Si2
Formula weight	671.5
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P $\bar{1}$ (No.2)
Unit cell dimensions	a = 8.744(4) Å alpha = 80.72(4) deg. b = 8.769(6) Å beta = 76.59(3) deg. c = 11.136(4) Å gamma = 76.23(5) deg.
Volume	801.6(7) $Å^3$
Z	1
Density (calculated)	1.39 Mg/m^3
Absorption coefficient	4.89 mm^{-1}
F(000)	342
Crystal size	0.30 x 0.20 x 0.08 mm
Theta range for data collection	2 to 25 deg.
Index ranges	0<=h<=10, -9<=k<=10, -12<=l<=13
Reflections collected	2827
Independent reflections	2827 [R(int) = 0.0000]
Reflections with I>2sigma(I)	2827
Structure solution	Direct methods
Refinement method	Full-matrix least-squares on all F^2
Data / restraints / parameters	2827 / 0 / 160
Goodness-of-fit on F^2	1.018
Final R indices [I>2sigma(I)]	R1 = 0.0218, wR2 = 0.0554
R indices (all data)	R1 = 0.0218, wR2 = 0.0554
Largest diff. peak and hole	0.85 and -1.30 $e.Å^{-3}$ (near Hg)
Abs.correction from psi scans	Tmax=1.00 ,Tmin=0.41
Maximum shift/e.s.d.	0.001

The molecule lies on a crystallographic inversion centre.

All non-H atoms were anisotropic. H's were included in riding

the torsion angle defining the H atom positions refined and Uiso(H) equal to 1.5Ueq(C).

Programs used were :

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

References :

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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)
Hg	0	0	0	24(1)
Si	2910(1)	-2445(1)	-1449(1)	24(1)
C(1)	1240(4)	-722(4)	-1775(3)	23(1)
C(2)	1590(4)	803(4)	-2467(3)	27(1)
C(3)	536(4)	1392(4)	-3226(3)	30(1)
C(4)	-544(4)	329(4)	-3093(3)	30(1)
C(5)	-147(4)	-934(4)	-2257(3)	27(1)
C(6)	2892(5)	1563(4)	-2304(4)	39(1)
C(7)	419(6)	2921(5)	-4078(4)	49(1)
C(8)	-1908(5)	649(5)	-3775(4)	47(1)
C(9)	-992(4)	-2298(5)	-1853(4)	38(1)
C(10)	4277(5)	-1836(5)	-623(4)	41(1)
C(11)	2082(5)	-4051(5)	-359(4)	44(1)
C(12)	4114(4)	-3280(4)	-2936(3)	32(1)
C(13)	3004(5)	-3880(5)	-3557(4)	43(1)
C(14)	4825(5)	-2014(6)	-3856(4)	48(1)
C(15)	5475(6)	-4667(6)	-2640(5)	57(1)

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

Hg-C(1)	2.136(3)	Si-C(11)	1.873(4)
Si-C(10)	1.879(4)	Si-C(1)	1.889(4)
Si-C(12)	1.899(4)	C(1)-C(5)	1.495(4)
C(1)-C(2)	1.493(5)	C(2)-C(3)	1.351(5)
C(2)-C(6)	1.506(5)	C(3)-C(4)	1.446(5)
C(3)-C(7)	1.509(5)	C(4)-C(5)	1.360(5)
C(4)-C(8)	1.506(5)	C(5)-C(9)	1.507(5)
C(12)-C(14)	1.528(6)	C(12)-C(13)	1.539(5)
C(12)-C(15)	1.539(5)		
C(1)-Hg-C(1)'	180.0	C(11)-Si-C(10)	105.1(2)
C(11)-Si-C(1)	110.8(2)	C(10)-Si-C(1)	110.6(2)
C(11)-Si-C(12)	109.0(2)	C(10)-Si-C(12)	109.9(2)
C(1)-Si-C(12)	111.2(2)	C(5)-C(1)-C(2)	103.5(3)
C(5)-C(1)-Si	121.5(2)	C(2)-C(1)-Si	121.3(2)
C(5)-C(1)-Hg	99.6(2)	C(2)-C(1)-Hg	101.4(2)
Si-C(1)-Hg	105.5(2)	C(3)-C(2)-C(1)	109.2(3)
C(3)-C(2)-C(6)	126.2(3)	C(1)-C(2)-C(6)	124.6(3)
C(2)-C(3)-C(4)	109.3(3)	C(2)-C(3)-C(7)	127.6(3)
C(4)-C(3)-C(7)	123.1(3)	C(5)-C(4)-C(3)	109.5(3)
C(5)-C(4)-C(8)	127.1(3)	C(3)-C(4)-C(8)	123.4(3)
C(4)-C(5)-C(1)	108.5(3)	C(4)-C(5)-C(9)	125.8(3)
C(1)-C(5)-C(9)	125.6(3)	C(14)-C(12)-C(13)	107.8(3)
C(14)-C(12)-C(15)	109.6(4)	C(13)-C(12)-C(15)	109.0(3)
C(14)-C(12)-Si	111.1(3)	C(13)-C(12)-Si	109.5(3)

Symmetry transformations used to generate equivalent atoms:
' -x,-y,-z

Table 4. Anisotropic displacement parameters ($Å^2 \times 10^3$) 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
Hg	22(1)	27(1)	20(1)	-2(1)	-1(1)	-1(1)
Si	24(1)	24(1)	22(1)	-1(1)	-4(1)	-2(1)
C(1)	24(2)	25(2)	19(2)	0(1)	-4(1)	-6(1)
C(2)	28(2)	23(2)	28(2)	-3(1)	-1(1)	-4(1)
C(3)	33(2)	26(2)	28(2)	4(1)	-4(1)	-4(1)
C(4)	25(2)	34(2)	27(2)	-3(1)	-6(1)	-2(1)
C(5)	20(2)	29(2)	30(2)	-3(1)	-1(1)	-5(1)
C(6)	44(2)	31(2)	47(2)	0(2)	-13(2)	-17(2)
C(7)	54(3)	38(2)	50(3)	14(2)	-17(2)	-8(2)
C(8)	41(2)	53(2)	49(3)	3(2)	-22(2)	-7(2)
C(9)	31(2)	43(2)	43(2)	0(2)	-7(2)	-17(2)
C(10)	35(2)	48(2)	42(2)	-10(2)	-17(2)	0(2)
C(11)	47(2)	36(2)	39(2)	13(2)	-6(2)	-4(2)
C(12)	31(2)	33(2)	30(2)	-7(2)	-4(2)	1(1)
C(13)	54(2)	40(2)	39(2)	-15(2)	-12(2)	-5(2)
C(14)	43(2)	63(3)	34(2)	-11(2)	9(2)	-16(2)
C(15)	50(3)	58(3)	51(3)	-22(2)	-15(2)	24(2)

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

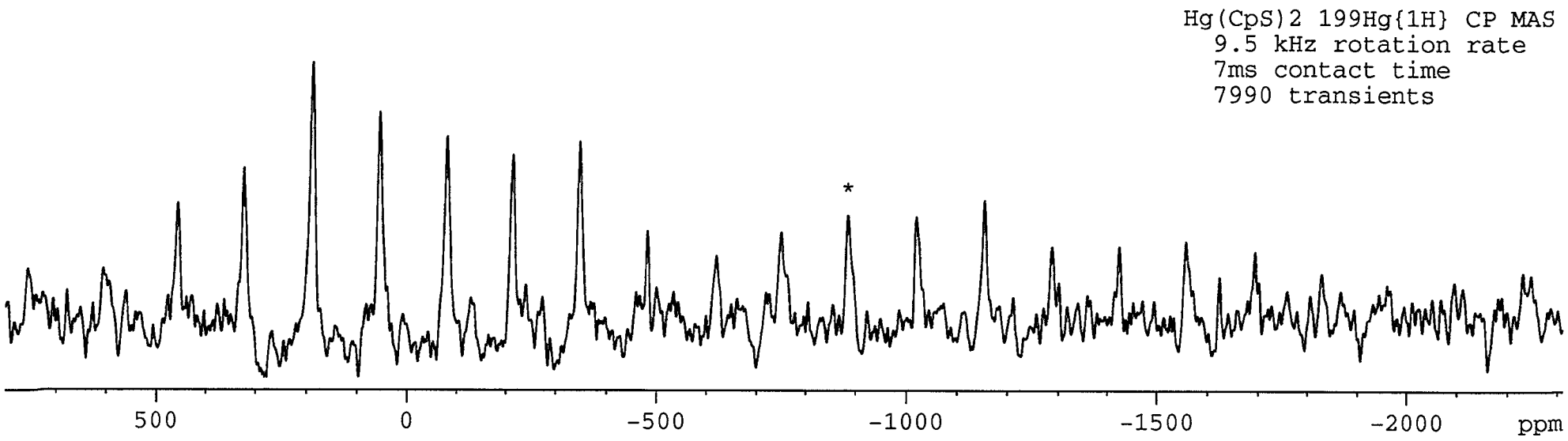
	x	y	z	U(eq)
H(6A)	3942(6)	983(23)	-2703(25)	58
H(6B)	2862(24)	1539(33)	-1416(4)	58
H(6C)	2719(22)	2661(12)	-2687(26)	58
H(7A)	-612(19)	3630(16)	-3801(19)	73
H(7B)	494(42)	2703(7)	-4928(7)	73
H(7C)	1300(25)	3423(21)	-4058(25)	73
H(8A)	-1478(6)	718(41)	-4672(4)	70
H(8B)	-2638(23)	1650(21)	-3567(25)	70
H(8C)	-2496(26)	-211(21)	-3528(25)	70
H(9A)	-1131(33)	-2557(24)	-951(5)	57
H(9B)	-347(18)	-3219(12)	-2263(22)	57
H(9C)	-2048(16)	-2004(14)	-2085(26)	57
H(10A)	4858(30)	-1085(30)	-1184(11)	62
H(10B)	5049(26)	-2770(7)	-365(27)	62
H(10C)	3637(6)	-1334(35)	110(17)	62
H(11A)	2966(6)	-4839(21)	-78(24)	66
H(11B)	1510(34)	-4557(26)	-788(10)	66
H(11C)	1337(31)	-3598(8)	360(15)	66
H(13A)	2567(33)	-4727(28)	-2999(14)	65
H(13B)	3619(11)	-4286(37)	-4336(16)	65
H(13C)	2120(23)	-3008(11)	-3732(29)	65
H(14A)	5576(31)	-1645(29)	-3496(14)	72
H(14B)	3959(7)	-1124(18)	-4032(25)	72
H(14C)	5398(35)	-2462(13)	-4628(12)	72
H(15A)	6193(28)	-4293(11)	-2250(34)	85
H(15B)	6085(31)	-5100(31)	-3410(6)	85
H(15C)	5014(6)	-5492(21)	-2070(30)	85

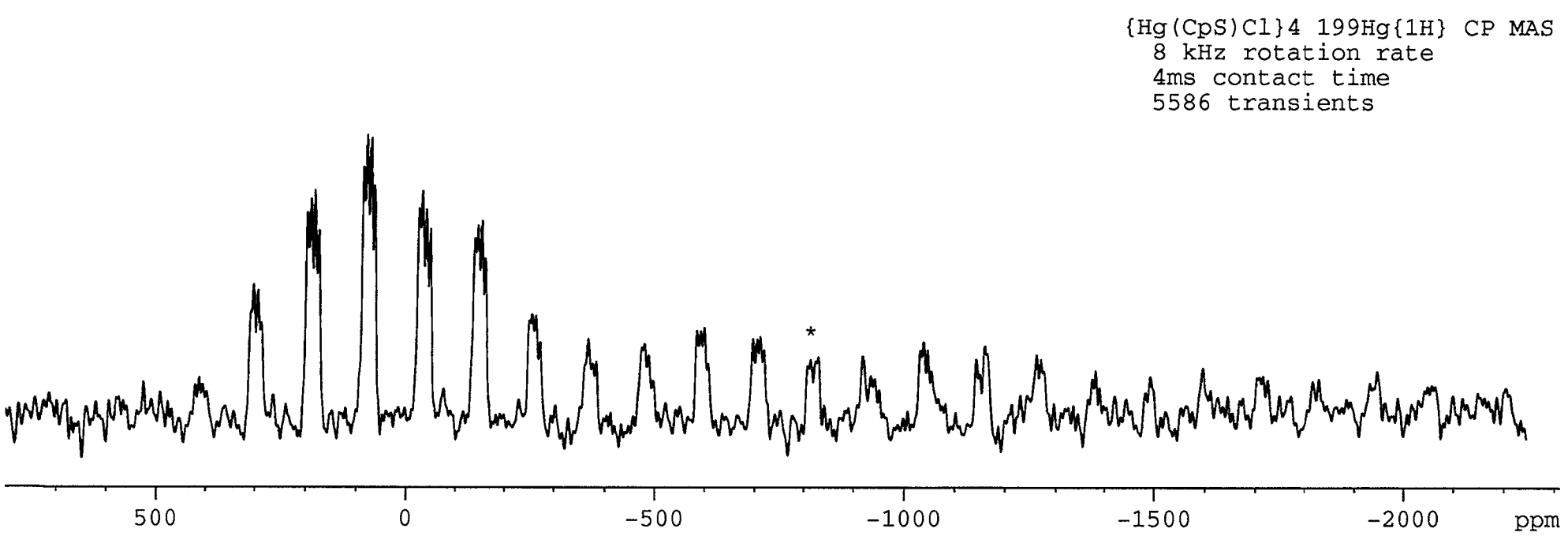
Least-squares planes (x,y,z in crystal coordinates) and deviations from them
(* indicates atom used to define plane)

3.195 (0.015) x + 4.143 (0.014) y + 7.628 (0.016) z = 2.054 (0.004)

*	-0.006 (0.002)	C1
*	0.003 (0.002)	C2
*	0.001 (0.002)	C3
*	-0.005 (0.002)	C4
*	0.007 (0.002)	C5
	0.993 (0.005)	Si
	-2.054 (0.004)	Hg

Rms deviation of fitted atoms = 0.005


Hg(CpS)2 199Hg{1H} CP MAS
9.5 kHz rotation rate
7ms contact time
7990 transients
*
500
0
-500
-1000
-1500
-2000
ppm


{Hg(CpS)Cl}4 199Hg{1H} CP MAS
8 kHz rotation rate
4ms contact time
5586 transients
*
500
0
-500
-1000
-1500
-2000
ppm