Table 3. *Planes, distances* (Å) *of* Sn *therefrom and dihedral angles* (°)

Planes are defined in terms of Cartesian coordinates by $Ax + By + Cz = D$; x is parallel to a, y is in the plane ab, and z is parallel to c^*; A, B, and C are the direction cosines of the normal to the plane and D is the distance of the plane from the origin. The values for A, B, and C are multiplied by 10^4.

Plane		A	B	C	D (Å ×10²)	Distance of Sn from plane (Å ×10²)
(I)	C(1) to H(6)	−974	−9872	−1259	−78·5	0·8 (1)
(II)	C(7) to H(12)	9449	−3147	−901	−44·3	−2·7 (1)
(III)	C(13) to H(18)	2121	3372	−9172	−251·1	−13·2 (1)
(IV)	C(19) to H(24)	3193	−4387	−8400	−54·2	−9·4 (1)
(V)	C(25) to H(30)	−445	9861	−1602	−82·3	1·4 (1)
(VI)	C(31) to H(36)	9305	3649	−317	−946·0	−1·9 (1)
(VII)	Sn(1), Br(1), C(1)	1317	−5958	−7923	−277·9	0·0
(VIII)	Sn(1), Br(1), C(7)	8155	−5773	−412	−46·3	0·0
(IX)	Sn(1), Br(1), C(13)	−6209	−794	−7799	−243·9	0·0
(X)	Sn(2), Br(2), C(19)	−5944	321	−8036	−836·7	0·0
(XI)	Sn(2), Br(2), C(25)	2412	5619	−7913	−62·3	0·0
(XII)	Sn(2), Br(2), C(31)	8389	5441	−114	−896·7	0·0

The sequence of atoms in planes I to VI is according to Table 1.

Dihedral angles

∠(I)/(VII)	47·5	∠(II)/(VIII)	17·1
∠(III)/(IX)	56·2	∠(V)/(XI)	47·9
∠(VI)/(XII)	11·6	∠(IV)/(X)	61·9

1977). Details of the least-squares planes in Ph_3SnBr are given in Table 3.

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Dibenzylmercury

BY PETER B. HITCHCOCK

School of Molecular Sciences, University of Sussex, Brighton BN1 9QJ, England

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Abstract. $C_{14}H_{14}Hg$, $M_r = 382·9$, tetragonal, $P4_2/n$, $a = 12·881$ (5), $c = 7·076$ (3) Å, $U = 1174·1$ Å^3, $Z = 4$, $D_c = 2·17$ Mg m^{-3}, $F(000) = 712$. Mo $K\alpha$ radiation, $\mu = 12·59$ mm^{-1}. $R_F = 0·044$ for 586 counter reflections. The molecule lies on a crystallographic twofold axis and has linear coordination at Hg, with Hg–C 2·07 (2) Å, and no abnormal intramolecular contacts.

Introduction. Studies of the thermal decomposition of dibenzylmercury (Jackson & O'Neill, 1978) raise the possibility that there may be some interaction of the Hg atom with the phenyl ring as in Zr and Hf benzyls (Davies, Jarvis & Kilbourn, 1971). The structure of benzyl(triphenylmethylthio)mercury (Bach, Weibel, Schmonsees & Glick, 1974) shows no such interaction

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but this could be due to steric effects. The structure of the title compound, for which only a preliminary investigation has been reported (Bain, Calvert & Killean, 1965), was determined as a check.

A crystal 0·4 × 0·15 × 0·15 mm was used for data collection on a Hilger & Watts Y290 four-circle diffractometer at room temperature. Cell dimensions were calculated from the setting angles for 12 reflections. Intensities for the 2384 reflections in the quadrant $h, \pm k, l$ with $2<\theta<25°$ were collected by an $\omega/2\theta$ step scan with Mo $K\alpha$ radiation and a graphite-crystal monochromator, over a period of 20 h. Three standard reflections remeasured after 100 reflections showed no significant variation. The data were corrected for Lorentz, polarization and absorption effects and, after averaging equivalent reflections, 586 reflections with $I > 3\sigma(I)$ were used in the analysis.

The Hg and C atoms were located by heavy-atom methods. H atoms were placed at idealized positions (C—H 1·08 Å) with U_{iso} values equal to those of the C atoms to which they were attached, and constrained to ride on these atoms. Full-matrix least-squares refinement with Hg and C anisotropic converged at $R_F = 0·044$, $R_{wF} = 0·067$ with a maximum shift to error of 0·003. The weights were $w = 1/[\sigma^2(F) + 0·004F^2]$. A final difference map had peaks of 1·5 e Å^{-3} near Hg but was elsewhere <0·7 e Å^{-3}. Scattering factors for neutral atoms were taken from Cromer & Mann (1968) for Hg and C, and Stewart, Davidson & Simpson (1965) for H, with dispersion corrections from Cromer & Liberman (1970). The structure refinement was performed with the *SHELX* program system of G. M. Sheldrick. Final atom positions are listed in Table 1.*

Discussion. The crystal structure contains discrete molecules whose conformation is shown in Fig. 1, with relevant parameters listed in Table 2. The coordination at Hg is linear and the Hg—C(1)—C(2) angle of 117 (1)° and Hg—C(1) length of 2·065 (17) Å are close to those (112° and 2·10 Å) in benzyl(triphenylmethylthio)mercury (Bach *et al.*, 1974) and show no indication of interaction of the Hg atom with either the π orbitals or the H atoms of the phenyl rings. The dihedral angle of 98° for Hg—C(1)—C(2)—C(3) is in agreement with that found in benzyl(triphenylmethylthio)mercury (87°) and is likewise close to the 90° predicted theoretically for benzylmercury bromide (Bach *et al.*, 1974).

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* Lists of structure factors, anisotropic thermal parameters and hydrogen atom parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34137 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Atomic fractional coordinates* (×10⁴) *with e.s.d.'s in parentheses*

	x	*y*	*z*
Hg	7500	2500	6046 (1)
C(1)	6002 (13)	1931 (13)	5988 (19)
C(2)	5377 (12)	2020 (13)	7761 (25)
C(3)	4672 (12)	2867 (11)	7943 (28)
C(4)	4190 (14)	3010 (13)	9533 (28)
C(5)	4294 (14)	2369 (14)	11114 (25)
C(6)	4883 (14)	1524 (12)	10928 (30)
C(7)	5502 (15)	1383 (12)	9292 (25)

Table 2. *Interatomic distances* (Å), *angles* (°) *and selected torsion angles* (°) *with e.s.d.'s in parentheses*

Hg—C(1)	2·065 (17)	C(4)—C(5)	1·40 (2)
C(1)—C(2)	1·50 (2)	C(5)—C(6)	1·33 (2)
C(2)—C(3)	1·43 (2)	C(6)—C(7)	1·42 (3)
C(3)—C(4)	1·30 (2)	C(2)—C(7)	1·37 (2)
Hg···C(2)	3·06 (2)		

C(1)—Hg—C(1)′	177·7 (16)	C(4)—C(5)—C(6)	117·3 (19)
Hg—C(1)—C(2)	117·3 (11)	C(5)—C(6)—C(7)	120·3 (19)
C(1)—C(2)—C(3)	118·6 (17)	C(6)—C(7)—C(2)	120·3 (17)
C(2)—C(3)—C(4)	119·5 (19)	C(7)—C(2)—C(3)	117·5 (18)
C(3)—C(4)—C(5)	124·3 (17)	C(7)—C(2)—C(1)	123·7 (16)

C(2)—C(1)—Hg—C(1)′	−163 (2)
C(2)—C(1)—C(1)′—C(2)′	35 (2)
Hg—C(1)—C(2)—C(3)	98 (2)

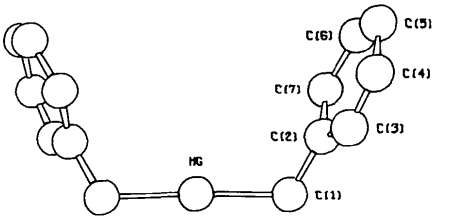

Fig. 1. The conformation and atom numbering for dibenzylmercury.

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