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Di(2-furyl)mercury

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Abstract. $C_8H_6HgO_2$, $[Hg(C_4H_3O)_2]$, monoclinic, $P2_1/n$, $a = 5{\cdot}444\,(2)$, $b = 7{\cdot}556\,(3)$, $c = 9{\cdot}515\,(5)$ Å, $\beta = 91{\cdot}90\,(2)^\circ$, $V = 391{\cdot}18$ Å^3, $Z = 2$, $D_m = 2{\cdot}85$, $D_x = 2{\cdot}85$ Mg m^{-3}, $\mu(\text{Mo } K\alpha) = 20{\cdot}03$ mm^{-1}. The structure was refined to $R = 0{\cdot}026$ for 1013 independent reflexions measured with an automatic single-crystal diffractometer. The molecule of di(2-furyl)mercury is centrosymmetric with an Hg—C bond length of 2·059 (5) Å.

Introduction. Prismatic needle-shaped crystals of di-(2-furyl)mercury (Gilman & Wright, 1933) were obtained from an acetone–water solution by slow evaporation at room temperature. The dimensions of the crystal used were 0·150 × 0·165 × 0·555 mm. The unit-cell dimensions were determined by least-squares refinement of the angular settings of 20 reflexions at room temperature with graphite-monochromatized Mo $K\alpha$ radiation ($\lambda = 0{\cdot}7107$ Å) by means of a Philips PW 1100 four-circle automatic diffractometer. The systematic absences were $h0l$, $h + l = 2n$ and $0k0$, $k = 2n$, indicating space group $P2_1/n$ (No. 14). The intensities and ω angles of three reference reflexions ($20\bar{6}$, $\bar{2}20$, $0\bar{4}2$), measured periodically every two hours, showed no appreciable variation during the course of data collection. The intensities of 1013 independent reflexions with $I > 3\sigma(I)$, collected within the range $2 < 2\theta < 68^\circ$, corrected for absorption (Harkema, 1979), polarization and Lorentz effects, were used for the structure determination by the heavy-atom method. Weights of $1/\sigma F_o$ were allotted to all reflexions. The structure was refined by the full-matrix least-squares method with anisotropic thermal parameters for all non-hydrogen atoms to $R = 0{\cdot}026$. The XRAY 72 computing program was used (Stewart, Kruger, Ammon, Dickinson & Hall, 1972). Neutral-atom scattering factors for Hg, C, O were taken from Cromer & Mann (1968) and the anomalous-dispersion correction from Cromer & Liberman (1970). All calculations were performed on the Univac 1110 computer of Zagreb University Computing Centre (SRCE). The final atomic coordinates with their standard deviations are given in Table 1.* Interatomic distances and bond angles are listed in Table 2.

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2 × 10^3) *with e.s.d.'s in parentheses*

$$U_{eq} = \tfrac{1}{3}(U_{11} + U_{22} + U_{33} + 2U_{13}\cos\beta).$$

	x	y	z	U_{eq}
Hg	0	0	0	37·4 (3)
C(1)	0·713 (1)	0·119 (1)	0·099 (1)	36 (4)
C(2)	0·588 (1)	0·084 (1)	0·215 (1)	44 (5)
C(3)	0·395 (1)	0·207 (1)	0·225 (1)	41 (5)
C(4)	0·411 (1)	0·316 (1)	0·114 (1)	44 (5)
O	0·607 (1)	0·266 (1)	0·035 (1)	44 (4)

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

Hg^{i}–C(1)	2·059 (5)	$Hg^{i}\cdots$O	2·961 (5)
C(1)–C(2)	1·336 (8)	O$\cdots$Hg	3·868 (5)
C(2)–C(3)	1·409 (9)	C(4)$\cdots$Hg	3·423 (6)
C(3)–C(4)	1·347 (8)	C(3)$\cdots$Hg	3·371 (6)
O–C(1)	1·388 (7)	C(3)$\cdots Hg^{iii}$	3·459 (6)
O–C(4)	1·377 (8)	C(4)$\cdots Hg^{iii}$	3·944 (6)
C(1)–Hg^{i}–C(1^{ii})	180	C(1)–O–C(4)	107·1 (4)
Hg^{i}–C(1)–O	117·1 (4)	O–C(4)–C(3)	109·5 (5)
Hg^{i}–C(1)–C(2)	134·9 (5)	C(4)–C(3)–C(2)	106·3 (5)
C(2)–C(1)–O	108·0 (5)	C(3)–C(2)–C(1)	109·1 (5)

Symmetry code: (i) $1 + x, y, z$; (ii) $2 - x, -y, -z$; (iii) $\tfrac{1}{2} + x, \tfrac{1}{2} - y, \tfrac{1}{2} + z$.

Discussion. The molecule of di(2-furyl)mercury is exactly centrosymmetric as required by the $P2_1/n$ space-group symmetry for the special positions $2(a)$. Consequently, the Hg—C bonds are equal and strictly collinear and the O atoms necessarily in the *anti* conformation (Fig. 1). This is completely analogous to

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36387 (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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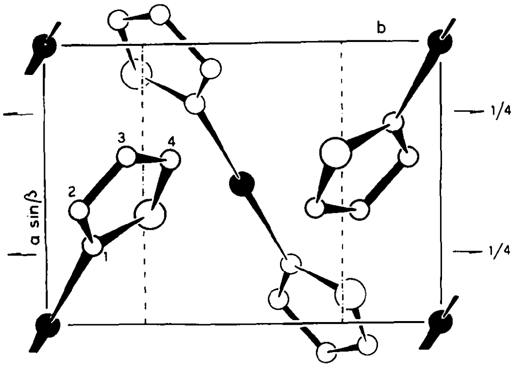

Fig. 1. Molecules of di(2-furyl)mercury in the crystal structure viewed along the *c*-axis direction.

the molecular structure of di(2-thienyl)mercury (Grdenić, Kamenar & Žeželj, 1979) but not to the crystal structure, which is rather similar to that of diphenylmercury (Grdenić, Kamenar & Nagl, 1977), as far as the space group and the molecular packing are concerned. As in diphenylmercury and di(2-thienyl)mercury, in di(2-furyl)mercury also the molecule as a whole is not strictly planar. The Hg atom is out of the furyl-ring plane by 0·11 Å, so that the angle between the Hg—C(1) bond and the normal to the furyl-ring plane is 87·0°. The Hg—C bond length of 2·059 (5) Å is almost equal to the 2·06 (2) Å in di(2-thienyl)mercury (Grdenić, Kamenar & Žeželj, 1979) and slightly shorter than the 2·085 (7) Å found in diphenylmercury (Grdenić, Kamenar & Nagl, 1977). It belongs to the group of shorter Hg—C bond lengths, *i.e.* of about 2·05 Å as compared with the larger values of about 2·10 Å (Grdenić, 1977). It supports the charge-transfer interaction between the 2-furyl (and 2-thienyl) ring and the Hg atom, revealed recently from the analysis of the ultraviolet photoelectron spectra (Colonna, Distefano, Guerra, Jones & Modelli, 1979).

The furyl ring is planar, the deviations of the atom positions from the least-squares plane being less than the e.s.d.'s of the O and C atom coordinates. The geometry of the furyl ring, as follows from the bond-length and bond-angle data in Table 2, is in good agreement with that formerly observed in other 2-substituted furan derivatives, *e.g.* in 6-furfurylaminopurine (Soriano-Garcia & Parthasarathy, 1977), where the 'single' C—C bond of 1·407 Å differs from the 'double'-bond values of 1·334 and 1·328 Å, as compared with the present values of 1·409 (9), 1·347 (8) and 1·336 (8) Å, respectively. The same is true for the C—O—C bond angle of 106·2° compared with the present value of 107·1 (4)°. The 2-furyl bond, *i.e.* the C(1)—Hg bond in the present case, is again significantly inclined towards the C—O bond, being 117·1 (4)° as in other α-substituted furans, *e.g.* 120° in 2-furoic acid (Hudson, 1962), 111·2 (7)° in *anti*-furfuraldoxime (Jensen & Jerslev, 1967), 117·6 (3)° in *trans*-*β*-2-furfurylacrylamide (Leiserowitz & Rabinovich, 1969) and 117·2° in 6-furfurylaminopurine (Soriano-Garcia & Parthasarathy, 1977). Consequently, the deviation of the C(1)—Hg bond from the O—C(1)—C(2) bissectrix direction is not due to an Hg···O attraction but is appropriate to the 2-furyl bond. The Hg···O contact of 2·961 (5) Å, longer than the sum of the van der Waals radii (Grdenić, 1965), and its direction do not indicate any significant mercury-to-oxygen interaction. The intermolecular contacts (Table 2) are as expected, taking into account the H atoms.

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