

(different CH<sub>2</sub>-N-CH<sub>2</sub>-CH<sub>3</sub> torsion angles). The N(1) cation (Fig. 2) has approximate  $D_{2d}$  ( $42m$ ) symmetry, making all methyl C atoms approximately coplanar with N(1). The N(2) cation (Fig. 3) has approximate  $S_4$  ( $4$ ) symmetry, with the methyl groups widely separated.

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## The Structure of Benzamido(phenyl)mercury(II)

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**Abstract.** [Hg(C<sub>6</sub>H<sub>5</sub>)(C<sub>7</sub>H<sub>6</sub>NO)], C<sub>13</sub>H<sub>11</sub>HgNO, monoclinic,  $P2_1/c$ ,  $a = 14.44$  (1),  $b = 9.69$  (1),  $c = 8.60$  (1) Å,  $\beta = 105.9$  (1)°,  $D_m = 2.22$ ,  $D_x = 2.28$  Mg m<sup>-3</sup> with  $Z = 4$ . The structure was determined from 1112 diffractometer-measured intensities and refined by least squares to  $R = 0.076$ . Hg is two-coordinated, Hg-C = 2.02 (2), Hg-N = 2.04 (2) Å,  $\angle C-Hg-N = 179$  (1)°. There are no other contacts to Hg; a weak hydrogen bond N...O = 3.15 (3) Å between screw-axis-related molecules is suggested.

**Introduction.** Crystals of the title compound, kindly supplied by Dr F. G. Thorpe, were thin plates somewhat elongated parallel to **b** with {100} as the principal form. The space group and cell dimensions were obtained from Weissenberg photographs taken with Cu  $K\alpha$  radiation ( $\lambda = 1.542$  Å). From one crystal of dimensions 0.012 × 0.50 × 0.32 mm, mounted with **b** aligned on the  $\omega$  axis of the Stoe STADI-2 automatic two-circle diffractometer, 1380 unique intensities were measured using graphite-monochromatized Mo  $K\alpha$  radiation ( $\lambda = 0.7107$  Å). Absorption corrections ( $\mu = 14.36$  mm<sup>-1</sup>) were made with the *SHELX* program (Sheldrick, 1976). The structure determination and refinement were performed using XRAY 72 (Stewart, Kruger, Ammon, Dickinson & Hall, 1972), only 1112 reflexions for which  $I \geq 3\sigma(I)$  being included.

Coordinates of Hg, obtained from a Patterson map, were refined together with  $U_{ij}$  values and used to phase

an ( $F_o - F_c$ ) map which gave the positions of all the remaining non-H atoms. Refinement of atomic parameters proceeded using anisotropic  $U_{ij}$  for Hg and isotropic  $U$  for C, N and O. At an intermediate stage of refinement individual scale factors for the intensity layers  $k = 0$  to 8 were refined with  $U_{22}$  restrained at a constant value to avoid excessive correlation. When the shifts on all parameters were less than 0.05 of the e.s.d. and there were no significant features on the ( $F_o - F_c$ )

Table 1. Fractional atomic parameters ( $\times 10^3$ , for Hg  $\times 10^4$ ) and thermal parameters ( $\times 10^3$ )

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> (Å <sup>2</sup> )
N	33 (1)	537 (3)	290 (2)	34 (6)
O	53 (1)	742 (2)	184 (2)	53 (6)
C(1)	4 (2)	630 (4)	182 (4)	40 (8)
C(2)	-91 (2)	619 (3)	56 (3)	26 (6)
C(3)	-113 (2)	723 (4)	-64 (3)	45 (8)
C(4)	-205 (2)	718 (4)	-181 (3)	45 (8)
C(5)	-269 (2)	607 (4)	-175 (3)	48 (8)
C(6)	-245 (2)	516 (4)	-55 (4)	56 (9)
C(7)	-158 (1)	507 (3)	62 (2)	17 (6)
C(8)	288 (2)	581 (3)	632 (3)	37 (7)
C(9)	303 (2)	694 (3)	737 (3)	38 (7)
C(10)	397 (2)	713 (4)	852 (3)	50 (8)
C(11)	473 (2)	624 (4)	852 (3)	45 (8)
C(12)	459 (2)	515 (4)	742 (4)	57 (9)
C(13)	363 (2)	496 (4)	635 (4)	62 (10)
Hg	1617 (1)	5572 (1)	4615 (1)	*

\* Anisotropic thermal parameters for Hg ( $\times 10^4$ )

$U_{11}$	$U_{22}$	$U_{33}$	$U_{12}$	$U_{13}$	$U_{23}$
476 (7)	204 (9)	530 (7)	26 (6)	97 (5)	74 (6)

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map, the refinement was terminated with  $R = 0.076$ . Atomic scattering factors for Hg including anomalous scattering were taken from Cromer & Mann (1968) and Cromer & Liberman (1970); those for all other atoms were from *International Tables for X-ray Crystallography* (1962). Final atomic coordinates and temperature factors are listed in Table 1.\*

**Discussion.** The bonds from Hg to C(8) and N, Fig. 1, are collinear within the limits of error and their lengths indicate typical covalent bonds. The amide group behaves as a unidentate ligand since the angle Hg–N–C(1) is  $121(2)^\circ$  and the distance Hg...O,  $3.05(2) \text{ \AA}$ , is too long to be considered as contributing to the bonding. The distances C(1)–N,  $1.28(4)$ , and C(1)–O,  $1.30(4) \text{ \AA}$ , are both significantly shorter than single bonds, a typical feature of amide groups. Within the limits of error ( $0.02 \text{ \AA}$ ) the atoms C(2), C(1), N, O, Hg are coplanar. The Hg may be described as *cisoid* relative to O in the N-substituted amide group, as is the case in the structure of bis(benzamido)Hg<sup>II</sup> (Halfpenny & Small, 1980). A further common feature of these two structures is the relatively small angle of twist between the amide group and its attached phenyl,  $8(1)^\circ$  in the present structure and  $7^\circ$  in one of the amide groups of bis(benzamido)Hg<sup>II</sup>. These values may be compared with angles in excess of  $22^\circ$  for all other benzamide derivatives, and the suggestion here is that, as in the bis(benzamido)Hg<sup>II</sup> structure, the amide group could be in the enol form.

\* A list of structure factors and a table of bond lengths and angles have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35529 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

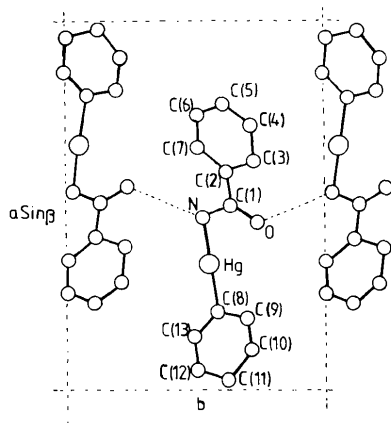


Fig. 1. Projection of part of the unit cell along  $c$ .

Apart from the covalently attached N and C(1) there are no close contacts to Hg; usually in structures of this type, Hg is bound intermolecularly to as many available O as possible. In this structure there is a close intermolecular N...O contact of  $3.15(3) \text{ \AA}$  to a screw-axis-related molecule which is short enough to be a weak hydrogen bond; the expected positions of a H atom attached to either O or N (for the enol and keto forms respectively) would both lie near the N...O vector. This type of bonding is in fact one of those expected in a typical mono-N-substituted amide. In the nomenclature of Leiserowitz & Tuval (1978) it is the twofold-screw-axis motif; a similar arrangement has been found in acetanilide (Brown, 1966). This structure may be compared with the arrangement in bis(benzamido)Hg<sup>II</sup> where both N...O and Hg...O associations are found. In the present structure, intermolecular association by N...O rather than Hg...O suggests that interaction by hydrogen bonds is energetically more favourable than that involving Hg. The difference in the type of association found in these two structures may arise from the additional benzamido group which replaces phenyl in the present compound. The benzamido group, being more electronegative than the phenyl, would enhance the acidity of Hg causing it to be a more effective acceptor of lone-pair electrons from adjacent O atoms.

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