

The Crystal Structures of Disordered Crystals of Adducts of Diphenylmercury with Bidentate Ligands

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The crystal structures of two adducts of diphenylmercury with neutral bidentate nitrogen donor atom ligands have been determined. The crystals are disordered in a manner giving rise to diffuse reflexions for which k is odd. The crystal of diphenylbis-(2,4,7,9-tetramethyl-1,10-phenanthroline)mercury(II) studied has $a = 21.09$, $b = 14.54$, $c = 14.65 \text{ \AA}$, $\beta = 120^\circ 34'$, $Z = 4$, and space group Cm . Crystals of diphenylbis-(2,9-dimethyl-1,10-phenanthroline)mercury(II) have $a = 15.42$, $b = 14.28$, $c = 14.55 \text{ \AA}$, $\alpha \approx \beta \approx \gamma \approx 90^\circ$, $Z = 4$, and space group $P1$ with approximate Pm symmetry. Both adducts have their planar ligands in (040) with the C-Hg-C units of Ph_2Hg moieties aligned in the [010] direction. Each Ph_2Hg moiety has one ligand adjacent to it with Hg-N distances of 2.8–3.0 Å, and one-half of the ligands in the crystals do not have a mercury atom adjacent to their nitrogen atoms. Within the unit cell of each adduct every second (040) plane has 0.5 occupancy for two Ph_2Hg moieties with mercury atoms in those planes, and every other (040) plane has 0.8 and 0.2 occupancy for two Ph_2Hg moieties in those planes, giving one Ph_2Hg for every two ligands.

Introduction

The adducts Ph_2HgL_2 [$L = 1,10\text{-phenanthroline}$, 2,9-dimethyl-1,10-phenanthroline (dmp), and 2,4,7,9-tetramethyl-1,10-phenanthroline (tmp)] have stoichiometry suggesting six-coordination for mercury (Deacon & Canty, 1969), whereas coordination numbers lower than six are found for isolable complexes of diarylmercury compounds forming more stable complexes in solution with the same ligands (see e.g. Canty & Deacon, 1971). Deacon & Canty (1969) commented that no definite evidence for coordination of ligands could be found and that the adducts may well be 'lattice compounds'. Uncertainty of the nature of the adducts has prompted this study.

Preliminary experimental results

An infrared spectrum and melting point confirmed that crystals of $\text{Ph}_2\text{Hg}(\text{tmp})_2$, $(\text{C}_6\text{H}_5)_2\text{Hg}(\text{C}_{10}\text{H}_{16}\text{N}_2)_2$, grown from benzene/hexane were identical with the pure compound. Crystals of $\text{Ph}_2\text{Hg}(\text{dmp})_2$, $(\text{C}_6\text{H}_5)_2\text{Hg}(\text{C}_{14}\text{H}_{12}\text{N}_2)_2$, were obtained from an analytically pure sample of the adduct dissolved in benzene, and had melting point and powder photographs identical with those of the sample. Crystals of both adducts have similar crystal habit, being colourless and elongated in the [001] direction, and all crystals chosen for X-ray studies extinguished polarized light when viewed normal to the two pairs of crystal faces parallel to the needle axis.

(a) Diphenylbis-(2,9-dimethyl-1,10-phenanthroline)-mercury(II)

Crystals of $\text{Ph}_2\text{Hg}(\text{dmp})_2$ mounted about the needle axis gave oscillation photographs with streaking normal to layer lines but not passing through all reflexions. Equi-inclination Weissenberg photographs for reciprocal lattice levels $hk0-h,k,12$ and $0kl-2kl$ have diffuse lines through reflexions along festoons with odd k and extending in the a^* and c^* directions respectively (Fig. 1). Each reflexion with odd k is present as a maximum in a diffuse line whereas all even k reflexions are sharp and generally of higher intensity.

Weissenberg photographs indicate triclinic symmetry, although cell angles of ca. 90° and similar intensities of reflexions in each octant of reciprocal space suggest that the structure has symmetry close to orthorhombic. The crystals have unit-cell dimensions $a = 15.42$, $b = 14.28$, $c = 14.55$, $\alpha \approx \beta \approx \gamma \approx 90^\circ$, $U = 3203.9 \text{ \AA}^3$, and $D_{\text{meas}} = 1.60 \text{ g.cm}^{-3}$ (by flotation), $D_{\text{calc}} = 1.59 \text{ g.cm}^{-3}$ for $Z = 4$. The cell angles are only $8'$, $8'$, and $5'$ ($\pm 4'$) removed from 90° for α , β , and γ respectively. Since the differences in intensity of equivalent reflexions for monoclinic symmetry are slight, it was not possible to decide whether $90^\circ < \alpha, \beta$, or $\gamma > 90^\circ$ from Weissenberg photographs obtained with the crystal oscillated about different axes. The conditions for reflexions to be observed:

$$hk0: h+k=2n$$

$$0k0: k=4n$$

$$00l: l=2n$$

are not all required together for space groups of orthorhombic or lower symmetry.

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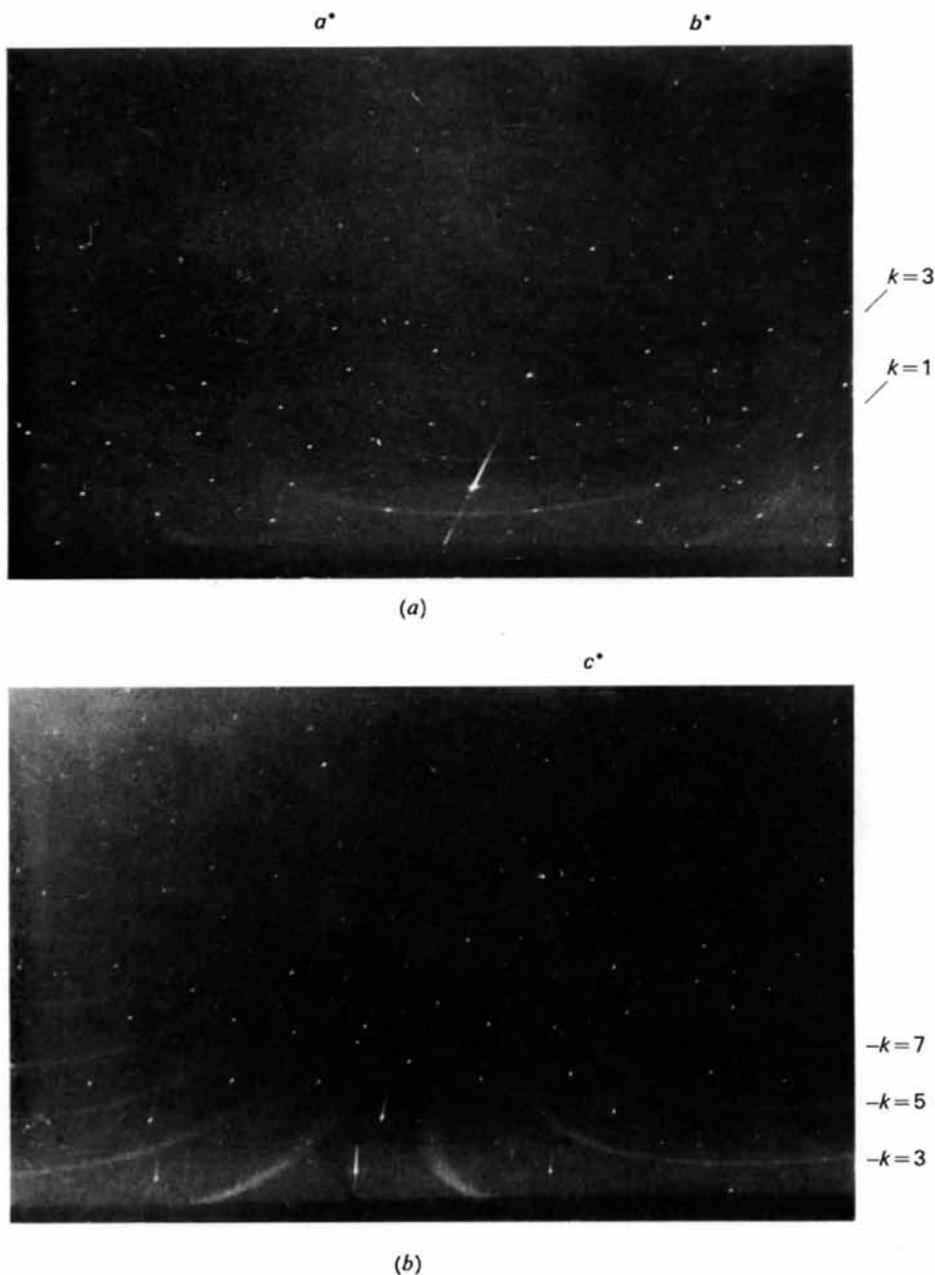


Fig. 1. Weissenberg photographs from a crystal of $\text{Ph}_2\text{Hg}(\text{dmp})_2$. (a) A region of the reciprocal lattice layer $hk0$. (b) A region of the reciprocal lattice layer $2kl$.

Table 1. Comparison of F_o and F_c for $\text{Ph}_2\text{Hg}(\text{tmp})_2$

Sharp reflexions are presented first. Unobserved reflexions are indicated with an asterisk.

H	K	F _O	F _C	H	K	F _O	F _C	H	K	F _O	F _C	H	K	F _O	F _C	H	K	F _O	F _C	H	K	F _O	F _C		
$\leftarrow\leftarrow\leftarrow L = 0 \rightarrow\rightarrow\rightleftharpoons$																									
8	4	79	17*	-6	10	84	161	-2	8	95	131	-8	2	93	97*	-1	5	39	79*	-1	5	62	62*		
10	6	80	133*	8	6	141	195	-6	0	266	237	-4	0	386	371	-10	0	92	71*	-1	9	39	57		
4	2	92	22	10	4	155	149	-8	2	265	224	-4	2	262	219	-12	0	131	114	-3	3	35	90*		
8	0	186	233	12	2	66	34	-6	6	159	176	-4	6	102	110	-12	2	94	31	-3	5	68	82		
10	0	110	99	-2	4	118	138	-10	0	67	30*	-6	0	67	25*	-18	2	240	235	-2	9	39	74		
12	0	80	133*	-2	6	35	56*	-10	2	92	55	-6	2	100	18*	-10	0	22	55	-5	1	112	80		
14	0	159	133*	-2	6	74	49	-10	2	71	51	-6	0	100	68*	-10	0	53	53	-5	3	53	53*		
12	2	217	195	-4	0	111	116	-12	2	202	294	-4	8	507	316	73	170	-4	7	48	63*	-7	7	62	97*
-2	4	92	44	-4	2	204	163	-12	8	179	225	-4	8	222	205	0	0	120	274	-7	1	94	76		
-2	6	33	62*	-4	4	81	93	-14	2	190	109	-8	4	122	124	-4	0	100	66*	-7	1	75	63		
-2	4	34	64*	-4	8	193	232	-14	2	190	109	-8	4	102	107	-4	0	100	66*	-7	1	75	63		
-4	2	10	48	-4	8	44	47*	-8	8	141	175	-4	8	120	102	-14	2	240	235	-2	9	39	74		
-4	2	225	189	-4	10	92	143	-8	8	141	175	-8	8	118	155	-6	0	99	83*	-7	7	59	59*		
-4	4	49	32*	-6	0	267	234	$\leftarrow\leftarrow\leftarrow L = 5 \rightarrow\rightarrow\rightleftharpoons$	-10	0	100	68*	-6	0	100	68*	-10	0	194	195	-7	9	61	92*	
-4	6	141	188	-6	2	247	157	-10	0	100	68*	-10	0	148	136	-12	0	97	107	-9	5	61	56*		
-4	10	73	86	-6	4	159	181	-10	0	100	68*	-10	0	76	110	-14	0	98	39*	-9	0	70	43*		
-6	2	79	29	-6	8	110	154	-4	2	193	253	-12	0	76	35*	-16	0	141	111	-11	5	78	59*		
-6	0	67	79	-6	8	273	291	-8	8	193	253	-12	4	82	34*	-8	0	141	142	-11	0	60	41*		
-6	2	174	241	-8	4	228	201	-8	8	97	144	-12	4	141	165	$\leftarrow\leftarrow\leftarrow L = 13 \rightarrow\rightarrow\rightleftharpoons$	-8	0	88	18*	-1	5	70	86	
-6	4	276	296	-8	6	62	49*	-9	10	70	65*	-14	0	171	129	-10	0	100	68*	-1	7	78	45*		
-6	4	181	154	-8	8	161	232	-10	0	100	68*	-10	0	100	68*	-10	0	100	68*	-1	5	70	86		
-6	6	135	128	-10	2	350	255	-2	4	210	210	-10	4	162	175	-4	0	64	86*	-1	5	70	86		
-10	2	135	104	-10	4	143	80	-7	8	127	179	-10	4	148	136	-4	4	82	34*	-1	5	51	88*		
-10	4	79	79*	-12	0	148	187	-4	0	100	68*	-10	0	100	68*	-10	0	120	74*	1	3	51	88*		
-10	6	91	164*	-12	0	111	102	-4	2	111	81	-12	0	100	68*	-10	0	100	68*	1	3	51	88*		
-12	4	90	88*	-12	0	122	134	-4	2	111	81	-12	0	100	68*	-10	0	100	68*	1	3	51	88*		
-12	6	90	88*	-12	4	82	68*	-4	8	82	67*	-12	4	141	165	$\leftarrow\leftarrow\leftarrow L = 0 \rightarrow\rightarrow\rightleftharpoons$	-8	0	88	18*	-1	5	70	86	
-14	2	169	187	-14	4	130	179	-6	8	102	105	-10	0	100	68*	-10	0	100	68*	-1	5	70	86		
-14	4	101	142	-14	4	130	179	-6	8	102	105	-10	0	100	68*	-10	0	100	68*	-1	5	70	86		
-14	6	134	184	-14	8	208	270	-6	8	86	84*	-12	0	100	68*	$\leftarrow\leftarrow\leftarrow L = 3 \rightarrow\rightarrow\rightleftharpoons$	-8	0	88	18*	-1	5	70	86	
$\leftarrow\leftarrow\leftarrow L = 1 \rightarrow\rightarrow\rightleftharpoons$																									
0	0	51	24	0	4	307	267	-2	10	65	55*	-2	4	141	165	$\leftarrow\leftarrow\leftarrow L = 8 \rightarrow\rightarrow\rightleftharpoons$	-8	0	88	18*	-1	5	70	86	
0	2	403	388	0	8	49	58*	-4	2	181	197	-4	2	195	185	0	0	88	18*	$\leftarrow\leftarrow\leftarrow L = 3 \rightarrow\rightarrow\rightleftharpoons$	1	5	70	86	
0	4	138	184	0	8	147	197	-4	2	181	197	-4	2	195	185	0	0	88	18*	1	5	51	88*		
0	6	457	457	0	10	94	21*	-4	6	216	271	-4	6	178	197	9	9	97	94*	1	3	51	88*		
0	10	114	239	0	2	207	274	-2	4	6	60	-15	0	262	276	0	0	88	18*	1	3	51	88*		
2	0	414	418	2	2	273	281	-10	8	108	176	-2	4	105	157	-7	8	207	227	1	9	22	77*		
2	2	38	34*	2	4	179	149	-6	0	370	314	-2	4	140	165	1	3	51	88*	1	5	70	86		
2	6	220	213	2	4	120	143	-6	0	208	213	-2	4	177	197	1	3	51	88*	1	5	70	86		
2	6	41	20*	2	8	120	143	-4	2	201	174	-6	0	209	216	9	9	97	94*	1	5	51	88*		
2	8	116	172	2	10	108	116	-4	8	143	156	-6	2	140	116	1	3	51	88*	1	5	51	88*		
2	10	45	13*	4	0	167	94	-4	8	67	102	-6	4	152	134	1	3	51	88*	1	5	51	88*		
2	4	109	170	4	2	140	146	-4	8	120	143	-6	2	177	197	1	3	51	88*	1	5	51	88*		
2	4	31	31	4	2	172	172	-4	8	143	156	-6	2	140	116	1	3	51	88*	1	5	51	88*		
2	4	102	92	4	6	114	114	-4	8	64	67*	-10	2	21	225	-1	3	51	88*	1	5	51	88*		
4	6	168	214	4	6	70	13*	-10	2	172	172	-12	0	100	68*	-10	0	100	68*	1	3	51	88*		
4	6	79	80	6	0	363	271	-10	2	172	172	-12	0	100	68*	-10	0	100	68*	1	3	51	88*		
4	10	58	97*	-6	0	134	134	-10	2	172	172	-12	0	100	68*	-10	0	100	68*	1	3	51	88*		
4	6	124	124	-6	0	241	234	-10	2	172	172	-12	0	100	68*	-10	0	100	68*	1	3	51	88*		
6	2	345	388	8	2	149	134	-1	8	153	165	-6	4	124	124	$\leftarrow\leftarrow\leftarrow L = 1 \rightarrow\rightarrow\rightleftharpoons$	-8	0	88	18*	1	3	51	88*	
6	4	88	70	8	2	146	125	-10	2	155	157	-10	2	140	125	1	3	51	88*	1	3	51	88*		
6	6	183	219	10	0	141	141	-10	2	155	157	-10	2	140	125	1	3	51	88*	1	3	51	88*		
6	10	97	107	-10	2	151	151	-10	2	151	151	-10	2	140	125	1	3	51	88*	1	3	51	88*		
8	0	203	198	-12	0	169	178	-4	2	173	126	-6	0	100	68*	-10	0	100	68*	1	3	51	88*		
8	2	86	86	-2	2	241	20*	-10	8	166	166	-12	0	100	68*	-10	0	100	68*	1	3	51	88*		
8	4	185	134	-6	0	175	202	-10	8	166	166	-12	0	100	68*	-10	0	100	68*	1	3	51	88*		
8	6	166	271	-6	0	166	271	-10	8	166	166	-12	0	100	68*	-10	0	100	68*	1	3	51	88*		
10	2	113	199	-6	0	164	177	-7	15	98	104	-6	4	143	113	1	3	51	88*	1	3	51	88*		
10	4	459	399	-6	0	232	226	-10	8	166	166	-12	0	100	68*	-10	0	100	68*	1	3	51	88*		
12	4	200	217	-6	0	165	243	-4	2	211	203	-6	0	100	68*	-10	0	100	68*	1	3	51	88*		
12	6	44	33*	-6	0	165	243	-4	2	211	203	-6	0	100	68*	-10	0	100	68*	1	3	51	88*		
14	0	123	188	-6	0	161	243	-4	8	99	9	-4	2	178	96	-1	3	51	88*	1	3	51			

A powder photograph can be indexed with the above unit-cell dimensions, and upon estimation of intensities of reflexions it was revealed that the most intense reflexions are accounted for by the powder lines.

(b) *Diphenylbis-(2,4,7,9-tetramethyl-1,10-phenanthroline)mercury(II)*

Oscillation photographs obtained from crystals of $\text{Ph}_2\text{Hg}(\text{tmp})_2$ have diffuse lines in the same orientation as in photographs of $\text{Ph}_2\text{Hg}(\text{dmp})_2$. The $hk0$ reciprocal lattice level is similar to that of $\text{Ph}_2\text{Hg}(\text{dmp})_2$, having identical requirements for reflexions to be observed $-hk0:h+k=2n$ and $0k0:k=4n$, but $hk1$ and $h0l$ Weissenberg photographs revealed the crystals to be twinned, with components of monoclinic symmetry having diffuse lines for odd k extending in the a^* and c^* directions of reciprocal space. Four crystals were examined and found to be twinned in this manner.

A very small crystal of habit different from that of the other crystals was found to have cell dimensions and intensities of reflexions similar ($\pm 0.1 \text{ \AA}$, $\pm 20^\circ$) to those of the twin components. The crystal was mounted about the b axis and since it was a very small crystal is proved too difficult to mount about another direct axis, so the b -axis length was determined from an oscillation photograph. The crystal has $a=21.09$, $b=14.54$, $c=14.65 \text{ \AA}$, $\beta=126^\circ 34'$, $U=3607.8 \text{ \AA}^3$, D_{meas} (twinned crystals, by flotation)= 1.52 g.cm^{-3} , $D_{\text{calc}}=1.52 \text{ g.cm}^{-3}$ for $Z=4$, requirements for reflexions to be observed $hk1:h+k=2n$, and gave an oscillation photograph symmetrical about the $h0l$ layer line, indicating one of the C -centred monoclinic space groups $C2$, Cm , or $C2/m$.

All except one line (of medium intensity) of a powder photograph can be indexed with the unit cell of the single crystal. The line not indexed does not result from either free ligand or diphenylmercury.

(c) *The diffuse lines*

The presence of diffuse lines usually indicates micro-synthetic twinning, often resulting from mistakes in crystal growth of layer structures. When twinning in this way leads to ordered regions displaced by $\frac{1}{2}b$ from each other, there is a lowering in intensity of odd k reflexions, and if the regions are small enough, diffuse streaks are observed through odd k reflexions (Dornberger-Schiff & Dunitz, 1965). Diffuse lines may be caused by the mode of disorder found in the urea-hydrocarbon (Smith, 1952) and urea-di-n-alkylmercury inclusion compounds (Bähr & Meier, 1958). In crystals of these compounds, the urea molecules form an ordered structure with channels of appropriate diameter for the inclusion of n-alkanes or di-n-alkylmercurials. One-dimensional disorder giving rise to diffuse lines occurs when the n-alkanes are randomly distributed along the channels. If discrete spots occur in the diffuse lines, then the hydrocarbon chains are partially ordered in their positions in the channels.

Diffuse lines may also arise from thermal diffuse scattering, particularly for structures involving large planar molecules. Thermal diffuse scattering resulting from vibrations of molecules is expected to be temperature dependent (see e.g. Wooster, 1962). With a crystal of $\text{Ph}_2\text{Hg}(\text{dmp})_2$ mounted about the needle axis an oscillation photograph obtained at a temperature below -115°C had diffuse lines of the same intensity relative to sharp reflexions, as diffuse lines in a photograph obtained at ca. 20°C . In addition, the Patterson syntheses for each adduct indicate that the planar aromatic ligands are in ac planes and the diffuse lines are observed to lie parallel to these planes in reciprocal space ($k=1, 3, 5, 7, \dots$) instead of normal to them as expected for thermal diffuse scattering.

Since the low temperature study of $\text{Ph}_2\text{Hg}(\text{dmp})_2$ shows that the diffuse lines probably result from dis-

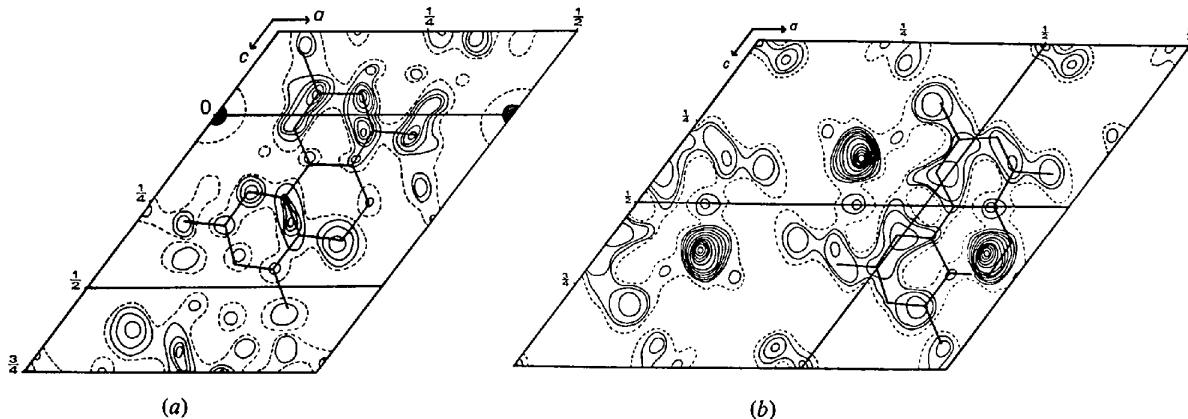


Fig. 2. Patterson syntheses for $\text{Ph}_2\text{Hg}(\text{tmp})_2$. The contours are evenly spaced on an arbitrary scale. Negative regions are bounded by broken lines. (a) The plane $y=0$. A skeleton of the ligand is placed to coincide with vectors near the origin. The asymmetric section is bounded by $x=0 \rightarrow \frac{1}{2}$, $z=0 \rightarrow \frac{1}{2}$. (b) The plane $y=\frac{1}{2}$. Mercury-ligand atom vectors are shown for mercury and ligand atoms separated by x , $\frac{1}{2}$, z , together with the large mercury-mercury vector at $0.33, \frac{1}{2}, 0.36$.

order, structure solution for both adducts was initially sought with all atoms fully occupied until packing requirements indicated the presence of partial occupancy. The observed data represents the sum of diffraction from all ordered regions of the crystal, and the structure solution obtained by this procedure will be referred to as the superposition structure. The possible structures of ordered regions have been estimated from the superposition structure.

Structure solutions

(1) Solution of the superposition structure for $\text{Ph}_2\text{Hg}(\text{tmp})_2$

From the very small monoclinic crystal of dimensions $0.05 \times 0.05 \times 0.025$ mm (absorption coefficient $\mu(\text{Cu } K\alpha) = 8.47 \text{ mm}^{-1}$, $t_{\text{opt}} = 0.236 \text{ mm}$) mentioned earlier, 414 independent non-zero reflexions were recorded photographically for reciprocal lattice levels $h0l-h, 10, l$ with an Enraf-Nonius equi-inclination Weissenberg camera. Reflexions of odd k index are so weak that only 36 reflexions of this type were observed, and no odd k reflexions were observed for $k > 3$. Reflexion intensities were measured visually by comparison with a standard strip of twenty spots.

After Lorentz and polarization corrections had been applied, a Patterson synthesis was calculated. Vector peaks were found to be predominantly in the (040)

planes with very few vectors between these planes. The (010) plane has mercury-ligand vectors grouped near the origin [Fig. 2(a)]. The positions of these vectors reveal that the ligands are oriented with $\text{N}(1)-\text{N}(10)$ parallel to the [001] direction and lie in ac planes (the atom numbering scheme for 2,4,7,9-tetramethyl-1,10-phenanthroline is given in Fig. 3). The only other vector in (010) is a peak at $\frac{1}{2}, 0, 0$ almost as large as the origin, suggesting that it is not only a mercury-mercury vector or vectors, but also a sum of smaller vectors between light atoms separated by $\frac{1}{2}a$. The $y=\frac{1}{4}$ plane has one large peak at $0.33, \frac{1}{4}, 0.36$ [Fig. 2(b)]. Both $C2$ and $C2/m$ space groups require a Harker plane ($2x, 0, 2z$) in the Patterson synthesis. Since the peak $0.33, \frac{1}{4}, 0.36$ is almost certainly a mercury-mercury vector, a large vector in (010) is expected in addition to the peak at $\frac{1}{2}, 0, 0$ for $C2$ or $C2/m$ space groups.

The space group was assumed to be Cm and a mercury atom was placed at $\frac{1}{4}, \frac{1}{4}, 0$ satisfying the Patterson peak at $\frac{1}{2}, 0, 0$ and consistent with space groups Cm , $C2$, and $C2/m$. The residual index $R = \sum |F_o| - |F_c| / \sum |F_o|$ was 0.33 and a difference Fourier synthesis had four large peaks at $0.08, 0, 0.36; \frac{1}{2} + 0.08, 0, 0.36; \frac{1}{2} - 0.08, 0, 1 - 0.36$ and $1 - 0.08, 0, 1 - 0.36$. Vectors from $\frac{1}{4}, \frac{1}{4}, 0$ to each of these positions satisfy the vector at $0.33, \frac{1}{4}, 0.36$ but vectors between all of these positions are not present. The coordinates $0.08, 0, 0.36$ were chosen for a mercury atom position, R was reduced to 0.24, and a subsequent difference Fourier synthesis revealed positions of ligand (Fig. 4) and phenyl group atoms. The phenyl groups lie immediately above and below each mercury atom, and the $\text{C}-\text{Hg}-\text{C}$ skeleton is linear and in the [010] direction.

No improvement in phasing of light atom positions occurred on adding ligand atoms singly to the structure factor calculation. Consequently, coordinates of ligand and phenyl group atoms were chosen to coincide with peaks in difference Fourier syntheses as closely as possible, maintaining $\text{C}-\text{C}$ and $\text{C}-\text{N}$ bond lengths within the range $1.29-1.52 \text{ \AA}$, $\text{Hg}-\text{C}$ bond lengths of $2.0-2.15 \text{ \AA}$, and planar phenyl rings.

The difference syntheses of Fig. 4 indicate eight ligands per unit cell as required from the density of the crystals. Ligands were added singly to the structure factor calculation. When the ligand in (010) with x coordinates $< \frac{1}{2}$ is added peaks corresponding to the ligand with $x > \frac{1}{2}$ disappear from the synthesis as well as those of the ligand added. However, when both of these ligands are added the subsequent difference synthesis is devoid of negative regions, confirming the presence of both ligands.

At this stage six mercury atoms had been placed in the unit cell (fourfold position $\frac{1}{4}, \frac{1}{4}, 0$; twofold $0.08, 0, 0.36$) whereas the measured density of the crystals suggests four. Phenyl group positions indicated in difference Fourier syntheses were confirmed by the Patterson synthesis. Mercury-phenyl-group atom vectors are present immediately below the origin of the synthesis. Vectors between mercury atoms and phenyl

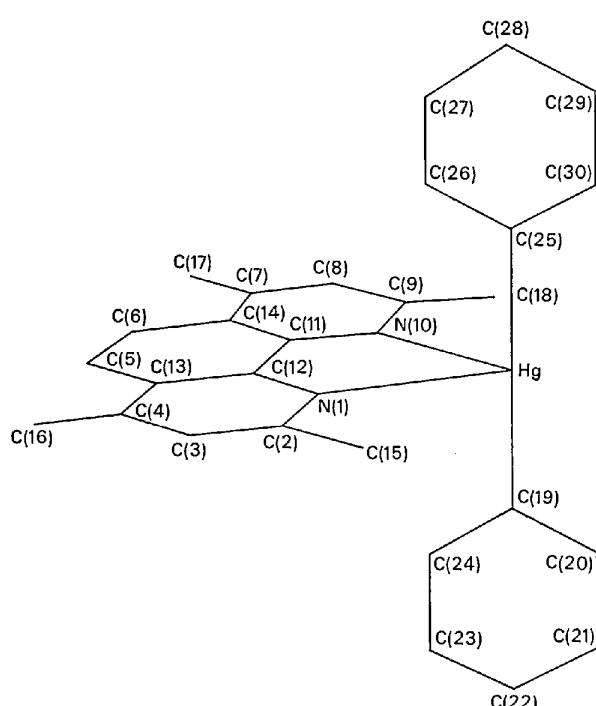


Fig. 3. Atom numbering scheme for $\text{Ph}_2\text{Hg}(\text{tmp})_2$. Adjacent ligand and Ph_2Hg moieties in the plane $y=\frac{1}{4}$ are shown. Adjacent ligand and Ph_2Hg moieties in (020) have an atom numbering scheme related by a twofold axis about the $\text{C}-\text{Hg}-\text{C}$ unit.

group atoms attached to mercury atoms in adjacent (040) planes are also present, being situated immediately above and below the mercury–mercury vector 0·33, $\frac{1}{4}$, 0·36. All peaks in the Patterson synthesis are now accounted for, and all calculated Hg–light-atom vectors are present. However, phenyl groups of mercury atoms at $x, \frac{1}{4}, z$ overlap with phenyl groups of mercury atoms at $x, \frac{3}{4}, z$.

The coincidence of phenyl groups is so close that atoms of separate groups cannot be distinguished in difference syntheses. A mirror plane in (020) is required for *Cm* symmetry, but whenever a Ph₂Hg moiety is placed at $x, \frac{1}{4}, z$ (e.g. $\frac{1}{4}, \frac{1}{4}, 0$) a Ph₂Hg moiety cannot be present at $x, \frac{3}{4}, z$ (e.g. $\frac{1}{4}, \frac{3}{4}, 0$) as required for space group *Cm*. With the fourfold Ph₂Hg moieties half-occupancy to maintain a mirror plane in the superposition structure in (020) and prevent overlap of phenyl groups, and with the Ph₂Hg moiety in (010) fully occupied, there are four formula units of Ph₂Hg(tmp)₂ in the unit cell as required.

The residual index *R* was 0·19 for the sharp reflexions and 0·57 for the diffuse reflexions. A small peak was present in a subsequent difference synthesis at $\frac{1}{2} + 0\cdot08$, 0, 0·36 suggesting the presence of a mercury atom in position for coordination of the ligand in (010) with *x* coordinates $> \frac{1}{2}$ [Fig. 4(a)]. Placing a Ph₂Hg moiety at this position requires partial occupancy, since overlap of phenyl groups occurs with Ph₂Hg moieties having mercury atoms in the $y = \frac{1}{2}$ plane. A mercury atom was placed at $\frac{1}{2} + 0\cdot08$, 0, 0·36 and the occupancies of Ph₂Hg moieties in the (020) planes varied such that with an occupancy of *m* for one Ph₂Hg moiety in (010) the occupancy of the other is $1 - m$, since it is translated to a position $\frac{1}{2}b$ removed from the Ph₂Hg moiety of occupancy *m* ($\frac{1}{2}, \frac{1}{2}, 0$ operation). Several models were tried, best agreement being obtained for *m* = 0·8. The calculated structure factors for diffuse reflexions are more sensitive than the sharp reflexions to occupancy variations since only the Ph₂Hg moieties with mercury atoms in (020) contribute to these re-

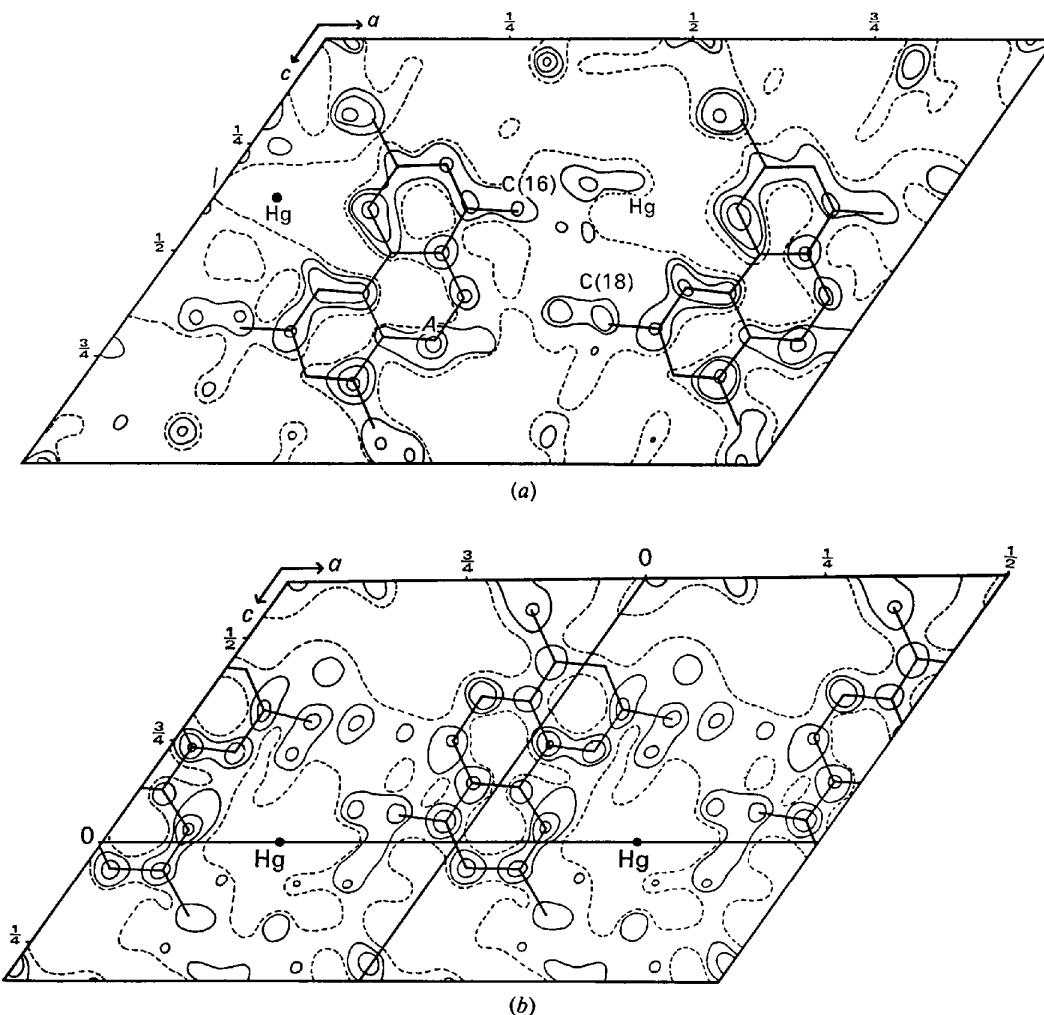


Fig. 4. Difference Fourier syntheses for Ph₂Hg(tmp)₂ with mercury atoms at $\frac{1}{2}, \frac{1}{4}, 0$ and 0·08, 0, 0·36 as the phasing atoms.
(a) The plane $y=0$. (b) The plane $y=\frac{1}{4}$.

flexions, the remainder of the cell contents conforming to a subcell of dimensions $a, \frac{1}{2}b, c$.

With occupancies of 0.8 and 0.2 for the Ph_2Hg

moieties in (020) R was 0.17 for both the 378 sharp and 36 diffuse reflexions and 0.25 for all reflexions, including 424 unobserved reflexions. A structure factor

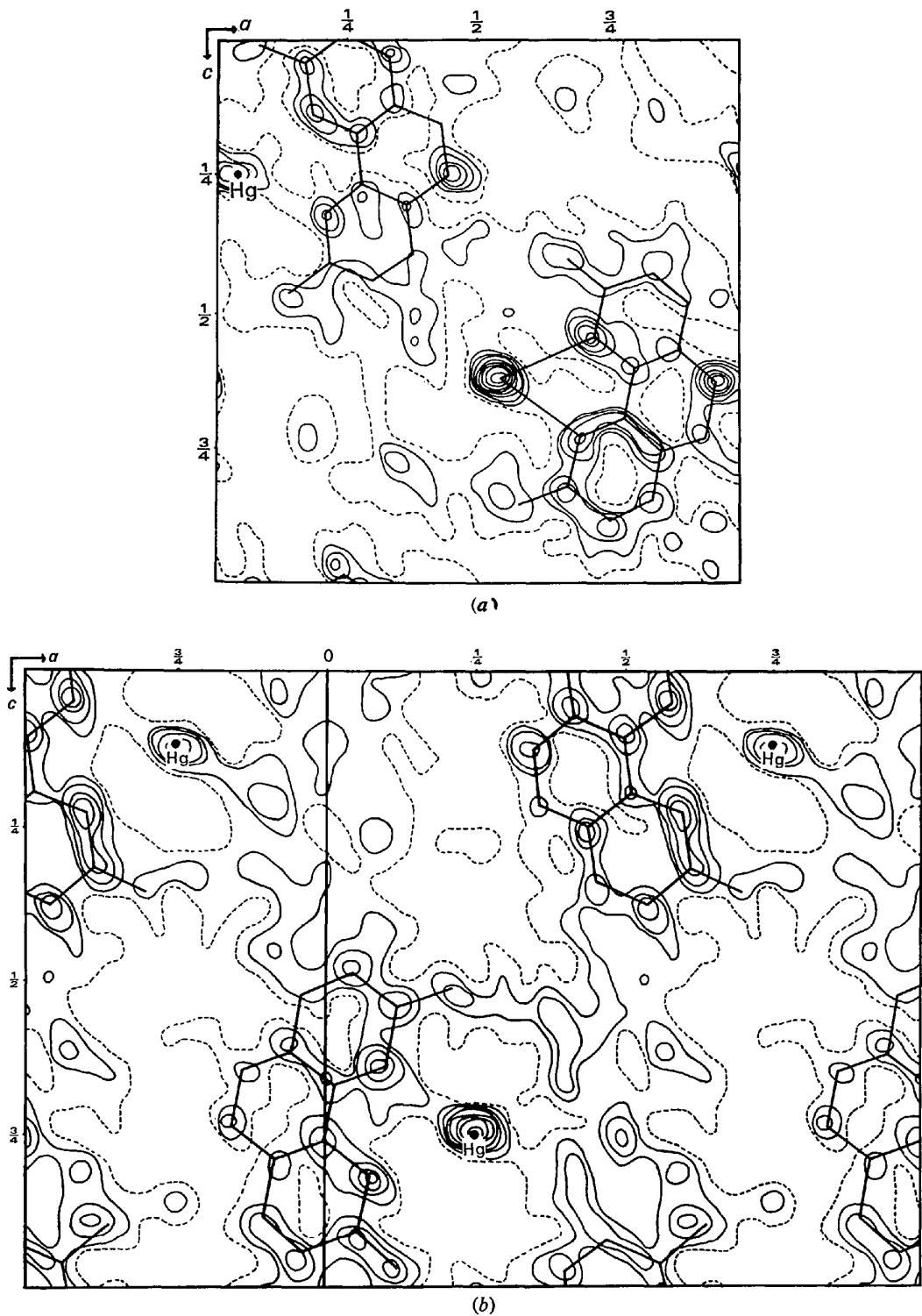


Fig. 5. Difference Fourier syntheses for $\text{Ph}_2\text{Hg}(\text{dmp})_2$ with mercury atoms at $\frac{1}{2}, \frac{1}{4}, \frac{3}{4}; \frac{1}{2}, \frac{1}{4}, \frac{3}{4}; \frac{1}{2}, \frac{1}{4}, \frac{3}{4}; 0.04, 0, \frac{1}{2};$ and $0.54, \frac{1}{2}, \frac{3}{4}$ as the phasing atoms calculated in space group $P1$. The contours are evenly spaced on an arbitrary scale. Negative regions are bounded by broken lines. (a) The plane $y=0$. (b) The plane $y=\frac{1}{4}$.

list is given in Table 1. A final difference Fourier synthesis calculated using observed reflexions has no peaks $> \frac{1}{2}$ or $< -\frac{1}{2}$ of a carbon atom, and difference syntheses calculated with mercury atoms only given the occupancy values of the final model are virtually identical with those shown in Fig. 4, which were calculated with an incomplete mercury atom contribution to the structure factor expression. Tables 2, 3 and 4 show the atomic coordinates, bond lengths and bond angles in $\text{Ph}_2\text{Hg}(\text{tmp})_2$.

Refinement was not attempted with 81 atoms in the asymmetric unit and only 414 observed reflexions.

Table 2. Coordinates of atoms of $\text{Ph}_2\text{Hg}(\text{tmp})_2$ within the asymmetric unit of space group Cm

	x/a	y/b	z/c	Occupancy
Hg(1)	0.2500	0.2500	0	0.5
Hg(2)	0.0839	0	0.3584	0.8
Hg(3)	0.5839	0	0.3584	0.2

Ligand coordinated to Hg(1)

N(1)	0.1062	0.2500	-0.0250	1.0
N(10)	0.1000	0.2500	-0.2240	1.0
C(2)	0.1125	0.2500	0.0692	1.0
C(3)	0.0387	0.2500	0.0615	1.0
C(4)	-0.0362	0.2500	-0.0481	1.0
C(5)	-0.1062	0.2500	-0.2531	1.0
C(6)	-0.1094	0.2500	-0.3565	1.0
C(7)	-0.0425	0.2500	-0.4481	1.0
C(8)	0.0250	0.2500	-0.4327	1.0
C(9)	0.0975	0.2500	-0.3250	1.0
C(11)	0.0312	0.2500	-0.2346	1.0
C(12)	0.0325	0.2500	-0.1346	1.0
C(13)	-0.0375	0.2500	-0.1461	1.0
C(14)	-0.0400	0.2500	-0.3442	1.0
C(15)	0.1937	0.2500	0.1808	1.0
C(16)	-0.1125	0.2500	-0.0673	1.0
C(17)	-0.1244	0.2500	-0.5596	1.0
C(18)	0.1775	0.2500	-0.2961	1.0

Ligand coordinated to Hg(2)

N(1)	0.2325	0	0.3904	1.0
N(10)	0.2375	0	0.5865	1.0
C(2)	0.2200	0	0.2885	1.0
C(3)	0.2850	0	0.2885	1.0
C(4)	0.3550	0	0.3904	1.0
C(5)	0.4412	0	0.6106	1.0
C(6)	0.4387	0	0.7048	1.0
C(7)	0.3812	0	0.8000	1.0
C(8)	0.3112	0	0.7961	1.0
C(9)	0.2437	0	0.6827	1.0
C(11)	0.3025	0	0.5961	1.0
C(12)	0.3000	0	0.4961	1.0
C(13)	0.3662	0	0.4923	1.0
C(14)	0.3750	0	0.7038	1.0
C(15)	0.1425	0	0.1846	1.0
C(16)	0.4312	0	0.4038	1.0
C(17)	0.4525	0	0.9231	1.0
C(18)	0.1700	0	0.6769	1.0

Atoms of ligand coordinated to Hg(3) have coordinates of atoms of ligand coordinated to Hg(2) + $\frac{1}{2}, 0, 0$ and occupancy 1.0.

Phenyl groups bonded to Hg(1)

C(19)	0.2500	0.3946	0.0000	0.5
C(20)	0.3228	0.4482	0.0625	0.5
C(21)	0.3228	0.5445	0.0625	0.5
C(22)	0.2500	0.5870	0.0000	0.5

Table 2 (cont.)

	x/a	y/b	z/b	Occupancy
C(23)	0.1815	0.5445	-0.0481	0.5
C(24)	0.1815	0.4482	-0.0481	0.5
C(25)	0.2500	0.1054	0.0000	0.5
C(26)	0.1815	0.0518	-0.0481	0.5
C(27)	0.1815	-0.0445	-0.0481	0.5
C(28)	0.2500	-0.0870	0.0000	0.5
C(29)	0.3228	-0.0445	0.0625	0.5
C(30)	0.3228	0.0518	0.0625	0.5

Phenyl groups bonded to Hg(2)

C(19)	0.0856	0.1462	0.3650	0.8
C(20)	0.0125	0.1979	0.3125	0.8
C(21)	0.0125	0.2911	0.3125	0.8
C(22)	0.0856	0.3446	0.3650	0.8
C(23)	0.1519	0.2911	0.4154	0.8
C(24)	0.1519	0.1979	0.4154	0.8

Atoms of phenyl groups bonded to Hg(3) have coordinates of atoms of phenyl groups bonded to Hg(1) + $\frac{1}{2}, 0, 0$ and occupancy 0.2.

Table 3. Bond lengths in $\text{Ph}_2\text{Hg}(\text{tmp})_2$

(a) Mercury stereochemistry	Hg(1)	Hg(2)
	Hg-N(1)	2.83 Å
	Hg-N(10)	2.90
	Hg-C(19)	2.10
	Hg-C(25)	2.13

(b) Ligands	Ligand coordinated to:	Hg(1)	Hg(2)
	N(1)—C(2)	1.31 Å	1.35 Å
	N(1)—C(12)	1.42	1.34
	C(2)—C(3)	1.49	1.37
	C(3)—C(4)	1.43	1.34
	C(4)—C(13)	1.42	1.37
	C(5)—C(6)	1.48	1.41
	C(5)—C(13)	1.36	1.50
	C(6)—C(14)	1.36	1.34
	C(7)—C(8)	1.30	1.44
	C(7)—C(14)	1.49	1.34
	C(8)—C(9)	1.40	1.40
	C(9)—N(10)	1.45	1.34
	N(10)—C(11)	1.36	1.29
	C(11)—C(12)	1.45	1.43
	C(11)—C(14)	1.40	1.40
	C(12)—C(13)	1.38	1.43
	C(2)—C(15)	1.51	1.42
	C(4)—C(16)	1.46	1.50
	C(7)—C(17)	1.51	1.51
	C(9)—C(18)	1.48	1.51

(c) Phenyl groups	For	For	
	Hg(1)	Hg(2)	
	C(19)—C(20)	1.46	1.46
	C(19)—C(24)	1.41	1.36
	C(20)—C(21)	1.40	1.36
	C(21)—C(22)	1.38	1.47
	C(22)—C(23)	1.32	1.37
	C(23)—C(24)	1.40	1.36
	C(25)—C(26)	1.41	
	C(25)—C(30)	1.46	
	C(26)—C(27)	1.40	
	C(27)—C(28)	1.32	
	C(28)—C(29)	1.38	
	C(29)—C(30)	1.40	

Table 4. Bond angles in $\text{Ph}_2\text{Hg}(\text{tmp})_2$

(a) Mercury stereochemistry

	Hg(1)	Hg(2)
N(1)—Hg—N(10)	59°	57°
C(19)—Hg—C(25)	180	
N(1), N(10)—Hg—C(19), C(25)	90	90

(b) Ligands

Ligand coordinated to:	Hg(1)	Hg(2)
Hg—N(1)—C(2)	115°	110°
Hg—N(1)—C(12)	121	120
C(2)—N(1)—C(12)	123	130
N(1)—C(2)—C(3)	119	118
N(1)—C(2)—C(15)	119	122
C(3)—C(2)—C(15)	123	121
C(2)—C(3)—C(4)	119	116
C(3)—C(4)—C(13)	118	125
C(3)—C(4)—C(16)	125	122
C(13)—C(4)—C(16)	117	112
C(6)—C(5)—C(13)	123	120
C(5)—C(6)—C(14)	118	128
C(8)—C(7)—C(14)	117	120
C(8)—C(7)—C(17)	128	108
C(14)—C(7)—C(17)	115	131
C(7)—C(8)—C(9)	123	110
N(10)—C(9)—C(8)	120	130
N(10)—C(9)—C(18)	112	120
C(8)—C(9)—C(18)	128	111
Hg—N(10)—C(9)	120	123
Hg—N(10)—C(11)	120	120
C(9)—C(10)—C(11)	120	117
N(10)—C(11)—C(12)	120	120
N(10)—C(11)—C(14)	118	120
C(12)—C(11)—C(14)	121	120
N(1)—C(12)—C(11)	119	123
N(1)—C(12)—C(13)	120	110
C(11)—C(12)—C(13)	120	127
C(4)—C(13)—C(5)	122	130
C(4)—C(13)—C(12)	120	120
C(5)—C(13)—C(12)	118	110
C(6)—C(14)—C(7)	119	122
C(6)—C(14)—C(11)	119	115
C(7)—C(14)—C(11)	121	123

(c) Phenyl groups

	Hg(1)	Hg(2)
Hg—C(19)—C(20)	122°	120°
Hg—C(19)—C(24)	124	124
C(20)—C(19)—C(24)	114	115
C(19)—C(20)—C(21)	122	121
C(20)—C(21)—C(22)	117	122
C(21)—C(22)—C(23)	125	113
C(22)—C(23)—C(24)	118	125
C(19)—C(24)—C(23)	124	124
Hg—C(25)—C(26)	124	
Hg—C(25)—C(30)	122	
C(26)—C(25)—C(30)	114	
C(25)—C(26)—C(27)	124	
C(26)—C(27)—C(28)	118	
C(27)—C(28)—C(29)	114	
C(28)—C(29)—C(30)	122	
C(25)—C(30)—C(29)	117	

(2) Solution of the superposition structure for $\text{Ph}_2\text{Hg}(\text{dmp})_2$

A crystal of dimensions $0.05 \times 0.08 \times 0.2$ mm, less than optimum size (absorption coefficient $\mu(\text{Cu } K\alpha) = 9.53 \text{ mm}^{-1}$, $t_{\text{opt}} = 0.21 \text{ mm}$) was chosen and mounted about the needle axis; a total of 1868 independent

non-zero reflexions (including 537 diffuse reflexions) were collected for reciprocal lattice levels $hk0-hk12$. Since only very small variations from monoclinic symmetry could be seen in intensities of reflexions, structure solution was sought with a monoclinic data set in space group $P1$ until the appropriate monoclinic space group became apparent. All calculations were carried out in $P1$ except for the final occupancy determination and structure factor list.

A three-dimensional Patterson synthesis calculated in $P\bar{1}$ has $P2/m$ symmetry and only vectors within the asymmetric unit of $P2/m$ are discussed. The synthesis has a large number of peaks in (040) and a small number of peaks between these planes, as observed for $\text{Ph}_2\text{Hg}(\text{tmp})_2$. Very large peaks are present in the synthesis at $\frac{1}{2}, 0, \frac{3}{8}$; $\frac{1}{2}, 0, \frac{5}{8}$; $0.21, \frac{1}{4}, \frac{1}{2}$; $0.29, \frac{1}{4}, \frac{1}{8}$; and $0.29, \frac{1}{4}, \frac{5}{8}$. With b and c axis lengths almost identical with that of $\text{Ph}_2\text{Hg}(\text{tmp})_2$, and vectors almost entirely in (040), similarities between mercury–mercury vectors in Patterson syntheses were sought. Coincidence of b and c axes in Patterson syntheses brings one large vector at $\frac{1}{2}, 0, \frac{5}{8}$ almost into coincidence with the $\frac{1}{2}, 0, 0$ vector in the Patterson synthesis of $\text{Ph}_2\text{Hg}(\text{tmp})_2$, and there are many smaller vectors near the origin at about the correct distance from it for mercury–ligand vectors.

Using this orientation of the Patterson syntheses, and hence unit cells, an initial mercury atom position was chosen to satisfy the Patterson synthesis and coincide as closely as possible with the initial mercury position used for $\text{Ph}_2\text{Hg}(\text{tmp})_2$.

With Hg(1) at $\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ R was 0.53 and a difference synthesis had strong peaks at $0.04, 0, \frac{1}{4}$ (A); $\frac{1}{2} - 0.04, 0, \frac{1}{4}$ (B); $\frac{1}{2} + 0.04, 0, \frac{5}{8}$ (C); $\frac{1}{2} + 0.04, 0, \frac{7}{8}$ (D); $\frac{3}{4}, \frac{1}{4}, \frac{1}{8}$ (E) and $\frac{3}{4}, \frac{1}{4}, \frac{5}{8}$ (F). The $y = \frac{1}{2}$ and $\frac{3}{4}$ planes are identical to the $y = 0$ and $\frac{1}{2}$ planes respectively, except for a peak at $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ corresponding to Hg(1) translated $\frac{1}{2}b$. Vectors from $\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ to E and F satisfy the Patterson synthesis peaks $\frac{1}{2}, 0, \frac{3}{8}$ and $\frac{1}{2}, 0, \frac{5}{8}$ respectively. Position E [Hg(2)] was added ($R = 0.50$) and peak F , together with the peak of the same x and z coordinates in the $y = \frac{3}{4}$ plane, was absent from a subsequent difference synthesis. Peaks at $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ and $\frac{3}{4}, \frac{1}{4}, \frac{1}{8}$ became more intense, and mercury atoms were added with these coordinates together with $0.04, 0, \frac{1}{4}$ [Hg(3)]. A structure factor calculation had $R = 0.32$ and a difference synthesis had only one strong peak at $\frac{1}{2} + 0.04, \frac{1}{2}, \frac{5}{8}$. This position [Hg(4)] was added to the structure factor calculation ($R = 0.26$), and subsequent difference Fourier syntheses are shown in Fig. 5. The $y = \frac{1}{4}$ and $\frac{3}{4}$ planes are identical, as also are the $y = 0$ and $\frac{1}{2}$ planes but with a small peak in the $y = 0$ plane having the same x and z coordinates as the mercury position in the $y = \frac{1}{2}$ plane [Hg(4)], and a small peak in $y = \frac{1}{2}$ corresponding to the mercury position in $y = 0$ [Hg(3)].

As for $\text{Ph}_2\text{Hg}(\text{tmp})_2$ the planar ligands lie in (040). The ligands were added singly to the structure factor calculation and all ligands were found to be present, difference syntheses having only very small

DISORDERED CRYSTALS OF ADDUCTS OF DIPHENYLMERCURY

Table 5. Comparison of F_o and F_c for $\text{Ph}_2\text{Hg}(\text{dmp})_2$

Sharp reflexions are presented first. Unobserved reflexions are indicated with an asterisk.

H	K	F _O	F _C	H	K	F _O	F _C	H	K	F _O	F _C	H	K	F _O	F _C	H	K	F _O	F _C				
<<<	L = 0 >>>	-9	2	43	12*	+3	8	298	345	10	10	54	8*	4	2	665	699	-13	4	54	109*		
-9	4	45	10*	-9	10	90	110	-10	12	127	85	-9	4	236	176	-13	6	54	79*				
-10	0	36	41	-5	12	175	225	-11	2	250	269	-4	4	415	386	-14	0	54	50*				
0	2	18	0*	-10	6	28*	28*	-5	12	140	111	-6	72	140	111	-4	8	213	199	-14	2	120	108
0	6	33	0*	-10	4	284	319	-4	2	140	172	-11	6	217	287	-4	10	244	234	-14	4	53	28*
0	8	518	946	-10	6	51	37*	-4	4	31	8*	-11	8	54	105*	-4	12	120	129	-14	6	134	184
0	10	49	0*	-10	8	220	267	-4	6	137	142	-11	10	156	181	-4	14	157	154	-14	10	106	112
0	12	49	530	-10	10	50	159	-4	4	41	41	-11	10	127	127	-4	14	230	241	-14	10	106	112
0	14	54	0*	-10	12	159	159	-5	0	128	107	-4	9	97	76	-4	15	77	94	-15	0	53	15*
0	16	289	313	-11	0	49	23*	-5	2	720	698	-12	8	171	203	-5	6	171	163	-15	2	52	55*
1	4	26	14*	-11	2	49	9*	-5	4	34	82*	-12	8	84	120	-5	6	46	23*	-15	0	51	6*
1	6	34	19*	-11	4	51	16*	-5	6	446	500	-13	4	54	54	-5	10	12	19	-15	0	51	6*
1	8	41	11*	-11	5	51	59*	-5	6	44	51*	-13	4	124	124	-5	6	437	479	-16	0	129	147
1	10	49	14*	-12	2	115	37	-5	10	200	213	-14	2	124	154	-5	6	68	78	-16	2	49	83*
1	12	52	56	-12	2	233	169	-5	12	55	43*	-14	4	54	71*	-6	6	326	337	-16	4	86	104
2	2	223	164	-12	4	53	26*	-5	14	163	187	-14	6	53	84*	-6	6	230	189	-16	4	44	66*
2	4	131	63	-12	6	272	291	-6	0	111	127	-15	2	124	124	-6	6	155	153	-16	8	85	95
2	6	20	14*	-12	8	14	14*	-6	6	111	127	-6	4	50	94*	-6	6	129	132	-16	8	106	112
2	8	76	50	-12	10	186	170	-5	4	62	105	-16	4	48	54*	-6	14	109	130	-<<<	L = 4 >>>		
2	10	154	154	-13	0	54	13*	-5	6	131	163	-16	2	83	146	-7	2	253	166	-<<<	L = 4 >>>		
2	12	54	46*	-13	2	54	17*	-6	8	122	134	-17	2	83	146	-7	4	163	165	-<<<	L = 4 >>>		
2	14	130	170	-13	4	24	14*	-7	6	131	160	-17	2	76	124	-7	8	142	175	-<<<	L = 4 >>>		
2	16	34	3*	-13	5	55	11*	-7	7	211	200	-18	1	6	287	237	-8	2	275	260	-<<<	L = 4 >>>	
3	4	136	13*	-13	8	199	169	-7	4	319	319	-11	6	287	237	-8	4	235	179	-<<<	L = 4 >>>		
3	6	36	14*	-12	2	55	38*	-7	5	385	368	-11	10	153	145	-8	6	192	189	-<<<	L = 4 >>>		
3	8	42	12*	-14	4	121	200	-7	6	121	124	-12	4	54	10*	-8	8	272	232	-<<<	L = 4 >>>		
3	10	140	14*	-14	6	124	124	-7	6	124	124	-12	4	54	10*	-10	10	137	152	-<<<	L = 4 >>>		
4	2	229	234	-14	8	104	139	-7	12	243	261	-12	0	17	30*	-8	10	180	184	-<<<	L = 4 >>>		
4	4	203	278	-15	0	54	10*	-8	0	100	127	-12	2	419	359	-8	12	179	160	-<<<	L = 4 >>>		
4	6	167	202	-15	2	54	8*	-8	2	178	162	-12	4	24	24*	-9	2	100	122	-<<<	L = 4 >>>		
4	8	373	329	-15	4	53	10*	-7	6	124	124	-12	4	54	10*	-10	10	156	156	-<<<	L = 4 >>>		
4	10	131	14*	-15	6	104	104	-7	6	107	117	-12	4	54	8*	-9	6	96	98	-<<<	L = 4 >>>		
4	12	243	217	-16	0	52	100*	-6	0	133	160	-12	10	252	251	-10	2	263	247	-12	12	164	187
5	2	30	34*	-16	2	132	123	-9	2	264	288	-12	12	54	10*	-10	4	49	65*	-12	14	148	138
5	4	34	10*	-16	4	49	70*	-6	4	131	107	-12	14	118	165	-10	6	249	275	-12	16	103	111
5	6	32	12*	-16	8	116	120	-7	6	253	259	-12	14	116	124	-10	8	154	154	-12	14	96	97
5	8	478	457	-17	0	47	24*	-9	8	96	105	-13	0	350	305	-10	10	137	152	-12	14	26	33*
6	4	321	310	-17	2	46	28*	-10	0	122	122	-3	4	180	173	-10	12	119	161	-12	14	157	97
6	6	356	329	-17	4	44	2*	-10	0	83	81	-3	6	339	367	-10	14	97	118	-12	14	32	24*
6	8	295	284	-17	6	40	18*	-10	2	84	78	-5	8	110	128	-11	2	100	122	-12	14	45	45*
6	10	137	125	-18	0	41	45*	-10	6	90	95	-6	6	125	125	-12	6	55	55	-12	14	252	216
6	12	199	225	-18	2	104	120	-10	6	122	124	-12	3	154	252	-13	2	92	77*	-12	14	178	142
6	14	195	123	-19	0	252	252	-3	0	252	252	-13	3	14	152	-14	2	388	374	-12	14	54	297
7	2	36	12*	-11	2	92	79	-11	2	92	79	-4	2	38	104	-12	6	54	62*	-12	14	253	215
7	4	20	10*	-<<<	-11	4	111	-13	-4	2	104	113	-12	10	149	139	-3	12	97	97	-<<<	L = 1 >>>	
7	6	44	8*	-<<<	-11	8	99	-101	-4	6	97	111	-12	10	149	139	-3	14	245	185	-<<<	L = 1 >>>	
7	8	49	8*	-<<<	-11	8	99	-101	-4	6	97	111	-12	10	149	139	-3	14	245	185	-<<<	L = 1 >>>	
8	2	411	488	0	2	281	278	-12	0	249	295	-4	10	267	240	-12	12	119	161	-12	14	157	97
8	4	42	47*	0	4	26	0*	-12	2	95	73	-4	10	50	46*	-13	2	54	11*	-12	14	32	42*
8	6	350	382	-17	0	363	344	-12	4	182	217	-12	17	158	158	-13	4	86	176	-<<<	L = 1 >>>		
8	8	132	83	-17	0	363	344	-12	4	182	217	-12	17	158	158	-13	4	86	176	-<<<	L = 1 >>>		
8	10	198	176	-19	0	363	344	-12	4	182	217	-12	17	158	158	-13	4	86	176	-<<<	L = 1 >>>		
8	12	129	182	-19	2	76	91	-15	2	122	135	-7	0	79	49	-12	16	162	182	-<<<	L = 1 >>>		
8	14	99	9*	-3	2	195	188	-15	4	53	44*	-7	2	259	285	-14	4	144	126	-<<<	L = 1 >>>		
8	16	51	16*	-3	4	376	361	-15	4	61	91	-7	4	242	272	-14	8	85	58	-<<<	L = 1 >>>		
8	18	53	15*	-3	6	272	202	-15	4	61	72	-7	6	124	124	-15	6	93	74	-<<<	L = 1 >>>		
8	20	55	38*	-3	6	74	109	-15	4	61	72	-7	6	124	124	-15	6	93	74	-<<<	L = 1 >>>		
8	22	100	84	-3	6	177	177	-15	4	61	72	-7	6	124	124	-15	6	93	74	-<<<	L = 1 >>>		
8	24	14*	73	-3	6	177	177	-15	4	61	72	-7	6	124	124	-15	6	93	74	-<<<	L = 1 >>>		
8	26	14*	73	-3	6	177	177	-15	4	61	72	-7	6	124	124	-15	6	93	74	-<<<	L = 1 >>>		
8	28	14*	73	-3	6	177	177	-15	4	61	72	-7	6	124	124	-15	6	93	74	-<<<	L = 1 >>>		
8	30	274	13*	-3	6	136	118	-5	6	72	86	-10	2	368	375	-<<<	L = 1 >>>						
8	32	10	344	-2	2	55	66*	-5	6	862	375	-10	2	170	200	-12	16	224	275	-<<<	L = 1 >>>		
8	34	14*	73	-3	6	177	177	-15	4	61	72	-7	6	124	124	-15	6	93	74	-<<<	L = 1 >>>		
8	36	39	20*	-3	6	53	64*	-5	12	222	239	-11	8	112	105	-2	0	112	105	-<<<	L = 1 >>>		
8	38	45	44*	-3	6	9																	

Table 5 (cont.)

K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC		
5	14	49	29	12	4	135	146	3	12	121	121	-12	4	92	284	-5	6	435	
5	17	108	62	12	6	93	47	2	4	249	125	-12	8	197	249	-5	8	47	
5	15	60	23	12	6	106	28	6	17	152	152	-12	0	126	165	5	12	49	
5	14	38	230	12	12	67	62	4	8	257	209	-12	10	119	98	-5	14	153	
5	6	123	101	13	2	53	23	4	10	62	74	-13	2	22	72	-6	12	83	
5	6	48	64	13	2	135	121	4	12	133	120	-13	10	100	90	-6	12	34	
5	7	12	10	13	2	135	121	4	12	133	120	-13	8	63	100	-5	12	66	
5	7	973	551	14	4	91	11*	5	6	244	181	-14	0	131	199	-7	0	312	
5	7	40	264	14	4	179	192	5	6	41	22*	-14	2	21	24	-7	2	64	
5	7	8	360	14	6	45	6*	5	6	743	225	-14	4	87	244	-7	4	14	
5	7	8	36	14	10	156	152	5	12	135	135	-14	6	47	30*	-7	6	66	
5	7	12	104	12	12	116	116	5	12	132	132	-15	8	77	86	-7	12	21	
5	7	12	94	12	2	194	105	6	4	324	329	-15	0	125	143	-7	10	50	
5	7	12	166	12	12	148	136	6	4	159	234	-15	2	48	13*	-7	12	192	
5	7	12	72	12	12	211	176	6	4	230	176	-15	0	104	125	-7	2	57	
5	7	12	41	12	12	104	104	6	4	105	102	-15	0	44	93*	-6	2	77	
5	7	47	174	12	12	109	109	6	10	104	102	-16	2	91	81	-6	4	63	
5	7	4	972	698	7	2	331	293	-16	4	58	74	-6	6	67	79	-2	12	48
5	7	0	378	382	7	4	42	6*	-16	6	82	84	-6	0	159	159	-5	12	125
5	7	2	152	144	7	4	53	53	-16	2	29	25	-7	0	309	309	-5	12	100
5	7	2	124	124	7	4	116	116	-16	2	29	25	-7	4	86	75	-3	2	111
5	7	6	119	193	7	4	339	269	-16	4	81	81	-7	14	35	12*	-6	3	34
5	7	8	271	264	7	4	70	69	-16	2	104	224	-17	6	83	104	-7	8	51
5	7	12	93	12	12	192	177	7	4	86	102	-16	0	44	12	-7	12	133	
5	7	12	120	120	7	4	115	109	-16	2	104	102	-16	0	304	304	-5	12	103
5	7	12	49	12	12	112	101	7	4	67	67	-16	4	116	115	-7	2	283	
5	7	2	47	47	7	2	274	261	8	14	85	84	-16	0	47	47	-4	4	287
5	7	0	229	269	3	2	35	56	9	2	103	94	-16	2	119	90	-5	12	211
5	7	2	127	152	3	4	228	183	9	6	71	104	-16	4	119	109	-5	12	225
5	7	12	93	12	12	143	143	9	6	163	143	-16	8	78	91	-7	12	224	
5	7	12	183	12	12	197	162	9	10	51	48*	-16	4	43	17*	-11	2	114	
5	7	12	147	12	12	50	42*	9	12	117	97	-16	2	195	141	-7	11	4	
5	7	12	113	12	12	66	59	9	12	117	97	-16	2	195	141	-7	12	142	
5	7	12	70	12	12	55	57	9	12	117	97	-16	2	195	141	-7	12	143	
5	7	12	52	12	12	259	434	9	12	220	212	-16	6	142	172	-9	12	119	
5	7	12	52	12	12	372	372	10	6	163	178	-16	12	120	103	-11	12	62	
5	7	12	4	52	12	12	104	45	10	10	210	172	-16	12	72	70	-6	2	304
5	7	12	4	53	12	12	234	226	10	10	45	50*	-16	12	82	72	-7	12	151
5	7	12	6	52	12	12	110	110	10	10	110	109	-16	2	304	304	-5	12	152
5	7	12	121	121	12	12	91	107	10	12	204	204	-16	2	304	304	-5	12	153
5	7	12	137	12	12	152	146	11	4	110	111	-16	2	304	304	-5	12	154	
5	7	12	97	12	12	67	60	11	6	9	138	-16	2	180	180	-7	12	119	
5	7	12	6	122	12	12	218	218	12	2	178	178	-16	2	180	180	-7	12	155
5	7	12	53	12	12	54	52	12	2	178	178	-16	2	180	180	-7	12	156	
5	7	12	52	12	12	44	44	12	2	204	212	-16	2	211	211	-7	9	72	
5	7	12	6	42	12	12	294	294	12	8	4	103	-16	3	211	183	-7	4	150
5	7	12	2	44	12	12	104	95	12	6	82	146	-16	3	211	183	-7	4	151
5	7	12	2	44	12	12	222	248	12	2	52	244	-16	3	211	183	-7	4	152
5	7	12	17	12	12	95	95	12	2	91	107	-16	3	211	183	-7	4	153	
5	7	12	12	12	345	303	17	4	35	24*	-16	3	12	219	201	-7	12	147	
5	7	12	3	26	12	12	206	165	17	6	85	90	-16	2	180	180	-7	12	148
5	7	12	3	26	12	12	218	233	17	6	85	90	-16	2	180	180	-7	12	149
5	7	12	3	26	12	12	244	258	17	6	85	90	-16	2	180	180	-7	12	150
5	7	12	10	12	12	53	54**	17	6	316	292	-16	6	44	304	-7	12	151	
5	7	12	12	176	12	12	181	181	18	6	45	48*	-16	6	293	272	-7	12	152
5	7	12	12	150	12	12	73	73	18	6	45	50*	-16	7	211	199	-7	12	153
5	7	12	4	85	59	12	12	14	14	91	97	-16	7	211	199	-7	12	154	
5	7	12	4	85	59	12	12	20	20	91	97	-16	7	211	199	-7	12	155	
5	7	12	4	85	59	12	12	36	36	91	97	-16	7	211	199	-7	12	156	
5	7	12	12	53	12	12	252	192	12	6	92	85*	-16	7	211	199	-7	12	157
5	7	12	12	183	12	12	163	163	12	6	92	85*	-16	7	211	199	-7	12	158
5	7	12	12	143	12	12	109	124	12	6	92	85*	-16	7	211	199	-7	12	159
5	7	12	12	204	12	12	167	167	12	6	92	85*	-16	7	211	199	-7	12	160
5	7	12	42	12	12	50	50**	12	4	91	70	-16	7	211	199	-7	12	161	
5	7	12	10	89	12	12	111	111	12	6	80	80	-16	7	211	199	-7	12	162
5	7	12	12	249	12	12	52	52**	12	6	80	80	-16	7	211	199	-7	12	163
5	7	12	12	195	12	12	244	244	12	6	80	80	-16	7	211	199	-7	12	164
5	7	12	12	249	12	12	125	125	12	6	80	80	-16	7	211	199	-7	12	165
5	7	12	12	213	12	12	50	50**	12	6	80	80	-16	7	211	199	-7	12	166
5	7	12	12	299	12	12	52	52**	12	6	80	80	-16	7	211	199	-7	12	167
5	7	12	12	271	12	12	52	52**	12	6	80	80	-16	7	211	199	-7	12	168
5	7	12	12	287	12	12	176	220	12	6	80	80	-16	7	211	199	-7	12	169
5	7	12	4	45	8	12	152	151	8	6	144	188	-16	1	211	199	-7	12	170
5	7	12	12	234	12	12	152	152	12	4	241	234	-16	4	144	188	-7	12	171
5	7	12	12	173	12	12	50	55**	12	4	241	234	-16	4	144	188	-7	12	172
5	7	12	12	125	12	12	152	152	12	4	241	234	-16	4	144	188	-7	12	173
5	7	12	12	165	12	12	48	48**	12	4	241	234	-16	4	144	188	-7	12	174
5	7	12	5	61	8	12	49	92*	12	4	241	234	-16	4	144	188	-7	12	175
5	7	12	4	59	8	12	104	118	8	6	167	181	-16	6	144	188	-7	12	176
5	7	12	4	71	8	12	46	65**	8	6	167	181	-16	6	144	188	-7	12	177
5	7	12	4	71	8	12	50	57**	8	6	167	181	-16	6	144	188	-7	12	178
5	7	12	2	320	12	12	104	104	7	2	331	295	-16	1	194	160	-7	2	292
5	7	12	12	117	12	12	42	42**	7	4	241	193	-16	4	144	188	-7	2	292
5	7	12	22	22	12	12	250	247	7	4	144	188	-16	4	144	188	-7	2	293
5	7	12	12	125	12	12	147	147	7	4	144	188	-16	4	144	188	-7	2	294
5	7																		

DISORDERED CRYSTALS OF ADDUCTS OF DIPHENYLMERCURY

Table 5 (cont.)

H	K	F0	FC	H	K	F0	FC	H	K	F0	FC	H	K	F0	FC	H	K	F0	FC	H	K	F0	FC		
8	8	137	171	10	6	49	43*	11	4	41	28*	-1	8	115	136	44444	L = 0	>>>	>	1	94	126			
9	2	118	142	11	8	43	93*	11	6	39	15*	-1	10	85	102	0	3	22	0*	0	3	80	116		
9	4	46	63*	11	6	73	53	12	2	41	8*	-1	12	87	92	0	3	22	0*	0	3	84	101		
9	6	135	152	12	4	46	66*	12	2	41	8*	-1	12	87	92	0	3	22	0*	0	3	87	104		
10	2	47	59*	12	6	43	30*	12	8	36	7*	-2	0	48	2	0	3	30	0*	0	3	47	3*		
10	4	47	19*	12	6	66	98	12	8	66	112	-2	0	36	45	0	7	37	0*	0	7	95	102		
10	6	47	54*	13	2	77	92	13	2	38	7*	-2	6	37	48*	0	9	44	0*	0	7	93	94		
11	2	103	79	13	4	46	66*	13	4	36	47*	-3	0	115	88	0	11	51	0*	0	9	55	44		
11	7	49	13*	13	6	11	13	13	2	35	35*	-2	2	142	171	0	13	55	0*	0	11	52	41		
11	6	70*	106	-1	2	163	299	14	2	52	55*	-1	3	143	187*	-1	3	91	0*	0	11	50	40		
12	2	47	18*	-1	2	163	112	14	4	31	33*	-3	4	170	190	1	3	143	187*	-1	3	91	60		
12	4	65	114	-1	6	197	183	14	6	62	123	-3	6	73	44	1	3	188	187	-1	3	92	84		
12	6	45*	158*	-1	6	197	183	14	6	62	123	-3	10	70	108	1	9	141	187	-1	9	97	84		
13	4	102	126	15	6	156	121	14	6	31	15*	-2	0	100	110	1	11	72	63	-1	11	93	101		
13	6	79	96	-1	10	108	109	14	6	63	95	-2	0	137	127	1	13	94	63	-1	13	94	90		
-1	0	259	257	-1	12	85	82	-2	0	346	378	-4	4	84	122	1	13	94	63	-1	13	95	102		
-1	2	246	241	-1	16	62	73	-2	2	80	76	-4	6	87	99	2	1	18	17	-1	7	95	102		
-1	4	329	299	-1	2	122	147	-2	6	54	80	-4	8	33	39	2	11	94	63	-1	11	95	80		
-1	6	313	89	-2	6	102	99	-2	8	164	179	-4	244	293	2	7	38	60	-1	13	94	76			
-1	10	197	-2	6	213	186	-10	9	43	56*	-9	39	25*	6	9	45	95	-1	13	9	55	67			
-1	12	71	11	-2	6	44	40*	-12	110	122	-5	9	231	209	2	11	92	39	-1	14	1	59	1		
-1	14	99	150	-1	12	154	119	-1	12	110	122	-5	9	231	209	2	13	95	39	-1	14	1	59	1	
-1	2	266	274	-1	12	84	42*	-5	12	126	156	-5	12	126	201	3	1	162	177	-1	14	9	54	6	
-1	2	133	28	-1	16	86	83	-3	4	34	26*	-6	0	36	25*	3	3	194	170	-1	14	7	52	6	
-1	2	421	19	-1	16	127	92	-3	5	66	59	-6	2	36	24*	3	5	145	181	-1	14	9	54	63	
-1	4	114	127	-1	16	207	192	-1	16	127	152	-4	4	34	32*	2	7	17	12	-1	14	9	55	63	
-1	6	420	408	-1	6	192	207	-1	6	51	31	-9	35	39*	4	11	71	88	-1	14	1	51	1		
-1	8	313	89	-2	6	102	99	-2	8	164	179	-4	244	293	2	7	38	60	-1	14	1	51	1		
-1	10	197	-2	6	213	186	-10	9	43	56*	-9	39	25*	6	9	45	95	-1	13	9	55	67			
-1	12	71	11	-2	6	44	40*	-12	110	122	-5	9	231	209	2	11	92	39	-1	14	1	59	1		
-1	14	99	150	-1	12	84	42*	-5	12	126	156	-5	12	126	201	3	1	162	177	-1	14	9	54	6	
-1	2	236	233	-1	14	59	92	-1	12	126	156	-5	12	126	201	3	3	194	170	-1	14	7	52	6	
-1	4	47	34*	-1	0	142	136	-14	9	77	126	-8	2	40	31*	4	9	47	67	-1	14	7	52	46*	
-1	12	143	157	-1	6	31	39*	-5	0	161	139	-8	4	40	36*	4	11	53	47	-1	14	1	51	1*	
-1	4	126	77	-1	6	44	47*	-5	2	110	76	-8	6	40	26*	5	1	165	178	-1	14	9	55	67	
-1	4	34	52*	-1	8	100	98	-5	8	67	67	-8	2	167	172	4	9	149	134	-1	14	1	51	1	
-1	6	106	76	-1	6	270	250	-5	8	96	101	-8	4	126	131	5	7	109	117	-1	14	1	51	1	
-1	8	85	64	-1	2	35	15*	-5	0	59	49	-9	0	39	37*	6	1	32	44	-1	14	1	51	1	
-1	10	12	221	-1	2	221	233	-5	2	123	239	-5	0	80	49	6	3	155	167	-1	14	1	51	1	
-1	2	294	270	-1	4	125	154	-5	4	125	154	-5	0	80	49	6	3	155	167	-1	14	1	51	1	
-1	4	38	7*	-1	8	202	229	-5	6	154	183	-10	4	40	23*	4	7	44	29	-1	14	9	55	67	
-1	6	234	222	-1	5	10	45	-3*	12	126	157	-7	0	39	74*	10	6	37	17*	8	11	54	10	1	
-1	8	46	6*	-1	5	12	126	-7	0	39	74*	-2	2	20	38*	11	0	0	71	134	10	5	42	62	
-1	10	102	94	-1	6	151	141	-1	6	151	141	-1	2	20	38*	12	7	27	80	-1	14	9	55	67	
-1	12	14	54*	-1	6	151	141	-1	6	151	141	-1	2	20	38*	13	7	27	80	-1	14	9	55	67	
-1	14	74	64	-1	6	143	136	-1	6	143	136	-1	2	20	38*	14	7	27	80	-1	14	9	55	67	
-1	16	64	53*	-1	6	151	141	-1	6	151	141	-1	2	20	38*	15	7	27	80	-1	14	9	55	67	
-1	0	373	354	-7	2	266	305	-8	8	161	183	-10	4	40	23*	8	3	41	20*	-1	14	9	55	67	
-1	2	240	26*	-7	4	95	96	-8	10	37	45*	-12	6	31	22*	8	5	44	20*	-1	14	9	55	67	
-1	7	292	301	-7	6	216	229	-9	12	120	130	-13	0	33	80*	8	7	49	20*	-1	14	9	55	67	
-1	7	8	207	-7	6	240	192	-9	12	120	130	-13	0	33	80*	8	7	49	20*	-1	14	9	55	67	
-1	10	46	10*	-6	4	44	45*	-9	4	43	43*	-12	6	31	22*	9	8	55	47*	-1	14	9	55	67	
-1	12	181	257	-9	6	160	138	-10	0	61	81	-12	2	12	131	-1	13	114	114	-1	14	9	55	67	
-1	14	200	219	-9	6	151	141	-10	2	12	131	-12	6	31	22*	10	7	55	47*	-1	14	9	55	67	
-1	6	121	113	-9	6	211	113	-10	6	161	141	-10	2	12	131	-1	13	114	114	-1	14	9	55	67	
-1	10	137	198	-9	6	111	111	-10	6	161	141	-10	2	12	131	-1	13	114	114	-1	14	9	55	67	
-1	10	45*	62*	-9	0	2	292	183	-1	4	117	155	-10	2	12	131	-1	13	114	114	-1	14	9	55	67
-1	12	78	103	-9	0	4	31	2*	-1	4	184	202	-10	2	12	131	-1	13	114	114	-1	14	9	55	67
-1	2	110	114	-9	0	4	38	274	-1	6	117	155	-10	2	12	131	-1	13	114	114	-1	14	9	55	67
-1	6	185	182	-9	0	4	38	156	-1	6	117	155	-10	2	12	131	-1	13	114	114	-1	14	9	55	67
-1	8	158	125	-9	0	39	0*	-12	7	97	77	-12	2	25	33*	-1	13	114	114	-1	14	9	55	67	
-1	10	83	109	-9	0	14	97	126	-12	2	25	33*	-12	2	24	33*	-1	13	114	114	-1	14	9	55	67
-1	11	62	85	-1	2	23	49	-2	4	32	30*	-12	2	24	33*	-1	13	114	114	-1	14	9	55	67	

Table 5 (cont.)

x	y	z	fo	fc	x	y	z	fo	fc	x	y	z	fo	fc	x	y	z	fo	fc	x	y	z	fo	fc
1	1	93	93	1	8	78	109	10	13	44	154	4	9	135	138	14	9	44	45	15	7	49	418	
1	1	92	92	1	7	119	92	11	13	49	845	4	7	131	119	17	1	43	47	18	11	52	389	
1	1	91	91	1	6	111	92	11	13	50	865	4	9	67	105	17	3	42	56	20	11	52	297	
1	1	90	90	1	5	112	92	11	13	52	875	4	11	30	74	17	5	56	59	21	11	52	184	
1	1	89	89	1	4	112	92	11	13	53	245	4	1	33	48	17	3	56	59	21	11	52	85	
1	1	88	88	1	3	112	92	11	13	54	245	4	1	37	10	18	9	24	57	19	11	52	74	
1	1	87	87	1	2	9	83	12	5	54	245	4	9	27	45	15	7	44	46	10	11	47	507	
1	1	86	86	1	1	12	83	12	5	54	245	4	11	9	45	15	7	44	46	10	11	47	446	
1	1	85	85	1	0	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	84	84	1	-1	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	83	83	1	-2	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	82	82	1	-3	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	81	81	1	-4	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	80	80	1	-5	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	79	79	1	-6	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	78	78	1	-7	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	77	77	1	-8	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	76	76	1	-9	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	75	75	1	-10	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	74	74	1	-11	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	73	73	1	-12	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	72	72	1	-13	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	71	71	1	-14	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	70	70	1	-15	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	69	69	1	-16	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	68	68	1	-17	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	67	67	1	-18	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	66	66	1	-19	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	65	65	1	-20	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	64	64	1	-21	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	63	63	1	-22	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	62	62	1	-23	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	61	61	1	-24	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	60	60	1	-25	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	59	59	1	-26	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	58	58	1	-27	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	57	57	1	-28	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	56	56	1	-29	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	55	55	1	-30	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	54	54	1	-31	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	53	53	1	-32	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	52	52	1	-33	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	51	51	1	-34	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	50	50	1	-35	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	49	49	1	-36	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	48	48	1	-37	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	47	47	1	-38	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	46	46	1	-39	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	45	45	1	-40	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	44	44	1	-41	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	43	43	1	-42	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	42	42	1	-43	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	41	41	1	-44	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	40	40	1	-45	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	39	39	1	-46	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	38	38	1	-47	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	37	37	1	-48	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	36	36	1	-49	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	35	35	1	-50	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	34	34	1	-51	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	33	33	1	-52	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	32	32	1	-53	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	31	31	1	-54	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	30	30	1	-55	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	29	29	1	-56	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	28	28	1	-57	12	83	12	5	54	245	4	11	11	45	15	7	44	46	10	11	47	446	
1	1	27	27	1	-58	12	83	12</td																

DISORDERED CRYSTALS OF ADDUCTS OF DIPHENYLMERCURY

Table 5 (cont.)

H	K	F0	FC	H	K	F0	FC	H	K	F0	FC	H	K	F0	FC	H	K	F0	FC	H	K	F0	FL	
-2	8	74	79	11	1	49	204	5	3	102	109	1	9	48	58*	2	9	40	63*	10	1	43	12*	
-2	7	87	67	11	3	50	19*	5	3	102	81	1	11	47	53*	2	9	44	37*	10	3	43	12*	
-2	9	86	91	11	4	50	17*	5	7	102	81	1	13	43	23*	2	9	49	36*	10	7	42	14*	
-2	11	53	45*	11	7	50	17*	6	1	56	14*	2	2	1	104	100	9	11	43	25*	10	7	40	14*
-2	12	51	33*	11	8	50	17*	5	3	56	13*	2	3	2	98	93	6	11	57	78*	10	9	35	21*
-3	3	118	104	12	3	51	61*	5	3	56	13*	2	3	2	98	93	6	11	57	78*	11	3	42	35*
-3	4	104	100	12	5	50	57*	6	7	49	11*	2	7	2	74	74	6	7	49	93*	11	9	40	46*
-3	5	99	82	13	1	50	18*	6	9	49	8*	3	3	1	42	48*	6	7	49	93*	11	1	33	16*
-3	6	97	80	13	3	50	18*	6	11	49	8*	3	3	3	42	48*	6	7	49	93*	11	3	35	10*
-3	7	97*	80	13	7	48	14*	6	13	49	8*	3	3	3	42	48*	7	1	42	48*	11	7	40	14*
-3	8	51	43*	13	9	48	14*	7	3	47	98*	2	9	47	44*	2	9	44	61*	12	7	34	9*	
-3	9	50	43*	13	9	48	11*	7	3	68	93	2	9	47	27*	2	8	3	42	13*	13	3	37	8*
-4	0	125	81	14	1	49	49*	7	5	72	108	2	4	1	108	93	8	11	43	55*	13	1	37	26*
-4	1	80	74	14	3	48	49*	7	7	73	108	2	4	1	108	93	8	11	43	55*	13	3	37	26*
-4	2	82	72	14	3	48	49*	8	1	44	12*	2	4	4	93	93	9	11	43	55*	13	3	37	26*
-4	3	60	66	15	1	46	11*	8	3	44	12*	2	4	4	93	93	9	11	43	55*	13	3	37	26*
-4	4	66	62	15	3	45	49*	8	5	46	10*	9	3	3	53	51*	9	9	43	59*	14	3	33	14*
-4	5	65*	62	15	3	45	49*	8	7	46	10*	9	3	3	53	51*	9	9	43	59*	14	3	33	14*
-4	6	96	104	15	1	41	34*	8	9	46	8*	9	3	3	42	48*	9	7	42	48*	11	9	43	59*
-4	7	97*	80	15	3	40	34*	8	11	46	8*	9	3	3	42	48*	9	7	42	48*	11	7	40	14*
-4	8	51	43*	15	3	40	34*	8	13	46	8*	9	3	3	42	48*	9	7	42	48*	11	3	35	10*
-4	9	50	43*	15	3	40	34*	8	15	46	8*	9	3	3	42	48*	9	7	42	48*	11	3	35	10*
-4	10	101	80	16	3	38	38*	8	11	46	8*	9	3	3	42	48*	9	7	42	48*	11	3	35	10*
-4	11	80	76	16	3	38	38*	8	13	37	44*	9	9	47	55*	10	3	45	55*	11	3	35	10*	
-4	12	81	76	16	3	38	38*	8	15	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	13	81	76	16	3	38	38*	8	17	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	14	81	76	16	3	38	38*	8	19	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	15	81	76	16	3	38	38*	8	21	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	16	81	76	16	3	38	38*	8	23	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	17	81	76	16	3	38	38*	8	25	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	18	81	76	16	3	38	38*	8	27	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	19	81	76	16	3	38	38*	8	29	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	20	81	76	16	3	38	38*	8	31	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	21	81	76	16	3	38	38*	8	33	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	22	81	76	16	3	38	38*	8	35	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	23	81	76	16	3	38	38*	8	37	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	24	81	76	16	3	38	38*	8	39	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	25	81	76	16	3	38	38*	8	41	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	26	81	76	16	3	38	38*	8	43	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	27	81	76	16	3	38	38*	8	45	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	28	81	76	16	3	38	38*	8	47	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	29	81	76	16	3	38	38*	8	49	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	30	81	76	16	3	38	38*	8	51	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	31	81	76	16	3	38	38*	8	53	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	32	81	76	16	3	38	38*	8	55	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	33	81	76	16	3	38	38*	8	57	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	34	81	76	16	3	38	38*	8	59	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	35	81	76	16	3	38	38*	8	61	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	36	81	76	16	3	38	38*	8	63	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	37	81	76	16	3	38	38*	8	65	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	38	81	76	16	3	38	38*	8	67	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	39	81	76	16	3	38	38*	8	69	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	40	81	76	16	3	38	38*	8	71	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	41	81	76	16	3	38	38*	8	73	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	42	81	76	16	3	38	38*	8	75	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	43	81	76	16	3	38	38*	8	77	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	44	81	76	16	3	38	38*	8	79	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	45	81	76	16	3	38	38*	8	81	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	46	81	76	16	3	38	38*	8	83	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	47	81	76	16	3	38	38*	8	85	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	48	81	76	16	3	38	38*	8	87	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	49	81	76	16	3	38	38*	8	89	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	50	81	76	16	3	38	38*	8	91	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	51	81	76	16	3	38	38*	8	93	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	52	81	76	16	3	38	38*	8	95	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	53	81	76	16	3	38	38*	8	97	37	44*	10	3	45	55*	11	3	45	55*	11	3	35	10*	
-4	54	81	76	16	3	38	38*	8	99	37	44*	10	3	45	55*	11	3	45	55*	11	3</td			

positive or negative regions at ligand atom positions as each ligand was added to the calculation.

Phenyl groups are located immediately above and below each mercury atom, and overlap for mercury atoms in the $y=\frac{1}{4}$ and $\frac{3}{4}$ planes. Difference Fourier syntheses indicate that the appropriate monoclinic space group is Pm , having mirror planes in (020). Ph_2Hg moieties in $y=\frac{1}{4}$ and $\frac{3}{4}$ were given half-occupancy and a subsequent difference synthesis had a larger peak in $y=0$ at $x>\frac{1}{2}$ [Fig. 5(a)], and in $y=\frac{1}{2}$ at $x<\frac{1}{2}$ than previously. Packing requirements again indicate the presence of partial occupancy for the Ph_2Hg moieties with mercury atoms in (020), and best agreement between calculated and observed structure factors was obtained with Ph_2Hg occupancies of 0.8 and 0.2, as found for $\text{Ph}_2\text{Hg}(\text{tmp})_2$.

This model has a unit cell with the required number of four formula units of $\text{Ph}_2\text{Hg}(\text{dmp})_2$, and for structure factors calculated for space group Pm , $R=0.16$ for both the 1331 sharp reflexions and the 537 diffuse reflexions, and 0.24 when 1981 unobserved reflexions are included. The structure factor list (Table 5) includes both $hk0$ and $h\bar{k}0$ reflexions, which must be identical for Pm symmetry, to indicate their similarity. Refinement was not attempted with 150 atoms in the asymmetric unit of space group Pm (232 in $P1$). Tables 6, 7 and 8 show the atomic coordinates, bond lengths and bond angles in $\text{Ph}_2\text{Hg}(\text{dmp})_2$.

Table 6. Coordinates of atoms of $\text{Ph}_2\text{Hg}(\text{dmp})_2$ within the asymmetric unit of space group Pm

The atom numbering scheme is similar to that of $\text{Ph}_2\text{Hg}(\text{tmp})_2$ (Fig. 2), with methyl groups having carbon atoms C(15) and C(16) and phenyl groups commencing with C(17) and C(23).

	x/a	y/b	z/c	Occupancy
Mercury positions				
Hg(1)	0.25	0.25	0.75	0.5
Hg(2)	0.75	0.25	0.1196*	0.5
Hg(3)	0.0433	0	0.25	0.8
Hg(4)	0.5433	0.50	0.6196†	0.8
Hg(5)	0.5433	0	0.6196†	0.2
Hg(6)	0.0433	0.50	0.25	0.2

* Given as ca. $\frac{1}{8}$ in discussing the structure solution.

† Given as ca. $\frac{3}{8}$ in discussing the structure solution.

Ligand coordinated to Hg(1)

N(1)	0.0683	0.25	0.8179	1.0
N(10)	0.0958	0.25	0.6384	1.0
C(2)	0.0500	0.25	0.9107	1.0
C(3)	-0.0417	0.25	0.9375	1.0
C(4)	-0.1083	0.25	0.8804	1.0
C(5)	-0.1667	0.25	0.7357	1.0
C(6)	-0.1458	0.25	0.6429	1.0
C(7)	-0.0433	0.25	0.5179	1.0
C(8)	0.0417	0.25	0.4875	1.0
C(9)	0.1200	0.25	0.5429	1.0
C(11)	0.0125	0.25	0.6679	1.0
C(12)	-0.0067	0.25	0.7571	1.0
C(13)	-0.0917	0.25	0.7857	1.0
C(14)	-0.0583	0.25	0.6125	1.0
C(15)	0.1167	0.25	0.9777	1.0
C(16)	0.2125	0.25	0.5134	1.0

Table 6 (cont.)

	x/a	y/b	z/c	Occupancy
Ligand coordinated to Hg(2)				
N(1)	0.6000	0.25	0.2321	1.0
N(10)	0.5800	0.25	0.0491	1.0
C(2)	0.6117	0.25	0.3214	1.0
C(3)	0.5433	0.25	0.3804	1.0
C(4)	0.4583	0.25	0.3446	1.0
C(5)	0.3583	0.25	0.2161	1.0
C(6)	0.3467	0.25	0.1250	1.0
C(7)	0.4033	0.25	-0.0232	1.0
C(8)	0.4750	0.25	-0.0768	1.0
C(9)	0.5633	0.25	-0.0393	1.0
C(11)	0.5050	0.25	0.1071	1.0
C(12)	0.5167	0.25	0.1964	1.0
C(13)	0.4433	0.25	0.2536	1.0
C(14)	0.4167	0.25	0.0714	1.0
C(15)	0.7000	0.25	0.3571	1.0
C(16)	0.6333	0.25	-0.0982	1.0
Ligand coordinated to Hg(3)				
N(1)	0.1917	0	0.1339	1.0
N(10)	0.2133	0	0.3250	1.0
C(2)	0.1733	0	0.0446	1.0
C(3)	0.2500	0	-0.0089	1.0
C(4)	0.3333	0	0.0268	1.0
C(5)	0.4250	0	0.1518	1.0
C(6)	0.4500	0	0.2500	1.0
C(7)	0.3792	0	0.3982	1.0
C(8)	0.3125	0	0.4553	1.0
C(9)	0.2292	0	0.4196	1.0
C(11)	0.2833	0	0.2678	1.0
C(12)	0.2667	0	0.1741	1.0
C(13)	0.3417	0	0.1205	1.0
C(14)	0.3700	0	0.3071	1.0
C(15)	0.0833	0	0.0089	1.0
C(16)	0.1458	0	0.4732	1.0
Ligand coordinated to Hg(4)				
N(1)	0.7233	0.5	0.5464	1.0
N(10)	0.6967	0.5	0.7321	1.0
C(2)	0.7500	0.5	0.4554	1.0
C(3)	0.8367	0.5	0.4241	1.0
C(4)	0.9017	0.5	0.4839	1.0
C(5)	0.9517	0.5	0.6304	1.0
C(6)	0.9333	0.5	0.7277	1.0
C(7)	0.8333	0.5	0.8464	1.0
C(8)	0.7500	0.5	0.8839	1.0
C(9)	0.6717	0.5	0.8250	1.0
C(11)	0.7800	0.5	0.6982	1.0
C(12)	0.8000	0.5	0.6027	1.0
C(13)	0.8800	0.5	0.5714	1.0
C(14)	0.8500	0.5	0.7571	1.0
C(15)	0.6750	0.5	0.4018	1.0
C(16)	0.5767	0.5	0.8536	1.0
Atoms of ligand coordinated to Hg(5) have coordinates of atoms of ligand coordinated to Hg(3) + 0, $\frac{1}{2}$, 0 and occupancy 1.0.				
Atoms of ligand coordinated to Hg(6) have coordinates of atoms of ligand coordinated to Hg(4) + 0, $\frac{1}{2}$, 0 and occupancy 1.0.				
Phenyl groups bonded to Hg(1)				
C(17)	0.25	0.3967	0.75	0.5
C(18)	0.3283	0.4467	0.7571	0.5
C(19)	0.3283	0.5433	0.7571	0.5
C(20)	0.25	0.5933	0.75	0.5
C(21)	0.1767	0.5433	0.7429	0.5
C(22)	0.1767	0.4467	0.7429	0.5
C(23)	0.25	0.1033	0.75	0.5

Table 6 (cont.)

	<i>x/a</i>	<i>y/b</i>	<i>z/c</i>	Occupancy
C(24)	0.1767	0.0533	0.7429	0.5
C(25)	0.1767	-0.0433	0.7429	0.5
C(26)	0.25	-0.0933	0.75	0.5
C(27)	0.3283	-0.0433	0.7571	0.5
C(28)	0.3283	0.0533	0.7571	0.5
Phenyl groups bonded to Hg(2)				
C(17)	0.75	0.3967	0.1196	0.5
C(18)	0.8283	0.4467	0.1196	0.5
C(19)	0.8283	0.5433	0.1196	0.5
C(20)	0.75	0.5933	0.1196	0.5
C(21)	0.6733	0.5433	0.1196	0.5
C(22)	0.6733	0.4467	0.1196	0.5
C(23)	0.75	0.1033	0.1196	0.5
C(24)	0.6733	0.0533	0.1196	0.5
C(25)	0.6733	-0.0433	0.1196	0.5
C(26)	0.75	-0.0933	0.1196	0.5
C(27)	0.8283	-0.0433	0.1196	0.5
C(28)	0.8283	0.0533	0.1196	0.5
Phenyl groups bonded to Hg(3)				
C(17)	0.0433	0.1467	0.2500	0.8
C(18)	-0.0417	0.1967	0.2500	0.8
C(19)	-0.0417	0.2933	0.2500	0.8
C(20)	0.0433	0.3433	0.2500	0.8
C(21)	0.1167	0.2933	0.2500	0.8
C(22)	0.1167	0.1967	0.2500	0.8
Phenyl groups bonded to Hg(4)				
C(17)	0.5433	0.6467	0.6196	0.8
C(18)	0.4633	0.6967	0.6161	0.8
C(19)	0.4633	0.7933	0.6161	0.8
C(20)	0.5433	0.8433	0.6196	0.8
C(21)	0.6233	0.7933	0.6232	0.8
C(22)	0.6233	0.6967	0.6232	0.8

Atoms of phenyl groups bonded to Hg(5) have coordinates of the phenyl groups of Hg(3)+0, $\frac{1}{2}$, 0 and occupancy of 0.2.

Atoms of phenyl groups bonded to Hg(6) have coordinates of the phenyl groups of Hg(4)+0, $\frac{1}{2}$, 0 and occupancy of 0.2.

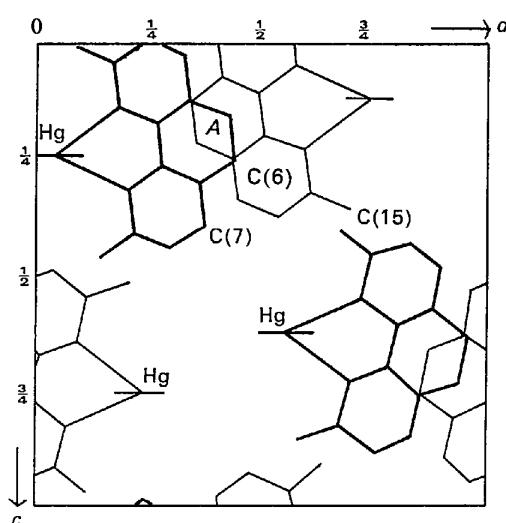


Fig. 6. Projection of the structure of $\text{Ph}_2\text{Hg}(\text{dmp})_2$ onto (010). The ligand and Ph_2Hg moieties in (020) are shown by bold lines.

Table 7. Bond lengths in $\text{Ph}_2\text{Hg}(\text{dmp})_2$

(a) Mercury stereochemistry				
	Hg(1)	Hg(2)	Hg(3)	Hg(4)
Hg-N(1)	2.97 Å	2.83 Å	2.84 Å	2.97 Å
Hg-N(10)	2.88	2.82	2.84	2.88
Hg-C(17)	2.10	2.10	2.10	2.10
Hg-C(23)	2.10	2.10		
(b) Ligands				
	Hg(1)	Hg(2)	Hg(3)	Hg(4)
N(1)—C(2)	1.38 Å	1.31 Å	1.33 Å	1.39 Å
N(1)—C(12)	1.46	1.39	1.30	1.44
C(2)—C(3)	1.47	1.36	1.42	1.41
C(3)—C(4)	1.32	1.41	1.39	1.33
C(4)—C(13)	1.40	1.34	1.37	1.32
C(5)—C(6)	1.39	1.34	1.48	1.44
C(5)—C(13)	1.37	1.42	1.36	1.40
C(6)—C(14)	1.42	1.33	1.49	1.35
C(7)—C(8)	1.38	1.35	1.32	1.40
C(7)—C(14)	1.40	1.39	1.33	1.33
C(8)—C(9)	1.45	1.47	1.39	1.48
C(9)—N(10)	1.44	1.31	1.40	1.41
N(10)—C(11)	1.35	1.43	1.36	1.38
C(11)—C(12)	1.33	1.31	1.39	1.42
C(11)—C(14)	1.36	1.46	1.45	1.38
C(12)—C(13)	1.38	1.41	1.40	1.32
C(2)—C(15)	1.42	1.46	1.48	1.40
C(9)—C(16)	1.49	1.38	1.50	1.52
(c) Phenyl groups				
	For Hg(1)	For Hg(2)	For Hg(3)	For Hg(4)
C(17)—C(18)	1.41 Å	1.40 Å	1.34 Å	1.43 Å
C(17)—C(22)	1.34	1.38	1.49	1.43
C(18)—C(19)	1.38	1.38	1.38	1.38
C(19)—C(20)	1.41	1.40	1.34	1.43
C(20)—C(21)	1.34	1.38	1.49	1.43
C(21)—C(22)	1.38	1.38	1.38	1.38
C(23)—C(24)	1.34	1.38		
C(23)—C(28)	1.41	1.40		
C(24)—C(25)	1.38	1.38		
C(25)—C(26)	1.34	1.38		
C(26)—C(27)	1.41	1.40		
C(27)—C(28)	1.38	1.38		

In both structure determinations all atoms were given isotropic temperature factors of 3.0 Å² and scattering factors given by Cromer & Waber (1965) were used. No corrections were made for anomalous dispersion. The full-matrix least-squares program used was that of Busing & Levy (1962) modified by White (1965) to operate on the Monash University CDC 3200 computer. The function minimized was $\sum_{hkl} w_{hkl}(|F_o| - |kF_c|^2)$

for which all reflexions were given unit weight and an overall scale used. Unobserved reflexions were assigned an arbitrary intensity value of one-half of the weakest observed reflexions. The Fourier program was written by White (1965). Powder photographs were obtained using a Philips Debye-Scherrer 114.6 mm powder camera with nickel-filtered Cu K α radiation.

(a) The superposition structures

Within their respective unit cells, each adduct has two ligands in each (040) plane with Ph_2Hg moieties in

Table 8. Bond angles in $\text{Ph}_2\text{Hg}(\text{dmp})_2$

(a) Mercury stereochemistry

	Hg(1)	Hg(2)	Hg(3)	Hg(4)
N(1)—Hg—N(10)	54°	57°	59°	56°
C(17)—Hg—C(23)	90	90		
N(1), N(10)—Hg—C(17), C(23)	90	90		

(b) Ligands

	Ligands coordinated to:			
	Hg(1)	Hg(2)	Hg(3)	Hg(4)
Hg—N(1)—C(2)	121°	117°	114°	128°
Hg—N(1)—C(12)	123	123	117	124
C(2)—N(1)—C(12)	116	120	129	107
N(1)—C(2)—C(3)	117	121	111	126
N(1)—C(2)—C(15)	122	119	123	107
C(3)—C(2)—C(15)	121	120	126	127
C(2)—C(3)—C(4)	126	119	125	120
C(3)—C(4)—C(13)	118	122	117	116
C(6)—C(5)—C(13)	109	120	125	117
C(5)—C(6)—C(14)	122	118	109	120
C(8)—C(7)—C(14)	118	117	123	124
C(7)—C(8)—C(9)	128	123	119	122
N(10)—C(9)—C(8)	109	123	122	110
N(10)—C(9)—C(16)	122	117	111	122
C(8)—C(9)—C(16)	129	120	127	129
Hg—N(10)—C(9)	109	123	123	109
Hg—N(10)—C(11)	127	123	120	124
C(9)—N(10)—C(11)	123	115	117	127
N(10)—C(11)—C(12)	121	118	117	123
N(10)—C(11)—C(14)	125	123	119	121
C(12)—C(11)—C(14)	114	119	124	116
N(1)—C(12)—C(11)	115	120	127	112
N(1)—C(12)—C(13)	125	122	119	125
C(11)—C(12)—C(13)	120	118	113	123
C(4)—C(13)—C(5)	112	122	115	113
C(4)—C(13)—C(12)	118	116	119	125
C(5)—C(13)—C(12)	130	121	127	122
C(6)—C(14)—C(7)	118	117	118	120
C(6)—C(14)—C(11)	125	123	123	123
C(7)—C(14)—C(11)	117	119	119	117

(c) Phenyl groups

	For Hg(1)	For Hg(2)	For Hg(3)	For Hg(4)
Hg—C(17)—C(18)	121°	121°	119°	120°
Hg—C(17)—C(22)	122	121	122	120
C(18)—C(17)—C(22)	117	118	119	120
C(17)—C(18)—C(19)	121	121	119	120
C(18)—C(19)—C(20)	121	121	119	120
C(19)—C(20)—C(21)	117	118	119	120
C(20)—C(21)—C(22)	122	121	122	120
C(17)—C(22)—C(21)	122	121	122	120
Hg—C(23)—C(24)	122	121		
Hg—C(23)—C(28)	121	121		
C(24)—C(23)—C(28)	117	118		
C(23)—C(24)—C(25)	122	121		
C(24)—C(25)—C(26)	122	121		
C(25)—C(26)—C(27)	117	118		
C(26)—C(27)—C(28)	121	121		
C(23)—C(28)—C(27)	121	121		

position for coordination of each ligand to form a 1:1 complex [Figs. 4 and 6]. Every second (040) plane has 0.5 occupancy for two Ph_2Hg moieties, and every other (040) plane has 0.8 and 0.2 occupancy for two Ph_2Hg moieties in that plane, giving one Ph_2Hg for every two ligands.

Molecular groups are packed at approximately van

der Waals distances from each other, with ligand planes separated by 3.63 Å in $\text{Ph}_2\text{Hg}(\text{tmp})_2$ and 3.57 Å in $\text{Ph}_2\text{Hg}(\text{dmp})_2$. Methyl groups in adjacent planes have slightly different x and z coordinates allowing closer approach in the b direction, but their x and z coordinates are closer in $\text{Ph}_2\text{Hg}(\text{tmp})_2$ than in $\text{Ph}_2\text{Hg}(\text{dmp})_2$, possibly accounting for the greater distance between planes in $\text{Ph}_2\text{Hg}(\text{tmp})_2$.

Excluding Hg—N distances closest approaches of adjacent mercury and/or ligand carbon atoms in the same (040) plane are 4.17 Å [C(16)—C(18)] and 3.66 Å [C(16)—Hg] in $\text{Ph}_2\text{Hg}(\text{tmp})_2$ [Fig. 4(a)], and 4.10 Å [C(6)—C(15) and C(7)—Hg] in $\text{Ph}_2\text{Hg}(\text{dmp})_2$ (Fig. 6).

(b) The structures of possible ordered regions

The derivation of possible ordered regions from the superposition structure must account for the diffuse lines and Ph_2Hg occupancies. With this requirement, the superposition structure can be most readily discussed in terms of disorder arising from a channel structure similar to the urea-di-n-alkylmercury inclusion compounds.

Inspection of a projection diagram of $\text{Ph}_2\text{Hg}(\text{dmp})_2$ (Fig. 6) and Fig. 4 indicate that for both adducts there are channels through the ligand structure perpendicular to the planes containing the ligands, and that the channels have appropriate dimensions to allow inclusion of Ph_2Hg moieties aligned with the C—Hg—C unit along the [010] direction. A random distribution of Ph_2Hg moieties, with the constraint that weak Hg—N interaction causes the mercury atoms to lie in (040), would lead to the presence of diffuse lines but without maxima in the lines since this structure would have cell dimensions $a, \frac{1}{2}b, c$. Some degree of ordering of Ph_2Hg occupancies in (020) causes the appearance of maxima in the lines, which have been used to determine occupancies in these planes.

Disordering of crystals is consistent with the solution stability of the adducts. The adducts are completely dissociated in benzene and this may indicate that crystal growth occurs by addition of ligand and Ph_2Hg moieties, rather than addition of complexes. Failure of a Ph_2Hg molecule to add to the growth plane would hardly affect the packing of ligand groups, since the presence of Ph_2Hg does not affect the distance between planes, and the ligands themselves are fairly closely packed in the (040) planes (Fig. 6), and thus mistakes may occur readily with a new ordered region extending from each mistake in crystal growth. A possible ordered region containing one Ph_2Hg moiety in each (040) plane is illustrated in Fig. 7. Ordered regions of this structure have space group P1 for both adducts.

There is no apparent reason why the crystals of each adduct selected for structure determination have the same set of occupancies for Ph_2Hg moieties in (040) when the disorder is explained by either a channel structure or ordered regions related by translations of $\frac{1}{2}b$. One possible explanation is that the composition of each channel is influenced, but not determined, by the

composition of neighbouring channels during crystal growth (channel model), or that mistakes during crystal growth have a fixed probability for each adduct. The close similarity of each model is apparent since mistakes in addition of Ph_2Hg moieties give essentially the same result – either a new ordered region displaced by $\frac{1}{2}b$ with ligand positions coincident, or a new channel with Ph_2Hg positions displaced by $\frac{1}{2}b$ but with ligand positions unaltered.

(c) *Twining of disordered crystals of $\text{Ph}_2\text{Hg}(\text{tmp})_2$*

Preliminary X-ray photographs indicated that disordered crystals of $\text{Ph}_2\text{Hg}(\text{tmp})_2$ readily form twins, with components related by a mirror plane in a^*b . Fig. 8 indicates that reflection in this plane followed by translation in ac leads to perfect coincidence of atom positions within the unit cell of one component.

(d) *Symmetry of the molecular packing*

The requirements for reflexions to be observed for $\text{Ph}_2\text{Hg}(\text{dmp})_2$, none of which are required for space group Pm , are explained from the molecular packing. The requirement $hk0:h+k=2n$ results from the presence of an n glide in projection on (001), and the requirement $00l:l=2n$ results from every ab plane having a neighbouring plane $\frac{1}{2}c$ removed containing exactly the same total contribution of C, N, and Hg electron density to the structure factor expression for Pm . The requirement $0k0:k=4n$ results from a similar situation in all ac planes separated by $\frac{1}{4}b$, even though a fourfold screw axis which normally causes this requirement is not present. Inspection of Weissenberg photographs of twinned crystals of $\text{Ph}_2\text{Hg}(\text{tmp})_2$ (the data crystal was only mounted about b) reveals the requirement $0k0:k=4n$ for the components, but since there is no periodicity of $\frac{1}{2}c$ in content of ab planes (Fig. 4) the requirement $001:l=2n$ does not occur.

If the origin of the unit cell is moved to A and translated $\frac{1}{2}b$ for both superposition structures [Fig. 4(a) and Fig. 6] maintaining the directions of axes as before, then atom positions conform to $P\bar{1}$, although atoms of different occupancy are related by centres of inversion.

The molecular structure

In both adducts the C–Hg–C unit of the diphenylmercury moieties is linear, as in the parent mercurial. Mercury–nitrogen distances are 2.8–3.0 Å for both adducts. For ligands having mercury atoms close to their nitrogen atoms the N–Hg–N angle is ca. 54–59°. Since the accuracy of Hg–N distances determined from difference Fourier syntheses is uncertain, it is not possible to ascertain whether the nitrogen atoms are definitely within the sum of van der Waals radii from mercury (3.0 Å with mercury radius of 1.50 Å, or 3.23 Å with the upper limit of 1.73 Å suggested by Grdenic (1965) as a criterion to indicate some form of bonding) and thus whether a mercury–nitrogen interaction is present in the adducts.

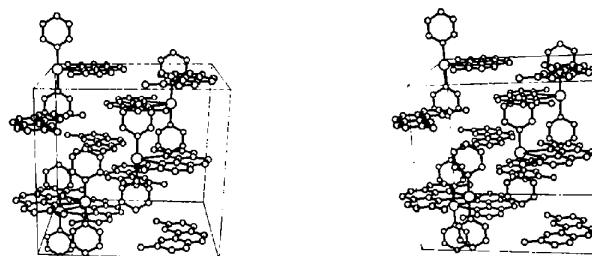


Fig. 7. Stereoscopic illustration of a possible ordered cell of $\text{Ph}_2\text{Hg}(\text{dmp})_2$ containing a 1:1 'complex' and uncoordinated ligand in each (040) plane. The unit cell is viewed almost normal to (001). The figure was drawn by a Fortran thermal ellipsoid plot program for crystal structure illustrations (Johnson, 1965).

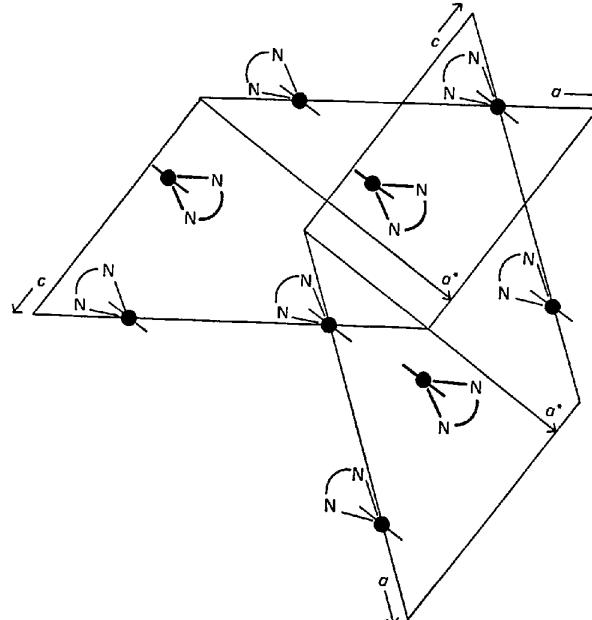


Fig. 8. Orientation of components of twinned crystals of $\text{Ph}_2\text{Hg}(\text{tmp})_2$. The (010) projection is shown with ligand and Ph_2Hg moieties in (020) drawn with bold lines.

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