1122. *Complexes of Mercury. Part I. X-Ray Analysis of 1,6-Dithiacyclodeca-*cis-3,cis-8-*dienebis(mercuric Chloride)*

By K. K. Cheung and G. A. Sim

1,6-Dithiacyclodeca-*cis*-3,*cis*-8-dienebis(mercuric chloride) crystallises in the monoclinic system, space group $P2_1/m$, with two molecules of $C_8H_{12}S_2Hg_2Cl_4$ in a cell of dimensions $a = 7{\cdot}29$, $b = 17{\cdot}01$, $c = 6{\cdot}20$ Å, $\beta = 92°\ 43'$. One mercury atom, Hg(2), is tetrahedrally co-ordinated by two sulphur atoms at 2·53 Å and two chlorine atoms, Cl(2) and Cl(3), at 2·51 Å. The other mercury atom, Hg(1), is in an only slightly distorted mercuric chloride molecule with Hg–Cl bond length of 2·30 Å and $Cl(1)Hg(1)Cl(1)_{V}$ * valency angle of 168°. A very distorted tetrahedral co-ordination around Hg(1) is completed by $Cl(2)_{I}$ and $Cl(3)_{II}$ at 3·02 and 2·93 Å, respectively, with $Cl(2)_{I}Hg(1)Cl(3)_{II}$ angle of 92°. When $Cl(2)_{II}$ and $Cl(3)_{III}$ at 3·21 and 4·44 Å, respectively, are also considered, the co-ordination of Hg(1) can be described as distorted octahedral. The relationship of valency angles and bond lengths to hybridisation in mercury(II) complexes is discussed.

It is generally accepted that the bonding in most mercury(II) compounds has appreciable covalent character.[1-3] One notable feature of covalent bonding is the variation of single-bond atomic radius with the state of hybridisation; for example, in the case of carbon, single-bond covalent radii for sp^3, sp^2, and sp hybridised states are about 0·77, 0·74, and

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* For explanation of the subscripts see Table 2.

[1] J. D. Dunitz and L. E. Orgel, *Adv. Inorg. Chem. Radiochem.*, 1960, **2**, 1.

[2] R. S. Nyholm, *Proc. Chem. Soc.*, 1961, 273.

[3] F. A. Cotton and G. Wilkinson, "Advanced Inorganic Chemistry," Interscience, New York, 1962.

0·69 Å, respectively.[4] In our investigation of the crystal structure of the alkaloid salt, perloline tetrachloromercurate(II), we obtained an Hg–Cl separation of 2·50 Å for the tetrahedral $HgCl_4^{2-}$ anion,[5] whereas the Hg–Cl bond length in the linear molecule CH_3HgCl is about 2·28 Å [6] and in the mercuric chloride–cyclohexane-1,4-dione adduct is 2·30 Å.[7] In the yellow modification of mercuric iodide [8] the mercury atom has two short collinear bonds of 2·62 Å, whereas in the red, low-temperature form [9] the mercury atom is tetrahedrally co-ordinated, with an Hg–I separation of 2·78 Å. The HgI_3^- ion in trimethylsulphonium tri-iodomercurate(II) is almost planar (the mercury atom thus uses orbitals which are almost sp^2) and the average Hg–I distance is 2·69 Å.[10] Mercuric sulphide is dimorphic; one form has the tetrahedrally co-ordinated sphalerite structure with d(Hg–S) = 2·53 Å and the other, cinnabar, contains nearly collinear (*i.e.*, *sp*) Hg–S bonds of length 2·36 Å.[11] These results demonstrate that the variation in bond lengths involving mercury(II) and a given type of ligand is appreciably greater than that shown by a light atom such as carbon. That the variation of bond length is a function of hybridisation type (degree of *s*-character of the bond) and not simply of co-ordination number is readily shown by examination of the interatomic distances in, for example, dichlorobisthioureamercury(II) [12] and dichlorobis(triphenylarsine oxide)mercury(II).[13] The comparison of mercury with a light atom such as carbon is complicated, of course, by the great importance of the ionic contribution in the longer metal–ligand bonds and the possible involvement of *d*-orbitals.

The preferred co-ordination number of an atom decreases as the separation between the energy levels of the orbitals involved in covalent bond formation increases; with a large *s*–*p* separation *sp*-hybridisation is more favoured than sp^2 or sp^3. The greater tendency of Hg^{2+}, compared with Cd^{2+} and Zn^{2+}, to form two short collinear bonds is attributable, at least in part, to the greater *s*–*p* separation in Hg^{2+}.[1,2] Bent has pointed out [14] that when a number of different substituents are covalently bonded to an atom the amount of *s*-character in the orbital directed towards a particular substituent is a function of the electronegativity of the substituent. Since *s*-electrons in an atom are held more tightly than *p*-electrons (*s*-electrons penetrate the inner core of electrons more than *p*-electrons do and hence experience a greater effective nuclear charge) it follows that if substituents of different electron-withdrawing power are attached to the atom it is more favourable energetically to have orbitals with greater than average *s*-character directed towards the least electron-withdrawing (most electropositive) substituents and orbitals with less than average *s*-character directed towards the most electron-withdrawing (most electronegative) substituents, rather than to have a set of entirely equivalent orbitals. Bent has discussed the geometry of a number of simple inorganic compounds in terms of this effect.[14] The greater the *s*–*p* energy separation the more marked the effect should be.

If the deviations from tetrahedral symmetry in a molecule MX_2Y_2, which, to a first approximation might be said to have covalent sp^3 bonds, are to be interpreted in terms of different degrees of *s*-character in the MX and MY bonds, the valency angles XMX (2θ) and YMY (2α) should be related by the equation $\tan\alpha = (1 - \cot^2\theta)^{-\frac{1}{2}}$. The mutual variation of 2θ and 2α is shown in Figure 1. In the case of metal complexes it is reasonable to ascribe deviations from ideal tetrahedral bonding in d^{10} ions to the electronegativity/

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[4] L. E. Sutton, *Tetrahedron*, 1959, **5**, 118; M. J. S. Dewar and H. N. Schmeising, *ibid.*, p. 166.

[5] J. A. D. Jeffreys, G. A. Sim, R. H. Burnell, W. I. Taylor, R. E. Corbett, J. Murray, and B. J. Sweetman, *Proc. Chem. Soc.*, 1963, 171.

[6] W. Gordy and J. Sheridan, *J. Chem. Phys.*, 1954, **22**, 92.

[7] P. Groth and O. Hassel, *Acta Chem. Scand.*, 1964, **18**, 1327.

[8] W. Gorskii, *Phys. Z. Sovietunion*, 1934, **5**, 367.

[9] J. M. Bijvoet, A. Classen, and A. Karssen, *Proc. k. ned. Akad. Wetenschap.*, 1926, **29**, 529.

[10] R. H. Fenn, J. W. Oldham, and D. C. Phillips, *Nature*, 1963, **198**, 381.

[11] K. L. Aurivillius, *Acta Chem. Scand.*, 1950, **4**, 1413.

[12] K. K. Cheung, R. S. McEwen, and G. A. Sim, *Nature*, 1965, **205**, 383.

[13] C.-I. Brändén, *Acta Chem. Scand.*, 1963, **17**, 1363.

[14] H. A. Bent, *J. Inorg. Nuclear Chem.*, 1961, **19**, 43.

hybridisation correlation, particularly if steric effects cannot reasonably be invoked. In dichlorobisthioureazinc,[15] for example, the SZnS and ClZnCl valency angles are 111·5 and 107·3°, respectively, satisfying the angular relationship given above to within 0·5° and corresponding to orbitals with 27% *s*-character directed towards the sulphur atoms and with 23% *s*-character directed towards the chlorine atoms (in ideal sp^3-bonding all four orbitals have 25% *s*-character); the *s*–*p* separation in Zn is about 7 ev and it is not unreasonable to ascribe greater electron-donor properties to the thiourea sulphur atom than to the chloride ion. In dichlorobis(triphenylarsine oxide)mercury(II) [13] the effect is particularly striking; the OHgO and ClHgCl valency angles are 92·5 and 146·5°, respectively, implying that the orbitals directed towards the chlorine atoms have 45·5% *s*-character while those directed towards the oxygen atoms have only 4·5% *s*-character. In keeping with these assignments the Hg–Cl distance in dichlorobis(triphenylarsine oxide)mercury(II) is 2·33 Å, only slightly longer than the value appropriate to *sp*-bonding, *ca.* 2·30 Å.

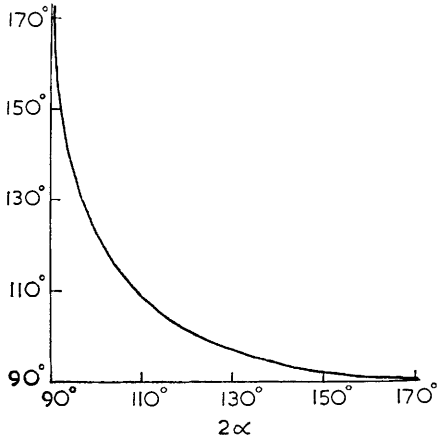
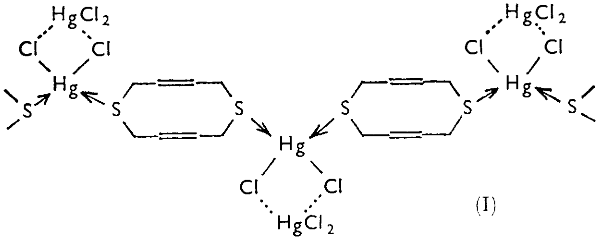


FIGURE 1. The mutual variation of the XMX (2θ) and YMY (2α) valency angles in a molecule MX_2Y_2 in which the valency orbitals of M are orthogonal *s*–*p* hybrids constructed from one *s* and three *p* orbitals

Because of the large *s*–*p* energy separation in mercury the hybridisation effect should play an important role in mercury complexes. It follows that, by judicious variation of the molecular and hence electronic structures of a given type of ligand (*e.g.*, sulphur derivatives), the correlation of mercury–ligand separation with hybridisation should be accessible to measurement in some detail. Accordingly, we have determined by *X*-ray-crystallographic methods the molecular structures of a number of complexes of mercury(II).[12]

1,6-Dithiacyclodeca-*cis*-3,*cis*-8-diene [16] forms a bis(mercuric chloride) complex on treatment with mercuric chloride in ethanol. We initially assumed that each mercury atom



(I)

in the complex would be in three-fold co-ordination and that a crystal-structure determination would therefore lead to a value for the Hg–Cl separation appropriate to sp^2-type bonds. In fact, the *X*-ray analysis shows that the complex has a polymeric structure of the type (I); one mercury atom is tetrahedrally co-ordinated by two sulphur and two

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[15] N. R. Kunchur and M. R. Truter, *J.*, 1958, 3478.
[16] G. Eglinton, I. A. Lardy, R. A. Raphael, and G. A. Sim, *J.*, 1964, 1154.

chlorine atoms while the other mercury atom is in an only slightly distorted mercuric chloride molecule.

The arrangement of molecules in the crystal as viewed in projections along the *a* and *c* axes is shown in Figure 2. The packing within one layer of mercury atoms and the attached chlorine and sulphur atoms is shown in Figure 3.

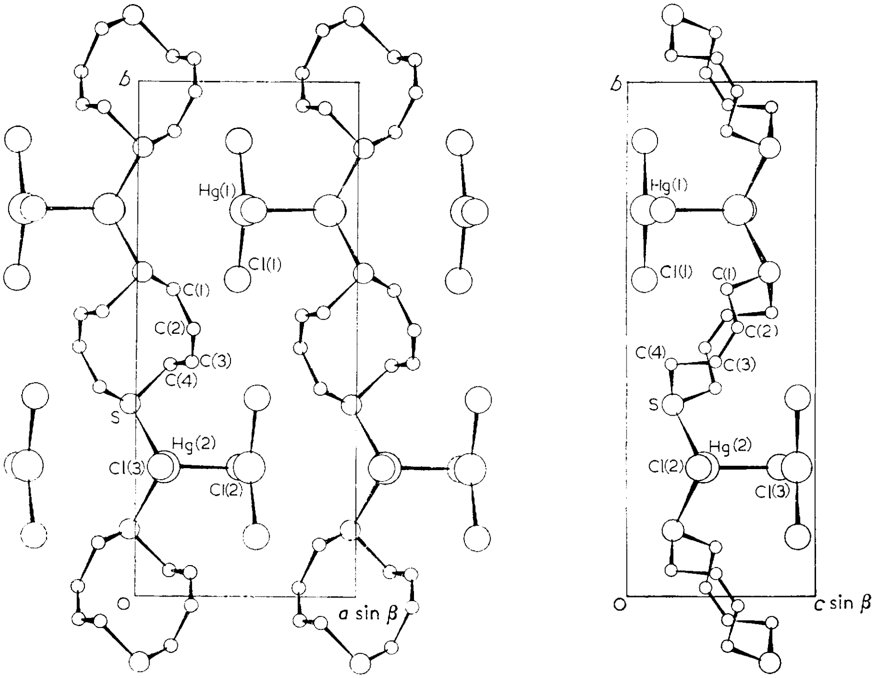

FIGURE 2a FIGURE 2b

FIGURE 2. The arrangement of molecules in the crystal as seen when viewed along (a) the *c*-axis, (b) the *a*-axis

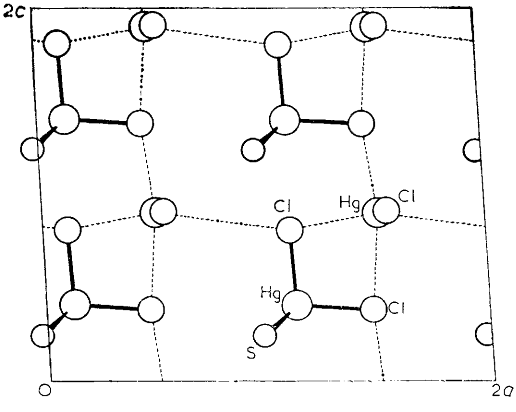

FIGURE 3. The packing of the atoms within one layer of mercury atoms and the attached chlorine and sulphur atoms

The atomic parameters were refined extensively by three-dimensional Fourier and least-squares methods; the final atomic co-ordinates and the estimated standard deviations of these co-ordinates are given in Table 1. The various interatomic distances and valency angles derived from the final atomic co-ordinates are listed in Table 2. The final electron-density distribution is shown in Figure 4 as superimposed contour sections drawn parallel to (001).

TABLE 1

Atomic co-ordinates and their standard deviations (Å)

Atom	x/a	$\sigma(x)$	y/b	$\sigma(y)$	z/c	$\sigma(z)$
Hg(1)	0·48740	0·002	0·75000	0	0·10023	0·003
Hg(2)	0·12956	0·002	0·25000	0	0·40675	0·003
Cl(1)	0·45384	0·011	0·61547	0·011	0·09586	0·014
Cl(2)	0·47042	0·014	0·25000	0	0·38134	0·017
Cl(3)	0·11405	0·016	0·25000	0	0·81076	0·022
S	−0·02476	0·009	0·37141	0·009	0·24616	0·012
C(1)	0·16419	0·036	0·59632	0·043	0·53083	0·050
C(2)	0·25480	0·039	0·51821	0·039	0·58579	0·054
C(3)	0·25100	0·036	0·45439	0·041	0·47044	0·053
C(4)	0·15541	0·038	0·44965	0·038	0·23401	0·054

TABLE 2

Interatomic distances (Å) and angles

Interatomic distances

C(4)–S	1·87	C(3)–C(4)	1·60	C(2) ··· C(1)$_{\mathrm{IX}}$	3·67
C(1)–S$_{\mathrm{IX}}$	1·84	C(3) ··· C(1)$_{\mathrm{IX}}$	3·15	C(3) ··· C(2)$_{\mathrm{IX}}$	3·72
C(1)–C(2)	1·52	C(4) ··· C(2)$_{\mathrm{IX}}$	3·29	C(3) ··· S$_{\mathrm{IX}}$	3·85
C(2)–C(3)	1·30				
Hg(1)–Cl(1)	2·30	C(4) ··· Hg(2)$_{\mathrm{VI}}$	3·57	Cl(3) ··· Cl(2)$_{\mathrm{VI}}$	3·81
Hg(2)–Cl(2)	2·50	C(3) ··· Hg(2)$_{\mathrm{VI}}$	3·60	C(2) ··· C(2)$_{\mathrm{VII}}$	3·83
Hg(2)–Cl(3)	2·51	C(2) ··· Cl(1)$_{\mathrm{VII}}$	3·63	C(1) ··· Cl(3)$_{\mathrm{III}}$	3·88
Hg(2)–S	2·53	C(3) ··· C(2)$_{\mathrm{VII}}$	3·67	Cl(1) ··· Cl(3)$_{\mathrm{II}}$	3·91
Hg(1) ··· Cl(3)$_{\mathrm{II}}$	2·93	C(3) ··· C(3)$_{\mathrm{VII}}$	3·95	Cl(1) ··· Cl(2)$_{\mathrm{II}}$	3·98
Hg(1) ··· Cl(2)$_{\mathrm{I}}$	3·02	S ··· Cl(1)$_{\mathrm{VIII}}$	3·70	Hg(2) ··· Hg(1)$_{\mathrm{IV}}$	4·04
Hg(1) ··· Cl(2)$_{\mathrm{II}}$	3·21	C(1) ··· Cl(2)$_{\mathrm{II}}$	3·75	Hg(1) ··· Hg(2)$_{\mathrm{I}}$	4·30
C(1) ··· Hg(2)$_{\mathrm{III}}$	3·41	Cl(1) ··· C(2)$_{\mathrm{X}}$	3·80	Hg(1) ··· S$_{\mathrm{VIII}}$	4·42
C(3) ··· Cl(1)$_{\mathrm{VII}}$	3·57	Cl(1) ··· Cl(2)$_{\mathrm{I}}$	3·80	Hg(1) ··· Cl(3)$_{\mathrm{III}}$	4·44

The subscripts here and in the text refer to the positions:

I	$1-x$,	$\frac{1}{2}+y$,	$-z$	VI	x,	$\frac{1}{2}-y$,	z
II	$1-x$,	$\frac{1}{2}+y$,	$1-z$	VII	$1-x$,	$1-y$,	$1-z$
III	$-x$,	$\frac{1}{2}+y$,	$1-z$	VIII	$-x$,	$1-y$,	$-z$
IV	$1-x$,	$-\frac{1}{2}+y$,	$1-z$	IX	$-x$,	$1-y$,	$1-z$
V	x,	$1\frac{1}{2}-y$,	z	X	x,	y,	$1+z$
				XI	$1+x$,	y,	z

Valency angles

C(1)C(2)C(3)	128°	Cl(2)Hg(2)Cl(3)	99°	Cl(3)Hg(1)$_{\mathrm{IV}}$Cl(2)$_{\mathrm{X}}$	92°
C(2)C(3)C(4)	123	SHg(2)Cl(2)	114	Cl(3)Hg(1)$_{\mathrm{IV}}$Cl(2)	76
C(3)C(4)S	106	SHg(2)Cl(3)	111	Cl(1)$_{\mathrm{IV}}$Hg(1)$_{\mathrm{IV}}$Cl(3)	96
C(2)C(1)S$_{\mathrm{IX}}$	110	SHg(2)S$_{\mathrm{VI}}$	109	Cl(1)$_{\mathrm{IV}}$Hg(1)$_{\mathrm{IV}}$Cl(2)	91
C(4)SC(1)$_{\mathrm{IX}}$	103	Cl(2)Hg(1)$_{\mathrm{IV}}$Cl(3)$_{\mathrm{XI}}$	86	Hg(2)Cl(2)Hg(1)$_{\mathrm{IV}}$	89
Cl(1)Hg(1)Cl(1)$_{\mathrm{V}}$	168	Cl(3)Hg(1)$_{\mathrm{IV}}$Cl(3)$_{\mathrm{XI}}$	162		

The environment of Hg(2) is not ideally tetrahedral; whereas the angle SHg(2)S$_{\mathrm{VI}}$ is 109°, the angle Cl(2)Hg(2)Cl(3) is only 99°. In this case the deviation of the angle Cl(2)Hg(2)Cl(3) from the tetrahedral value cannot be attributed to the hybridisation/electron-donor-capacity correlation, for there is no corresponding increase beyond tetrahedral of the angle SHg(2)S$_{\mathrm{VI}}$. The reduction of the angle Cl(2)Hg(2)Cl(3) from tetrahedral to 99° can probably be ascribed to the involvement of the chlorine atoms in bonding with Hg(1)$_{\mathrm{IV}}$; a value of 109° for Cl(2)Hg(2)Cl(3) would necessarily involve unreasonably small values for the other angles in the ring Cl(2)Hg(2)Cl(3)Hg(1)$_{\mathrm{IV}}$ (since the sum of the internal angles in a planar four-membered ring must equal 360°) and might bring the two non-bonded mercury atoms too close together. It is possible that we have here an example of bent bonds[17] with the chlorine atoms Cl(2) and Cl(3) displaced slightly from the sp^3-orbitals of Hg(2). The Hg(2)–Cl(2) and Hg(2)–Cl(3) distances of 2·50 and 2·51 Å, respectively, are in excellent agreement with the average Hg–Cl separation of 2·50 Å in the tetrahedral anion $HgCl_4^{2-}$.[5] The Hg(2)–S distance of 2·53 Å is in good agreement

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[17] W. H. Flygare, *Science*, 1963, **140**, 1179.

with the values of 2·53 Å in metacinnabarite [11] and 2·55 Å in bis(ethylenediamine)copper(II) tetrathiocyanatomercurate(II).[18]

The mercury atom Hg(1) is in an only slightly distorted mercuric chloride molecule. The Cl(1)Hg(1)Cl(1)$_V$ angle of 168° corresponds to mercury orbitals with 49·4% *s*-character, *i.e.*, very close to ideal *sp*-bonding, and the Hg–Cl distance of 2·30 Å does not differ significantly from the values reported for *sp*-Hg–Cl bonds.[6,7,19] The value of 168° for the angle Cl(1)Hg(1)Cl(1)$_V$ implies that the valency angle Cl(2)Hg(1)Cl(3)$_{II}$ should be 90·4° and the metal orbitals directed towards Cl(2)$_I$ and Cl(3)$_{II}$ should have 0·6% *s*-character; the experimental value for the angle is 92° and the Hg(1)–Cl(2)$_I$ and Hg(1)–Cl(3)$_{II}$ bridging distances of 3·02 and 2·93 Å, respectively, are in accord with the vanishingly small degree of *s*-character associated with these bonds (cf. values of 2·50 and 2·56 Å for Hg–Cl bonds of, respectively, 25% and 23% *s*-character [5,12]). When two other contacts Hg(1) · · · Cl(2)$_{II}$,

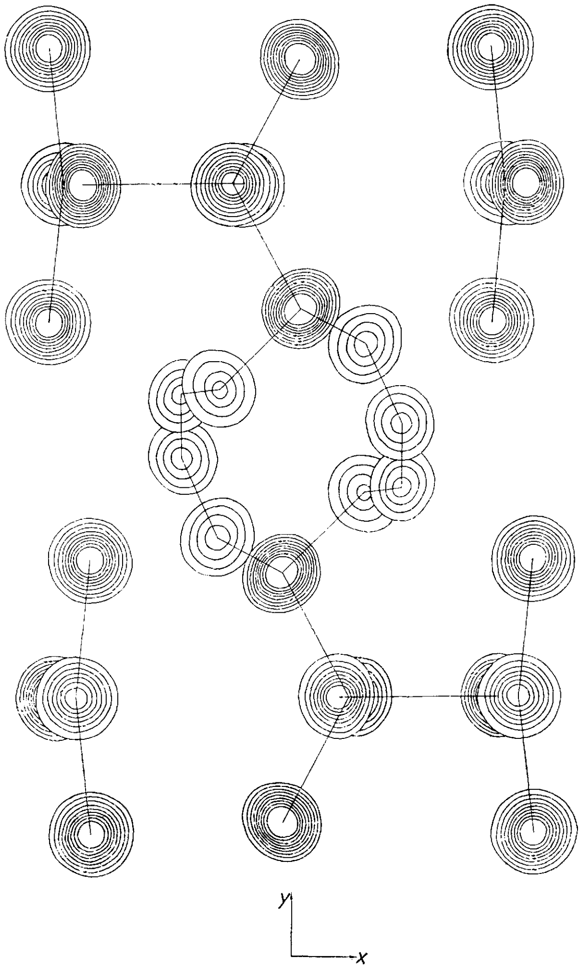

FIGURE 4. The final three-dimensional electron-density distribution shown by means of superimposed contour sections drawn parallel to (001). Contour interval 12 eÅ^{-3} around the mercury atoms, 2 eÅ^{-3} around the chlorine and sulphur atoms, and 1·5 eÅ^{-3} around the carbon atoms

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[18] H. Scouloudi, *Acta Cryst.*, 1953, **6**, 651.

[19] A. F. Wells, " Structural Inorganic Chemistry," Oxford University Press, Oxford, 1962.

TABLE 3

Measured and calculated values of the structure factors

h	k	l	F_o	F_c	h	k	l	F_o	F_c
0	1	4	87.0	112.9			4	37.6	38.7
0	2	2	37.4	-58.8	0	18	0	104.4	-97.9
		3	11.0	5.9			1	28.6	27.7
		4	89.8	138.1			2	23.0	-21.2
0	3	1	36.6	-41.8			4	31.0	41.5
		2	164.8	-226.8	0	19	1	10.3	9.6
		3	52.7	61.0			2	66.8	-72.0
		4	55.3	-63.9			3	21.7	27.4
0	4	0	190.9	256.1	0	20	0	79.2	74.8
		1	52.3	-61.5			1	22.5	-21.8
		2	76.6	92.0			2	28.3	32.2
		3	9.0	-4.8	0	21	2	46.2	67.0
		4	117.5	-140.9	1	0	0	18.6	-35.2
0	5	2	212.0	237.8			2	25.6	-15.9
		3	58.8	-57.2			3	70.9	-60.5
		4	84.5	88.4			4	117.6	116.0
0	6	0	281.4	-318.5			-1	126.9	-163.4
		1	7.6	5.1			-2	136.7	-138.1
		2	72.6	-77.1			-3	128.8	104.6
		3	27.2	28.3			-4	78.5	78.5
		4	112.1	122.7	1	1	0	72.6	-105.8
0	7	1	19.8	-16.9			1	48.8	-64.7
		2	246.1	-242.4			2	81.8	-95.7
		3	22.2	-23.1			3	177.7	-164.8
		4	89.8	-93.8			4	13.8	1.2
0	8	0	281.7	318.0			-1	212.9	256.3
		1	15.0	10.7			-2	65.4	62.5
		2	42.5	43.7			-3	170.2	144.2
		3	21.2	-14.7			-4	75.7	65.4
		4	114.4	-108.6	1	2	0	44.0	55.3
0	9	1	36.4	-26.8			1	183.6	206.2
		2	197.9	204.9			2	82.9	-82.5
		4	90.4	79.6			3	73.6	70.6
0	10	0	232.2	-218.2			4	76.6	-72.2
		1	32.3	27.3			-1	94.6	117.0
		2	38.9	-34.1			-2	103.9	113.6
		3	10.3	5.7			-3	123.6	-122.3
		4	87.5	79.5			-4	16.0	-11.8
0	11	2	163.7	-141.6	1	3	0	93.0	129.3
		3	54.2	41.3			1	43.3	-50.3
		4	55.7	-46.1			2	42.9	50.9
0	12	0	143.9	137.8			3	131.7	155.3
		1	39.7	-30.8			4	25.0	-24.2
		2	72.5	64.9			-1	101.7	-124.1
		4	92.7	-99.2			-2	22.6	15.4
0	13	1	24.6	18.3			-3	143.6	-142.7
		2	171.8	146.5			-4	53.1	-55.6
		3	57.6	-43.9	1	4	0	37.6	-49.5
		4	59.4	60.3			1	108.9	-164.7
0	14	0	187.1	-172.1			2	101.7	112.0
		1	14.4	9.6			3	42.4	-41.6
		2	60.7	-54.5			4	32.7	32.4
		3	21.7	15.7			-1	44.1	-69.1
		4	72.7	81.7			-2	54.1	-59.6
0	15	1	17.5	8.0			-3	77.6	82.7
		2	136.2	-126.5			-4	27.2	-29.3
		3	10.2	-10.1	1	5	0	105.9	-136.9
		4	57.9	-61.4			1	26.7	24.8
0	16	0	158.5	153.8			2	37.8	-45.9
		4	46.3	-53.6			3	127.9	-148.3
0	17	1	27.3	-22.8			-1	101.6	140.6
		2	94.7	96.2			-2	9.8	15.5

TABLE 3 (*Continued*)

h	*k*	*l*	F_o	F_c
		- 3	117.8	148.3
		- 4	28.2	35.3
1	6	0	43.3	50.8
		1	136.6	215.3
		2	54.1	- 64.5
		3	94.3	59.4
		4	62.9	- 70.1
		- 1	68.5	104.1
		- 2	68.1	86.4
		- 3	75.6	- 95.0
		- 4	11.8	- 19.3
1	7	0	52.5	61.4
		1	42.2	46.1
		2	77.2	81.2
		3	143.1	161.0
		4	13.1	- 12.0
		- 1	136.9	-191.6
		- 2	51.2	- 50.3
		- 3	108.9	-121.9
		- 4	59.2	- 63.9
1	8	0	35.7	- 33.9
		1	161.3	-182.2
		2	16.8	8.5
		3	56.9	- 53.5
		4	93.1	82.9
		- 1	106.5	-121.6
		- 2	102.4	- 99.1
		- 3	112.4	98.4
		- 4	50.0	51.8
1	9	0	81.1	- 79.7
		1	40.4	- 32.4
		2	66.3	- 62.8
		3	108.7	-100.4
		- 1	185.8	177.1
		- 2	18.5	14.8
		- 3	108.1	95.3
		- 4	51.5	42.7
1	10	0	10.5	3.0
		1	132.0	141.1
		2	60.6	- 51.5
		3	48.6	42.7
		4	60.7	- 58.6
		- 1	67.4	52.0
		- 2	110.4	83.9
		- 3	99.5	- 80.7
1	11	0	111.9	90.8
		1	26.2	- 20.8
		2	24.6	23.4
		3	103.6	95.4
		4	30.3	- 22.4
		- 1	126.7	- 99.6
		- 2	26.2	18.0
		- 3	113.8	- 89.0
		- 4	36.8	- 32.4
1	12	0	40.5	- 28.5
		1	125.0	-112.4
		2	91.6	78.1
		3	32.2	- 29.6
		4	27.2	17.7
		- 1	69.6	- 58.1
		- 2	36.1	- 26.5
		- 3	70.2	59.5
		- 4	29.5	- 20.3
1	13	0	56.2	- 48.6
		1	11.3	6.1
		2	34.2	- 26.9
		3	123.1	-117.5
		4	15.5	16.1
		- 1	97.2	73.8
		- 3	110.4	93.3
		- 4	33.2	30.3
1	14	0	46.1	32.7
		1	145.7	126.3
		2	56.6	- 40.8
		3	34.7	34.7
		4	39.8	- 38.8
		- 1	79.0	57.2
		- 2	61.5	43.6
		- 3	69.8	- 59.0
1	15	0	69.1	59.2
		1	17.6	11.4
		2	54.6	47.4
		3	82.7	80.0
		- 1	159.5	-123.5
		- 2	22.3	- 16.9
		- 3	78.9	- 71.4
		- 4	15.3	- 23.1
1	16	1	115.0	- 97.9
		2	16.6	13.4
		3	26.4	- 33.7
		4	47.0	48.7
		- 1	57.0	- 45.1
		- 2	80.5	- 59.2
		- 3	61.4	55.8
1	17	0	43.8	- 34.3
		1	27.2	- 17.3
		2	25.6	- 21.2
		3	45.9	- 50.1
		- 1	108.0	83.9
		- 3	40.3	38.4
		- 4	15.3	23.0
1	18	0	9.4	- 9.9
		1	72.7	62.9
		2	35.7	- 31.8
		3	19.8	21.3
		- 1	40.6	32.6
		- 2	35.3	34.5
		- 3	48.2	- 42.6
1	19	0	48.2	43.2
		1	9.0	- 8.5
		3	39.3	48.4
		- 1	66.9	- 52.7
		- 2	22.4	17.1
		- 3	38.2	- 40.2
1	20	0	11.8	- 7.8
		1	67.2	- 65.1
		2	42.9	40.6
		- 1	27.2	- 21.0
		- 2	14.0	- 16.3
		- 3	19.8	32.9
1	21	0	33.2	- 29.9
		- 1	49.8	42.1
2	0	0	146.8	187.3
		1	110.2	144.8

TABLE 3 (*Continued*)

h	*k*	*l*	F_o	F_c	*h*	*k*	*l*	F_o	F_c
		2	114.5	132.0			3	85.9	-96.1
		3	86.2	-81.3			4	92.2	-116.9
		4	19.1	-14.4			-1	14.8	-4.1
		-1	167.2	182.3			-2	135.1	161.5
		-2	151.3	-153.1			-3	82.0	96.6
		-3	58.0	39.5	2	8	0	118.8	162.3
		-4	135.2	-119.9			1	62.1	81.4
2	1	0	129.4	-178.3			2	85.9	118.1
		1	82.9	111.7			3	79.4	-90.6
		2	101.8	96.5			-1	68.3	95.1
		3	133.0	127.2			-2	83.9	-109.7
		4	127.6	116.5			-3	29.3	37.0
		-2	166.8	-175.3			-4	76.1	-84.4
		-3	121.6	-116.2	2	9	0	93.9	-126.1
		-4	16.2	17.9			1	72.7	91.4
2	2	0	160.7	-182.9			2	39.3	42.9
		1	35.8	-37.3			3	76.8	92.2
		2	155.5	-165.8			4	75.0	77.5
		3	119.9	111.6			-1	23.9	31.3
		4	22.7	22.8			-2	94.3	-122.6
		-1	68.5	-83.6			-3	63.8	-80.5
		-2	90.2	86.4			-4	17.7	17.7
		-3	72.8	-59.0	2	10	0	88.1	-79.4
		-4	123.8	108.7			1	14.9	-11.9
2	3	0	137.9	156.3			2	95.2	-92.6
		1	134.6	-166.9			3	70.1	68.8
		2	69.0	-64.4			-1	78.9	-87.8
		3	45.5	-40.3			-2	70.6	70.7
		4	87.9	-73.8			-3	51.2	-56.2
		-1	44.2	-41.8			-4	83.8	80.6
		-2	157.3	142.6	2	11	0	99.7	99.2
		-3	24.6	29.0			1	109.6	-104.5
2	4	0	37.3	48.3			2	52.5	-43.1
		1	8.4	6.7			3	16.0	-20.5
		2	142.4	150.8			4	49.6	-45.1
		3	90.0	-93.7			-1	31.0	-27.2
		4	42.0	-36.5			-2	89.3	82.0
		-1	127.1	132.5			-3	17.8	19.5
		-2	57.3	-58.2	2	12	0	53.9	44.9
		-3	72.7	67.3			1	7.4	1.3
		-4	108.4	-112.4			2	112.7	103.1
2	5	0	126.1	-163.2			3	74.0	-66.0
		1	126.2	166.2			4	22.1	-22.1
		2	76.1	75.9			-1	75.2	70.2
		3	44.8	51.5			-2	45.2	-33.7
		4	60.8	62.0			-3	52.3	43.4
		-1	16.6	-10.2			-4	81.3	-74.0
		-2	86.5	-100.2	2	13	0	92.4	-87.8
		-3	39.7	-45.2			1	106.5	98.6
		-4	14.3	10.8			2	50.5	38.7
2	6	0	102.3	-130.5			3	23.2	28.2
		1	45.0	-54.8			4	52.8	52.9
		2	125.6	-145.2			-1	11.9	-5.6
		3	74.6	77.9			-2	83.9	-72.4
		4	32.8	34.9			-3	41.6	-37.8
		-1	87.3	-120.0			-4	18.3	12.6
		-2	74.9	79.7	2	14	0	86.2	-63.4
		-3	35.3	-38.9			1	39.2	-31.4
		-4	103.6	115.5			2	97.6	-91.6
2	7	0	109.6	133.4			3	50.5	47.9
		1	63.4	-88.9			4	20.5	19.1
		2	77.4	-80.3			-1	101.7	-81.4

TABLE 3 (*Continued*)

h	k	l	F_o	F_c
		-2	68.3	52.2
		-3	30.9	-23.1
		-4	76.9	78.3
2	15	0	100.2	89.4
		1	74.1	-61.9
		2	50.3	-37.6
		3	50.5	-50.8
		4	52.5	-63.0
		-1	12.3	-10.2
		-2	96.1	81.6
		-3	47.9	48.0
2	16	0	92.9	74.8
		1	20.3	20.9
		2	65.9	63.2
		3	51.7	-51.8
		-1	66.1	53.4
		-2	68.3	-59.6
		-3	24.5	26.0
		-4	39.8	-48.8
2	17	0	62.3	-57.6
		1	47.5	44.6
		2	15.2	8.5
		3	33.1	38.8
		4	31.1	42.7
		-1	42.2	34.8
		-2	75.0	-62.3
		-3	45.7	-40.6
2	18	0	39.7	-36.7
		2	45.6	-41.9
		3	40.8	43.9
		-1	49.7	-35.6
		-2	52.1	42.0
		-3	40.1	-39.0
		-4	22.5	32.2
2	19	0	49.2	46.7
		1	61.9	-50.4
		2	16.3	-15.7
		-1	19.0	-17.8
		-2	41.5	37.3
		-3	13.0	15.0
2	20	0	16.6	14.7
		2	50.5	50.7
		-1	48.2	43.0
		-2	18.9	-19.5
2	21	0	54.9	-49.1
		1	43.5	51.2
3	0	0	206.9	-245.1
		1	60.1	-68.2
		2	52.2	-52.5
		3	107.5	-95.3
		4	144.7	126.6
		-1	49.9	42.1
		-2	146.0	-128.6
		-3	136.7	140.3
		-4	121.7	114.4
3	1	0	38.2	-44.0
		1	58.1	57.1
		2	207.0	-207.8
		3	19.5	-12.2
		4	76.7	-54.7
		-1	149.9	135.1
		-2	188.1	187.6
		-3	22.0	-20.5
		-4	103.0	99.6
3	2	0	183.3	208.0
		1	43.1	42.8
		2	12.4	5.4
		3	80.1	66.7
		4	133.5	-113.1
		-1	40.8	-35.3
		-2	121.7	112.2
		-3	59.7	-86.5
		-4	90.6	-90.6
3	3	0	112.9	111.5
		1	82.5	-78.6
		2	162.9	170.3
		3	9.1	6.5
		4	50.7	38.2
		-1	56.2	-60.6
		-2	142.2	-144.2
		-4	101.4	-78.8
3	4	0	159.3	-215.3
		1	40.6	-46.5
		2	77.1	68.7
		3	55.6	-44.3
		4	103.1	90.8
		-1	67.7	55.5
		-2	96.2	-87.9
		-3	61.4	59.1
		-4	44.2	42.9
3	5	0	80.3	-91.3
		1	87.4	87.3
		2	136.6	-151.7
		3	36.2	-31.1
		4	49.6	-42.1
		-1	26.6	34.1
		-2	153.5	161.0
		-3	8.8	3.7
		-4	94.8	84.8
3	6	0	168.0	217.9
		1	45.0	46.3
		2	8.6	13.1
		3	59.8	55.5
		4	107.2	-91.2
		-1	46.3	-48.2
		-2	85.4	90.5
		-3	89.3	-86.4
		-4	67.4	-78.2
3	7	0	30.7	35.8
		1	46.4	-51.6
		2	159.7	183.3
		3	10.4	6.3
		4	56.5	54.7
		-1	104.3	-126.0
		-2	133.3	-157.6
		-3	18.7	20.0
		-4	74.1	-77.8
3	8	0	112.3	-158.3
		1	43.5	-49.8
		2	38.8	-41.5
		3	85.7	-86.6
		4	117.5	112.9
		-1	27.5	31.4
		-2	96.8	-112.2

TABLE 3 (*Continued*)

h	k	l	F_o	F_c	h	k	l	F_o	F_c
		-3	90.6	103.4			3	47.6	-48.4
		-4	82.4	98.0			4	48.4	62.7
3	9	0	40.6	-42.7			-1	28.5	23.0
		1	38.4	44.0			-2	65.2	-57.2
		2	120.5	-150.1			-3	49.8	47.7
		4	27.9	-28.9			-4	33.2	51.8
		-1	75.1	93.1	3	17	0	37.7	-30.9
		-2	86.5	117.3			1	33.1	28.8
		-3	22.0	-22.8			2	93.7	-84.3
		-4	61.0	78.3			3	10.9	15.8
3	10	0	107.4	138.5			-1	66.0	50.2
		1	14.3	22.5			-2	57.6	48.1
		2	16.1	-11.3			-3	21.3	-24.7
		3	52.7	45.0			-4	39.9	46.0
		4	89.1	-84.0	3	18	0	64.5	61.2
		-1	23.6	-28.6			2	11.1	-4.5
		-2	57.5	71.9			3	27.0	29.2
		-3	50.2	-55.6			-1	49.2	-25.6
		-4	34.8	-55.0			-2	61.8	54.2
3	11	0	64.7	64.2			-3	32.4	-32.9
		1	55.7	-55.9	3	19	0	36.4	31.0
		2	104.6	109.4			1	35.1	-31.7
		4	29.0	26.9			2	52.0	56.1
		-1	16.4	-19.9			-1	12.0	-7.1
		-2	77.8	-94.6			-2	45.9	-45.0
		-4	64.5	-66.1	3	20	0	80.7	-73.1
3	12	0	150.0	-139.5			1	10.7	-9.9
		1	26.6	-22.0			2	6.7	12.9
		2	43.3	29.8			-1	31.8	28.9
		3	35.7	-30.4			-2	16.7	-26.1
		4	62.6	64.1	4	0	0	34.0	25.8
		-1	51.4	48.4			1	199.5	203.3
		-2	73.1	-67.7			2	31.9	25.0
		-3	55.1	45.9			3	24.9	10.6
		-4	28.9	27.1			4	14.9	8.7
3	13	0	65.4	-59.3			-1	62.4	63.0
		1	69.2	65.1			-2	47.2	-38.5
		2	109.1	-107.8			-3	54.8	-53.1
		3	18.1	-14.6			-4	26.6	-20.7
		4	32.4	-33.6	4	1	0	18.5	-17.8
		-1	41.9	42.3			1	16.9	18.9
		-2	104.1	98.0			2	23.8	-20.0
		-4	61.3	53.1			3	190.7	169.1
3	14	0	144.2	126.6			4	31.6	26.3
		1	44.1	35.2			-1	131.5	-120.4
		3	41.5	42.1			-2	22.1	-21.4
		4	55.9	-57.5			-3	130.9	-126.0
		-1	42.1	-38.7			-4	18.4	11.8
		-2	66.4	52.1	4	2	0	32.4	28.9
		-3	60.2	-50.9			1	169.4	-172.6
		-4	41.0	-46.3			2	10.8	9.0
3	15	0	20.8	17.4			3	21.8	-17.1
		1	36.2	-37.2			4	13.4	8.4
		2	104.3	94.8			-1	113.5	-117.0
		3	13.5	11.4			-2	22.3	16.9
		4	21.9	29.1			-3	58.2	49.6
		-1	62.8	-51.9			-4	15.2	8.0
		-2	109.8	-91.7	4	3	0	7.2	-3.1
		-4	43.5	-46.0			1	65.0	-58.4
3	16	0	98.5	-79.9			2	15.5	-9.4
		1	26.7	-19.8			3	127.3	-121.3
		2	10.7	-15.2			4	30.2	21.4

TABLE 3 (*Continued*)

h	*k*	*l*	F_o	F_c
		- 1	115.7	116.5
		- 2	52.2	- 43.3
		- 3	106.5	105.0
		- 4	15.4	8.3
4	4	0	44.3	- 39.2
		1	111.3	109.6
		2	11.2	10.5
		3	15.0	11.7
		4	40.4	- 35.3
		- 1	94.8	100.6
		- 2	47.8	42.0
		- 3	41.7	- 46.3
4	5	1	68.2	66.0
		2	15.7	9.5
		3	105.3	106.2
		4	13.8	- 9.6
		- 1	117.0	-118.5
		- 2	18.4	14.5
		- 3	74.8	- 83.5
4	6	0	24.9	24.7
		1	148.9	-159.5
		2	17.6	- 14.9
		3	12.1	- 16.4
		4	13.9	9.2
		- 1	91.1	-100.2
		- 2	16.8	17.0
		- 3	47.9	49.8
4	7	0	27.1	28.9
		1	20.3	- 18.4
		2	24.4	22.0
		3	139.0	-156.4
		4	14.0	- 16.5
		- 1	101.6	106.0
		- 3	98.3	117.9
4	8	0	18.0	11.9
		1	145.9	163.2
		3	11.4	15.5
		4	14.0	9.4
		- 1	52.0	71.5
		- 2	37.5	- 43.3
		- 3	37.9	- 48.3
4	9	0	15.2	5.5
		1	9.1	9.2
		2	12.9	- 13.2
		3	104.9	118.7
		4	15.5	17.6
		- 1	69.2	- 85.1
		- 3	68.1	- 95.2
4	10	0	12.8	18.1
		1	96.1	-110.1
		- 1	43.5	- 58.7
		- 3	26.5	28.5
4	11	0	12.5	- 9.1
		1	53.1	- 51.2
		3	82.8	- 85.0
		4	16.1	22.3
		- 1	58.8	79.3
		- 2	20.8	- 26.1
		- 3	55.0	71.1
4	12	0	47.1	- 39.0
		1	93.0	85.1
		3	15.9	14.3
		4	18.7	- 20.0
		- 1	71.1	86.7
		- 3	27.0	- 28.2
4	13	0	24.9	- 18.3
		1	51.2	41.1
		2	10.5	4.2
		3	68.0	77.7
		- 1	74.3	- 77.6
		- 2	17.4	17.3
		- 3	55.9	- 57.0
4	14	0	18.4	13.9
		1	93.2	- 93.0
		2	16.0	- 14.3
		- 1	57.0	- 59.6
		- 2	10.6	8.8
		- 3	41.9	42.7
4	15	0	15.4	8.5
		1	20.0	- 14.4
		2	19.1	15.9
		3	76.7	- 81.9
		- 1	76.9	69.5
		- 3	80.0	66.5
4	16	1	101.4	88.9
		2	12.3	- 7.7
		- 1	41.7	37.0
		- 2	24.6	- 21.1
		- 3	26.1	- 25.9
4	17	0	15.5	8.6
		1	12.2	6.2
		2	15.3	- 15.0
		3	57.3	66.4
		- 1	43.6	- 38.0
		- 2	10.8	7.6
		- 3	57.9	- 57.1
4	18	0	16.1	14.7
		1	65.4	- 56.7
		2	15.3	17.8
		- 1	45.0	- 38.8
4	19	1	35.9	- 29.0
		- 1	38.5	39.3
		- 2	11.5	- 13.5
5	0	0	129.9	-117.1
		1	11.0	7.6
		2	136.4	-135.9
		3	13.8	- 3.6
		4	35.1	31.9
		- 1	40.2	- 33.6
		- 2	41.4	45.7
		- 3	26.6	22.1
		- 4	127.7	116.6
5	1	0	120.5	114.8
		1	41.9	- 36.1
		2	105.1	- 97.2
		4	78.0	- 72.5
		- 1	32.3	23.0
		- 2	127.0	124.2
		- 3	16.6	- 11.4
		- 4	18.4	2.1
5	2	0	144.4	132.7
		2	94.0	94.6
		3	37.7	- 36.6
		4	30.1	- 28.2

TABLE 3 (*Continued*)

h	*k*	*l*	F_o	F_c	*h*	*k*	*l*	F_o	F_c
		-1	18.8	13.0			-2	17.6	-20.0
		-2	41.2	-40.9			-4	64.5	-65.3
		-4	98.7	-88.1	5	11	0	45.1	-41.0
5	3	0	78.5	-63.3			1	29.2	27.8
		1	50.9	46.8			2	55.0	52.4
		2	64.9	62.7			4	46.1	48.7
		3	18.0	19.3			-1	23.9	31.4
		4	77.9	70.6			-2	69.5	-87.6
		-1	49.8	47.5	5	12	0	117.2	-94.3
		-2	147.1	-147.7			2	46.1	-46.7
		-3	15.7	-0.2			3	42.7	46.0
		-4	18.5	-9.9			4	11.7	12.5
5	4	0	152.9	-145.4			-2	28.3	33.9
		2	63.0	-67.1			-3	30.2	-31.9
		3	74.9	69.6			-4	50.7	47.7
		4	15.6	17.8	5	13	0	51.6	42.5
		-1	17.7	-12.8			1	19.5	-16.0
		-2	47.1	43.3			2	37.9	-35.0
		-3	37.7	-39.4			4	48.9	-59.0
		-4	72.1	71.0			-1	23.3	-24.8
5	5	0	73.3	61.8			-2	98.4	94.1
		1	28.5	-27.1	5	14	0	89.2	74.2
		2	75.5	-74.3			2	64.3	60.7
		3	11.6	-15.2			3	18.9	-14.6
		4	81.2	-76.9			-2	34.0	-30.3
		-1	25.4	-23.9			-4	50.8	-57.2
		-2	120.5	124.3	5	15	0	76.5	-58.2
5	6	0	118.7	118.4			1	14.4	11.7
		1	15.0	10.3			2	58.1	45.5
		2	81.9	87.1			-1	14.5	-6.0
		3	20.7	-21.0			-2	73.4	-65.5
		4	24.4	-23.1			-3	13.2	11.9
		-1	16.4	11.5	5	16	0	62.3	-48.8
		-2	35.7	-40.1			1	21.4	17.5
		-4	90.4	-84.3			2	69.9	-62.8
5	7	0	94.4	-95.5			-1	16.0	-10.3
		1	28.6	28.1			-2	17.3	15.4
		2	71.4	72.1	5	17	0	68.8	49.9
		4	69.4	65.9			1	35.3	-28.7
		-1	17.6	-17.0			2	36.2	-32.9
		-2	111.4	-118.3			-1	23.6	-16.2
		-3	12.1	10.5			-2	56.9	54.3
5	8	0	102.6	-94.2	5	18	0	58.4	45.4
		1	7.7	7.9			1	21.8	-17.9
		2	110.4	-113.5			-1	13.1	10.2
		4	21.0	22.5	6	0	0	73.9	68.6
		-1	17.9	-17.5			1	110.7	103.3
		-2	33.2	39.7			2	34.1	-29.4
		-4	94.3	96.0			3	67.3	67.2
5	9	0	94.9	92.6			4	29.7	-27.7
		1	43.0	-39.3			-1	65.8	-49.3
		2	68.9	-71.8			-2	40.6	36.2
		4	51.7	-52.9			-3	80.6	-82.3
		-2	80.6	96.3	6	1	0	80.0	62.7
		-3	16.3	-17.0			1	91.6	-82.4
		-4	17.8	11.7			2	50.8	44.8
5	10	0	94.4	91.8			3	52.9	49.3
		1	23.6	-21.0			4	21.0	21.7
		2	62.6	67.8			-1	99.9	-88.3
		3	22.2	-26.9			-2	54.1	-53.3
		4	21.6	-24.2			-3	16.4	-16.0
		-1	19.5	21.0			-4	45.1	-36.5

TABLE 3 (*Continued*)

h	k	l	F_o	F_c
6	2	0	84.9	-63.5
		1	68.6	-62.6
		2	26.4	22.8
		3	66.0	-67.8
		4	48.9	50.9
		-1	39.2	30.5
		-2	80.0	-78.4
		-3	91.9	80.4
6	3	0	83.8	-62.7
		1	45.0	39.0
		2	80.5	-82.6
		3	30.4	-28.7
		-1	103.2	91.7
		-2	27.2	27.2
		-4	72.9	58.2
6	4	0	44.6	38.5
		1	59.6	55.1
		2	42.3	-34.2
		3	69.7	71.6
		4	57.6	-64.5
		-1	12.2	10.7
		-2	89.0	81.0
		-3	71.3	-72.6
6	5	0	60.7	53.5
		1	49.7	-44.0
		2	73.6	71.4
		3	37.5	35.9
		4	14.1	-10.3
		-1	79.9	-85.4
		-2	24.9	-23.5
		-3	15.5	-14.5
		-4	56.4	-53.9
6	6	0	70.4	-61.5
		1	64.4	-60.4
		2	20.1	16.7
		3	69.6	-69.0
		4	45.4	44.6
		-1	35.8	30.4
		-2	68.3	-61.2
		-3	74.4	83.8
6	7	0	54.1	-46.8
		1	86.0	74.8
		2	48.2	-46.9
		3	34.5	-34.7
		-1	77.8	81.3
		-2	43.4	46.5
		-4	41.7	38.4
6	8	0	62.3	54.6
		1	84.3	75.2
		2	25.7	-19.5
		3	44.6	54.4
		4	17.7	-24.8
		-1	44.8	-45.0
		-2	40.5	42.3
		-3	62.4	-69.7
6	9	0	61.6	59.6
		1	57.4	-60.4
		2	30.6	31.4
		3	42.3	41.6
		-1	68.1	-67.7
		-2	26.8	-34.9
		-3	17.0	-17.6
		-4	24.6	-22.8
6	10	0	45.5	-40.5
		1	63.7	-60.4
		2	38.5	38.5
		3	38.5	-48.8
		4	38.4	42.1
		-1	16.7	17.2
		-2	43.2	-48.4
		-3	37.6	45.5
		-4	25.2	11.2
6	11	0	61.6	-52.1
		1	36.0	33.0
		2	64.6	-59.4
		3	25.3	-21.2
		-1	57.1	60.6
		-2	17.9	21.1
		-4	35.0	44.4
6	12	0	42.7	34.0
		1	32.7	27.7
		2	18.5	-13.7
		3	45.7	48.8
		4	26.1	-43.1
		-1	10.9	-7.5
		-2	71.8	69.1
		-3	63.6	-60.9
		-4	11.5	-12.8
6	13	0	35.9	28.1
		1	36.6	-30.6
		2	62.2	51.4
		3	22.0	19.3
		-1	63.3	-65.8
		-4	35.0	-39.0
6	14	0	47.4	-31.7
		1	55.7	-42.1
		2	18.4	12.3
		3	36.8	-50.8
		-1	24.4	18.4
		-2	40.6	-33.6
		-3	55.3	56.3
6	15	0	41.2	-31.5
		1	66.0	51.0
		2	30.2	-26.4
		-1	57.1	46.4
		-2	23.6	20.4
6	16	1	54.0	44.2
		-1	36.4	-26.7
		-2	24.3	21.8
6	17	0	18.4	38.9
7	0	0	43.9	33.5
		1	68.4	-59.8
		2	50.6	-49.4
		3	10.4	-11.7
		-1	65.7	-57.4
		-2	53.3	49.9
		-3	23.2	17.6
		-4	26.5	28.1
7	1	0	70.0	71.5
		1	44.7	-40.8
		2	15.3	16.1
		3	55.1	-63.5
		4	12.0	-4.5
		-1	59.0	47.1

TABLE 3 (*Continued*)

h	*k*	*l*	F_o	F_c	*h*	*k*	*l*	F_o	F_c
		-3	35.9	36.0			3	17.9	-17.5
		-4	17.7	-21.6			-1	37.8	46.5
7	2	0	11.4	-8.0			-2	27.4	-27.5
		1	73.2	62.2	7	11	0	26.2	-22.8
		2	34.9	33.6			1	43.3	37.5
		3	19.2	-16.8			2	17.4	-16.1
		-1	62.0	55.5			3	37.4	49.8
		-2	49.8	-45.4			-1	18.8	-16.3
7	3	0	26.3	-26.1			-2	7.1	-5.2
		1	37.1	36.2			-3	40.6	-43.9
		2	19.1	-14.7	7	12	1	60.3	-54.5
		3	60.8	68.9			2	11.4	-10.0
		4	12.7	22.0			-1	42.6	-36.4
		-1	38.3	-31.1			-2	33.1	33.0
		-3	66.7	-61.3	7	13	0	26.4	21.3
		-4	28.5	21.2			1	28.1	-21.7
7	4	1	84.1	-79.4			2	21.5	22.4
		2	17.5	-17.0			-1	27.0	20.7
		3	32.9	36.6			-2	5.8	5.4
		4	14.6	-9.4	7	14	0	17.1	-14.7
		-1	45.3	-44.4			1	45.9	42.6
		-2	37.1	34.0			-1	33.2	27.8
7	5	0	32.9	31.9			-2	17.6	-31.9
		1	45.1	-44.3	8	0	0	83.6	73.6
		2	31.3	28.8			2	32.5	34.1
		3	60.4	-71.4			3	7.5	4.0
		4	9.6	-18.3			-1	44.8	-43.4
		-1	37.6	30.2			-3	15.5	-16.0
		-2	14.9	16.6			-4	27.2	-37.6
		-3	40.6	46.8	8	1	0	13.7	-10.8
		-4	16.3	-25.7			1	27.0	-25.1
7	6	0	22.6	-16.1			2	33.4	34.7
		1	64.4	64.6			3	10.6	-12.2
		2	39.9	36.3			-2	67.7	-69.0
		3	16.2	-14.6			-3	16.5	20.3
		4	14.9	18.7			-4	11.0	-4.4
		-1	43.8	46.5	8	2	0	91.0	-63.4
		-2	50.5	-48.7			2	27.4	-28.3
		-4	14.3	-20.7			-1	14.9	16.6
7	7	0	68.3	-62.8			-4	34.0	42.8
		1	27.9	29.3	8	3	0	25.3	19.6
		2	15.4	-16.0			2	51.6	-56.0
		3	50.3	54.6			-2	63.5	66.4
		4	14.3	8.6			-3	17.8	-20.0
		-1	44.4	-40.7			-4	14.4	23.0
		-3	34.6	-34.1	8	4	0	73.9	74.2
		-4	19.0	22.8			1	26.7	-25.4
7	8	0	28.3	22.8			2	32.5	33.8
		1	45.2	-44.3			3	9.6	12.0
		2	32.3	-34.9			-2	15.2	16.8
		3	11.8	-9.6			-3	13.3	-19.2
		-1	40.7	-50.1			-4	32.6	-45.0
		-2	35.0	39.6	8	5	0	30.5	-24.5
		-3	19.6	23.0			1	12.2	-9.2
7	9	0	54.5	48.8			2	59.5	62.2
		1	33.3	-34.2			3	6.9	-12.6
		3	42.2	-47.1			-2	49.5	-55.1
		-1	34.5	37.7			-3	18.0	21.5
		-3	28.5	32.8			-4	13.9	-26.4
		-4	11.0	-14.1	8	6	0	63.9	-59.5
7	10	1	53.4	42.7			1	7.2	8.7
		2	27.1	25.2			2	25.8	-29.9

TABLE 3 (*Continued*)

h	*k*	*l*	F_o	F_c
		3	9.5	- 12.2
		- 1	17.8	16.8
		- 3	11.9	16.9
8	7	0	14.0	9.9
		1	27.6	23.5
		2	22.9	- 25.9
		- 2	48.9	57.2
		- 3	9.5	- 13.2
8	8	0	69.8	56.1
		1	8.9	3.2
		2	22.9	24.9
		- 1	30.9	- 35.9
8	9	0	12.0	- 7.3
		1	20.7	- 16.3
		2	29.5	28.7
		- 2	54.2	- 62.9
8	10	0	63.6	- 56.8
		1	18.2	12.5
		- 1	13.4	16.7
		- 2	10.0	- 10.2
8	11	0	18.5	13.5
9	0	0	11.6	9.1
		1	32.1	- 32.4
		2	6.3	11.4
		- 2	11.2	- 17.4
9	1	0	17.4	- 13.2
		1	26.7	26.4
		2	4.1	- 6.4
		- 1	43.0	48.9
		- 2	12.1	- 18.9
9	2	0	9.3	- 9.7
		1	26.4	48.7
		- 2	16.0	20.3
9	3	0	34.3	28.4
		1	14.2	- 15.0
		- 1	38.4	- 47.4
9	4	1	51.0	- 59.9
		- 1	6.2	2.4
		- 2	10.0	- 16.7
9	5	0	33.1	- 32.2
		1	19.1	22.5
		- 1	34.8	45.6

3·21 Å, and Hg(1) $\cdots$ $Cl(3)_{III}$, 4·44 Å, are taken into account the co-ordination of Hg(1) can be described as distorted octahedral (cf. crystalline mercuric chloride [20]).

In the 1,6-dithiacyclodeca-*cis*-3,*cis*-8-diene molecule the bond lengths and valency angles do not differ significantly from expected values.[21]

EXPERIMENTAL

Crystal Data.—1,6-Dithiacyclodeca-*cis*-3,*cis*-8-dienebis(mercuric chloride), $C_8H_{12}S_2Hg_2Cl_4$, $M = 714{\cdot}5$. Monoclinic, $a = 7{\cdot}29$, $b = 17{\cdot}01$, $c = 6{\cdot}20$ Å, $\beta = 92^\circ\ 34'$, $U = 768$ Å^3, $Z = 2$, $D_c = 3{\cdot}08$, $F(000) = 320$. Space group $P2_1/m$ (C_{2h}^2).

Crystallographic Measurements.—Rotation, oscillation, and Weissenberg photographs were taken with Cu-K_α radiation; precession photographs were taken with Mo-K_α radiation. Cell dimensions were obtained from precession photographs. The space group is not determined uniquely from systematic halvings in the intensities; the choice between $P2_1$ and $P2_1/m$ was settled in favour of the latter by the structure analysis. For the intensity measurements a small crystal was employed completely bathed in a uniform *X*-ray beam and no corrections for absorption were applied. The *X*-ray reflexions were recorded on multiple-film equi-inclination Weissenberg photographs and the intensities were estimated visually. The usual correction factors [22] were applied. In all, 1158 independent structure amplitudes (F_o) were evaluated.

The positions of the two independent mercury atoms were deduced from Patterson projections and sections through the three-dimensional Patterson function. When structure factors based on the mercury atoms alone were calculated the value of *R* was 31·2%. The structure factors used to calculate three-dimensional F_o and ($F_o - F_c$) syntheses in which two independent chlorine atoms, Cl(1) and Cl(2), the sulphur atom and the four carbon atoms were located. With the inclusion of these atoms in the structure-factor calculation the value of *R* decreased to 23·3%. Improved co-ordinates were obtained from the next F_o and ($F_o - F_c$) syntheses and the values of *R* fell to 20·9%. Three cycles of least-squares adjustment of positional and anisotropic thermal parameters then reduced *R* to 18·5% at which stage the remaining chlorine atom, Cl(3), was located in F_o and ($F_o - F_c$) syntheses. After five further rounds of least-squares calculations the parameters shifts became extremely small and refinement was terminated. The final value of *R* is 13·6%.

The final calculated structure factors are shown with the measured values of the structure

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[20] H. Braekken and W. Scholten, *Z. Krist.*, 1934, **89**, 448; D. Grdenić, *Arhiv Kemi*, 1950, **22**, 14.

[21] L. E. Sutton *et al.*, " Tables of Interatomic Distances and Configuration in Molecules and Ions," *Chem. Soc. Special Publ.*, No. 11, 1958.

[22] International Tables for X-Ray Crystallography," The Kynoch Press, Birmingham, 1962, vol. III.

amplitudes in Table **3**. The final three-dimensional electron-density distribution derived from the data in Table **3** is shown in Figure **4** by means of superimposed contour sections drawn parallel to (001). The atomic co-ordinates and interatomic distances are given in Tables **1** and **2**. The final anisotropic thermal parameters are in Table **4**; they are values of b_{ij} in the equation:

$$\exp(-B \sin^2\theta/\lambda^2) = 2^{-(b_{11}h^2 + b_{22}k^2 + b_{33}l^2 + b_{12}hk + b_{13}hl + b_{23}kl)}$$

The standard deviations of the final atomic co-ordinates were derived from the least-squares residuals by means of the equation

$$\sigma^2(x_i) = \sum_j w_j(\Delta F_j)^2/[(n - s)\sum w_j(\partial F_j/\partial x_i)^2]$$

The results are listed in Table **1**.

TABLE 4

Anisotropic temperature factors ($b_{ij} \times 10^5$)

Atom	b_{11}	b_{22}	b_{33}	b_{12}	b_{23}	b_{13}
Hg(1)	2649	368	2574	—	—	−226
Hg(2)	1638	224	3719	—	—	4
Cl(1)	2361	335	2595	−358	−110	−521
Cl(2)	1707	312	1516	—	—	−252
Cl(3)	1817	584	2820	—	—	906
S	1531	229	2086	310	−738	−1026
C(1)	1170	410	3252	51	−296	2595
C(2)	1622	351	2792	9	−832	−404
C(3)	1025	333	4358	89	−152	−72
C(4)	1866	251	4034	−235	226	2255

Most of the calculations were performed on the Glasgow University DEUCE computer with programmes devised by Dr. J. S. Rollett and Dr. J. G. Sime. Some of the later calculations were performed on the IBM 7094 computer at the University of Illinois. The work was supported in part by the U.S. National Science Foundation.

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[*Received, April* 22*nd*, 1965.]