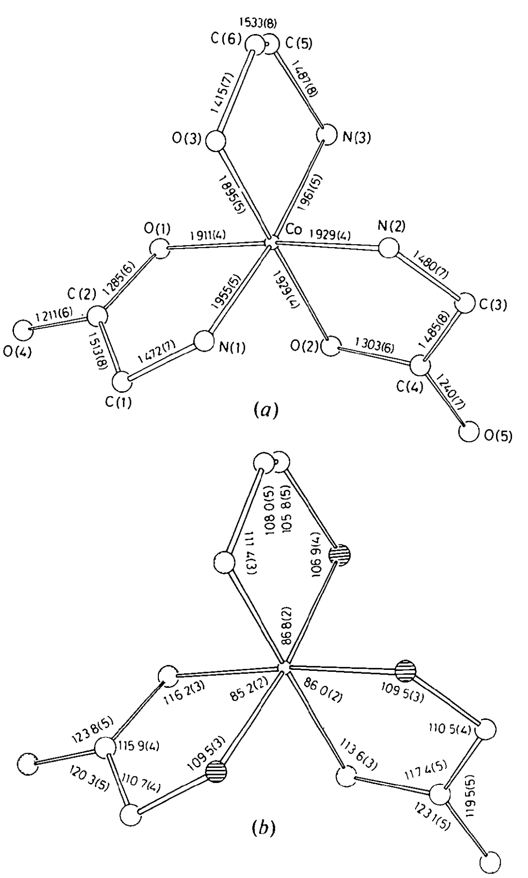

Fig. 2. Projection of the complex molecule on the N(1)–N(2)–O(3) plane with (*a*) interatomic distances (Å) and (*b*) bond angles (°).

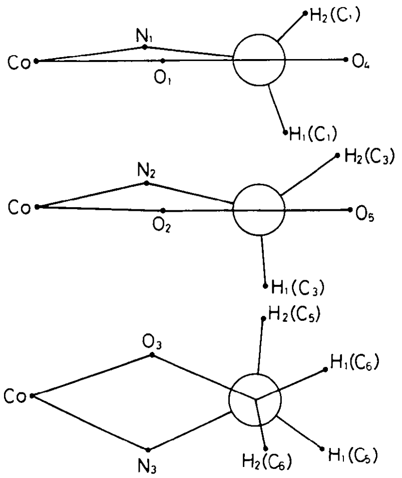

Fig. 3. Projections of the five-membered chelate rings along the central C–C bonds.

Fig. 3 shows projections of the three five-membered chelate rings along the central C–C bonds. The shapes and sizes of the two glycinato moieties are normal. The glycinato rings are nearly planar. N–C–C–O (ligating O atom) torsion angles are 11·4 and 14·1°.

In contrast, the dihedral angle N–C–C–O in eta is 49·7°, indicating a strain-free conformation of the chelate ring. The Co–O(eta) distance of 1·895 (5) Å is significantly shorter than the average Co–O(gly) distance of 1·920 (5) Å. This shorter Co–O(eta) distance may be ascribed to a greater charge localization on this O atom than on the carboxyl O atom.

Calculations were carried out on the FACOM 230/48 computer of this Institute.

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Polymeric (2,2'-trimethylenedipyridine 1,1'-dioxide)bis[dichloromercury(II)]

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Abstract. $C_{13}H_{14}N_2O_2Cl_4Hg_2$, M_r = 773·0, orthorhombic, *Fdd*2, a = 46·465 (21), b = 18·903 (12), c = 4·238 (5) Å, U = 3722·4 Å^3, Z = 8, d_c = 2·76, d_m = 2·72 (5) g cm^{-3}, Mo $K\alpha$ radiation, λ = 0·7107 Å, μ = 177·0 cm^{-1}. Each 2,2'-trimethylenedipyridine 1,1'-dioxide ligand is bonded through O to four $HgCl_2$

groups thus forming pairs of polymeric chains along **c**. Each Hg atom is bonded to two Cl [2·33 (1), 2·30 (1) Å] and two O atoms [2·64 (3), 2·65 (3) Å]. 887 independent reflections above background have been refined to $R = 0 \cdot 10$.

Introduction. The preparation and properties of the 1 : 1 complex between $HgCl_2$ and 2,2′-trimethylenedipyridine 1,1′-dioxide have been described previously (Alshaikh-Kadir & Holt, 1976). This compound was prepared by mixing warm methanolic solutions of equimolar quantities of $HgCl_2$ and the ligand. When the sample was left unfiltered for a week, the Hg complex was transformed to the 2 : 1 complex $(HgCl_2)_2$(ligand). Crystals of the 1 : 1 complex were unsuitable for X-ray work but those of the 2 : 1 complex were just adequate. A crystal of size 0·4 × 0·05 × 0·9 mm was mounted on a General Electric XRD 5 apparatus which was used to measure diffraction intensities and cell dimensions. It was equipped with a manual goniostat, scintillation counter and pulse-height discriminator. Zr-filtered Mo $K\alpha$ radiation was used. 1520 independent reflections with $2\theta < 50°$ were measured by the stationary-crystal–stationary-counter method with counts of 10s. 887 independent reflexions with $I > 2\sigma(I)$ were used in subsequent calculations. An absorption correction was applied using *ABSORB* (Stewart, Kruger, Ammon, Dickinson & Hall, 1972).

The positions of the Hg atoms were obtained from a Patterson function and a Fourier map gave the positions of the remaining atoms. The structure was refined by full-matrix least squares with Hg anisotropic and the remaining atoms isotropic. The pyridine ring was constrained to have the usual dimensions and the final R value was 0·10. (The opposite enantiomorph gave $R = 0 \cdot 11$ and was rejected.) The weighting scheme, chosen to give average values of $w\Delta^2$ for groups of reflections independent of values of F_o and $\sin\theta/\lambda$, was $w^{1/2} = 1$ for $F_o < 150$ and $w^{1/2} = 150/F_o$ for $F_o > 150$. Calculations were made on a CDC 7600 computer at the university of London Computer Centre using the XRAY (Stewart *et al.*, 1972) and *SHELX* (Sheldrick, 1976) sets of programs. Atomic scattering factors and corrections for anomalous dispersion were taken from *International Tables for X-ray Crystallography* (1974). For all zero-weighted reflections, I_c was no greater than $2I_o$. In a final difference Fourier map no peak was $> 0 \cdot 25h_C$ (where h_C is the height of a C atom) apart from some close (*ca* 1 Å) to the Hg atom which were *ca* $\frac{1}{2}h_C$. In the final cycle of refinement all shifts were $< 0 \cdot 02\sigma$. The final list of positions is given in Table 1, and bond lengths and angles around the Hg atom are given in Table 2.*

Table 1. *Positional parameters* ($\times 10^4$) *with estimated standard deviations in parentheses*

	x	y	z
Hg	349 (0)	2110 (1)	0*
Cl(1)	−132 (2)	1768 (4)	290 (29)
Cl(2)	806 (2)	2571 (5)	−272 (31)
O(1)	453 (5)	1312 (11)	4986 (81)
N(2)	636 (5)	764 (9)	5104 (68)
C(3)	891 (5)	825 (9)	3397 (68)
C(4)	1060 (5)	227 (9)	2825 (68)
C(5)	972 (5)	−431 (9)	3959 (68)
C(6)	717 (5)	−493 (9)	5665 (68)
C(7)	548 (5)	105 (9)	6238 (68)
C(8)	277 (7)	67 (17)	8031 (97)
C(9)	0*	0*	5852 (102)

* Parameter fixed.

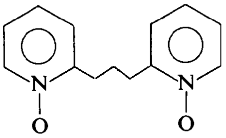
Table 2. *Mercury atom environment*

Hg–Cl(1)	2·33 (1) Å	Cl(1)–Hg–Cl(2)	173·8 (3)°
Hg–Cl(2)	2·30 (1)	Cl(1)–Hg–O(1)	88·6 (5)
Hg–O(1)	2·64 (3)	Cl(1)–Hg–O(1^{i})	93·4 (5)
Hg–O(1^{i})	2·65 (3)	Cl(2)–Hg–O(1)	95·0 (5)
Hg–Cl(1^{iv})	3·25 (1)	Cl(2)–Hg–O(1^{i})	90·4 (7)
Hg–Cl(1^{iii})	3·08 (1)	O(1)–Hg–O(1^{i})	106·4 (10)

Roman numerals as superscripts refer to the following equivalent positions relative to the reference set (x,y,z) in Table 1.

(i) $x, y, -1 + z$	(iii) $-x, \frac{1}{2} - y, -\frac{1}{2} + z$
(ii) $-x, -y, z$	(iv) $-x, \frac{1}{2} - y, \frac{1}{2} + z$

Discussion. We have studied the reactions of various metal chlorides with polymeric ligands such as poly(2-vinylpyridine 1-oxide), poly(4-vinylpyridine 1-oxide), poly(dimethylaminostyrene *N*-oxide) and some analogous alkyl-substituted ones (Alshaikh-Kadir & Holt, 1976, 1977). The dimeric ligand 2,2′-trimethylenedipyridine 1,1′-dioxide (I) has proved useful as a model for such ligands and we have prepared and report here the crystal structure of (2,2′-trimethylenedipyridine 1,1′-dioxide)bis[dichloromercury(II)].



(I)

Details of the structure are shown in Fig. 1. It contains two chains of Hg atoms parallel to **c**, linked by O atoms [2·64 (3), 2·65 (3) Å] and two Cl atoms [2·33 (1), 2·30 (1) Å] which are mutually *trans*, as is usual in $HgCl_2$ complexes. These four atoms occupy four sites of a distorted octahedron; in the other two sites there

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* Lists of structure factors, dimensions of the ligand and thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33179 (6 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

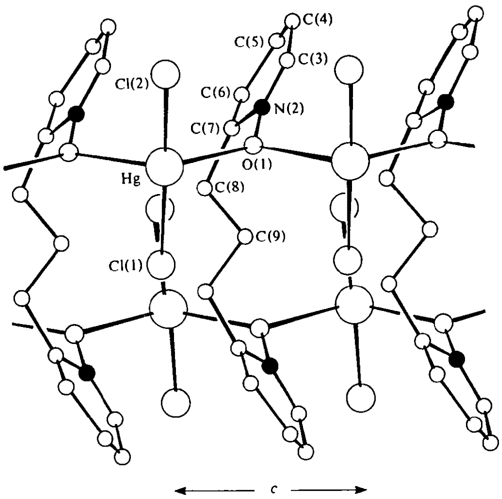

Fig. 1. The structure of the title compound ($c = 4{\cdot}238$ Å).

are two Cl atoms from another double chain that are weakly bonded to the metal atom [3·25 (1), 3·08 (1) Å]. The structure can be compared to that of dimeric $HgCl_2L$ (L = pyridine 1-oxide) (Sawitzki & von Schnering, 1974) in which the Hg atom is strongly bonded to two Cl atoms [2·316 (15), 2·339 (15) Å], weakly bonded to two others [3·185 (18), 3·318 (17) Å] and bridged to the adjacent Hg by O atoms of two ligands [Hg—O 2·59 (5), 2·60 (5) Å]. In this structure the Hg environment is also distorted octahedral with the strongly bonded Cl atoms in *trans* positions.

The poor quality of the data precludes any discussion of the ligand dimensions but from the torsion angles it is clear that the pyridine ring is approximately perpendicular to the planar C(7)—C(8)—C(9)—C(8^{ii})—C(9^{ii}) linkage.

Apart from the two weak Hg···Cl contacts already mentioned, there are no other distances significantly less than the sum of the van der Waals radii between atoms in the double chains.

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cis-Dichloro(ammine)(dimethyl sulphoxide)platinum(II)

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Abstract. $PtCl_2C_2H_9NSO$, M_r = 361·16, orthorhombic, $P2_12_12_1$, a = 8·889 (4), b = 9·042 (6), c = 10·475 (8) Å, Z = 4, V = 841·9 (9) Å^3, D_x = 2·849, D_m = 2·84 (1) g cm^{-3} (flotation); λ(Mo $K\alpha$) = 0·71069 Å, μ(Mo $K\alpha$) = 183·10 cm^{-1}, t = 22 °C. Positional and anisotropic thermal parameters were refined by full-matrix least-squares calculations to R = 0·036 and R_w = 0·029. The coordination around the Pt atom is planar. The compound has the *cis* configuration. The Pt—Cl bond which is *trans* to the dimethyl sulphoxide molecule seems slightly longer (2·321 Å) than the *cis* Pt—Cl bond (2·297 Å).

Introduction. Recently, we have studied the isomerization of complexes of the type [Pt(DMSO)(L)Cl_2] (where L = nucleoside, NH_3 or pyridine, and DMSO = dimethyl sulphoxide). In order to confirm the configurations of the isomers, some typical compounds were studied by X-ray diffraction. Here we report the crystal structure of *cis*-[Pt(DMSO)(NH_3)Cl_2].

cis-[Pt(NH_3)(DMSO)Cl_2] was prepared from the isomerization of the *trans* isomer as already described by Kong, Iyamuremye & Rochon (1976). A set of precession photographs indicated that the crystal belongs to the orthorhombic space group $P2_12_12_1$.