

Fig. 1. The structure of the title compound ($c = 4.238 \text{ \AA}$).

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'')—C(9'') 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) Å³, $D_x = 2.849$, $D_m = 2.84$ (1) g cm⁻³ (floatation); $\lambda(\text{Mo } K\alpha) = 0.71069$ Å, $\mu(\text{Mo } K\alpha) = 183.10$ cm⁻¹, $t = 22^\circ\text{C}$. 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 $[Pt(\text{DMSO})(L)\text{Cl}_2]$ (where $L =$ nucleoside, NH_3 or pyridine, and $\text{DMSO} =$ 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*- $[Pt(\text{DMSO})(\text{NH}_3)\text{Cl}_2]$.

cis- $[Pt(\text{NH}_3)(\text{DMSO})\text{Cl}_2]$ 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 $P2_12_12_1$.

The intensity data were collected from a crystal $0.08 \times 0.42 \times 0.06$ mm elongated along the **b** direction on a Syntex $P\bar{1}$ diffractometer using graphite-monochromatized Mo $K\alpha$ radiation. 1458 independent reflections were measured in the region of $2\theta < 60^\circ$ by the $2\theta/\theta$ scan technique at a variable speed (24 to 1° min^{-1}). Most of the reflections were measured at a speed of 1° min^{-1} . The background to scan time ratio was 0.40. The 1172 reflections for which the intensity was greater than $2.5\sigma(I)$ were considered as observed. The standard deviation $\sigma(I)$ was calculated as already described (Melanson & Rochon, 1975). An absorption correction based on the equation of the crystal faces was applied to all the reflections. The data were then corrected for the Lorentz and polarization effects. The scattering factors were those of Cromer & Waber (1965) and the anomalous-dispersions terms (Cromer, 1965) of Pt, Cl and S were included in the calculations.

The position of the Pt atom was easily located from the three-dimensional Patterson map. The positions of all other atoms except H were obtained by structure-factor and Fourier-map calculations. Individual weights, w , according to the equation $1/w = a + bF_o + cF_o^2$, were calculated. The constants in the equation were adjusted to make the distribution of $w|AF|^2$ practically constant with respect to $|F_o|$ and $\sin \theta/\lambda$ ($a = 30.0$, $b = -0.353$ and $c = 0.0011$). An isotropic secondary-extinction correction (Coppens & Hamilton, 1970) was also introduced. The H atoms on the methyl

and ammine groups could not be localized. The refinement of the scale factor, the coordinates and anisotropic temperature factors of all nonhydrogen atoms converged to a conventional $R = \Sigma (|F_o| - |F_c|)/|F_o|$ of 0.036 and a weighted residual $R_w = [\Sigma w(|F_o| - |F_c|)^2/\Sigma w|F_o|^2]^{1/2}$ of 0.029.* The refined parameters are given in Table 1.

The calculations were carried out with a CDC 6400 computer and the programs used have been described elsewhere (Melanson & Rochon, 1975).

Discussion. A stereoscopic view of the molecule is shown in Fig. 1. The bond lengths and angles are given in Table 2. Two Cl, one S and one N atom form the square-planar coordination expected for Pt^{II} complexes. The weighted best plane was calculated through the five atoms. The deviations from this plane are: Pt -0.0005 (6), Cl(1) 0.018 (5), Cl(2) 0.000 (5), S 0.011 (4) and N -0.003 (15) Å. The angles around the Pt atom are close to the expected 90 and 180° .

The compound has the *cis* configuration. The two Pt-Cl bond lengths [*cis* (related to DMSO) Pt-Cl = 2.297 Å, *trans* Pt-Cl = 2.321 Å] agree well with the

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33183 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 1. Final atomic parameters ($\times 10^4$)

Estimated standard deviations are given in parentheses.

	<i>x</i>	<i>y</i>	<i>z</i>
Pt	-1137.3 (6)	4880.7 (7)	1250.1 (6)
Cl(1)	-3543 (5)	4265 (6)	1928 (5)
Cl(2)	-925 (7)	6711 (6)	2760 (5)
S	1111 (5)	5426 (4)	548 (3)
O	1711 (13)	4383 (13)	-424 (11)
N	-1323 (19)	3261 (16)	-82 (15)
C(1)	1128 (32)	7238 (19)	-99 (22)
C(2)	2471 (17)	5597 (20)	1778 (17)

Table 2. Bond distances (Å) and bond angles ($^\circ$)

Pt-Cl(1)	2.321 (5)	Cl(1)-Pt-Cl(2)	92.2 (2)
Pt-Cl(2)	2.297 (5)	Cl(1)-Pt-S	178.0 (2)
Pt-S	2.186 (4)	Cl(1)-Pt-N	87.8 (5)
Pt-N	2.030 (15)	Cl(2)-Pt-S	89.7 (2)
S-O	1.487 (12)	Cl(2)-Pt-N	180.0 (5)
S-C(1)	1.773 (18)	S-Pt-N	90.3 (5)
S-C(2)	1.774 (17)	Pt-S-O	114.5 (5)
		Pt-S-C(1)	110.2 (8)
		Pt-S-C(2)	113.5 (6)
		C(1)-S-O	108.7 (9)
		C(1)-S-C(2)	101.0 (10)
		C(2)-S-O	107.0 (8)

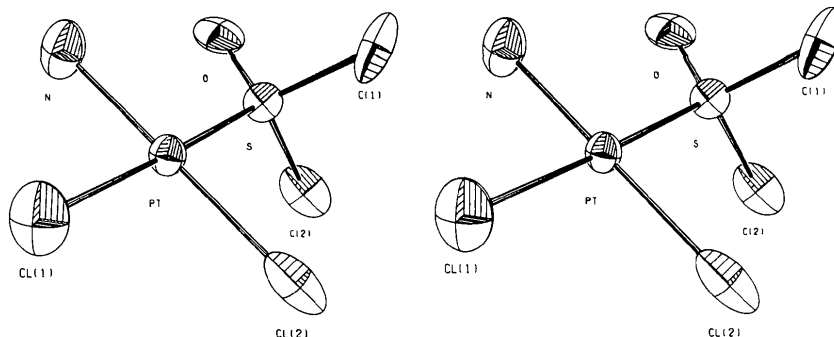


Fig. 1. Stereoscopic view of a molecule of *cis*-[Pt(DMSO)(NH₃)Cl₂].

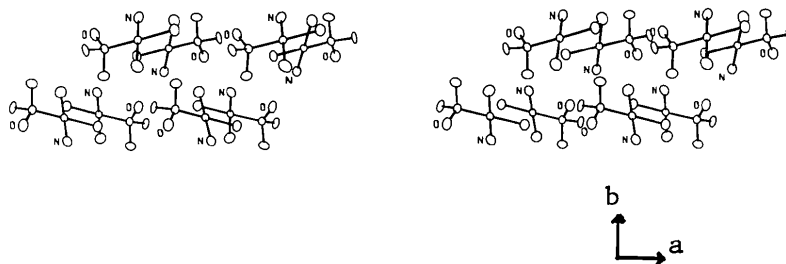


Fig. 2. Packing in the *cis*-[Pt(DMSO)(NH₃)Cl₂] crystal.

values found in K[Pt(DMSO)Cl₃] (*cis* Pt—Cl = 2.30 Å, *trans* Pt—Cl = 2.32 Å) (Melanson, Hubert & Rochon, 1976), *cis*-[Pt(DMSO)₂Cl₂] (2.31 Å, Melanson & Rochon, 1975), *trans*-{Pt[*S*-bis(isopropyl) sulphoxide](*N*-1-methylcytosine)Cl₂} (2.29 and 2.30 Å, Lock, Speranzini & Powell, 1976), *cis*-[Pt(DMSO)(2-picoline)Cl₂] (*cis* Pt—Cl = 2.288 Å, *trans* Pt—Cl = 2.307 Å, Melanson & Rochon, 1977) and *trans*-[Pt(DMSO)(2-picoline)Cl₂] (*cis* Pt—Cl = 2.282 and 2.295 Å, Melanson & Rochon, 1978). DMSO has a relatively high *trans* influence (Kukushkin, Stetsenko, Strelin & Duibanova, 1972; Kukushkin & Vyaz'menskii, 1970). In the above Pt dimethyl sulphoxide complexes, slightly higher values have been observed for bonds *trans* to DMSO (2.31–2.32 Å) compared with the *cis* bonds (2.28–2.30 Å), but, at the moment, we do not know if this is really significant.

The Pt—S bond (2.186 Å) is slightly shorter than the values (2.244 and 2.229 Å) found for *cis*-[Pt(DMSO)₂Cl₂] (Melanson & Rochon, 1975), and value (2.232 Å) found in *trans*-{PtCl₂[*S*-bis(isopropyl) sulphoxide](*N*-1-methylcytosine)} (Lock, Speranzini & Powell, 1976) and the value of 2.212 Å found in *trans*-[Pt(DMSO)(2-picoline)Cl₂] (Melanson & Rochon, 1978). It is close to the value of 2.193 Å found in K[Pt(DMSO)Cl₃] (Melanson, Hubert & Rochon, 1976) and the value of 2.200 Å found in *cis*-[Pt(DMSO)(2-picoline)Cl₂] (Melanson & Rochon, 1977). The S atom has an approximate tetrahedral environment with angles ranging from 101 to 114°. The distances and angles found in the DMSO ligand agree well with the equivalent values found in DMSO itself (Viswamitra & Kannan, 1966; Thomas, Shoemaker & Eriks, 1966) and in the Pt sulphoxide complexes mentioned above.

Fig. 2 illustrates the packing in the *cis*-[Pt(DMSO)(NH₃)Cl₂] crystal. It consists of layers of molecules parallel to the *ac* plane.

The environment of the N atom was closely examined for possible hydrogen bonding. Two short intermolecular contacts with favourable angles seem to

indicate that hydrogen bonding is important in the crystal. The N[x,y,z]...O[x - ½, ½ - y, -z] distance is 3.01 (2) Å and the Pt—N...O angle is 119.9 (7)°. The second hydrogen bond seems to involve the NH₃ molecule with Cl(2). The N[x,y,z]...Cl(2)[-½ - x, 1 - y, z - ½] distance is 3.33 (2) Å and the Pt—N...Cl(2) angle is 121.4 (6)°. There is no intramolecular hydrogen bonding.

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