

the α and β configurations (Bombieri *et al.*, 1981, 1983; Bombieri, Forsellini, Del Pra, Tobe & Henderson, 1979). Another common characteristic of such compounds is the expansion of the external angle at the 'flat' N(4), C(10)—N(4)—C(11) 119.2 (8)°. This, and the shorter Co—N(4) bond distance, could be a consequence of the reduction of angular strain at this centre. No other significant angular distortions are present in the polyamine ligand and the angles to the metal ions agree with the literature data. The Co—N(2) distance [1.941 (7) Å] *trans* to the Co—O(H₂O) is of the same order as Co—N [1.951 (7) Å] *trans* to the Co—N(NO₂) group in the nitro derivative [Co(picdien)(NO₂)(ClO₄)₂] (Bombieri *et al.*, 1983), showing a comparable *trans* influence by the NO₂ and H₂O groups. While the nitrate group shows regularity in bond distances and angles [angles around 120° and N—O 1.22 (1), 1.24 (1) Å], the perchlorate anions are rather disordered. The disorder has been described with two main orientations of the two ClO₄⁻ anions.

The crystal packing. Fig. 2 shows the packing diagram of the cationic and anionic units together with some details of the hydrogen-bonding scheme present in the structure.

There are some relatively short contacts between O(5)(water) and O(63ⁱ)(nitrate) [(i) at $x - \frac{1}{2}, \frac{3}{2} - y, z$] [O(5)···O(63ⁱ) 2.63 (1) Å], O(5)_{water} and O(3ⁱ)-(perchlorate) [O(5)···O(3ⁱ) 2.67 (2) Å], as well as between the nitrate O atoms O(61) and O(62) with N(2) of the adjacent cationic unit [N(2)···O(61) 3.16 (1), H(21)···O(61) 2.25 (3) Å, N(2)—H(21)···O(61) 162 (2)°; N(2)···O(62) 2.91 (1), H(21)···O(62) 2.12 (3) Å, N(2)—H(21)···O(62) 140 (2)°]. This suggests that the role of the nitrate group in the structure is to establish a hydrogen-bonding system between adjacent cationic units with the formation of chains running in the *a*-axis direction [the O atoms of the nitrate anion

are in contact with the coordinated water molecule of one cationic unit and N(2) of the adjacent cationic unit]. The other interactions with perchlorate anions are dealing with the two orientations of a disordered ClO₄ group {N(3)···O(24ⁱⁱ) [(ii) $1-x, 1-y, 1-z$] 2.95 (1), H(31)···O(24ⁱⁱ) 2.10 (4) Å, N(3)—H(31)···O(24ⁱⁱ) 147 (3)°; N(3)···O(224ⁱⁱ) 2.96 (2), H(31)···O(224ⁱⁱ) 2.25 (4) Å, N(3)—H(31)···O(24ⁱⁱ) 131 (3)°, N(4)···O(22ⁱⁱⁱ) [(iii) $\frac{3}{2}-x, \frac{1}{2}+y, 1-z$] 2.94 (2), H(4)···O(22) 2.12 (3) Å, N(4)—H(4)···O(22) 143 (3)°}.

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cis-Dichlorobis(di-*n*-propyl sulfoxide)platinum(II) and *cis*-Dichlorobis(ethyl methyl sulfoxide)platinum(II)

BY R. MELANSON AND F. D. ROCHON

Département de chimie, Université du Québec à Montréal, CP 8888, succ. A, Montréal, Canada H3C 3P8

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Abstract. [PtCl₂(C₆H₁₄OS)₂], $M_r = 534.48$, triclinic, $P\bar{1}$, $a = 8.274$ (5), $b = 11.256$ (6), $c = 11.949$ (7) Å, $\alpha = 115.92$ (4), $\beta = 98.30$ (5), $\gamma = 99.86$ (5)°, $V = 955.5$ (10) Å³, $Z = 2$, $D_x = 1.857$, $D_m = 1.83$ (3) Mg m⁻³, $\lambda(\text{Mo } K\alpha) = 0.71069$ Å, $\mu =$

7.91 mm⁻¹, $F(000) = 520$, $T = 295$ K, $R = 0.061$ for 2942 unique observed reflections. Pt has *cis* square-planar coordination to two Cl and to two S atoms of the dipropyl sulfoxide ligands. The bond distances are Pt—Cl = 2.289 (3), 2.302 (3) and Pt—S = 2.263 (3)

Table 1. *Experimental details of the two crystals*

	<i>cis</i> -[Pt(dpso) ₂ Cl ₂]	<i>cis</i> -[Pt(emso) ₂ Cl ₂]
Max. 2θ (°)	60	60
Quadrants	<i>h, ±k, ±l</i>	<i>h, k, ±l</i>
Scan technique	2θ/θ	2θ/θ
Scan speed (° min ⁻¹)	1.0–24.0	0.8–24.0
Standard reflections	020, 20 $\bar{1}$, 11 $\bar{3}$	400, 020, 0012
Variations (%)	<2.5	<2.0
No. of independent reflections	5597	3771
Observed reflections (<i>I</i> _{net} > 2.5σ)	2942	1660
<i>h, k, l</i>	0→11, -15→15, -16→16	0→11, 0→11, -28→26
μ (mm ⁻¹)	7.91	11.86
Crystal shape, faces and dimensions (mm)	platelet 012–0 $\bar{1}$ 2 (0.066) 100–100 (0.472) 01 $\bar{1}$ –011 (0.048)	hexagonal plate 102–102 (0.028) 011–0 $\bar{1}$ 1 (0.284) 133–1 $\bar{3}$ 3 (0.288) 104–104 (0.288)
Transmission factor range	0.1579–0.6462	0.0899–0.7199
Max. shift/e.s.d. in final cycle	0.11	0.21
Δρ _{max} (e Å ⁻³)	0.95 (close to Pt)	1.76 (close to Pt)
Δρ _{min} (e Å ⁻³)	0.73	0.77 (close to Pt)
<i>R</i>	0.061	0.069
<i>wR</i>	0.048	0.055
Weighting scheme	1/σ ² (<i>F</i>)	1/σ ² (<i>F</i>)

and 2.247 (3) Å. The O atoms are located in the same plane as the platinum coordination plane. [PtCl₂(C₃H₈OS)₂], *M_r* = 450.32, monoclinic, *P*2₁/*c*, *a* = 8.284 (8), *b* = 7.979 (6), *c* = 20.416 (10) Å, β = 109.59 (5)°, *V* = 1271 (2) Å³, *Z* = 4, *D_x* = 2.352, *D_m* = 2.33 (2) Mg m⁻³, λ(Mo *K*α) = 0.71069 Å, μ = 11.86 mm⁻¹, *F*(000) = 848, *T* = 295 K, *R* = 0.069 for 1660 unique observed reflections. Pt has a *cis* square-planar coordination with bond distances Pt–Cl = 2.312 (5), 2.317 (5) and Pt–S = 2.257 (5) and 2.272 (5) Å. The O atoms are also located in the Pt plane. The packing consists of layers of molecules parallel to the *ab* plane.

Introduction. We have been involved in a study of Pt–Me₂SO complexes for many years. The reaction of K₂PtCl₄ with Me₂SO in aqueous medium produces *cis*-[Pt(Me₂SO)₂Cl₂] (Melanson & Rochon, 1975). The corresponding palladium salt gives in the same conditions *trans*-[Pd(Me₂SO)₂Cl₂] (Bennett, Cotton, Weaver, Williams & Watson, 1967). The enhanced (*d-d*)π bonding is more effective in the *cis* Pt complexes, while in the Pd complexes it is probably insufficient to overcome the repulsions between the two sulfoxide ligands.

With other sulfoxides (*L*), IR data have shown that the [PdL₂Cl₂] complexes have the *trans* S-bonded configuration. In the corresponding Pt^{II} compounds, IR data support a *cis* configuration except when *L* is very bulky, as in bis(3-methylbutyl) sulfoxide (Price, Williamson, Schramm & Wayland, 1972). Sulfoxide ligands have a high *trans* effect and it has been shown in the reaction of K₂PtCl₄ with sulfoxides in aqueous

Table 2. *Positional parameters (× 10⁴) with their e.s.d.'s and temperature factors*

$$U_{eq} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq} (Å ²)
<i>cis</i> -[Pt(dpso) ₂ Cl ₂]				
Pt	759.1 (5)	2630.9 (5)	1336.8 (4)	328
Cl(1)	2928 (3)	2037 (3)	408 (3)	588
Cl(2)	-1048 (4)	1402 (4)	-681 (3)	595
S(1)	2686 (3)	3858 (3)	3254 (2)	356
S(2)	-1503 (3)	3113 (3)	2106 (3)	409
O(1)	4448 (7)	3843 (8)	3267 (6)	466
O(2)	-1164 (7)	4045 (7)	3490 (6)	462
C(1)	2136 (11)	3320 (11)	4382 (9)	376
C(2)	2292 (13)	1859 (12)	3976 (12)	534
C(3)	1775 (17)	1326 (16)	4890 (16)	735
C(4)	2618 (11)	5607 (10)	3962 (9)	396
C(5)	3163 (13)	6266 (13)	3153 (12)	526
C(6)	3083 (16)	7726 (15)	3702 (15)	647
C(7)	-3060 (11)	1586 (11)	1730 (11)	452
C(8)	-2537 (14)	933 (12)	2543 (11)	529
C(9)	-4003 (14)	-152 (13)	2481 (12)	601
C(10)	-2683 (12)	3796 (12)	1283 (11)	473
C(11)	-1699 (16)	5156 (17)	1483 (17)	744
C(12)	-2589 (25)	5952 (24)	1107 (26)	1242
<i>cis</i> -[Pt(emso) ₂ Cl ₂]				
Pt	2263.8 (8)	843.1 (7)	-1256.4 (4)	507
Cl(1)	-48 (5)	-608 (5)	-1160 (2)	591
Cl(2)	3511 (7)	-1706 (5)	-1324 (3)	689
S(1)	4670 (6)	2053 (5)	-1305 (3)	533
S(2)	890 (6)	3287 (5)	-1245 (2)	491
O(1)	4746 (15)	3880 (13)	-1340 (7)	680
O(2)	-868 (16)	3167 (16)	-1262 (7)	802
C(1)	6454 (20)	1336 (20)	-554 (9)	562
C(2)	5144 (31)	1319 (22)	-2052 (14)	999
C(3)	3748 (24)	1550 (26)	-2697 (9)	707
C(4)	877 (24)	4595 (20)	-1958 (9)	585
C(5)	2099 (22)	4491 (20)	-515 (10)	695
C(6)	2256 (26)	3623 (22)	213 (10)	731

medium that *trans*-[PtL₂Cl₂] is first formed. *trans*-[PtL₂Cl₂], where *L* = dipropyl sulfoxide (Price, Birk & Wayland, 1978) and benzyl methyl sulfoxide (Rochon, Kong & Girard, 1986), can be isolated after a few minutes of reaction. The *trans* compounds later isomerize to the more stable *cis* complexes.

A few years ago, we started to study the reactions of Pt complexes with sulfoxide ligands other than Me₂SO. In order to synthesize hydroxo-bridged platinum(II) dimers, we have synthesized as starting materials *cis*-[PtL₂Cl₂] (Rochon, Kong & Girard, 1986). In order to characterize all the compounds involved in these reactions, we have decided to determine the crystal structures of some of these compounds. We have recently published the structure of *cis*-[Pt(tetrahydrothiophene 1-oxide)Cl₂] (Melanson, de la Chevrotière & Rochon, 1985). We now report the crystal structure of *cis*-[Pt(dpso)₂Cl₂] [dpso = di(*n*-propyl) sulfoxide] and of *cis*-[Pt(emso)₂Cl₂] (emso = ethyl methyl sulfoxide).

Experimental. The two compounds *cis*-[Pt(dpso)₂Cl₂] (I) and *cis*-[Pt(emso)₂Cl₂] (II) were synthesized as already reported (Rochon, Kong & Girard, 1986) and were recrystallized by slow evaporation of aqueous solutions.

Table 3. Bond distances (Å) and angles (°)

<i>cis</i> -[Pt(dps _o) ₂ Cl ₂]			
Pt-Cl(1)	2.289 (3)	Cl(1)-Pt-Cl(2)	88.0 (1)
Pt-Cl(2)	2.302 (3)	Cl(1)-Pt-S(1)	88.3 (1)
Pt-S(1)	2.263 (3)	Cl(1)-Pt-S(2)	175.8 (1)
Pt-S(2)	2.247 (3)	Cl(2)-Pt-S(1)	175.9 (1)
S(1)-O(1)	1.458 (7)	Cl(2)-Pt-S(2)	87.8 (1)
S(2)-O(2)	1.471 (7)	S(1)-Pt-S(2)	95.9 (1)
S(1)-C(1)	1.79 (1)	Pt-S(1)-O(1)	117.4 (3)
S(1)-C(4)	1.79 (1)	Pt-S(2)-O(2)	116.4 (3)
S(2)-C(7)	1.79 (1)	Pt-S(1)-C(1)	110.8 (4)
S(2)-C(10)	1.78 (1)	Pt-S(1)-C(4)	110.1 (4)
C(1)-C(2)	1.53 (2)	Pt-S(2)-C(7)	111.6 (4)
C(4)-C(5)	1.53 (2)	Pt-S(2)-C(10)	111.5 (4)
C(7)-C(8)	1.51 (2)	O(1)-S(1)-C(1)	106.7 (5)
C(10)-C(11)	1.50 (2)	O(1)-S(1)-C(4)	107.4 (5)
C(2)-C(3)	1.54 (2)	O(2)-S(2)-C(7)	108.1 (5)
C(5)-C(6)	1.50 (2)	O(2)-S(2)-C(10)	107.5 (5)
C(8)-C(9)	1.54 (2)	C(1)-S(1)-C(4)	103.5 (5)
C(11)-C(12)	1.43 (3)	C(7)-S(2)-C(10)	100.4 (6)
		S(1)-C(1)-C(2)	110.4 (8)
		S(1)-C(4)-C(5)	110.8 (8)
		S(2)-C(7)-C(8)	112.3 (8)
		S(2)-C(10)-C(11)	112.5 (10)
		C(1)-C(2)-C(3)	112 (1)
		C(4)-C(5)-C(6)	112 (1)
		C(7)-C(8)-C(9)	113 (1)
		C(10)-C(11)-C(12)	118 (2)

<i>cis</i> -[Pt(emso) ₂ Cl ₂]			
Pt-Cl(1)	2.312 (5)	Cl(1)-Pt-Cl(2)	87.9 (2)
Pt-Cl(2)	2.317 (5)	Cl(1)-Pt-S(1)	174.7 (2)
Pt-S(1)	2.257 (5)	Cl(1)-Pt-S(2)	89.9 (2)
Pt-S(2)	2.272 (5)	Cl(2)-Pt-S(1)	87.4 (2)
S(1)-O(1)	1.47 (1)	Cl(2)-Pt-S(2)	176.4 (2)
S(2)-O(2)	1.46 (1)	S(1)-Pt-S(2)	95.0 (2)
S(1)-C(1)	1.83 (2)	Pt-S(1)-O(1)	119.0 (6)
S(1)-C(2)	1.80 (3)	Pt-S(2)-O(2)	116.6 (6)
S(2)-C(4)	1.79 (2)	Pt-S(1)-C(1)	108.1 (6)
S(2)-C(5)	1.78 (2)	Pt-S(1)-C(2)	110.3 (8)
C(2)-C(3)	1.45 (3)	Pt-S(2)-C(4)	111.3 (6)
C(5)-C(6)	1.60 (3)	Pt-S(2)-C(5)	109.4 (6)
		O(1)-S(1)-C(1)	109 (1)
		O(1)-S(1)-C(2)	105 (1)
		O(2)-S(2)-C(4)	107 (1)
		O(2)-S(2)-C(5)	110 (1)
		S(1)-C(2)-C(3)	113 (2)
		S(2)-C(5)-C(6)	113 (1)
		C(1)-S(1)-C(2)	105 (1)
		C(4)-S(2)-C(5)	102 (1)

The experimental details of the two crystals are shown in Table 1. Density by flotation in thallos malonate aqueous solution for (I) and dibromomethane-ethylene bromide for (II); space groups determined by precession photographs; Syntex P1 diffractometer; graphite-monochromatized Mo K α radiation; cell parameters from refined angles of 15 centered reflections; $\sigma(I)$ calculated as in Melanson & Rochon (1975); absorption correction based on equations of crystal faces; data corrected for Lorentz and polarization effects; atomic scattering factors of Cromer & Waber (1965) for Pt, Cl, S, O, C and of Stewart, Davidson & Simpson (1965) for H; anomalous-dispersion terms of Pt, Cl and S from Cromer (1965).

Patterson map showed position of Pt; other non-hydrogen atoms located by structure factors and Fourier-map calculations; isotropic secondary-extinction correction (Coppens & Hamilton, 1970); H atoms fixed at calculated positions (C-H = 0.95 Å and N-H = 0.85 Å) with isotropic $B = 6.0 \text{ \AA}^2$. Cal-

culations on a Cyber 830 with programs of Melanson & Rochon (1975).*

Discussion. The refined atomic parameters are listed in Table 2. A labeled diagram of the two molecules is shown in Fig. 1. The coordination around the Pt atom is square planar and the angles around the Pt atom are close to the expected values of 90 and 180°. As expected from IR spectroscopy, the compounds are the *cis* isomers (Rochon, Kong & Girard, 1986) and the sulfoxide ligands are bonded to Pt through their S atom. Bond distances and angles are reported in Table 3.

The weighted best coordination plane was calculated through the five atoms. The deviations are for (I): Pt, -0.0013 (6); Cl(1), -0.010 (4); Cl(2), 0.040 (4); S(1), 0.027 (3); S(2), -0.006 (4) Å; and for (II): Pt, -0.0002 (7); Cl(1), -0.044 (4); Cl(2), 0.065 (5); S(1), -0.050 (5); S(2), 0.048 (5) Å. The O atoms of the sulfoxide ligands are also located in the same plane as the platinum coordination plane. The deviations are for (I): O(1), 0.003 (9) and O(2), 0.063 (9) Å and for (II): O(1), 0.004 (13) and O(2), 0.180 (14) Å.

* Lists of structure factors, anisotropic thermal parameters, H coordinates, equations and deviations from weighted best planes, and Figs. 2 and 3 have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44064 (42 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

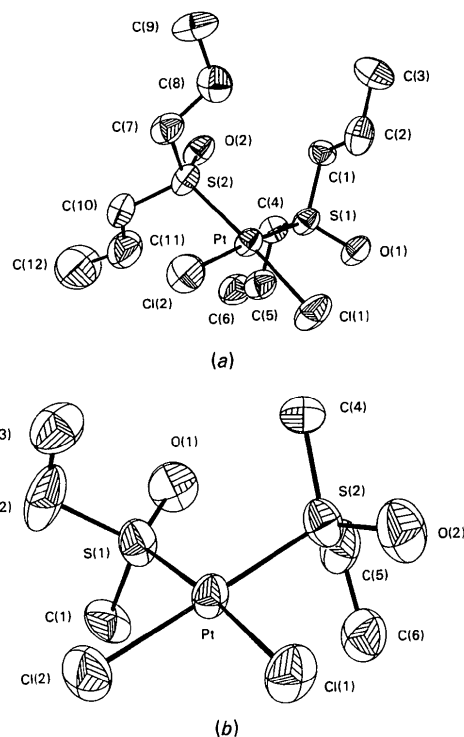


Fig. 1. Labeled diagram of the molecules (a) *cis*-[Pt(dps_o)₂Cl₂] and (b) *cis*-[Pt(emso)₂Cl₂].

The Pt—Cl bonds [2.289 (3), 2.302 (3) Å for (I) and 2.312 (5), 2.317 (5) Å for (II)] and the Pt—S bond distances [2.263 (3), 2.247 (3) Å for (I) and 2.257 (5), 2.272 (5) Å for (II)] are normal [the standard deviations calculated as in Melanson & Rochon (1975) are probably underestimated] and agree well with the values found in *cis*-[Pt(Me₂SO)₂Cl₂] (Melanson & Rochon, 1975) and *cis*-[Pt(tetrahydrothiophene sulfoxide)₂Cl₂] (Melanson, de la Chevrotière & Rochon, 1985). The S atoms in the sulfoxide ligands are in a tetrahedral environment. The Pt—S—O angles [117.4 (3), 116.4 (3)° for (I) and 119.0 (6), 116.6 (6)° for (II)] are larger than the tetrahedral value as observed in the Pt—sulfoxide structures described above and other published structures (Rochon & Guay, 1987, and references therein). The Pt—S—C angles [110.1 (4)—111.6 (4)° for (I) and 108.1 (6)—111.3 (6)° for (II)] are normal as in Pt—Me₂SO complexes (Melanson & Rochon, 1975; Rochon, Kong & Melanson, 1985). The S—O, S—C and C—C bond distances agree well with published values except for a few terminal C—C bonds. The thermal factors of most terminal C atoms are high, indicating some disorder. All the C—C—C angles in *cis*-[Pt(dpso)₂Cl₂] are slightly larger than expected [112 (1)—118 (2)°], resulting in a flattening of the propyl groups.

The density of the crystal *cis*-[Pt(dpso)₂Cl₂] (1.857 Mg m⁻³) is smaller than expected. The corresponding densities for *cis*-[Pt(Me₂SO)₂Cl₂], *cis*-[Pt(tetrahydrothiophene sulfoxide)₂Cl₂] and *cis*-[Pt(emso)₂Cl₂] are 2.620, 2.381 and 2.352 Mg m⁻³. The low density in *cis*-[Pt(dpso)₂Cl₂] results in high thermal factors of the carbon atoms, which tend to occupy more space, resulting in a flattening of the propyl groups.

The packing of the molecules is shown in Figs. 2 and 3.* No hydrogen bonding is expected for these compounds. In *cis*-[Pt(dpso)₂Cl₂], the propyl groups are almost perpendicular to the platinum plane which also contains the O atoms. The propyl groups are also almost parallel to the *b* axis. In *cis*-[Pt(emso)₂Cl₂], the platinum planes with the O atoms are nearly parallel to the *ab* plane.

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* See deposition footnote.

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Structure of Pentaqua(hypoxanthine)nickel(II) Sulfate*

BY ERICH DUBLER, GABY HÄNGGI AND HELMUT SCHMALLE

Institute of Inorganic Chemistry, University of Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland

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Abstract. [Ni(C₅H₄N₄O)(H₂O)₅]₂SO₄, *M_r* = 380.96, triclinic, *P* $\bar{1}$, *a* = 7.498 (1), *b* = 12.901 (2), *c* = 6.633 (1) Å, α = 92.77 (1), β = 90.15 (1), γ = 92.23 (1)°, *V* = 640.4 (3) Å³, *Z* = 2, *D_m* = 1.98 by flotation, *D_x* = 1.98 g cm⁻³, $\lambda(\text{Mo } K\alpha)$ = 0.71073 Å, μ = 17.4 cm⁻¹, *F*(000) = 392, room temperature, *R* = 0.032 for 5408 observed unique reflections. The

structure contains [Ni(hypoxanthine)(H₂O)₅]²⁺ cations and non-coordinating sulfate anions. Nickel(II) exhibits a slightly distorted octahedral coordination by five water molecules and a monodentate hypoxanthine ligand binding through N(7). Hypoxanthine is protonated at N(1) and N(9); metal coordination at N(7) induces about 30% of the shifts in the bonding angles of the imidazole ring compared to the shifts by protonation of guanine derivatives at N(7). The structure is

* Hypoxanthine is 1,7-dihydro-6*H*-purin-6-one.