SHORT STRUCTURAL PAPERS

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trans-(Dithiocyanato)(bispyridine)platinum (II)

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Abstract. *trans*-[Pt(II) $(py)_2(SCN)_2$]: triclinic, space group $P\bar{1}$, $a=5{\cdot}377$ (5), $b=10{\cdot}568$ (5), $c=6{\cdot}820$ (5) Å, $\alpha=96{\cdot}8$ (1), $\beta=107{\cdot}2$ (1), $\gamma=99{\cdot}7$ (1)°, $Z=1$, $M=469{\cdot}0$, $D_m=2{\cdot}15$, $D_c=2{\cdot}17$ g cm^{-3}. The platinum atom is in square-planar coordination.

Introduction. Weissenberg photographs, taken about the three principal axes, showed no systematic absences, indicating that the space group was either $P1$ or $P\bar{1}$. The latter was chosen for the structural determination, the choice being vindicated by the successful refinement of the structure. The crystal used for data collection was a cube of size 0·25 mm and the cell parameters were obtained from least-squares analysis of the settings of 25 reflexions measured on a four-circle Philips PW 1100 diffractometer.

Intensities were measured with graphite-monochromated Mo $K\alpha$ radiation ($\lambda=0{\cdot}7107$ Å), ω–2θ scan mode (scan width $1{\cdot}6°\theta$, scan speed $0{\cdot}05°\theta$ s^{-1}). 1259 reflexions were collected in the 2θ range 6° to 50°. All reflexions had $I>1{\cdot}65\sigma(I)$ and were classified as 'observed'. Lorentz and polarization corrections were applied; no corrections for absorption were made. An electron density map, based on structure factors calculated by placing Pt at the origin, yielded the positions of all the non-hydrogen atoms. After two cycles of isotropic and four cycles of anisotropic least-squares refinement, a difference map yielded the positions of all the hydrogen atoms. Finally three cycles of refinement were carried out in which the positions of the H atoms were allowed to vary, and their temperature factors were fixed as the isotropic U values of the atoms to which they were bonded. The final R was 0·035 with unit weight for each reflexion. The scattering factors for Pt, S, C and N were those of Cromer & Mann (1960), and for H, those of Stewart, Davidson & Simpson (1965). Anomalous dispersion corrections were applied to the Pt and S scattering curves (*International Tables for X-ray Crystallography*, 1968). Table 1 lists the final parameters of the heavy atoms and Table 2 those of the light atoms. Fig. 1 shows the molecular configuration and atomic nomenclature. Tables 3 and 4 list the principal bond lengths and angles.*

Discussion. There is great interest at present in platinum(II) compounds owing to their anti-tumour activity (Cleare, 1974). The compound was prepared by

* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 30720 (13 pp., 1 microfiche). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 1. *Fractional atomic coordinates and thermal parameters and their e.s.d.'s for the heavy atoms*

Coordinates are $\times 10^3$. Thermal parameters are of the form $T=\exp[-2\pi^2(U_{11}h^2a^{*2}+U_{22}k^2b^{*2}+U_{33}l^2c^{*2}+2U_{12}hka^*b^*+2U_{13}hla^*c^*+2U_{23}klb^*c^*)\times 10^3]$.

	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pt	0	0	0	36 (0)	18 (0)	35 (0)	8 (0)	14 (0)	15 (0)
N(1)	47 (2)	−160 (1)	135 (1)	33 (5)	26 (4)	42 (5)	1 (4)	1 (4)	18 (4)
C(1)	188 (2)	−240 (1)	72 (2)	45 (6)	32 (6)	59 (7)	16 (5)	23 (6)	20 (5)
C(2)	215 (3)	−354 (1)	153 (2)	47 (7)	27 (6)	62 (8)	16 (5)	7 (6)	13 (5)
C(3)	90 (3)	−385 (1)	293 (2)	57 (7)	27 (6)	51 (7)	3 (5)	0 (6)	23 (5)
C(4)	−56 (3)	−304 (1)	353 (2)	62 (8)	46 (7)	56 (8)	13 (6)	23 (7)	34 (6)
C(5)	−73 (2)	−190 (1)	271 (2)	46 (7)	40 (6)	46 (7)	17 (5)	19 (6)	18 (5)
S	374 (1)	107 (0)	278 (1)	58 (2)	29 (1)	51 (2)	3 (1)	−1 (1)	20 (1)
C(6)	415 (2)	266 (1)	255 (2)	47 (7)	33 (6)	38 (6)	4 (5)	4 (5)	10 (5)
N(2)	453 (2)	373 (1)	243 (2)	78 (8)	27 (6)	65 (7)	4 (5)	3 (6)	13 (5)

Table 2. *Final hydrogen atom positional and thermal parameters (both* $\times 10^2$*)*

	x	y	z	U_{iso} (Å^2)
H(1)	27 (2)	−22 (1)	−4 (2)	3·9
H(2)	32 (2)	−40 (1)	10 (2)	4·5
H(3)	10 (2)	−47 (1)	35 (2)	4·6
H(4)	−15 (2)	−32 (1)	46 (2)	5·1
H(5)	−16 (2)	−15 (1)	32 (2)	3·6

Table 3. *Bond lengths* (Å) *and their e.s.d.'s*

Pt—N(1)	2·041 (9)	S—C(6)	1·69 (1)
Pt—S	2·322 (5)	C(6)–N(2)	1·14 (2)
N(1)–C(1)	1·34 (2)	C(1)–H(1)	1·0 (1)
C(1)–C(2)	1·39 (2)	C(2)–H(2)	0·9 (1)
C(2)–C(3)	1·37 (2)	C(3)–H(3)	1·0 (1)
C(3)–C(4)	1·36 (2)	C(4)–H(4)	1·0 (1)
C(4)–C(5)	1·39 (2)	C(5)–H(5)	0·8 (1)
C(5)–N(1)	1·32 (2)		

Table 4. *Bond angles* (°) *and their e.s.d.'s*

N(1)–Pt—N(1^i)	180·0	Pt—N(1)–C(5)	120·8 (8)
S—Pt—S^i	180·0	C(1)–N(1)–C(5)	120 (1)
S—Pt—N(1)	84·7 (2)	N(1)–C(1)–C(2)	121 (1)
S^i—Pt—N(1)	95·3 (2)	C(1)–C(2)–C(3)	119 (1)
Pt—S—C(6)	105·4 (4)	C(2)–C(3)–C(4)	119 (1)
S—C(6)–N(2)	177 (1)	C(3)–C(4)–C(5)	120 (1)
Pt—N(1)–C(1)	118·8 (9)	C(4)–C(5)–N(1)	121 (1)

heating a mixture of K_2PtCl_4 and KSCN in aqueous solution, followed by the addition of pyridine. The yellow product was recrystallized from acetone containing an excess of pyridine. The structure was investigated because from the infrared spectra it could not be unambiguously established whether the compound had the *cis-* or *trans-* configuration and whether the SCN ligand was bonded *via* nitrogen or sulphur. The lengths Pt–N [2·041 (9) Å] and Pt–S [2·322 (5) Å] are comparable to those found in other Pt(II) structures (Stephenson, 1962; Bleĭdelis & Bokii, 1957). Plane I, defined by Pt, N(1), N(1^i), S and S^i intersects plane II, the plane through the pyridine moiety, at an angle of 89·0°. Plane III, defined by Pt, S and C(6), intersects plane I at 5·3°. There are no short non-bonded distances.

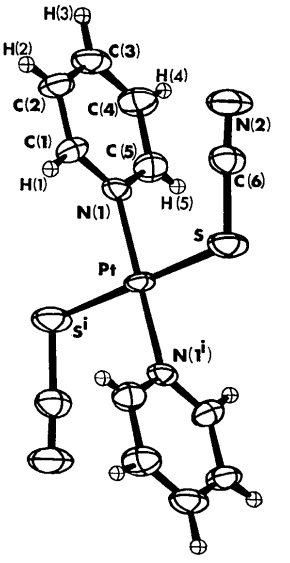

Fig. 1. Molecular structure showing the atomic nomenclature. The thermal ellipsoids are drawn at the 50% probability level. Superscripted atoms are centrosymmetrically related to the atoms without superscripts.

All calculations were performed on the University of Cape Town's Univac 1106 computer with the X-RAY program system (1972).

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