

(Deacon, Patrick, Skelton, Thomas & White, 1984), the terpyridine ligand was bonded in a bidentate fashion.

References

- CROMER, D. T. (1974). *International Tables for X-ray Crystallography*, Vol. IV, Table 2.3.1. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)
- DEACON, G. B., PATRICK, J. M., SKELTON, B. W., THOMAS, N. C. & WHITE, A. H. (1984). *Aust. J. Chem.* **37**, 929–945.
- SHEDRICK, G. M. (1986). *SHELXTL*. Crystallographic computing system. Nicolet Instruments Division, Madison, WI, USA.

Acta Cryst. (1990). **C46**, 1107–1108

Structure of Bis(ethylenediamine)platinum(II) Dichloride

BY SHOICHI SATO

The Institute for Solid State Physics, The University of Tokyo, Roppongi 7-22-1, Minato-ku, Tokyo 106, Japan

AND MIKAKO HARUKI* AND SUSUMU KURITA

Faculty of Engineering, Yokohama National University, Tokiwadai 156, Hodogaya-ku, Yokohama 240, Japan

(Received 4 December 1989; accepted 23 January 1990)

Abstract. $[\text{Pt}(\text{C}_2\text{H}_8\text{N}_2)_2]\text{Cl}_2$, $M_r = 386.2$, triclinic, $P\bar{1}$, $a = 6.918(4)$, $b = 8.378(5)$, $c = 4.951(2)\text{\AA}$, $\alpha = 98.00(6)$, $\beta = 100.15(6)$, $\gamma = 108.57(6)^\circ$, $V = 261.8(2)\text{\AA}^3$, $Z = 1$, $D_x = 2.25\text{ Mg m}^{-3}$, $\lambda(\text{Ag } \text{K}\alpha) = 0.56087\text{\AA}$, $\mu = 7.5\text{ mm}^{-1}$, $F(000) = 180$, $T = 298\text{ K}$. $R = 0.022$ for 3111 unique reflections. The ethylenediamine moieties coordinate in a square planar manner with amino N atoms attached to the Pt atom at the center of symmetry. The five-membered chelate rings adopt the *meso* form with the ligands in almost symmetric *gauche* (synclinal) conformations. The C atoms are shifted about 0.35\AA above and below the PtNN plane. The complex cations are linked two-dimensionally along the (010) plane by N—H \cdots Cl hydrogen bonds. No short contacts are observed along **b**.

Experimental. Crystals prepared by recrystallization from an aqueous solution of the title compound (Bekaroglu, Breer, Endres, Keller & Nam Gung, 1977). The details of data collection and structure refinement are summarized in Table 1. The structure was solved by the heavy-atom method, and refined by full-matrix least squares. The H atoms were deduced clearly from difference Fourier maps, and included in the refinement. Thermal parameters were anisotropic for the non-H atoms and isotropic for the H atoms. Since two space groups, *P*1 and $P\bar{1}$, were possible, refinements were attempted for both space groups; they converged in quite similar

structures with nearly the same R values. Therefore, the centrosymmetric space group $P\bar{1}$ was selected.

A projection of the structure along **c** (in which direction the cations are obliquely stacked) is shown in Fig. 1. The final atomic coordinates and equivalent isotropic thermal parameters are listed in Table 2.^f Bond lengths, angles, hydrogen bonds and torsion angles are tabulated in Table 3.

Atomic form factors and f' , f'' values taken from *International Tables for X-ray Crystallography* (1974). Calculations performed on a FACOM

^f Lists of structure factors, anisotropic thermal parameters, H-atom parameters and bond lengths involving H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52624 (8 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Experimental details*

Crystal	Colourless, transparent, plate like; shaped to a sphere ($d = 0.37\text{ mm}$)
Diffractometer	Rigaku AFC-3, graphite monochromator
Scan	ω mode, width $(2.4 + 0.8\tan\theta)^\circ$, speed 2°min^{-1} , $2\theta < 60^\circ$
Standards	062, 054, 710, 374, 483; every 50 reflections, no significant fluctuation
Range of hkl	$h 0 \rightarrow 12$, $k -14 \rightarrow 14$, $l -8 \rightarrow 8$
Reflections	Measured 3113
Corrections	Observed 3111, $ F_o > 3\sigma(F_o)$
Transmission	Lp, absorption ($\mu r = 1.39$)
Unit cell	$0.15 - 0.19$
Function minimized	68 reflections, $19.5 < \theta < 21.5^\circ$
Parameters refined	$\sum w(F_o - F_c)^2$, $w = [\sigma^2(F_o) + (0.015 F_o)^2]^{-1}$
R , wR , S	66
Max. Δ/σ	0.022, 0.028, 1.04
Min. and max. $\Delta\rho$	0.04
	-1.8 and 3.0 e \AA^{-3} near the Pt atom (-0.5 and 0.4 e \AA^{-3} elsewhere)

* Present address: Laboratorium für Festkörperphysik, ETH-Hönggerberg, CH-8093, Zürich, Switzerland.

Table 2. Positional and thermal parameters with e.s.d.'s in parentheses

	x	y	z	$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j$
Pt	0.0	0.0	0.0	0.02110 (4)
N(1)	-0.0283 (4)	0.2332 (3)	-0.0207 (5)	0.0307 (7)
N(2)	0.2755 (4)	0.1077 (3)	-0.1136 (6)	0.0308 (7)
C(1)	0.1778 (6)	0.3583 (4)	-0.0316 (8)	0.0386 (10)
C(2)	0.2724 (6)	0.2642 (4)	-0.2196 (7)	0.0372 (10)
Cl	0.6806 (1)	0.2601 (1)	0.4178 (2)	0.0390 (3)

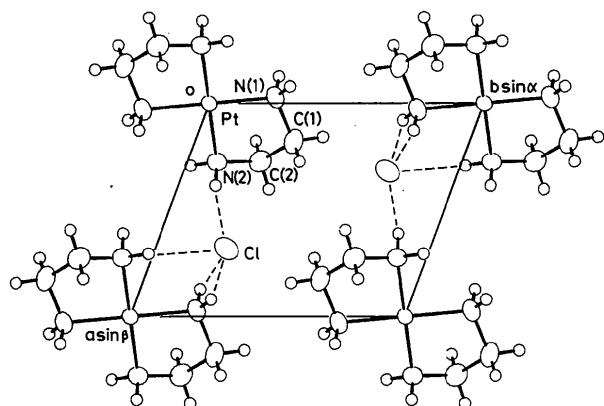


Fig. 1. A projection of the structure along c with the atomic numbering scheme. Thermal ellipsoids are drawn at the 60% probability level; a value of 0.8 \AA^2 is given for the B_{iso} of the H atoms in this figure. Broken lines indicate N—H···Cl hydrogen bonds.

M-380R computer at ISSP, The University of Tokyo. Computational programs used were UNICSI (Sakurai, 1967), RADIEL (Coppens, Guru Row, Leung, Stevens, Becker & Yang, 1979) and ORTEPII (Johnson, 1971).

Table 3. Bond lengths (\AA), angles ($^\circ$), N—H···Cl hydrogen bonds (\AA) and torsion angles ($^\circ$)

Pt—N(1)	2.039 (3)	Pt—N(2)	2.046 (3)
N(1)—C(1)	1.492 (4)	N(2)—C(2)	1.483 (5)
C(1)—C(2)	1.502 (6)		
N(1)···Cl ⁱ	3.242 (4)	N(1)···Cl ⁱⁱ	3.213 (3)
N(2)···Cl	3.255 (4)	N(2)···Cl ⁱⁱⁱ	3.365 (4)
N(1)—Pt—N(2)	83.1 (1)	Pt—N(1)—C(1)	109.3 (2)
Pt—N(2)—C(2)	109.0 (2)	N(1)—C(1)—C(2)	107.3 (3)
N(2)—C(2)—C(1)	107.5 (3)		
N(2)—Pt—N(1)—C(1)	14.0	N(1)—Pt—N(2)—C(2)	15.2
Pt—N(1)—C(1)—C(2)	-40.2	Pt—N(2)—C(2)—C(1)	-41.2
N(1)—C(1)—C(2)—N(2)	53.4		

Symmetry operations: (i) $-1 + x, y, z$; (ii) $-1 + x, y, -1 + z$; (iii) $1 - x, -y, -z$.

Related literature. The geometry and conformation of the en ring (en = ethylenediamine) are very similar to those in [PtCl₂(en)]₂(ClO₄)₂ (Sato, Haruki, Wachter & Kurita, 1990).

References

- BEKAROGLU, O., BREER, H., ENDRES, H., KELLER, H. J. & NAM GUNG, H. (1977). *Inorg. Chim. Acta*, **21**, 183–186.
- COPPENS, P., GURU ROW, T. N., LEUNG, P., STEVENS, E. D., BECKER, P. J. & YANG, Y. W. (1979). *Acta Cryst. A35*, 63–72. *International Tables for X-ray Crystallography* (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)
- JOHNSON, C. K. (1971). Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
- SAKURAI, T. (1967). Editor. UNICSI. *Universal Crystallographic Computation Program System*. The Crystallographic Society of Japan, Tokyo, Japan.
- SATO, S., HARUKI, M., WACHTER, P. & KURITA, S. (1990). *Acta Cryst.* In the press.

Structure of an Optically Active Organoaluminium Naphthylethylamine Dimer

BY WILLIAM T. PENNINGTON,* GREGORY H. ROBINSON* AND SAMUEL A. SANGOKOYA

Department of Chemistry, Clemson University, Clemson, SC 29634–1905, USA

(Received 15 September 1989; accepted 2 January 1990)

Abstract. Bis- μ -[1-(1-naphthyl)ethylaminato-*N*]-bis[dimethylaluminium(III)], [Al₂(CH₃)₄(C₁₀H₁₂N)₂], $M_r = 454.62$, monoclinic, $P2_1$, $a = 10.925 (4)$, $b = 11.129 (4)$, $c = 11.212 (4) \text{ \AA}$, $\beta = 94.18 (3)^\circ$, $V = 1359.6 (8) \text{ \AA}^3$, $Z = 2$, $D_x = 1.11 \text{ g cm}^{-3}$, Mo $K\alpha$, $\lambda = 0.71073 \text{ \AA}$, $\mu = 1.19 \text{ cm}^{-1}$, $F(000) = 488$, $T = 294 \text{ K}$, $R = 0.0355$ for 1615 observed reflections. The reaction of trimethylaluminium with (*R*)-(+)1-(1-naph-

thyl)ethylamine involves cleavage of Al—C_{Me} and N—H bonds resulting in elimination of methane and formation of an asymmetric Al₂N₂ fragment, as the core of a dimeric molecule consisting of two (C₁₀H₇)CH(CH₃)NHAl(CH₃)₂ units. The molecule has approximate C_2 symmetry, with an average Al—N bond distance of 1.96 (1) \AA .

Experimental. The title compound results from the slow addition of a trimethylaluminium/toluene solu-

* To whom correspondence should be addressed.