

Table 3. Selected bond lengths (Å) and bond angles (°) (with e.s.d.'s)

	(A)*	(B)†
Ru1—Ru2	2.558 (1)	2.560 (1)
Ru1—P1	2.372 (3)	2.382 (1)
Ru1—N1	2.167 (8)	2.163 (2)
Ru1—N2	2.149 (8)	2.161 (2)
Ru1—C11	1.87 (1)	1.866 (3)
Ru1—C12	1.85 (1)	1.858 (3)
P1—C31	1.83 (1)	1.834 (2)
P1—C41	1.81 (1)	1.835 (3)
P1—C51	1.83 (1)	1.825 (3)
C11—O11	1.13 (1)	1.140 (3)
C12—O12	1.15 (1)	1.143 (3)
N1—C1	1.44 (1)	1.419 (4)
N2—C2	1.42 (1)	1.431 (4)
C1—C2	1.41 (1)	1.403 (5)
C2—C3	1.37 (1)	1.364 (5)
C3—C4	1.40 (2)	1.407 (6)
C4—C5	1.33 (2)	1.357 (6)
C5—C6	1.41 (2)	1.404 (6)
C6—C1	1.37 (1)	1.376 (5)
Ru2—Ru1—P1	150.7 (1)	151.3 (1)
Ru2—Ru1—N1	53.8 (2)	53.7 (1)
Ru2—Ru1—N2	53.5 (2)	53.7 (1)
Ru2—Ru1—C11	104.5 (3)	106.2 (1)
Ru2—Ru1—C12	105.6 (4)	102.9 (1)
P1—Ru1—N1	105.2 (2)	104.8 (1)
P1—Ru1—N2	102.4 (2)	103.4 (1)
P1—Ru1—C11	94.2 (3)	92.7 (1)
P1—Ru1—C12	96.2 (4)	98.5 (1)
N1—Ru1—N2	69.1 (3)	68.6 (1)
N1—Ru1—C11	158.3 (4)	159.7 (1)
N1—Ru1—C12	96.1 (4)	97.8 (1)
N2—Ru1—C11	97.6 (4)	97.6 (1)
N2—Ru1—C12	158.7 (4)	156.6 (1)
C11—Ru1—C12	91.4 (5)	89.7 (1)

*Averaged values.

†Mirror plane related.

A comparison of bond distances and angles for molecules (A) and (B) shows that both are virtually identical, with normal differences derived from distinct packings due to different solvents. All this information allows us to conclude that molecules of structures (A) and (B) are of the same compound, mentioned in the title of this paper, and therefore structure (C) should be substituted by structure (B) of the present communication.

Acta Cryst. (1990). **C46**, 2046–2049

Structure of *cis*-Tetrachlorobis(1-ethylimidazole- κN^3)platinum(IV)

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(Received 25 July 1989; accepted 5 February 1990)

Abstract. [PtCl₄(C₅H₈N₂)₂], $M_r = 529.2$, monoclinic, $P2_1/n$, $a = 12.749$ (4), $b = 9.217$ (3), $c = 14.898$ (5) Å, $\beta = 110.06$ (5)°, $V = 1644.4$ (9) Å³, $Z = 4$, $D_m = 2.12$ (3), $D_x = 2.14$ Mg m⁻³, Mo $K\alpha$, $\lambda = 0.71069$ Å,

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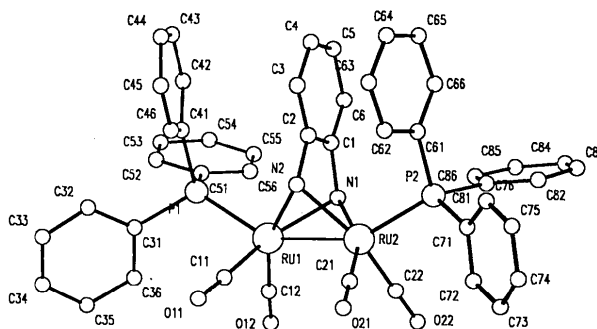


Fig. 1. *PLUTO* (Motherwell, 1976) diagram showing the atomic arrangement and numbering for molecule (A); molecule (B) follows a similar labelling.

The molecule shows a mirror plane containing the diimine ring, which is a crystallographic mirror plane for structure (B).

The distance between the two ruthenium atoms, 2.559 (1) Å, is significantly short for a single Ru^I—Ru^I bond.

Both ruthenium atoms exhibit a significantly distorted octahedral environment due to the very diverse nature of the ligands.

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$\mu = 9.61$ mm⁻¹, $F(000) = 1000$, $T = 294$ (2) K, $R = 0.036$ for 2110 unique observed reflections. The complex consists of mononuclear PtCl₄(1-ethylimidazole)₂ units. The coordination around Pt^{IV} is

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octahedral with the two 1-ethylimidazole ligands mutually *cis*. The Pt—N distances are 2.007 (10) and 2.055 (11) Å. The Pt—Cl distances [2.304 (4) to 2.326 (4) Å] are typical for platinum(IV) complexes.

Introduction. Although neutral platinum(IV) complexes are known to be cytotoxically active, they have been rather neglected compared with platinum(II) species in the search for new anti-cancer drugs and only relatively few reports of tests of platinum(IV) derivatives have appeared (Pendyala, Cowens & Creaven, 1982; Rotondo, Fimiani, Cavallaro & Ainis, 1983). This neglect reflects the conviction that octahedral platinum complexes cannot be intrinsically biologically active because of structural hindrance and their slow rates of ligand exchange *in vivo* (Thomson, Williams & Reslova, 1972).

The biological activity noted in some neutral platinum(IV) complexes is attributed to reduction *in vivo* to the corresponding platinum(II) species with simultaneous removal of the axial ligands (Cleare, 1977). However, it has been found that active antitumour platinum(IV) complexes can react *in vitro* with DNA without prior reduction to the bivalent state and that they may induce in DNA conformational alterations similar to those produced by bivalent complexes (Brabec, Vrana & Kleinwachter, 1986).

It is therefore of interest to investigate the relationship between antineoplastic activity and oxidation state by comparing platinum(IV) derivatives with their platinum(II) analogues.

Previously we synthesized and tested *in vitro* some platinum(II) complexes with 1-ethylimidazole and 1-propylimidazole ligands (Kuduk-Jaworska & Jeżowska-Trzebiatowska, 1983). We also described the structure of a platinum(IV) analogue with 1-propylimidazole (Kuduk-Jaworska, Kubiak & Głowiak, 1988). Here we report the structure of a new neutral platinum(IV) complex with 1-ethylimidazole as part of our structure-activity study on platinum complexes.

Experimental. A mixture of 0.46 g (1 mmol) of *cis*-dichlorobis(1-ethylimidazole)platinum(II) and 10 ml 30% H₂O₂ was boiled until a clear solution was obtained. Then 10 ml 1M HCl was added and the solution boiled for a further 30 min. After cooling, by-products were removed by extraction with CH₂Cl₂. The water phase was evaporated and the precipitate was crystallized from dimethylformamide-ethyl acetate [m.p. 505 K; IR—far IR: 1690, 1610, 1545, 1520 ($\nu_{C=C}$, $\nu_{C=N}$), 340 (ν_{Pt-Cl}) cm⁻¹; $A_M(\text{DMF}) = 8.5 \Omega^{-1} \text{cm}^2 \text{mol}^{-1}$].

Infrared spectra were obtained with a Perkin Elmer 180 spectrophotometer (Nujol mulls between KBr and polyethylene disc).

Conductivity was measured on the Radelkis OK-102/1 conductometer. Yellow crystal, dimensions 0.12 × 0.12 × 0.20 mm; D_m by flotation in CCl₄/1,2-dibromoethane, monoclinic from Weissenberg photographs; Syntex P2₁ computer-controlled four-circle diffractometer; scintillation counter, graphite monochromator; cell parameters by least squares from setting angles of 15 reflections with $15 < 2\theta < 24^\circ$ measured on the diffractometer; 2267 independent reflections measured; $2\theta_{\text{max}} = 50^\circ$; variable ω - 2θ scans, scan rate 2.0 - $29.3^\circ \text{min}^{-1}$ depending on intensity, two standards measured every 50 reflections, variation in their intensities $\pm 4\%$; corrections for Lorentz and polarization effects, but not for extinction; calculations performed on a NOVA 1200 computer with programs supplied by Syntex (1976), scattering factors for neutral atoms, corrected for anomalous dispersion (for Pt and Cl) from *International Tables for X-ray Crystallography* (1974); for structure solution and refinement 2110 amplitudes with $F \geq 6\sigma(F)$ used, $h0 \rightarrow 15$, $k0 \rightarrow$, $l-17 \rightarrow 16$, Patterson synthesis and difference Fourier methods; full-matrix least-squares refinement minimizing $\sum w(|F_o| - |F_c|)^2$; $w = 1/\sigma^2(F)$; H atoms included in calculated positions (with $B = 6.5 \text{ \AA}^2$), non-H atoms refined with anisotropic thermal parameters, absorption correction following the *DIFABS* procedure (Walker & Stuart, 1983) was applied; max. and min. absorption factors 1.396 and 0.734, respectively; $(\Delta/\sigma)_{\text{max}} = 0.1$; residual electron density in final difference map within -0.20 and 0.30 e \AA^{-3} , $R = 0.036$, $wR = 0.046$, $S = 2.716$.

Discussion. The positional parameters are reported in Table 1 and the relevant bond distances and angles in Table 2.*

As can be seen in Fig. 1, the complex consists of mononuclear [PtCl₄(C₂H₅N₂)₂] units. The Pt atom is octahedrally coordinated by four Cl atoms, and by mutually *cis* N atoms from two 1-ethylimidazole ligands.

The Pt—Cl distances [2.304 (4) to 2.326 (4) Å] are similar to those observed in [PtCl₄(1-propylimidazole)₂] [2.310 (3)–2.322 (3) Å; Kuduk-Jaworska, Kubiak & Głowiak, 1988] and other six-coordinate Pt^{IV} complexes: 2.314 (1) Å in K₂PtCl₆ (Ohba & Saito, 1984), 2.318 (2) Å in 9-methylguaninium hexachloroplatinate(IV) dihydrate (Terzis & Mentzafos, 1983) and 2.313 to 2.323 (6) Å in the mixed-valence complex Pt(*N*-methylimidazole)₄.PtCl₆ (Biagini Cingi, Manotti Lanfredi, Tiripicchio, van Kralingen

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53026 (20 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. Fractional atomic coordinates and equivalent isotropic thermal parameters (\AA^2) with e.s.d.'s in parentheses

$$B_{\text{eq}} = 1/3(B_{11} + B_{22} + B_{33}).$$

	x	y	z	B_{eq}
Pt	0.36457 (4)	0.12634 (6)	0.13801 (4)	2.03 (2)
Cl(1)	0.1941 (3)	0.0527 (4)	0.1462 (2)	3.0 (3)
Cl(2)	0.2990 (3)	0.0769 (4)	-0.0240 (2)	3.2 (3)
Cl(3)	0.3006 (3)	0.3616 (4)	0.1096 (3)	3.8 (3)
Cl(4)	0.5335 (3)	0.1979 (4)	0.1245 (3)	3.4 (3)
N(11)	0.4223 (9)	0.1727 (11)	0.2817 (7)	2.7 (9)
N(12)	0.4350 (11)	0.1955 (17)	0.4300 (8)	4.8 (12)
N(21)	0.4219 (8)	-0.0777 (11)	0.1644 (7)	2.5 (8)
N(22)	0.5054 (9)	-0.2831 (12)	0.1520 (8)	3.0 (9)
C(11)	0.3732 (11)	0.1462 (22)	0.3414 (10)	4.9 (15)
C(12)	0.5199 (13)	0.2452 (20)	0.3284 (11)	4.9 (16)
C(13)	0.5230 (13)	0.2583 (20)	0.4199 (11)	4.8 (16)
C(14)	0.4101 (16)	0.1682 (28)	0.5183 (13)	6.4 (23)
C(15)	0.3057 (14)	0.2279 (24)	0.5297 (12)	6.7 (23)
C(21)	0.4877 (11)	-0.1449 (14)	0.1258 (9)	2.8 (10)
C(22)	0.3968 (11)	-0.1793 (14)	0.2227 (9)	2.9 (11)
C(23)	0.4470 (12)	-0.3083 (16)	0.2157 (10)	3.7 (12)
C(24)	0.5748 (13)	-0.3902 (17)	0.1244 (11)	4.4 (14)
C(25)	0.6854 (15)	-0.4123 (23)	0.2028 (15)	6.7 (20)

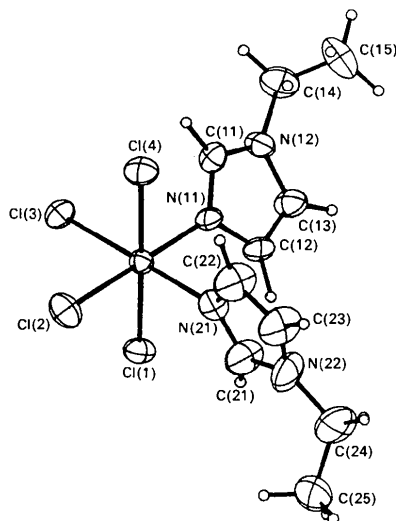


Fig. 1. A view of the complex showing the atom-numbering scheme.

& Reedijk, 1980). The Pt—N(11) and Pt—N(21) bond distances of 2.055 (11) and 2.007 (10) Å are practically identical to those observed in the 1-propylimidazole Pt^{IV} complex and in other compounds of Pt^{IV} with nitrogen-donor ligands (Fanizzi, Natile, Maresca, Manotti Lanfredi & Tiripicchio, 1984). The bond lengths and angles of the two imidazole rings are very similar and are in good agreement with corresponding values in [PtCl₄(1-propylimidazole)₂] and related complexes (Brouant, Barbe, Marsura & Luu-Duc, 1985). Both imidazole rings are planar; the ethyl-group conformation is defined by the torsion angles C(15)—C(14)—N(12)—C(11) = -65 (4) and C(25)—C(24)—N(22)—C(21) = 102 (5)°. The dihedral angle between the planes of the two imidazole

Table 2. Bond distances (Å) and angles (°) with e.s.d.'s in parentheses

Pt—Cl(1)	2.320 (4)	Pt—Cl(2)	2.313 (3)
Pt—Cl(3)	2.304 (4)	Pt—Cl(4)	2.326 (4)
Pt—N(11)	2.055 (11)	Pt—N(21)	2.007 (10)
N(11)—C(11)	1.275 (19)	N(21)—C(21)	1.322 (17)
N(11)—C(12)	1.374 (21)	N(21)—C(22)	1.387 (17)
N(12)—C(11)	1.362 (20)	N(22)—C(21)	1.329 (17)
N(12)—C(13)	1.316 (23)	N(22)—C(23)	1.413 (19)
N(12)—C(14)	1.477 (23)	N(22)—C(24)	1.475 (20)
C(12)—C(13)	1.354 (22)	C(22)—C(23)	1.371 (20)
C(14)—C(15)	1.503 (30)	C(24)—C(25)	1.504 (26)
Cl(1)—Pt—Cl(2)	89.3 (1)	Cl(3)—Pt—N(11)	88.5 (3)
Cl(1)—Pt—Cl(3)	90.4 (1)	Cl(4)—Pt—N(11)	91.2 (3)
Cl(1)—Pt—Cl(4)	178.1 (1)	Cl(1)—Pt—N(21)	90.1 (3)
Cl(2)—Pt—Cl(3)	90.0 (1)	Cl(2)—Pt—N(21)	89.8 (3)
Cl(2)—Pt—Cl(4)	88.8 (1)	Cl(3)—Pt—N(21)	179.2 (3)
Cl(3)—Pt—Cl(4)	89.8 (1)	Cl(4)—Pt—N(21)	89.8 (3)
Cl(1)—Pt—N(11)	90.8 (3)	N(11)—Pt—N(21)	90.8 (4)
Cl(2)—Pt—N(11)	179.3 (3)		
Pt—N(11)—C(11)	127.0 (10)	Pt—N(21)—C(21)	126.6 (9)
Pt—N(11)—C(12)	124.6 (10)	Pt—N(21)—C(22)	127.4 (9)
N(11)—C(11)—N(12)	110.7 (14)	N(21)—C(21)—N(22)	113.0 (12)
C(11)—N(12)—C(13)	105.6 (14)	C(21)—N(22)—C(23)	106.2 (11)
N(12)—C(13)—C(12)	110.1 (15)	N(22)—C(23)—C(22)	106.0 (12)
C(13)—C(12)—N(11)	105.2 (14)	C(23)—C(22)—N(21)	108.9 (12)
C(11)—N(11)—C(12)	108.4 (13)	C(21)—N(21)—C(22)	105.8 (11)
N(12)—C(14)—C(15)	120.5 (17)	N(22)—C(24)—C(25)	111.4 (14)

rings is 79 (4)° and these planes make dihedral angles of 99 (2) and 126 (2)°, respectively with the plane Pt, N(11), N(21), Cl(2) and Cl(3).

The crystal structure consists of discrete molecules held together by van der Waals forces.

This work was supported by the Polish Academy of Sciences (Project CPBP.01.12).

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Acta Cryst. (1990). **C46**, 2049–2051

Structure of (*N,N*-Dipropyldithiocarbamato)[tris(3,5-dimethyl-1-pyrazolyl)-hydroborato]oxovanadium(IV)

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Abstract. [VO(C₁₅H₂₂BN₆)(C₇H₁₄NS₂)], *M_r* = 540.46, monoclinic, *P*₂₁/*n*, *a* = 9.838 (2), *b* = 20.683 (6), *c* = 14.029 (2) Å, β = 106.365 (2)°, *V* = 2739.1 Å³, *Z* = 4, *D_m* = 1.32, *D_x* = 1.31 g cm⁻³, Mo *K*α, λ = 0.71073 Å, μ = 5.24 cm⁻¹, *F*(000) = 1140, *T* = 295 K, *R* = 0.049, *wR* = 0.060 for 2070 reflections. The central V atom adopts a distorted-octahedral coordination geometry in which one face of the octahedron is occupied by the tridentate tris(3,5-dimethyl-1-pyrazolyl)hydroborate ligand and the opposite face by oxo and dipropyldithiocarbamato ligands. The structure of the mononuclear complex is compared with that of the analogous diethyldithiocarbamato complex.

Introduction. Interest in metal oxo compounds has gained considerable momentum in recent years due to the role of metal-oxo species in certain catalytic processes of biological (Spiro, 1985) and industrial importance (Nugent & Mayer, 1988). These include the presence of mononuclear oxomolybdenum species in molybdenum hydroxylases (Bray, 1980; Spence, 1983). The bulky tris(3,5-dimethyl-1-pyrazolyl)hydroborate ligand (*L*) has been utilized to prepare oxomolybdenum complexes with unusual structural features and to prevent the formation of polynuclear species. Compounds such as *LMoOX*₂ (*X* = halide, pseudohalide, alkoxide, thiolate) (Cleland, Barnhart, Yamanouchi, Collison, Mabbs, Ortega & Enemark, 1987) and *LMoO(S₂CNR₂)* (*R* = Me, Et, Pr, Bu) (Young, Roberts, Ortega & Enemark, 1987) have been prepared and characterized. We have recently prepared a series of vanadyl complexes of the form *LVO(S₂CNR₂)* (*R* = Me, Et, Pr, Bu) (Sit, Collison, Mabbs & Cleland,

1989) and are investigating the detailed electron-spin-resonance spectra of these species in dilute single crystals. Crystals of the analogous *LMoO(S₂CNR₂)* complexes serve as diamagnetic host lattices for these studies. We herein report the structure of one of these complexes, *LVO(S₂CNPr₂)*.

Experimental. The complex was prepared by the method of Sit *et al.* (1989). Violet crystals obtained by liquid–liquid diffusion of methanol into a methylene chloride solution of *LVO[S₂CN(C₃H₇)₂]* at 298 K, dimensions 0.30 × 0.25 × 0.10 mm, mounted on a glass fiber with cyanoacrylate glue, *D_m* by flotation (ZnBr₂ and H₂O). Monoclinic crystal class, limiting conditions identified space group *P*₂₁/*n* (*h*0*l*: *h* + *l* = 2*n*; 0*k*0: *k* = 2*n*), 25 reflections for measuring lattice parameters, 13 ≤ 2θ ≤ 28°. Enraf–Nonius CAD-4 diffractometer, graphite-monochromated Mo *K*α, no absorption correction applied. θ–2θ scans, 2θ_{max} = 50°, 0 ≤ *h* ≤ 11, 0 ≤ *k* ≤ 24, −16 ≤ *l* ≤ 15, standard reflection $\bar{2}20$, decay of 1%, no correction made. 4667 unique reflections, 2070 with *F_o* > 3σ(*F_o*) used in refinement. *R*_{int} = 0.028. Coordinates of V from Patterson, 34 non-H atoms from difference electron-density maps. Disorder was found in the last C atom of one of the propyl groups of the dithiocarbamate. Atom C47' was added at 0.50 occupancy; (Δ/σ) for this atom was zero after three cycles of refinement. Full-matrix least squares on *F*, all non-H atoms anisotropic. H atoms included at calculated positions but not refined. Final refinement of *F* (2070 reflections, 317 parameters) resulted in *R* = 0.049, *wR* = 0.060, where *w* = 4*F_o*²/[σ²(*I*) + (*pF_o*²)²] with *p* set to 0.06, (Δρ)_{max} = 0.34, (Δρ)_{min} = −0.38 e Å⁻³, (Δ/σ)_{max} = 0.08. Atomic scattering factors from Cromer & Waber (1974) and anomalous-dispersion factors from Cromer (1974). Programs *SDP* (Frenz, 1978) run on a MicroVAX II.

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