

The  $[\text{PtBr}_3(\text{CH}_3\text{CN})]^-$  unit has square-planar geometry about the Pt, with no atom deviating from the least-squares plane by more than 0.069 (10) Å [ $\chi^2 = 5.0$ ]. The acetonitrile is coordinated to the Pt in a nearly linear manner, with a Pt–N bond length of 1.961 (10) Å and Pt–N(1)–C(1) angle of 171.5 (1.0)°. The C(1) and C(2) atoms deviate from the  $\text{PtNBr}_3$  plane by 0.24 (1) and 0.46 (1) Å respectively. The closest intramolecular contact involving the non-H atoms of acetonitrile is 2.60 (2) Å [N(1)···C(2)]. Bond lengths and angles for coordinated acetonitrile are similar to those reported for complexes of  $\text{Zn}^{\text{II}}$  and  $\text{Cu}^{\text{II}}$  ( $\langle\text{N}-\text{C}\rangle$  1.15,  $\langle\text{C}-\text{C}\rangle$  1.48 Å and  $\langle\text{N}-\text{C}-\text{C}\rangle$  173°) (*Molecular Structures and Dimensions*, 1972). The Pt–Br(3) bond length is about 0.04 Å shorter than the other two Pt–Br lengths. This may be explained in terms of the higher *trans* influence of Br compared to acetonitrile. This effect increases the bond distances of the two Br *trans* to the Pt compared to the distance of the Br *trans* to the N.

This complex resulted from our attempt to prepare a platinum(II) complex with an ambidentate styrylbenzothiazole derivative, using acetonitrile as solvent. Acetonitrile, as well as dimethyl sulfoxide (Price, Williamson, Schramm & Wayland, 1972), has a high coordinating ability toward platinum(II) and competes with other potential ligands for coordination. It is evident from this study that acetonitrile competes with the ligand during the reaction. On the other hand, the styrylbenzothiazole derivative provides more steric hindrance than the acetonitrile.

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## Monoclinic Anhydrous Zinc(II) Acetate

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**Abstract.** *catena*-Bis- $\mu$ -acetato-(*O,O'*)-dizinc(II),  $\text{C}_4\text{H}_6\text{O}_4\text{Zn}$ ,  $M_r = 183.47$ ,  $C2/c$ ,  $a = 30.237$  (2),  $b = 4.799$  (1),  $c = 9.260$  (1) Å,  $\beta = 99.49$  (1)°,  $V = 1325.3$  (3) Å<sup>3</sup>,  $Z = 8$ ,  $D_x = 1.839$  Mg m<sup>-3</sup>,  $\lambda(\text{Mo } K\alpha) = 0.71073$  Å,  $\mu = 3.74$  mm<sup>-1</sup>,  $F(000) = 736$ ,  $T = 293$  K,  $R = 0.025$  for 1066 unique observed reflections. The structure consists of polymeric two-dimensional sheets in which tetrahedrally coordinated Zn atoms are connected by acetate bridges in a *syn-anti* arrangement. The geometry of coordination is similar to that in the orthorhombic form of zinc acetate, which,

Distances and angles within the tetraethylammonium cation are all normal. The closest intramolecular contact involving the non-H atoms is 2.41 (2) Å [C(6)···C(3)].

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however, forms a three-dimensional network. The methyl-group H atoms are disordered.

**Introduction.** Capilla & Aranda (1979) reported the crystal structure of anhydrous zinc(II) acetate, in which Zn is tetrahedrally coordinated and the acetate ligands act as *syn-anti* bridges to form a three-dimensional polymeric network. A spectroscopic study of anhydrous zinc(II) acetate, however, led to the suggestion of a mononuclear structure, with chelating ligands, on the basis of the vibrational spectrum (Johnson, Powell &

Cannon, 1981). Such characteristics are found, in fact, in the dihydrate (van Niekerk, Schoening & Talbot, 1953). In the course of a study of various zinc carboxylates, we have prepared a monoclinic form of anhydrous zinc(II) acetate, and have determined its crystal structure in order to compare it with the orthorhombic form and with the proposed mononuclear structure.

Table 1. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic thermal parameters ( $\text{\AA}^2 \times 10^4$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{eq}$
Zn	6256 (1)	5456 (1)	6790 (1)	360 (1)
O(11)	6412 (1)	9390 (4)	7067 (2)	472 (7)
O(12)	6789 (1)	13270 (4)	7532 (2)	450 (7)
C(11)	6745 (1)	10685 (6)	7702 (3)	383 (9)
C(12)	7108 (1)	9245 (7)	8724 (4)	641 (13)
O(21)	5713 (1)	4139 (4)	7471 (2)	463 (7)
O(22)	6100 (1)	4726 (5)	9647 (2)	455 (7)
C(21)	5767 (1)	3747 (6)	8826 (3)	382 (10)
C(22)	5433 (1)	1981 (9)	9433 (3)	602 (13)

$$U_{eq} = \frac{1}{3}(\text{trace of the orthogonalized } U_{ij} \text{ matrix}).$$

Table 2. Bond lengths ( $\text{\AA}$ ) and angles ( $^\circ$ )

Zn—O(11)	1.952 (2)	Zn—O(21)	1.960 (2)
Zn—O(12 <sup>b</sup> )	1.949 (2)	Zn—O(22 <sup>b</sup> )	1.965 (2)
O(11)—C(11)	1.246 (3)	O(12)—C(11)	1.260 (4)
C(11)—C(12)	1.495 (4)	O(21)—C(21)	1.253 (3)
O(22)—C(21)	1.248 (3)	C(21)—C(22)	1.497 (5)
O(11)—Zn—O(21)	117.8 (1)	O(11)—Zn—O(12 <sup>b</sup> )	107.9 (1)
O(21)—Zn—O(12 <sup>b</sup> )	113.7 (1)	O(11)—Zn—O(22 <sup>b</sup> )	100.8 (1)
O(21)—Zn—O(22 <sup>b</sup> )	103.6 (1)	O(12 <sup>b</sup> )—Zn—O(22 <sup>b</sup> )	112.3 (1)
Zn—O(11)—C(11)	134.6 (2)	C(11)—O(12)—Zn <sup>III</sup>	118.4 (2)
O(11)—C(11)—O(12)	121.7 (2)	O(11)—C(11)—C(12)	121.4 (3)
O(12)—C(11)—C(12)	116.9 (3)	Zn—O(21)—C(21)	113.0 (2)
C(21)—O(22)—Zn <sup>IV</sup>	129.3 (2)	O(21)—C(21)—O(22)	120.9 (3)
O(21)—C(21)—C(22)	118.4 (2)	O(22)—C(21)—C(22)	120.7 (2)

Symmetry code: (i) *x*,  $-1 + y$ , *z*; (ii) *x*,  $-y$ ,  $-\frac{1}{2} + z$ ; (iii) *x*,  $1 + y$ , *z*; (iv) *x*,  $-y$ ,  $\frac{1}{2} + z$ .

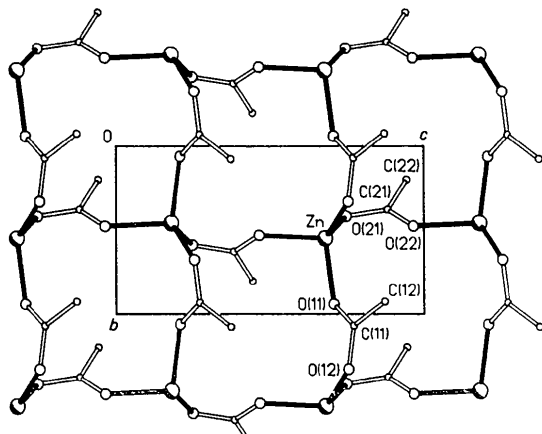


Fig. 1. Part of a polymeric sheet, seen in projection along the *a* axis. H atoms are omitted; independent atoms are labelled.

**Experimental.** Compound prepared from the dihydrate by recrystallization from ethanol solution. Crystal  $0.17 \times 0.37 \times 0.57$  mm; Siemens AED2 diffractometer; cell parameters from  $2\theta$  values of 32 reflections measured at  $\pm\omega$  ( $20 < 2\theta < 25^\circ$ ). Data collected in  $\omega/\theta$  scan mode, scan width =  $1.53^\circ + \alpha$ -doublet splitting, scan time 17.5–70.0 s;  $2\theta_{max}$   $50^\circ$ ,  $h$   $-35 \rightarrow 35$ ,  $k$   $0 \rightarrow 5$ ,  $l$   $-11 \rightarrow 8$ ; no significant variations for three standard reflections; semi-empirical absorption correction, transmission 0.176–0.286. 2237 reflections, 1168 unique, 1066 with  $F > 4\sigma(F)$  for structure determination and refinement,  $R_{int} = 0.022$ . Structure solution by Patterson and difference syntheses; blocked-cascade refinement to minimize  $\sum w\Delta^2$ ,  $\Delta = |F_o| - |F_c|$ ,  $w^{-1} = \sigma^2(F)$ ; anisotropic thermal parameters for non-H atoms; twofold torsional disorder of  $\text{CH}_3$  groups modelled by rigid hexagons of partially occupied H-atom positions constrained to give all C—H = 0.96  $\text{\AA}$ , H—C—H =  $109.5^\circ$  within each  $\text{CH}_3$ ; refined occupancy factors 0.65:0.35 (4) and 0.53:0.47 (3) for the two methyl groups;  $U(\text{H}) = 1.2U_{eq}(\text{C})$ ; this H-atom model was suggested by the presence of corresponding peaks in a difference synthesis. Isotropic extinction parameter  $x = 8.4 (6) \times 10^{-7} [F'_c = F_c / (1 + xF_c^2 / \sin 2\theta)^{1/4}]$ . Final  $R = 0.025$ ,  $wR = 0.027$ ;  $(\Delta/\sigma)_{max} = 0.039$ ,  $(\Delta/\sigma)_{mean} = 0.004$ ; slope of normal probability plot = 1.65;  $(\Delta\rho)_{max} = 0.34 \text{ e \AA}^{-3}$ ,  $(\Delta\rho)_{min} = -0.32 \text{ e \AA}^{-3}$ ; scattering factors from *International Tables for X-ray Crystallography* (1974). Program: *SHELXTL* (Sheldrick, 1985).\*

\* 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 43219 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

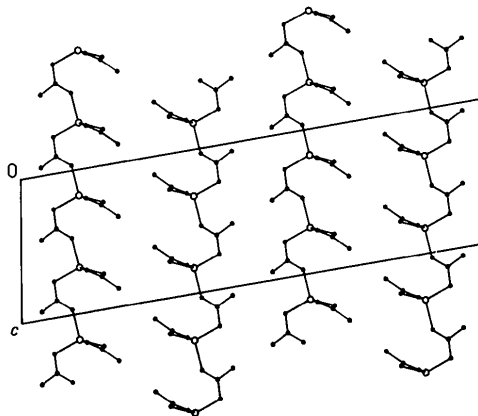


Fig. 2. Projection along the *b* axis, showing the arrangement of polymeric sheets in the unit cell.

**Discussion.** Final atomic parameters, bond lengths and angles are given in Tables 1 and 2. The structure consists of polymeric two-dimensional sheets, with *syn-anti* acetate bridges connecting tetrahedrally coordinated Zn atoms (Fig. 1). The geometry of the coordination and of the acetate bridges is very similar to that found in the orthorhombic form, in which the bridges connect the Zn atoms into a three-dimensional network rather than two-dimensional sheets (Capilla & Aranda, 1979). Neither of these observed structures is consistent with the proposal of Johnson, Powell & Cannon (1981).

There is no covalent bonding between sheets, the acetate methyl groups protruding from them on each side (Fig. 2).

A similar sheet structure is observed for zinc(II) propionate (Goldschmied, Rae & Stephenson, 1977). By contrast, zinc(II) 2-chlorobenzoate forms polymeric chains with pairs of *syn-syn* bridges linking Zn atoms (Nakacho, Misawa, Fujiwara, Wakahara & Tomita, 1976); a different type of polymeric chain is found for zinc(II) benzoate (Guseinov, Musaev, Usubaliev, Amiraslanov & Mamedov, 1984) and zinc(II) crotonate (Clegg, Little & Straughan, 1986), in which Zn<sub>2</sub>-(carboxylate)<sub>2</sub><sup>+</sup> binuclear units with three *syn-syn* bridges are connected by single *syn-anti* carboxylates. Thus anhydrous zinc(II) carboxylates have been

observed with one-, two- and three-dimensional polymeric structures of different types, with the acetate existing in (at least) two forms.

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## Structure of *cis*-Dichlorobis(4-vinylpyridine)platinum(II)

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**Abstract.** [PtCl<sub>2</sub>(C<sub>7</sub>H<sub>7</sub>N)<sub>2</sub>], *M<sub>r</sub>* = 476.3, monoclinic, space group *P*2<sub>1</sub>/*c*, *a* = 13.709 (4), *b* = 13.359 (4), *c* = 11.739 (4) Å, β = 133.72 (5)°, *V* = 1553.8 (9) Å<sup>3</sup>, *Z* = 4, *D<sub>x</sub>* = 2.04, *D<sub>m</sub>* = 2.00 (5) Mg m<sup>-3</sup>, Mo *K*α, λ = 0.71069 Å, μ = 9.8 mm<sup>-1</sup>, *F*(000) = 896, *T* = 294 (2) K, *R* = 0.059 for 2034 observed counter reflections. The Pt atom is coordinated to two N and two Cl atoms at the corners of a slightly distorted square with *cis* configuration. The Pt–Cl distances are 2.278 (7) and 2.301 (7) Å. The 4-vinylpyridine ligand is bonded to Pt through the N atom, Pt–N 1.969 (19) and 1.988 (23) Å.

**Introduction.** Since the discovery of the antitumour activity of Pt compounds, the importance of platinum metal has markedly increased in bio-inorganic chemistry. As studies of the structure–cytostatic activity

relationship show, only Pt complexes with *cis* configuration may afford potential drugs. Because *cis-trans* isomerization often occurs among complexes of pyridine derivatives, the precise determination of the configuration is necessary for the correlation between molecular structure and pharmacological activity.

As part of a programme directed towards the structural investigation of Pt<sup>II</sup> and Pd<sup>II</sup> complexes with pyridine derivatives, we present here the crystal structure of the title complex, obtained and characterized as described elsewhere (Kuduk-Jaworska, 1985).

**Experimental.** Yellow crystals, dimensions 0.12 × 0.14 × 0.20 mm; *D<sub>m</sub>* by flotation in CCl<sub>4</sub>/1,2-dibromoethane, monoclinic from Weissenberg photographs; Syntex *P*2<sub>1</sub> computer-controlled four-circle