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Bis[*trans*-2-(2-phenylethenyl)pyrazin-4-ium] tetrachlorozincate

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The title compound, $(C_{12}H_{11}N_2)_2[ZnCl_4]$, was prepared from $Zn(OAc)_2{\cdot}2H_2O$ and *trans*-2-(2-phenylethenyl)pyrazine in hydrochloric acid. The two *trans*-2-(2-phenylethenyl)pyrazin-4-ium cations combine with one $ZnCl_4^{2-}$ anion through N—H···Cl hydrogen bonds and C—H···Cl interactions. The Zn^{2+} species is situated on a twofold symmetry axis.

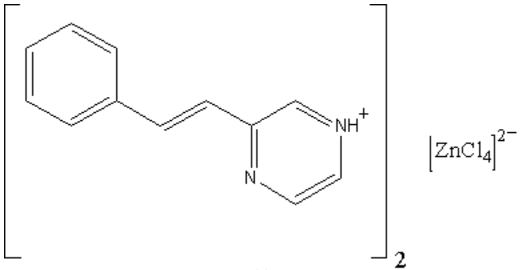
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.037
wR factor = 0.074
Data-to-parameter ratio = 17.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

The investigation of pyrazine derivatives for the treatment of diabetes mellitus is of increasing interest. As an analogue of pyrazine, *trans*-2-(2-phenylethenyl)pyrazine (PPz) acts as a potential *N*-donor ligand capable of coordinating to metal ions under certain conditions. Previous studies were predominantly focused on the synthesis of silver or copper complexes of some simple pyrazine derivatives (Vansant *et al.*, 1980; Amoroso *et al.*, 1995; Das *et al.*, 1993), but studies on metal complexes of the PPz have not been reported. Therefore, we set out to prepare a Zn^{II}–PPz complex from $Zn(OAc)_2{\cdot}2H_2O$ and PPz in hydrochloric acid. However, the title compound, (I) (Fig. 1), was obtained unexpectedly; this compound is similar to piperazinium tetrachlorocobaltate monohydrate (Tran Qui & Palacios, 1990). The syntheses and structures of the complexes of other pyrazine derivatives with transition metal ions will be presented in future work.



(I)

In the asymmetric unit of (I), there is one *trans*-2-(2-phenylethenyl)pyrazin-4-ium (PPzH) cation and half a tetrachlorozincate anion (Fig. 1), with the Zn^{2+} cation situated on a twofold axis. Only atom N2 in PPz is protonated, and the two PPzH molecules associated with each $[ZnCl_4]^{2-}$ anion are staggered, with a dihedral angle between the two pyrazinyl rings of 40.1 (3)°, while that of the two phenyl rings is 58.5 (4)°. Each Zn^{II} ion is in a tetrahedral coordination environment composed of four Cl anions, with Zn—Cl bond distances of 2.2368 (8) and 2.2871 (9) Å. The Cl—Zn—Cl bond angles range from 103.15 (5) to 111.55 (3)°. The pyra-

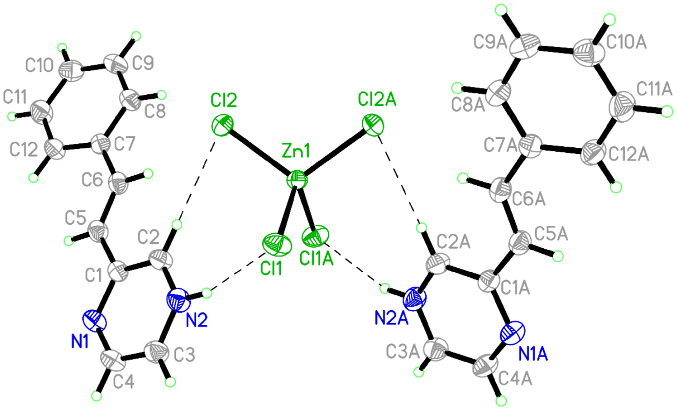


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids. H atoms are drawn as small spheres of arbitrary radii. Atoms with the suffix *A* are generated by the symmetry code ($-x$, y, $\frac{1}{2} - z$).

zinyl ring does not coordinate directly with the Zn^{II} ion through the N atoms, but connects with two Cl atoms of the tetrachlorozincate anion through N2—H2···Cl1 hydrogen bonds and C2—H2*A*···Cl2 interactions, resulting in a seven-membered ring, as illustrated in Fig. 1.

In the unit-cell packing of (I), four PPzH molecules are linked through the N—H···Cl and C—H···Cl bonds described above to form a star-like assembly, as depicted in Fig. 2. Weak face-to-face π–π stacking interactions are also observed between two antiparallel PPzH molecules, with the centroids of the phenyl and pyrazinyl rings separated by 4.032 (3) Å.

Experimental

To a mixture of PPz (0.36 g, 2 mmol) in acetonitrile (10 ml) and Zn(OAc)$_2$·2H$_2$O (0.22 g, 1 mmol) in acetone (10 ml) was added 20% hydrochloric acid until the pH was 3, during which the colorless solution turned yellow. The solution was stirred at room temperature for 30 min and then filtered. The filtrate was allowed to evaporate slowly at ambient temperature to give single crystals of (I) suitable for X-ray analysis (yield: 52%, m.p. 455–456 K). IR (KBr, ν, cm^{-1}): 2899 (*w*), 2806 (*w*), 2362 (*w*), 2035 (*w*), 1714 (*m*), 1634 (*s*), 1609 (*m*), 1496 (*s*), 1455 (*s*), 1334 (*w*), 1295 (*m*), 1260 (*s*), 1213 (*s*), 974 (*s*), 814 (*s*), 690 (*s*).

Crystal data

$(C_{12}H_{11}N_2)_2[ZnCl_4]$
$M_r = 573.63$
Monoclinic, $C2/c$
$a = 10.806\ (4)$ Å
$b = 11.777\ (4)$ Å
$c = 19.944\ (7)$ Å
$\beta = 97.660\ (5)^\circ$
$V = 2515.5\ (15)$ Å^3
$Z = 4$
$D_x = 1.515$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 739 reflections
$\theta = 2.6$–24.5°
$\mu = 1.42$ mm^{-1}
$T = 293\ (2)$ K
Block, yellow
0.20 × 0.18 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.755$, $T_{max} = 0.797$
7101 measured reflections
2576 independent reflections
1850 reflections with $I > 2\sigma(I)$
$R_{int} = 0.038$
$\theta_{max} = 26.4^\circ$
$h = -13 \rightarrow 12$
$k = -8 \rightarrow 14$
$l = -24 \rightarrow 21$

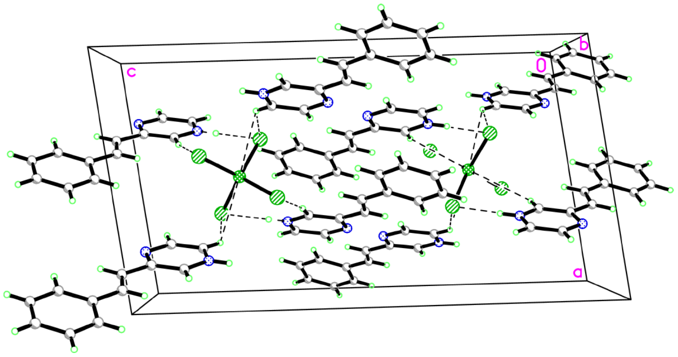


Figure 2
Packing diagram of (I) projected onto (010).

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.074$
$S = 1.02$
2576 reflections
150 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.03P)^2 + 0.5088P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—Cl2	2.2368 (8)	Zn1—Cl1	2.2871 (9)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···Cl1	0.86	2.31	3.147 (2)	163
C2—H2*A*···Cl2	0.93	2.65	3.569 (2)	169

H atoms were placed in calculated positions (C—H = 0.93–0.97 Å) and allowed to ride on the parent atoms, with U_{iso} values constrained to be $1.2U_{eq}$ of the parent atom.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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