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#### Key indicators

Single-crystal X-ray study T = 298 KMean  $\sigma$ (C–C) = 0.016 Å R factor = 0.084 wR factor = 0.209 Data-to-parameter ratio = 19.2

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

# Ethylenediaminium tetrachlorozincate

The title compound,  $(C_2H_{10}N_2)[ZnCl_4]$ , contains a network of ethylenediaminium cations and tetrahedral tetrachlorozincate anions. A three-dimensional network of N-H···Cl hydrogen bonds, some of which are bifurcated, helps to establish the crystal packing.

## Comment

The title compound, (I), (Fig. 1), contains a network of ethylenediaminium cations and tetrahedral tetrachlorozincate anions. The  $ZnCl_4^{2-}$  anion has been seen in many crystal structures and possesses (Table 1) typical Zn-Cl bond lengths (Deeth *et al.*, 1984), with a mean value of 2.268 (4) Å. The Cl-Zn-Cl bond angles in (I) indicate relatively little distortion from a regular tetrahedron [spread of values 104.78 (10)–115.57 (13)°].



To ensure charge balance for (I), the organic species must be doubly protonated. Each  $-NH_3$  group participates in  $N-H\cdots$ Cl hydrogen bonds (Table 2), three of which are bifurcated. These interactions help to establish a three-dimensional hydrogen-bond network (Fig. 2) in (I). Such  $N-H\cdots$ Cl and  $N-H\cdots$ (Cl,Cl) interactions have been discussed in the context of crystal engineering (Brammer *et al.*, 2002).

Compound (I) is clearly different from the phase described as  $(C_2H_{10}N_2)_2$ ·ZnCl<sub>6</sub> (Deeth *et al.*, 1984), which is probably better formulated as  $(C_2H_{10}N_2)_2$ ·ZnCl<sub>4</sub>·Cl<sub>2</sub>, *i.e.* it contains tetrachlorozincate anions, as does (I), as well as two 'free' Cl<sup>-</sup> ions, and not ZnCl<sub>6</sub><sup>4-</sup> moieties. Deeth *et al.* (1984) reported some basic geometric information for  $(C_2H_{10}N_2)_2$ ·ZnCl<sub>6</sub> and



# A view of (I), showing 30% probability displacement ellipsoids and arbitrary spheres for the H atoms. The hydrogen bond is indicated by dashed lines.

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Figure 2

The unit-cell packing in (I), viewed down [100], with hydrogen bonds indicated a dashed bond.

noted that other workers would report its full single-crystal structure in due course, but we have not been able to locate this paper. Based on similarities in cell parameters and space group,  $(C_2H_{10}N_2)_2$ ·HgCl<sub>6</sub> (Spengler *et al.*, 1998) probably has a close structural relationship to  $(C_2H_{10}N_2)_2$ ·ZnCl<sub>6</sub>. However, the detailed coordination about the metal atom is likely to be different in the two phases. As noted above, the zinc compound probably contains relatively regular tetrahedral coordination could be described as grossly distorted tetrahedral or possibly five-coordinate.

# **Experimental**

Acidified aqueous zinc chloride and ethylenediamine were mixed in a 1:1 ratio in a Petri dish, resulting in a clear solution. Rod and block-like crystals of (I) grew as the water evaporated over a few days at 298 K.

### Crystal data

$(C_2H_{10}N_2)[ZnCl_4]$	Mo $K\alpha$ radiation
$M_r = 269.29$	Cell parameters from 25
Orthorhombic, $P2_12_12_1$	reflections
a = 8.832 (4)  Å	$\theta = 10.0 - 15.0^{\circ}$
b = 9.811 (4) Å	$\mu = 3.60 \text{ mm}^{-1}$
c = 11.089 (5) Å	T = 298 (2) K
V = 960.9 (7) Å <sup>3</sup>	Rod, colourless
Z = 4	$0.40 \times 0.10 \times 0.10 \text{ mm}$
$D_x = 1.862 \text{ Mg m}^{-3}$	
Data collection	
Siemens P4 diffractometer	$R_{\rm int} = 0.114$
$\omega/2\theta$ scans	$\theta_{\rm max} = 26.0^{\circ}$
Absorption correction: $\psi$ scan	$h = 0 \rightarrow 10$
(XEMP; Siemens, 1990)	$k = 0 \rightarrow 12$
$T_{\min} = 0.327, T_{\max} = 0.715$	$l = -6 \rightarrow 13$
1744 measured reflections	3 standard reflections
1616 independent reflections	every 97 reflections
1383 reflections with $I > 2\sigma(I)$	intensity decay: none
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Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.1645P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.084$	where $P = (F_0^2 + 2F_c^2)/3$
$wR(F^2) = 0.209$	$(\Delta/\sigma)_{\rm max} = 0.001$
S = 1.05	$\Delta \rho_{\rm max} = 0.71 \ {\rm e} \ {\rm \AA}^{-3}$
1616 reflections	$\Delta \rho_{\rm min} = -1.09 \text{ e } \text{\AA}^{-3}$
84 parameters	Absolute structure: Flack (1983),
H-atom parameters constrained	with 507 Friedel pairs
	Flack parameter: $-0.01(5)$

 Table 1

 Selected bond lengths (Å).

Zn1-Cl3	2.240 (3)	Zn1-Cl4	2.275 (3)
Zn1-Cl2	2.262 (3)	Zn1-Cl1	2.296 (3)

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

$D - H \cdots A$	D-H	$H \cdots A$	$D \cdots A$	$D - \mathbf{H} \cdots A$
$\overline{N1-H1A\cdots Cl2^{i}}$	0.89	2.48	3.240 (10)	144
$N1 - H1A \cdots Cl4^{i}$	0.89	2.94	3.472 (9)	120
$N1 - H1B \cdot \cdot \cdot Cl4^{ii}$	0.89	2.40	3.185 (10)	147
$N1 - H1C \cdot \cdot \cdot Cl1$	0.89	2.29	3.173 (10)	169
$N2-H2C\cdots Cl2^{iii}$	0.89	2.47	3.239 (11)	146
$N2-H2C\cdots Cl4^{iv}$	0.89	2.83	3.381 (10)	121
$N2-H2D\cdots Cl1^{iv}$	0.89	2.46	3.242 (11)	148
$N2-H2E\cdots Cl1^{v}$	0.89	2.65	3.260 (9)	127
$N2-H2E\cdots Cl2^{v}$	0.89	2.85	3.618 (11)	146

Symmetry codes: (i)  $-x + \frac{3}{2}, -y + 1, z - \frac{1}{2}$ ; (ii)  $x - \frac{1}{2}, -y + \frac{1}{2}, -z + 1$ ; (iii) x - 1, y, z; (iv)  $-x + \frac{1}{2}, -y + 1, z - \frac{1}{2}$ ; (v)  $x - \frac{1}{2}, -y + \frac{3}{2}, -z + 1$ .

The H atoms were positioned geometrically, with N-H = 0.86 Å and C-H = 0.97 Å, and refined as riding, with  $U_{iso}(H) = 1.2U_{eq}(\text{carrier})$ , allowing for free rotation of the rigid -NH<sub>3</sub> groups about their C-N bonds.

Data collection: XSCANS (Siemens, 1990); cell refinement: XSCANS; data reduction: XSCANS; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP3 for Windows (Farrugia, 1997); software used to prepare material for publication: SHELXL97.

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