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(2-Aminoethan-1-aminium-κN^2)trichloridozinc(II)

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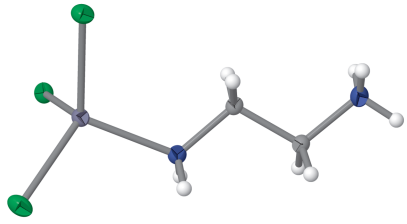
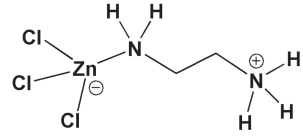
The mononuclear zwitterionic Zn^{II} complex, $[ZnCl_3(C_2H_9N_2)]$, contains a monodentate 2-ammonioethylamine moiety and three chloride anions coordinating to the central zinc atom in form of a distorted tetrahedron. The molecular packing shows amine and ammonium groups interacting through hydrogen-bonding interactions with chlorine atoms of symmetry-related complexes to form a supramolecular framework structure.

3D view



Chemical scheme



Structure description

Zwitterionic trichloridozinc(II) complexes with the metal additionally ligated in a monodentate manner by a protonated organic molecule are known (Clemente *et al.*, 2002; Maixner & Zachová, 1993; Purnell & Hodgson, 1976; Sheldrick, 1982; Steffen & Palenik, 1978; Zhu *et al.*, 2002), including a protonated quinine ligand (Kang *et al.*, 2013). The commonly used ethylenediamine (en) ligand acts primarily as a chelating ligand, and monodentate (Fanshawe *et al.*, 2000) or bridging forms (Çolak *et al.*, 2008) of en are rather rare. An example of a protonated and monodentate en ligand has been reported within a germanotungstate polyanion composed of two $[GeW_9O_{34}]^{10-}$ moieties sandwiching a rhomboid-like Zn_4 cluster, in which two central Zn^{II} atoms are coordinated by the N atom of the non-protonated amino group (Wang *et al.* 2010). In this context, we synthesized the title complex $[ZnCl_3(C_2H_9N_2)]$ using en, hydrochloric acid and zinc chloride as starting materials.

The molecular structure of $[ZnCl_3(C_2H_9N_2)]$ is characterized by a protonated en ligand, monodentately binding through the amine N atom (N1) to the central Zn^{II} atom. The tetrahedral coordination environment is completed by three Cl^- ligands (Fig. 1). The Zn—N bond length is 2.0345 (10) Å, much shorter than the values found in the Zn^{II}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···Cl1^{i}	0.883 (18)	2.636 (17)	3.3733 (11)	141.7 (14)
N1—H1B···Cl2^{ii}	0.828 (17)	2.678 (18)	3.4620 (11)	158.6 (17)
N2—H2A···Cl3^{ii}	0.85 (2)	2.46 (2)	3.2188 (12)	149.2 (17)
N2—H2B···Cl1^{iii}	0.87 (2)	2.566 (19)	3.2449 (11)	135.2 (16)
N2—H2C···Cl2^{i}	0.81 (2)	2.70 (2)	3.4526 (12)	154.2 (19)

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

complexes with chelating ethylendiamine (en) ligands, for example [Zn(en)(acetate)$_2$] (Kim *et al.*, 2007) where the Zn—N distance is 2.0784 (16) Å, or in the complex octahedral cation $[Zn(en)_3]^{2+}$ (Cheng *et al.*, 2008) with distances between 2.159 (2) and 2.220 (2). The present Zn—N bond length is also considerably shorter than in the germanotungstate cluster comprising a Zn^{II} atom bound to a monodentate en ligand [2.121 (16) Å; Wang *et al.*, 2010]. The three Zn—Cl bond lengths in the title complex range from 2.2600 (3) to 2.2686 (3) Å, which is comparable to those previously reported in the complexes having a $ZnCl_3$ moiety mentioned above. The present Cl—Zn—Cl and N—Zn—Cl bond angles vary from 104.52 (3) to 115.969 (12)°, indicating a considerable distortion from an ideal tetrahedron. The protonated en ligand has an *anti*-conformation with an N1—C1—C2—N2 torsion angle of 178.18 (10)°.

The molecular packing is stabilized by an intricate framework of intermolecular N—H···Cl hydrogen bonds involving both the amine (N1) and ammonium (N2) groups as donors and all three Cl ligands as acceptor atoms (Table 1). Part of the crystal packing is illustrated in Fig. 2.

Synthesis and crystallization

The title complex was obtained by addition of a methanolic solution (10 ml) of $ZnCl_2$ (0.136 g, 1 mmol) to a flask containing 10 ml of a methanolic solution of ethylenediamine, $C_2H_8N_2$ (0.06 g, 1 mmol) and 5 ml of hydrochloric acid HCl (1 *N*). The resulting mixture was stirred for 2 h at room temperature. A clear solution was obtained and left to evaporate slowly at room temperature, leading to colorless single crystals suitable for single-crystal X-ray diffraction after 24 h.

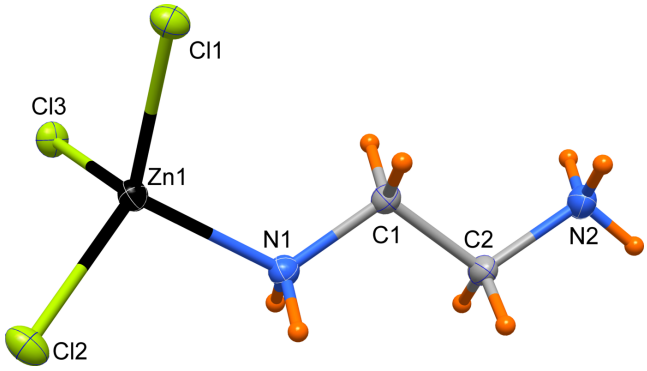


Figure 1
Molecular structure of the title complex with displacement ellipsoids drawn at the 50% probability level.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[ZnCl_3(C_2H_9N_2)]$
M_r	232.83
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	150
a, b, c (Å)	6.6669 (4), 8.1192 (4), 14.7559 (7)
V (Å^3)	798.74 (7)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	3.99
Crystal size (mm)	0.24 × 0.13 × 0.11
Data collection	
Diffractometer	Bruker *APEX* CCD area-detector
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.407, 0.520
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11232, 3036, 3017
R_{int}	0.020
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.770
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.012, 0.026, 1.12
No. of reflections	3036
No. of parameters	101
H-atom treatment	Only H-atom coordinates refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.29, −0.33
Absolute structure	Refined as an inversion twin Parsons *et al.*, 2013]
Absolute structure parameter	0.374 (5)

Computer programs: *SMART* and *SAINT* (Bruker, 2000), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 1999) and *WinGX* (Farrugia, 2012).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

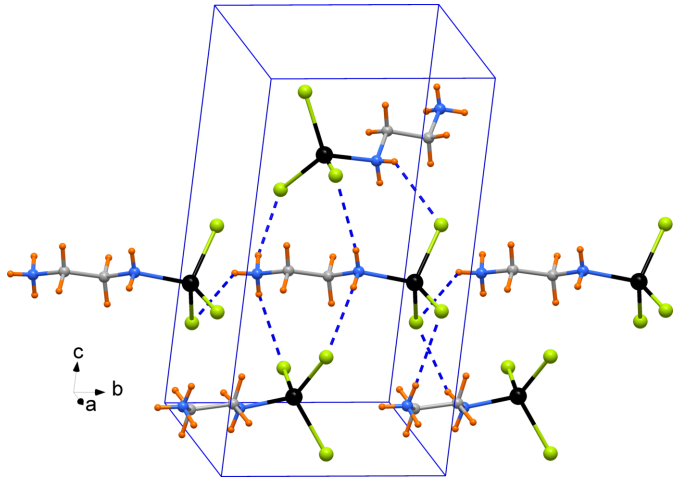


Figure 2
Partial view of the molecular packing in the crystal of the title complex with N—H···Cl hydrogen bonds indicated as dashed lines

Acknowledgements

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References

Brandenburg, K. & Putz, H. (1999). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2000). *SMART* and *SAINT*. Bruker AXS Analytic X-Ray Systems Inc., Madison, Wisconsin, UA.
Cheng, L., Sun, Y.-Y., Zhang, Y.-W. & Xu, G. (2008). *Acta Cryst.* E**64**, m1246.
Clemente, D. A., Marzotto, A. & Benetollo, F. (2002). *Polyhedron* **21**, 2161–2166.
Çolak, A. T., Yeşilel, O. Z., Hökelek, T. & Şahin, E. (2008). *Struct. Chem.* **19**, 285–290.
Fanshawe, R. L., Mobinikhaledi, A., Clark, C. R. & Blackman, A. G. (2000). *Inorg. Chim. Acta* **307**, 27–32.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Kang, J., Yun, H. & Do, J. (2013). *Z. Krist. New Cryst. Struct.* **228**, 57-58.
Kim, Y.-I., Lee, Y.-S., Seo, H.-J. & Kang, S. K. (2007). *Acta Cryst.* E**63**, m2239–m2240.
Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.
Maixner, J. & Zachová, J. (1993). *Acta Cryst.* C**49**, 927–929.
Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.
Purnell, L. G. & Hodgson, D. J. (1976). *Biochimic. Biophys. Acta* **447**, 117–119.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Sheldrick, W. S. (1982). *Z. Naturforsch. B* **37**, 653–656.
Steffen, W. L. & Palenik, G. J. (1978). *Inorg. Chem.* **17**, 1338–1340.
Wang, Y., Xu, L., Jiang, N., Liu, X., Li, F. & Li, Y. (2010). *Inorg. Chem. Commun.* **13**, 964–967.
Zhu, M.-L., Lu, L.-P., Jin, X.-L. & Yang, P. (2002). *Acta Cryst.* C**58**, m158–m159.

full crystallographic data

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(2-Aminoethan-1-aminium-κN^2)trichloridozinc(II)

Crystal data

$[ZnCl_3(C_2H_9N_2)]$
M_r = 232.83
Orthorhombic, $P2_12_12_1$
a = 6.6669 (4) Å
b = 8.1192 (4) Å
c = 14.7559 (7) Å
V = 798.74 (7) Å^3
Z = 4
$F(000)$ = 464
D_x = 1.936 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7854 reflections
θ = 1.9–25.0°
μ = 3.99 mm^{-1}
T = 150 K
Block, colorless
0.24 × 0.13 × 0.11 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min} = 0.407, T_{max} = 0.520
11232 measured reflections
3036 independent reflections
3017 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 33.2°, θ_{min} = 2.8°
h = −9→10
k = −12→12
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.012
$wR(F^2)$ = 0.026
S = 1.12
3036 reflections
101 parameters
0 restraints
Hydrogen site location: difference Fourier map
Only H-atom coordinates refined
$w = 1/[\sigma^2(F_o^2) + (0.0075P)^2 + 0.0649P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}
Absolute structure: Refined as an inversion twin Parsons *et al.*, 2013]
Absolute structure parameter: 0.374 (5)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refined as a 2-component inversion twin. H atoms were freely refined with U_{iso}(H) 1.2× or 1.5×U_{eq} of the parent atom. The crystal structure was refined as a two-component inversion twin [Flack parameter = 0.374 (5); Parsons *et al.*, 2013].

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.45714 (2)	0.91365 (2)	0.38549 (2)	0.01331 (3)
Cl1	0.29829 (4)	0.98873 (3)	0.25628 (2)	0.01659 (5)
Cl2	0.79364 (4)	0.95070 (4)	0.37517 (2)	0.01909 (5)
Cl3	0.30307 (5)	1.04462 (3)	0.50133 (2)	0.01698 (5)
N1	0.42319 (16)	0.66776 (12)	0.40719 (7)	0.01523 (18)
H1A	0.535 (3)	0.620 (2)	0.3886 (11)	0.018*
H1B	0.427 (3)	0.642 (2)	0.4615 (12)	0.018*
N2	0.08625 (17)	0.31486 (12)	0.33981 (8)	0.0185 (2)
H2A	−0.023 (3)	0.342 (2)	0.3659 (12)	0.028*
H2B	0.105 (3)	0.209 (2)	0.3455 (12)	0.028*
H2C	0.074 (3)	0.338 (2)	0.2865 (14)	0.028*
C1	0.25042 (17)	0.58592 (14)	0.36385 (7)	0.01499 (19)
H1C	0.260 (3)	0.612 (2)	0.2975 (11)	0.018*
H1D	0.129 (3)	0.631 (2)	0.3899 (11)	0.018*
C2	0.26187 (17)	0.40102 (13)	0.38011 (8)	0.01628 (19)
H2E	0.374 (3)	0.356 (2)	0.3522 (11)	0.020*
H2D	0.265 (3)	0.3787 (19)	0.4438 (12)	0.020*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.01369 (6)	0.01376 (5)	0.01250 (5)	−0.00133 (4)	−0.00035 (5)	0.00047 (4)
Cl1	0.01636 (12)	0.02048 (10)	0.01292 (10)	0.00025 (10)	−0.00161 (9)	0.00117 (8)
Cl2	0.01381 (11)	0.02772 (12)	0.01575 (11)	−0.00389 (10)	−0.00020 (9)	0.00146 (9)
Cl3	0.01857 (12)	0.01778 (10)	0.01460 (10)	−0.00088 (9)	0.00209 (9)	−0.00156 (8)
N1	0.0162 (5)	0.0142 (4)	0.0153 (4)	−0.0002 (3)	−0.0010 (3)	0.0007 (3)
N2	0.0190 (5)	0.0143 (4)	0.0222 (5)	−0.0001 (3)	−0.0010 (4)	−0.0024 (4)
C1	0.0161 (5)	0.0123 (4)	0.0165 (4)	0.0001 (4)	−0.0016 (3)	0.0011 (4)
C2	0.0162 (5)	0.0128 (4)	0.0198 (5)	−0.0001 (3)	−0.0024 (4)	0.0012 (4)

Geometric parameters (Å, º)

Zn1—N1	2.0345 (10)	N2—H2A	0.85 (2)
Zn1—Cl3	2.2600 (3)	N2—H2B	0.87 (2)
Zn1—Cl1	2.2646 (3)	N2—H2C	0.81 (2)
Zn1—Cl2	2.2686 (3)	C1—C2	1.5222 (15)
N1—C1	1.4755 (15)	C1—H1C	1.003 (16)
N1—H1A	0.883 (18)	C1—H1D	0.967 (18)
N1—H1B	0.828 (17)	C2—H2E	0.930 (18)
N2—C2	1.4879 (16)	C2—H2D	0.958 (17)

N1—Zn1—Cl3	106.99 (3)	C2—N2—H2C	110.9 (14)
N1—Zn1—Cl1	110.15 (3)	H2A—N2—H2C	107.2 (19)
Cl3—Zn1—Cl1	107.313 (12)	H2B—N2—H2C	109.4 (18)
N1—Zn1—Cl2	104.52 (3)	N1—C1—C2	109.68 (9)
Cl3—Zn1—Cl2	115.969 (12)	N1—C1—H1C	106.1 (10)
Cl1—Zn1—Cl2	111.728 (11)	C2—C1—H1C	110.9 (9)
C1—N1—Zn1	117.43 (7)	N1—C1—H1D	108.1 (10)
C1—N1—H1A	109.2 (11)	C2—C1—H1D	110.6 (10)
Zn1—N1—H1A	106.5 (11)	H1C—C1—H1D	111.2 (14)
C1—N1—H1B	109.4 (13)	N2—C2—C1	111.18 (9)
Zn1—N1—H1B	113.2 (11)	N2—C2—H2E	105.8 (11)
H1A—N1—H1B	99.6 (16)	C1—C2—H2E	111.0 (11)
C2—N2—H2A	112.0 (13)	N2—C2—H2D	108.7 (11)
C2—N2—H2B	108.0 (14)	C1—C2—H2D	110.0 (10)
H2A—N2—H2B	109.3 (19)	H2E—C2—H2D	110.1 (16)
Zn1—N1—C1—C2	174.46 (7)	N1—C1—C2—N2	178.18 (10)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···Cl1^{i}	0.883 (18)	2.636 (17)	3.3733 (11)	141.7 (14)
N1—H1*B*···Cl2^{ii}	0.828 (17)	2.678 (18)	3.4620 (11)	158.6 (17)
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