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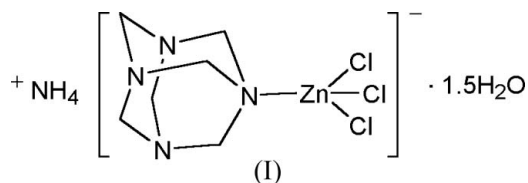
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**Key indicators**Single-crystal X-ray study  
 $T = 273$  K  
Mean  $\sigma(\text{N}-\text{C}) = 0.004$  Å  
H-atom completeness 95%  
Disorder in main residue  
 $R$  factor = 0.040  
 $wR$  factor = 0.093  
Data-to-parameter ratio = 16.8For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.**Ammonium trichloro(hexamethylene-  
tetramine)zincate(II) sesquihydrate**

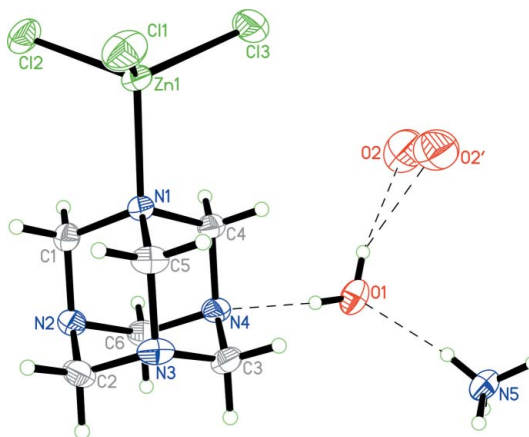
In the title compound,  $(\text{NH}_4)[\text{ZnCl}_3(\text{C}_6\text{H}_{12}\text{N}_4)] \cdot 1.5\text{H}_2\text{O}$ , the  $\text{Zn}^{\text{II}}$  atom is in a tetrahedral environment, coordinated by one N atom of the hexamethylenetetramine ligand and by three Cl atoms. The charge of the hexamethylenetetraminetrichlorozincate(II) anion is counter-balanced by an ammonium cation. Two water molecules, one of which shows disorder and is only partly occupied, are also present. The structure is stabilized by weak intermolecular  $\text{O}-\text{H} \cdots \text{N}$ ,  $\text{N}-\text{H} \cdots \text{O}$  and  $\text{N}-\text{H} \cdots \text{N}$  hydrogen bonds.

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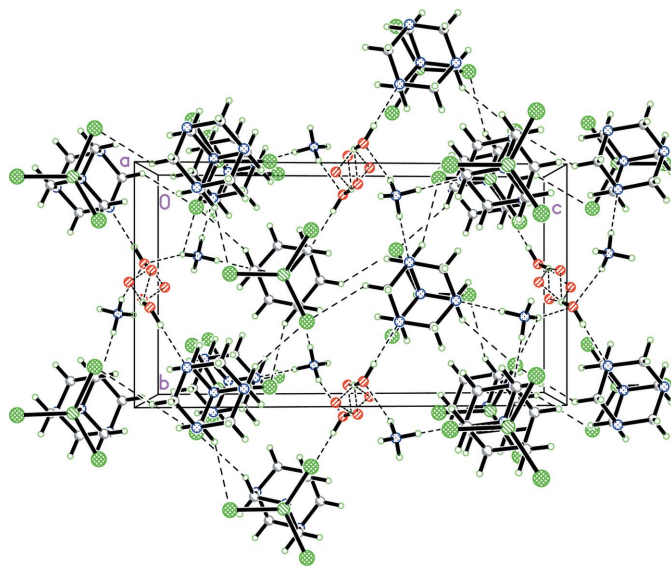
Various structures of hexamethylenetetramine (urotropine, UTP) metal complexes, *e.g.*  $(\text{UTP})\text{Ni}(\text{C}_9\text{H}_5\text{O}_6)_2$  (Gao *et al.*, 2005),  $(\text{UTP})\text{Cd}(\text{C}_9\text{H}_7\text{O}_3)_2$  (Cheng *et al.*, 2005),  $(\text{UTP})\text{-Cd}(\text{H}_2\text{O})_4$  (Zhou *et al.*, 2005),  $(\text{UTP})\text{Ni}_2(\text{C}_2\text{H}_3\text{O}_2)_4$  (Wang *et al.*, 2002), and  $(\text{Cd}_3\text{Br}_6)(\text{UTP})_2(\text{H}_2\text{O})_4$  (Tong *et al.*, 2000) have been published previously. We report here the synthesis and structure of a new urotropine–metal complex,  $(\text{NH}_4)[\text{ZnCl}_3(\text{C}_6\text{H}_{12}\text{N}_4)] \cdot 1.5\text{H}_2\text{O}$ , (I).



In the structure of compound (I), the  $\text{Zn}^{\text{II}}$  atom is in a tetrahedral environment, coordinated by one N atom of the

**Figure 1**

The asymmetric unit of (I), with displacement ellipsoids drawn at the 40% probability level. Hydrogen bonds are indicated by dashed lines. Both disorder components are shown.


**Figure 2**

The packing of the structural units in (I), viewed along the *a* axis. Hydrogen bonding is depicted by dashed lines. Colour code: O atoms red dashed spheres, N atoms blue dotted spheres, C atoms grey spheres, H atoms small green spheres, Cl atoms green checkered spheres, Zn atoms green dashed spheres.

urotropine ligand and by three Cl atoms. The tetrahedron around Zn is considerably distorted, with bond angles ranging from 105.41 (6) to 112.77 (4)° (Table 1). In (I), the Zn–N distance of 2.108 (2) Å is close to the value of 2.099 (3) Å observed for a comparable [ZnNCl<sub>3</sub>] tetrahedron in which the N atom belongs to a pyridine ligand (Wan *et al.*, 2005). The UTP–trichlorozincate anion is charge-balanced by an ammonium cation, and two water molecules, one of which shows disorder and is partly occupied, are also present in the structure (Fig. 1).

In addition to the O–H···N and N–H···N hydrogen bonds that link the UTP entities, ammonium cations and water molecules, there are several C–H···Cl intermolecular contacts in the structure of (I), which additionally contribute to the stabilization of the crystal structure (Table 2 and Fig. 2).

## Experimental

Compound (I) was synthesized by heating a mixture of UTP, ZnCl<sub>2</sub>·H<sub>2</sub>O and aqueous ammonia in a molar ratio of 1:2:2. The clear solution was then concentrated gradually at room temperature to afford colourless blocks after a couple of days. Elemental analysis confirmed the molecular formula.

### Crystal data

(NH <sub>4</sub> )[ZnCl <sub>3</sub> (C <sub>6</sub> H <sub>12</sub> N <sub>4</sub> )]·1.5H <sub>2</sub> O	<i>Z</i> = 4
<i>M<sub>r</sub></i> = 357.96	<i>D<sub>x</sub></i> = 1.650 Mg m <sup>-3</sup>
Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>c</i>	Mo <i>K</i> α radiation
<i>a</i> = 8.7692 (19) Å	<i>μ</i> = 2.26 mm <sup>-1</sup>
<i>b</i> = 9.621 (2) Å	<i>T</i> = 273 (2) K
<i>c</i> = 17.137 (4) Å	Block, colourless
<i>β</i> = 94.842 (4)°	0.37 × 0.35 × 0.32 mm
<i>V</i> = 1440.6 (5) Å <sup>3</sup>	

### Data collection

Bruker SMART APEX CCD area-detector diffractometer	8538 measured reflections
<i>φ</i> and <i>ω</i> scans	3136 independent reflections
Absorption correction: multi-scan (SADABS; Bruker, 2002)	2694 reflections with <i>I</i> > 2σ( <i>I</i> )
<i>T</i> <sub>min</sub> = 0.444, <i>T</i> <sub>max</sub> = 0.499	<i>R</i> <sub>int</sub> = 0.025
	<i>θ</i> <sub>max</sub> = 27.0°

### Refinement

Refinement on <i>F</i> <sup>2</sup>	$w = 1/[\sigma^2(F_o^2) + (0.0367P)^2 + 0.9695P]$
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )] = 0.040	where <i>P</i> = ( <i>F</i> <sub>o</sub> <sup>2</sup> + 2 <i>F</i> <sub>c</sub> <sup>2</sup> )/3
<i>wR</i> ( <i>F</i> <sup>2</sup> ) = 0.093	(Δσ) <sub>max</sub> = 0.001
<i>S</i> = 1.09	Δρ <sub>max</sub> = 0.33 e Å <sup>-3</sup>
3136 reflections	Δρ <sub>min</sub> = -0.35 e Å <sup>-3</sup>
187 parameters	
H atoms treated by a mixture of independent and constrained refinement	

**Table 1**

Selected geometric parameters (Å, °).

Zn1–N1	2.108 (2)	N2–C1	1.469 (3)
Zn1–Cl2	2.2335 (9)	N2–C6	1.476 (4)
Zn1–Cl1	2.2487 (10)	N3–C3	1.466 (4)
Zn1–Cl3	2.2500 (10)	N3–C5	1.469 (3)
N1–C4	1.494 (3)	N3–C2	1.474 (4)
N1–C5	1.496 (3)	N4–C4	1.464 (3)
N1–C1	1.498 (3)	N4–C3	1.471 (4)
N2–C2	1.468 (4)	N4–C6	1.477 (4)
N1–Zn1–Cl2	105.41 (6)	Cl1–Zn1–Cl3	112.77 (4)
N1–Zn1–Cl1	107.20 (6)	C4–N1–Zn1	109.81 (15)
Cl2–Zn1–Cl1	110.54 (3)	C5–N1–Zn1	111.01 (16)
N1–Zn1–Cl3	108.17 (6)	Cl1–N1–Zn1	112.80 (15)
Cl2–Zn1–Cl3	112.32 (4)		

**Table 2**

Hydrogen-bond geometry (Å, °).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
O1–H1WA···N4	0.823 (18)	2.012 (19)	2.834 (3)	176 (3)
O1–H1WB···O2	0.842 (19)	2.040 (19)	2.871 (17)	169 (3)
O1–H1WB···O2 <sup>i</sup>	0.842 (19)	2.279 (19)	3.002 (16)	144 (3)
O1–H1WB···O2 <sup>ii</sup>	0.842 (19)	2.538 (19)	3.225 (17)	139 (3)
O1–H1WB···O2 <sup>iii</sup>	0.842 (19)	2.245 (19)	3.043 (17)	158 (3)
N5–H5E···O1	0.82 (4)	2.05 (4)	2.838 (4)	160 (3)
N5–H5F···O1 <sup>iii</sup>	0.87 (4)	2.05 (4)	2.894 (4)	163
N5–H5C···N3 <sup>iii</sup>	0.97 (4)	2.08 (4)	3.040 (4)	176 (3)
N5–H5D···N2 <sup>iv</sup>	0.92 (5)	2.15 (5)	3.067 (4)	177 (4)
C1–H1A···Cl1 <sup>v</sup>	0.97	2.87	3.673 (3)	141
C5–H5A···Cl2 <sup>vi</sup>	0.97	2.90	3.679 (3)	138
C6–H6A···Cl2 <sup>vii</sup>	0.97	2.86	3.655 (3)	140

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

One of the two water molecules is disordered. The position of its O atom was split into two parts with an occupancies of 0.25 for both O2 and O2'. Because of the disorder, the H atoms attached to O2 and O2' could not be located. The other H atoms of the second water molecule and of the ammonium cation were found in difference Fourier maps. The O–H and H···H distances of this water molecule were restrained to 0.82 (2) and 1.39 (1) Å, respectively, whereas the H atoms of the ammonium cation were refined freely. All other H atoms

were positioned geometrically and refined using a riding model with their isotropic displacement parameters equal to  $1.2U_{\text{eq}}$  of their parent atoms. The C—H distances were fixed at 0.97 Å for methylene groups.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINTE* (Bruker, 2002); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXTL* (Bruker, 2002); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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