



# Crystal structure and Hirshfeld surface analysis of 8-azaniumylquinolinium tetrachloridozincate(II)

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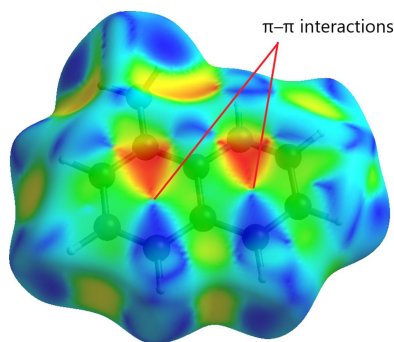
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The reaction of 8-aminoquinoline, zinc chloride and hydrochloric acid in ethanol yielded the title salt,  $(C_9H_{10}N_2)[ZnCl_4]$ , which consists of a planar 8-azaniumylquinolinium dication and a tetrahedral tetrachlorozincate dianion. The 8-aminoquinoline moiety is protonated at both the amino and the ring N atoms. In the crystal, the cations and anions are connected by intermolecular  $N-H\cdots Cl$  and  $C-H\cdots Cl$  hydrogen bonds, forming sheets parallel to (001). Adjacent sheets are linked through  $\pi$ - $\pi$  interactions involving the pyridine and arene rings of the 8-azaniumylquinolinium dication. Hirshfeld surface analysis indicates that the most important contributions to the crystal packing are from  $H\cdots Cl$  (48.1%),  $H\cdots H$  (19.9%),  $H\cdots C/C\cdots H$  (14.3%) (involving the cations) and  $H\cdots Cl$  (82.6%) (involving the anions) interactions.

## 1. Chemical context

Quinoline and its derivatives comprise an important group of heterocyclic compounds that exhibit a wide range of pharmacological properties, such as antimalarial (Shiraki *et al.*, 2011; Singh *et al.*, 2011; Murugan *et al.*, 2022), antibacterial (Upadhayaya *et al.*, 2009; Zeleke *et al.*, 2020), antimicrobial (Teja *et al.*, 2016), anti-inflammatory (Guirado *et al.*, 2012), anticancer (Abbas *et al.*, 2015), antidiabetic (Kulkarni *et al.*, 2012) and antihistaminic activities (Sridevi *et al.*, 2010). The quinoline moiety is found in many drugs and is useful in the rational design of novel bioactive molecules in medicinal chemistry. The interest in 8-aminoquinoline, which contains functional groups commonly involved in hydrogen bonding, is related to its genotoxic activities, such as mutagenicity (Takahashi *et al.*, 1987), and to its unusually low proton-acceptor ability in solution. Quinolines are also strongly fluorescent and have been employed in the analytical study of heavy metals (Fritsch *et al.*, 2006). They have also been used to prepare highly conducting copolymers (Li *et al.*, 2005). As a ligand, 8-aminoquinoline usually binds in a bidentate fashion via the two N-atom positions (Setifi *et al.*, 2016; Mao *et al.*, 2018; Yang *et al.*, 2019), although examples of bridging-binding modes are also known (Schmidbaur *et al.*, 1991). In addition, 8-aminoquinoline can form  $\pi$ - $\pi$  stacking interactions with (other) aromatic rings, thus controlling the intergrowth of interpenetrating networks (Khelfa *et al.*, 2021; Rahmati *et al.*, 2018). Zinc, an essential component of life, is an abundant ion in living organisms (Andreini *et al.*, 2006; Cuajungco *et al.*, 2021). A bioinformatics study found that over 50% of zinc-bound proteins are enzymes, and in the vast majority of them,



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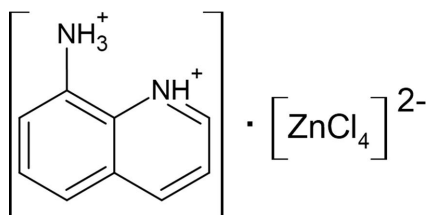
**Table 1**

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$           | $D-H$    | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-------------------------|----------|-------------|-------------|---------------|
| $N1-H1A\cdots Cl1$      | 0.88 (1) | 2.31 (1)    | 3.1309 (16) | 154 (2)       |
| $N1-H1B\cdots Cl2^i$    | 0.89 (1) | 2.39 (1)    | 3.1747 (17) | 148 (2)       |
| $N1-H1C\cdots Cl3^{ii}$ | 0.88 (2) | 2.48 (2)    | 3.2415 (16) | 145 (2)       |
| $N2-H2\cdots Cl4$       | 0.86 (2) | 2.25 (2)    | 3.0958 (16) | 166 (2)       |
| $C7-H7\cdots Cl1^{iii}$ | 0.93     | 2.71        | 3.584 (2)   | 157           |

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

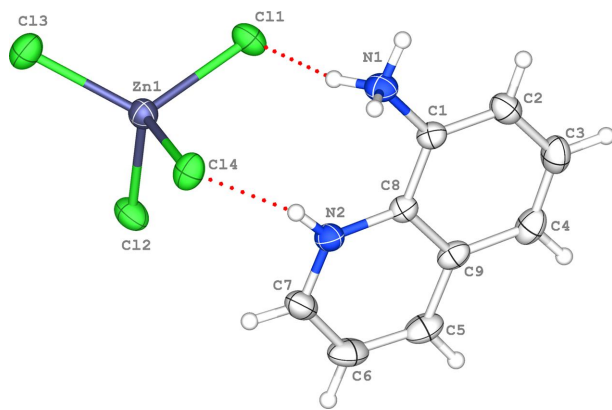
the metal plays a catalytic role (Andreini & Bertini, 2012). About 20% of them feature zinc as a structural component (Banci *et al.*, 2002; Andreini & Bertini, 2012). Zinc complexes exhibit a wide range of coordination numbers and coordination spheres, with tetrahedral (Ashurov *et al.*, 2018; Petrus *et al.*, 2020) and octahedral (Ashurov *et al.*, 2011) environments being the most frequently observed.



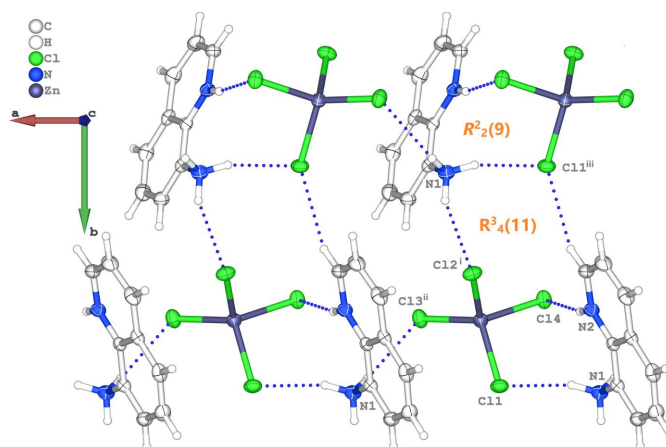
In the context given above, we report here the synthesis, crystal structure and Hirshfeld surface analysis of the organic-inorganic hyride salt  $(C_9H_{10}N_2)[ZnCl_4]$ .

## 2. Structural commentary

The title salt crystallizes with one  $(C_9H_{10}N_2)^{2+}$  dication and one  $[ZnCl_4]^{2-}$  dianion in the asymmetric unit (Fig. 1). The cation consists of an 8-aminoquinoline moiety that is protonated at both the amino and the ring N atoms. Protonation of the amino group results in a lengthening of the C–N( $sp^3$ ) bond from 1.377 (3) Å ( $sp^2$  N) in 8-aminoquinoline (Van

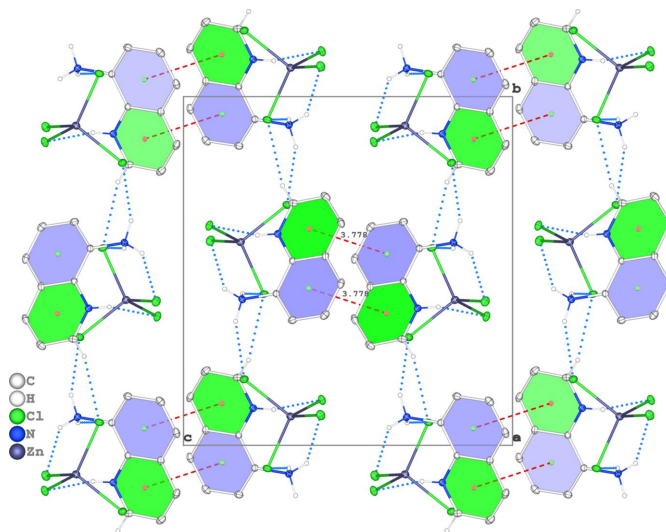

**Figure 1**

View of the asymmetric unit of the title salt, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radius and hydrogen bonds are shown as dashed lines.


**Figure 2**

The formation of  $N1-H1A\cdots Cl1$ ,  $N1-H1B\cdots Cl2^i$ ,  $N1-H1C\cdots Cl3^{ii}$ ,  $N2-H2\cdots Cl4$  and  $C7-H7\cdots Cl1^{iii}$  hydrogen bonds (dashed blue lines) in the crystal structure, leading to  $R_2^2(9)$  and  $R_4^3(11)$  graph-set motifs. The symmetry codes are as in Table 1.

Meervelt *et al.*, 1997) to 1.464 (2) Å. This reflects the loss of the conjugation between the aromatic ring and the lone-pair electrons of the amino N atom when the latter is protonated. The quinoline ring system (atoms C1–C9/N2) is essentially planar; the r.m.s. deviation for the non-H atoms is 0.017 (2) Å, with a maximum deviation from the mean plane of 0.022 (2) Å for the C7 atom. The azaniumyl N atom is almost coplanar with the quinoline plane, deviating from it by only 0.033 (2) Å. The coordination environment of the Zn atom in the  $[ZnCl_4]^{2-}$  dianion is slightly distorted tetrahedral ( $\tau^4 = 0.91$ ; Yang *et al.*, 2007). The mean value of the Zn–Cl bond lengths of the  $[ZnCl_4]^{2-}$  anion is 2.279 Å, which is in good agreement with the literature value [2.268 (4) Å; Harrison, 2005]. The Cl–Zn–Cl bond angles in the dianion indicate distortions from a regular tetrahedron (109.5°), with a spread of values


**Figure 3**

The crystal packing viewed along [100]. N–H $\cdots$ Cl and C–H $\cdots$ Cl hydrogen bonds are shown as blue dashed lines, while the  $\pi$ - $\pi$  stacking interactions are shown as red dashed lines.

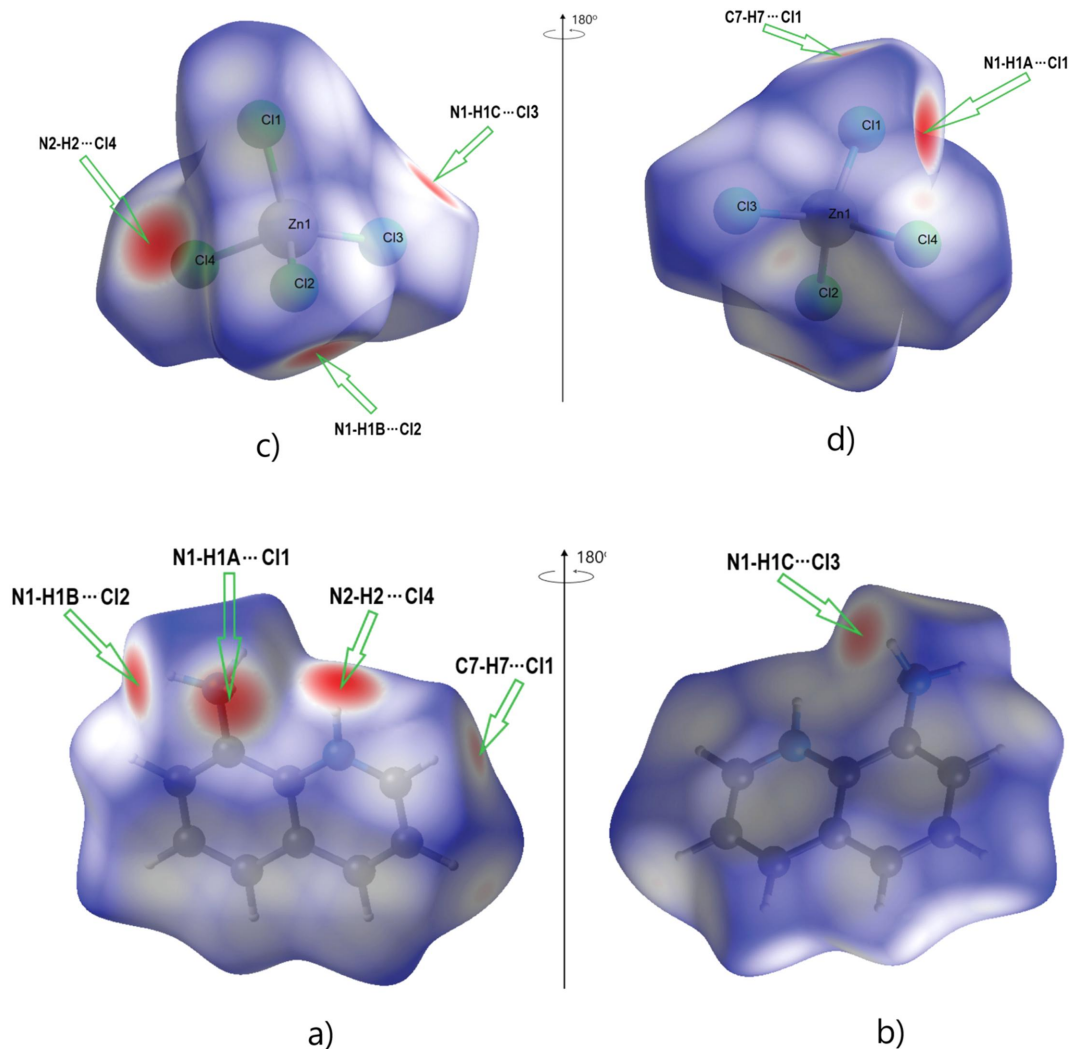
between  $103.058(19)$  and  $117.08(2)^\circ$ . The most acute angle of  $103.058(19)^\circ$  within the tetrachloridozincate dianion is subtended by atoms Cl1 and Cl4. These atoms are associated with the relatively long Zn–Cl bond lengths, which, in turn, are correlated with the most relevant intermolecular interactions in the structure; atom Cl4 is involved in the shortest and most linear N–H $\cdots$ Cl hydrogen bond (see Section 3) and thus represents the most distant ligand in the anion.

### 3. Supramolecular features and Hirshfeld surface analysis

Each  $[\text{ZnCl}_4]^{2-}$  dianion is connected to four neighbouring organic cations through N–H $\cdots$ Cl and C–H $\cdots$ Cl interactions involving all the Cl atoms (Table 1). Thus, the N1–H1A $\cdots$ Cl1, N2–H2 $\cdots$ Cl4 and N1–H1C $\cdots$ Cl3<sup>ii</sup> hydrogen bonds generate  $R_2^2(9)$  ring motifs (Bernstein *et al.*, 1995) and link the dications and anions into chains parallel to [100] (Fig. 2). These chains are interconnected by

N1–H1B $\cdots$ Cl2<sup>i</sup> and C7–H7 $\cdots$ Cl1<sup>iii</sup> hydrogen bonds, which generate  $R_4^3(11)$  ring motifs, forming sheets parallel to (001) (Fig. 2). In addition, the molecules are linked by pairs of  $\pi$ – $\pi$  interactions between the pyridine and arene rings of neighbouring dications. The molecules stack along [001] to consolidate the triperiodic supramolecular network (Fig. 3). The relevant centroid-to-centroid distance for  $\pi$ – $\pi$  stacking interaction between Cg1 (the centroid of pyridine ring C5–C7/N2/C8/C9) and Cg2 (the centroid of arene ring C1–C4/C9/C8) is  $Cg1\cdots Cg2^i = 3.7784(11)$  Å [symmetry code: (i)  $-x + 1, -y + 1, -z + 1$ ], with a slippage of 1.613 Å.

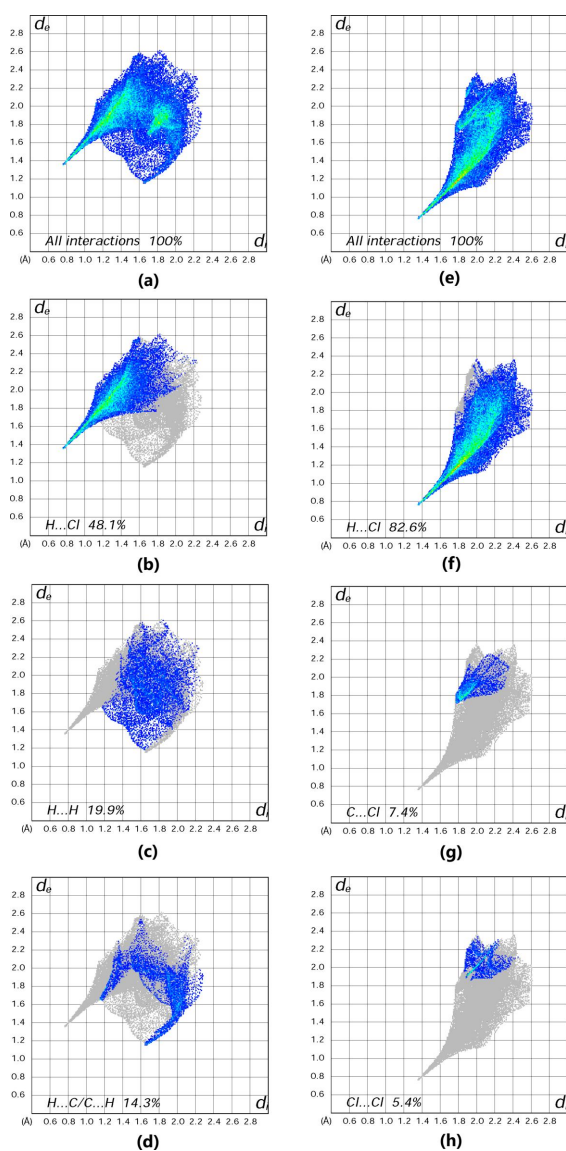
The supramolecular interactions were investigated quantitatively and visualized by Hirshfeld surface analysis performed with *CrystalExplorer21* (Spackman *et al.*, 2021). It should be noted that the Hirshfeld surfaces and fingerprint plots were calculated separately for the 8-azaniumylquinolinium dication and the  $[\text{ZnCl}_4]^{2-}$  dianion. The respective acceptor and donor atoms showing strong N–H $\cdots$ Cl intermolecular hydrogen bonds (for N1–H1A $\cdots$ Cl1, N1–H1B $\cdots$



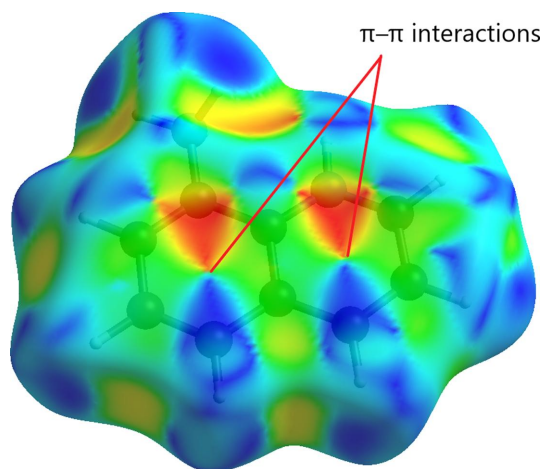
**Figure 4**

View of the three-dimensional Hirshfeld surface for the  $(\text{C}_9\text{H}_{10}\text{N}_2)^{2+}$  dication and the  $[\text{ZnCl}_4]^{2-}$  dianion plotted over  $d_{\text{norm}}$ . Parts (a) and (b) show the front and back sides, respectively, of the  $(\text{C}_9\text{H}_{10}\text{N}_2)^{2+}$  dication. Parts (c) and (d) show the front and back sides, respectively, of the  $[\text{ZnCl}_4]^{2-}$  dianion.

$\text{Cl2}^i$ ,  $\text{N1-H1C}\cdots\text{Cl3}^{ii}$  and  $\text{N2-H2}\cdots\text{Cl4}$  are indicated as bright-red spots on the Hirshfeld surface (Fig. 4). Classical  $\text{N-H}\cdots\text{Cl}$  hydrogen bonds correspond to  $\text{H}\cdots\text{Cl}$  contacts [with contributions of 82.6 and 48.1% to the Hirshfeld surface for the  $[\text{ZnCl}_4]^{2-}$  dianion and 8-azaniumylquinolinium dication, respectively; Figs. 5(f) and 5(b)]. These interactions can be seen as spikes with a sharp tip.  $\text{H}\cdots\text{H}$ ,  $\text{H}\cdots\text{C}/\text{C}\cdots\text{H}$  and  $\text{C}\cdots\text{C}$  interactions in the dication, and  $\text{C}\cdots\text{Cl}$  and  $\text{Cl}\cdots\text{Cl}$  interactions in the dianion follow with contributions of 19.9, 14.3, 6.7, 7.4 and 5.4%, respectively (Fig. 5). Other, minor, contributions are from  $\text{C}\cdots\text{Cl}$  (6.4%),  $\text{H}\cdots\text{N}/\text{N}\cdots\text{H}$  (2.6%),  $\text{H}\cdots\text{Zn}$  (0.7%),  $\text{N}\cdots\text{Cl}$  (0.6%) and  $\text{N}\cdots\text{C}/\text{C}\cdots\text{N}$  (0.1%) contacts in the dication, and from  $\text{Zn}\cdots\text{Cl}/\text{Cl}\cdots\text{Zn}$  (1.7%),  $\text{Zn}\cdots\text{H}$  (1.1%),  $\text{N}\cdots\text{Cl}$  (1.0%) and  $\text{Zn}\cdots\text{C}$  (0.8%) contacts in the dianion. The shape-index of the 8-azaniumylquinolinium



**Figure 5**  
 Two-dimensional Hirshfeld surface fingerprint plots for the  $(\text{C}_9\text{H}_{10}\text{N}_2)^{2+}$  dication [panels (a), (b), (c) and (d)] and the  $[\text{ZnCl}_4]^{2-}$  dianion [panels (e), (f), (g) and (h)]. The  $d_i$  and  $d_e$  values are the closest internal and external distances (in Å) from a given point on the Hirshfeld surface.



**Figure 6**  
 The Hirshfeld surface of the  $(\text{C}_9\text{H}_{10}\text{N}_2)^{2+}$  dication plotted over shape-index.

dication is a tool to visualize  $\pi$ - $\pi$  stacking by the presence of adjacent red and blue triangles. Fig. 6 gives clear evidence that these interactions exist, as discussed above.

#### 4. Database survey

A search of the Cambridge Structural Database (CSD, Version 2022.3.0; Groom *et al.*, 2016) revealed 114 compounds involving the 8-aminoquinoline moiety. Among them, 65 are metal complexes and 20 are organic salts and cocrystals. In all of these metal complexes, 8-aminoquinoline coordinates in a bidentate fashion, although there are examples of bridging-binding (CSD refcode VIZBIP; Schmidbaur *et al.*, 1991) and monodentate (MUDNEG; Xu *et al.*, 2015) modes. Only in the structure of 8-azaniumylquinolinium dichloride (PENHAR; Yan *et al.*, 1998) are both the amino group and the ring N atom protonated.

#### 5. Synthesis and crystallization

Commercially available starting materials were used without further purification. 8-Aminoquinoline (0.144 g, 1 mmol) was dissolved in 10 ml of an ethanol/HCl mixture (9:1 v/v) and added to a solution of  $\text{ZnCl}_2$  (0.136 g, 1 mmol) in 10 ml of the same ethanol/HCl mixed solvent. The mixture was heated under reflux and stirred for 30 min. A pale-yellow crystalline product was obtained at room temperature after 6 d by slow solvent evaporation [yield: 80%; elemental analysis calculated (%) for  $\text{C}_9\text{H}_{10}\text{Cl}_4\text{N}_2\text{Zn}$ : C 30.59, H 2.85, N 7.93; found: C 30.43, H 2.79, N 7.89].

#### 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. C-bound H atoms were placed in calculated positions and refined using the riding-model approximation, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  and  $\text{C-H} = 0.93$  Å for aromatic H atoms. Both the amino and the ring N-bound H

**Table 2**

Experimental details.

|   |  |
|---|--|
| Crystal data  |  |
| Chemical formula  | (C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> )[ZnCl <sub>4</sub> ]               |
| <i>M<sub>r</sub></i>  | 353.36   |
| Crystal system, space group   | Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>n</i>                                     |
| Temperature (K)   | 566  |
| <i>a</i> , <i>b</i> , <i>c</i> (Å)  | 7.52646 (6), 13.40703 (12),<br>12.65801 (11)                                       |
| $\beta$ (°)   | 92.8635 (8)  |
| <i>V</i> (Å <sup>3</sup> )  | 1275.69 (2)  |
| <i>Z</i>  | 4  |
| Radiation type  | Cu <i>K</i> $\alpha$   |
| $\mu$ (mm <sup>-1</sup> )   | 10.16  |
| Crystal size (mm)   | 0.24 × 0.21 × 0.15   |
| Data collection   |  |
| Diffraction   | Rigaku XtaLAB Synergy single<br>source diffractometer with a<br>HyPix3000 detector |
| Absorption correction   | Multi-scan ( <i>CrysAlis PRO</i> ; Rigaku<br>OD, 2020)                             |
| <i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>   | 0.491, 1.000   |
| No. of measured, independent and<br>observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections                          | 11239, 2474, 2341  |
| <i>R<sub>int</sub></i>  | 0.037  |
| ( <i>sin</i> $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )   | 0.615  |
| Refinement  |  |
| <i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i> | 0.023, 0.065, 1.06   |
| No. of reflections  | 2474   |
| No. of parameters   | 162  |
| No. of restraints   | 4  |
| H-atom treatment  | H atoms treated by a mixture of<br>independent and constrained<br>refinement       |
| $\Delta\rho_{\max}$ , $\Delta\rho_{\min}$ (e Å <sup>-3</sup> )  | 0.32, -0.28  |

Computer programs: *CrysAlis PRO* (Rigaku OD, 2020), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

atoms were located in a difference Fourier map and refined with bond-length restraints of 0.89 (1) and 0.86 (1) Å, respectively.

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## supporting information

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## Crystal structure and Hirshfeld surface analysis of 8-azaniumylquinolinium tetrachloridozincate(II)

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### Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2020); cell refinement: *CrysAlis PRO* (Rigaku OD, 2020); data reduction: *CrysAlis PRO* (Rigaku OD, 2020); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: SHELXL (Sheldrick, 2015b); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: *publCIF* (Westrip, 2010).

### 8-Azaniumylquinolinium tetrachloridozincate(II)

#### Crystal data

(C<sub>9</sub>H<sub>10</sub>N<sub>2</sub>)[ZnCl<sub>4</sub>]

$M_r = 353.36$

Monoclinic,  $P2_1/n$

$a = 7.52646$  (6) Å

$b = 13.40703$  (12) Å

$c = 12.65801$  (11) Å

$\beta = 92.8635$  (8)°

$V = 1275.69$  (2) Å<sup>3</sup>

$Z = 4$

$F(000) = 704$

$D_x = 1.840$  Mg m<sup>-3</sup>

Cu  $K\alpha$  radiation,  $\lambda = 1.54184$  Å

Cell parameters from 8253 reflections

$\theta = 3.3\text{--}71.4^\circ$

$\mu = 10.16$  mm<sup>-1</sup>

$T = 566$  K

Block, pale yellow

0.24 × 0.21 × 0.15 mm

#### Data collection

Rigaku XtaLAB Synergy single source diffractometer with a HyPix3000 detector

Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source

Mirror monochromator

Detector resolution: 10.0000 pixels mm<sup>-1</sup>

$\omega$  scans

Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2020)

$T_{\min} = 0.491$ ,  $T_{\max} = 1.000$

11239 measured reflections

2474 independent reflections

2341 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.037$

$\theta_{\max} = 71.4^\circ$ ,  $\theta_{\min} = 4.8^\circ$

$h = -9 \rightarrow 7$

$k = -16 \rightarrow 16$

$l = -15 \rightarrow 15$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.023$

$wR(F^2) = 0.065$

$S = 1.06$

2474 reflections

162 parameters

4 restraints

Primary atom site location: dual

Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0362P)^2 + 0.3283P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.32$  e Å<sup>-3</sup>

$$\Delta\rho_{\min} = -0.28 \text{ e } \text{\AA}^{-3}$$

Extinction correction: SHELXL (Sheldrick, 2015b),  $F_c^* = kF_c [1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$   
 Extinction coefficient: 0.00359 (19)

*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.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

|     | <i>x</i>    | <i>y</i>     | <i>z</i>     | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|--------------|--------------|----------------------------------|
| Zn1 | 0.92145 (3) | 0.41694 (2)  | 0.17409 (2)  | 0.02862 (11)                     |
| Cl4 | 0.66523 (6) | 0.36967 (4)  | 0.07893 (3)  | 0.03361 (13)                     |
| Cl1 | 0.84550 (6) | 0.56627 (3)  | 0.24448 (4)  | 0.03547 (13)                     |
| Cl2 | 0.95542 (7) | 0.31035 (3)  | 0.31521 (4)  | 0.03674 (14)                     |
| Cl3 | 1.16765 (6) | 0.41294 (4)  | 0.08236 (4)  | 0.03691 (14)                     |
| N2  | 0.4715 (2)  | 0.39322 (11) | 0.28755 (12) | 0.0269 (3)                       |
| N1  | 0.4398 (2)  | 0.58098 (12) | 0.17865 (12) | 0.0296 (4)                       |
| C1  | 0.3676 (2)  | 0.56492 (13) | 0.28262 (13) | 0.0245 (4)                       |
| C8  | 0.3848 (2)  | 0.47086 (13) | 0.33164 (13) | 0.0228 (3)                       |
| C9  | 0.3120 (2)  | 0.45601 (14) | 0.43180 (14) | 0.0275 (4)                       |
| C4  | 0.2233 (2)  | 0.53608 (16) | 0.47875 (15) | 0.0340 (4)                       |
| H4  | 0.173175    | 0.526950     | 0.543724     | 0.041*                           |
| C2  | 0.2837 (2)  | 0.64101 (14) | 0.33141 (16) | 0.0320 (4)                       |
| H2A | 0.274830    | 0.703201     | 0.299033     | 0.038*                           |
| C7  | 0.4940 (3)  | 0.30526 (14) | 0.33447 (16) | 0.0335 (4)                       |
| H7  | 0.556834    | 0.255296     | 0.301634     | 0.040*                           |
| C5  | 0.3326 (3)  | 0.36147 (16) | 0.47933 (15) | 0.0357 (4)                       |
| H5  | 0.282864    | 0.349307     | 0.543880     | 0.043*                           |
| C6  | 0.4245 (3)  | 0.28736 (16) | 0.43198 (17) | 0.0391 (5)                       |
| H6  | 0.440294    | 0.225711     | 0.464797     | 0.047*                           |
| C3  | 0.2103 (3)  | 0.62624 (16) | 0.43029 (16) | 0.0367 (5)                       |
| H3  | 0.152643    | 0.678533     | 0.462586     | 0.044*                           |
| H1A | 0.5529 (15) | 0.5639 (17)  | 0.179 (2)    | 0.042 (7)*                       |
| H1B | 0.434 (3)   | 0.6446 (9)   | 0.160 (2)    | 0.056 (8)*                       |
| H1C | 0.381 (3)   | 0.5492 (16)  | 0.1272 (14)  | 0.039 (6)*                       |
| H2  | 0.518 (3)   | 0.3968 (17)  | 0.2270 (11)  | 0.040 (6)*                       |

*Atomic displacement parameters ( $\text{\AA}^2$ )*

|     | $U^{11}$     | $U^{22}$     | $U^{33}$     | $U^{12}$      | $U^{13}$     | $U^{23}$      |
|-----|--------------|--------------|--------------|---------------|--------------|---------------|
| Zn1 | 0.02863 (16) | 0.02727 (16) | 0.03004 (16) | 0.00008 (9)   | 0.00209 (11) | -0.00273 (9)  |
| Cl4 | 0.0300 (2)   | 0.0444 (3)   | 0.0265 (2)   | -0.00244 (18) | 0.00214 (17) | -0.00831 (18) |
| Cl1 | 0.0422 (3)   | 0.0237 (2)   | 0.0402 (3)   | 0.00109 (18)  | -0.0005 (2)  | -0.00495 (17) |
| Cl2 | 0.0478 (3)   | 0.0272 (2)   | 0.0354 (2)   | 0.00672 (19)  | 0.0037 (2)   | 0.00296 (17)  |
| Cl3 | 0.0301 (2)   | 0.0450 (3)   | 0.0360 (3)   | -0.00615 (18) | 0.00597 (19) | -0.00603 (19) |
| N2  | 0.0301 (8)   | 0.0249 (7)   | 0.0258 (7)   | -0.0017 (6)   | 0.0042 (6)   | -0.0003 (6)   |



|    |             |             |             |             |             |             |
|----|-------------|-------------|-------------|-------------|-------------|-------------|
| N1 | 0.0371 (9)  | 0.0273 (9)  | 0.0244 (8)  | -0.0017 (7) | 0.0025 (7)  | 0.0033 (6)  |
| C1 | 0.0261 (8)  | 0.0257 (8)  | 0.0216 (8)  | -0.0030 (7) | 0.0006 (7)  | 0.0003 (6)  |
| C8 | 0.0233 (8)  | 0.0249 (9)  | 0.0203 (8)  | -0.0030 (7) | -0.0001 (6) | -0.0014 (6) |
| C9 | 0.0261 (8)  | 0.0333 (10) | 0.0231 (8)  | -0.0076 (7) | 0.0009 (7)  | 0.0000 (7)  |
| C4 | 0.0305 (9)  | 0.0469 (12) | 0.0250 (9)  | -0.0049 (8) | 0.0058 (7)  | -0.0074 (8) |
| C2 | 0.0340 (10) | 0.0265 (9)  | 0.0352 (10) | 0.0004 (7)  | -0.0006 (8) | -0.0025 (7) |
| C7 | 0.0315 (10) | 0.0242 (9)  | 0.0445 (11) | -0.0002 (7) | -0.0007 (8) | 0.0014 (8)  |
| C5 | 0.0367 (10) | 0.0440 (11) | 0.0266 (9)  | -0.0092 (9) | 0.0020 (8)  | 0.0100 (8)  |
| C6 | 0.0394 (11) | 0.0345 (10) | 0.0428 (11) | -0.0054 (9) | -0.0041 (9) | 0.0161 (9)  |
| C3 | 0.0337 (10) | 0.0391 (11) | 0.0376 (11) | 0.0012 (8)  | 0.0053 (8)  | -0.0129 (9) |

*Geometric parameters (Å, °)*

|             |              |           |             |
|-------------|--------------|-----------|-------------|
| Zn1—C14     | 2.3108 (5)   | C8—C9     | 1.420 (2)   |
| Zn1—C11     | 2.2759 (5)   | C9—C4     | 1.411 (3)   |
| Zn1—C12     | 2.2919 (5)   | C9—C5     | 1.408 (3)   |
| Zn1—C13     | 2.2360 (5)   | C4—H4     | 0.9300      |
| N2—C8       | 1.362 (2)    | C4—C3     | 1.357 (3)   |
| N2—C7       | 1.327 (2)    | C2—H2A    | 0.9300      |
| N2—H2       | 0.860 (10)   | C2—C3     | 1.407 (3)   |
| N1—C1       | 1.464 (2)    | C7—H7     | 0.9300      |
| N1—H1A      | 0.882 (10)   | C7—C6     | 1.385 (3)   |
| N1—H1B      | 0.884 (10)   | C5—H5     | 0.9300      |
| N1—H1C      | 0.877 (10)   | C5—C6     | 1.366 (3)   |
| C1—C8       | 1.409 (2)    | C6—H6     | 0.9300      |
| C1—C2       | 1.364 (3)    | C3—H3     | 0.9300      |
| C11—Zn1—C14 | 103.058 (19) | C4—C9—C8  | 118.77 (17) |
| C11—Zn1—C12 | 105.30 (2)   | C5—C9—C8  | 117.93 (18) |
| C12—Zn1—C14 | 107.04 (2)   | C5—C9—C4  | 123.31 (17) |
| C13—Zn1—C14 | 114.479 (19) | C9—C4—H4  | 119.6       |
| C13—Zn1—C11 | 117.08 (2)   | C3—C4—C9  | 120.82 (18) |
| C13—Zn1—C12 | 109.07 (2)   | C3—C4—H4  | 119.6       |
| C8—N2—H2    | 123.2 (16)   | C1—C2—H2A | 119.7       |
| C7—N2—C8    | 123.26 (16)  | C1—C2—C3  | 120.58 (18) |
| C7—N2—H2    | 113.6 (16)   | C3—C2—H2A | 119.7       |
| C1—N1—H1A   | 111.1 (17)   | N2—C7—H7  | 119.8       |
| C1—N1—H1B   | 111.1 (18)   | N2—C7—C6  | 120.47 (18) |
| C1—N1—H1C   | 113.6 (16)   | C6—C7—H7  | 119.8       |
| H1A—N1—H1B  | 107 (2)      | C9—C5—H5  | 119.5       |
| H1A—N1—H1C  | 109 (2)      | C6—C5—C9  | 120.96 (18) |
| H1B—N1—H1C  | 105 (2)      | C6—C5—H5  | 119.5       |
| C8—C1—N1    | 119.84 (15)  | C7—C6—H6  | 120.4       |
| C2—C1—N1    | 119.86 (16)  | C5—C6—C7  | 119.13 (18) |
| C2—C1—C8    | 120.31 (17)  | C5—C6—H6  | 120.4       |
| N2—C8—C1    | 122.61 (15)  | C4—C3—C2  | 120.33 (18) |
| N2—C8—C9    | 118.20 (16)  | C4—C3—H3  | 119.8       |
| C1—C8—C9    | 119.18 (16)  | C2—C3—H3  | 119.8       |

|             |              |             |              |
|-------------|--------------|-------------|--------------|
| N2—C8—C9—C4 | 179.45 (15)  | C8—C9—C4—C3 | -1.2 (3)     |
| N2—C8—C9—C5 | -0.5 (2)     | C8—C9—C5—C6 | 2.0 (3)      |
| N2—C7—C6—C5 | 0.0 (3)      | C9—C4—C3—C2 | 0.7 (3)      |
| N1—C1—C8—N2 | 1.9 (2)      | C9—C5—C6—C7 | -1.8 (3)     |
| N1—C1—C8—C9 | -179.12 (16) | C4—C9—C5—C6 | -177.92 (18) |
| N1—C1—C2—C3 | 178.65 (17)  | C2—C1—C8—N2 | -178.25 (16) |
| C1—C8—C9—C4 | 0.5 (2)      | C2—C1—C8—C9 | 0.7 (3)      |
| C1—C8—C9—C5 | -179.45 (16) | C7—N2—C8—C1 | 177.61 (17)  |
| C1—C2—C3—C4 | 0.5 (3)      | C7—N2—C8—C9 | -1.3 (3)     |
| C8—N2—C7—C6 | 1.6 (3)      | C5—C9—C4—C3 | 178.74 (18)  |
| C8—C1—C2—C3 | -1.2 (3)     |             |              |

*Hydrogen-bond geometry (Å, °)*

| <i>D—H...A</i>             | <i>D—H</i> | <i>H...A</i> | <i>D...A</i> | <i>D—H...A</i> |
|----------------------------|------------|--------------|--------------|----------------|
| N1—H1A...C11               | 0.88 (1)   | 2.31 (1)     | 3.1309 (16)  | 154 (2)        |
| N1—H1B...C12 <sup>i</sup>  | 0.89 (1)   | 2.39 (1)     | 3.1747 (17)  | 148 (2)        |
| N1—H1C...C13 <sup>ii</sup> | 0.88 (2)   | 2.48 (2)     | 3.2415 (16)  | 145 (2)        |
| N2—H2...C14                | 0.86 (2)   | 2.25 (2)     | 3.0958 (16)  | 166 (2)        |
| C7—H7...C11 <sup>iii</sup> | 0.93       | 2.71         | 3.584 (2)    | 157            |

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