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Synthesis, crystal structure and Hirshfeld surface analysis of a dinuclear zinc(II) complex with 1-[3-(pyridin-2-yl)-1*H*-1,2,4-triazol-5-yl]methanamine

Tetyana V. Bondarchuk,[a] Mariia B. Struhatska,[a]* Dmytro M. Khomenko,[a,b] Alexandra Bargan[c] and Oleksandr V. Vaschenko[a]

[a]Department of Chemistry, Taras Shevchenko National University of Kyiv, 12 Hetman Pavlo Skoropadsky Str., Kyiv 01033, Ukraine, [b]Enamine Ltd (www.enamine.net), Winston Churchill Str. 78, 02094 Kyiv, Ukraine, and [c]'PetruPoni' Institute of Macromolecular Chemistry, Aleea Gr., Ghica Voda 41A, 700487 Iasi, Romania. *Correspondence e-mail: mariia.struhatska@knu.ua

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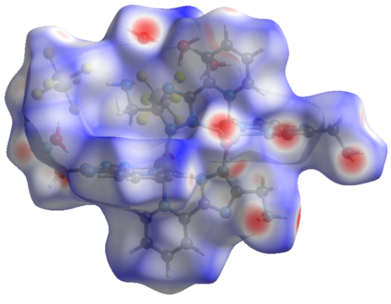
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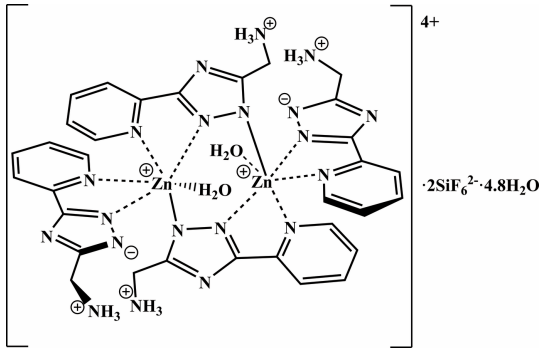
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The asymmetric unit of the title compound, bis[μ-5-(azaniumylmethyl)-3-(pyridin-2-yl)-1*H*-1,2,4-triazol-1-ido]bis{aqua[5-(azaniumylmethyl)-3-(pyridin-2-yl)-1*H*-1,2,4-triazol-1-ido]zinc(II)} bis(hexafluoridosilicate) 4.8-hydrate, $[Zn_2(C_8H_9N_5)_4(H_2O)_2](SF_6)_2\cdot 4.8H_2O$, consists of a centrosymmetric dinuclear complex cation, two hexafluoridosilicate anions and two water molecules of crystallization. Each Zn^{2+} ion adopts a distorted octahedral ZnN_5O coordination geometry, being coordinated by five N atoms from three anionic 1-[3-(pyridin-2-yl)-1*H*-1,2,4-triazol-5-yl]methanamine ligands and one water molecule. Two triazole-based ligands bridge the two Zn^{2+} centres, giving rise to a dinuclear unit. Hirshfeld surface analysis revealed that the most important contributions to the crystal packing are from H···H (35.2%), F···H/H···F (28.0%) and C···H/H···C (13.3%) interactions.

1. Chemical context

Polynuclear zinc(II) complexes have been actively investigated for their enzyme-inhibitory and anticancer activities (Zhang *et al.*, 2021; Su *et al.*, 2025), as well as for their potential applications as luminescent materials (Zhang *et al.*, 2013; Wang *et al.*, 2018*b*) and photoluminescent sensors (Wang *et al.*, 2018*a*; Cao *et al.*, 2020). The properties of zinc-based materials are largely determined by the nature of the organic ligand. Coordination of ligands to metal centers increases the overall rigidity of the framework, thereby minimizing non-radiative energy losses and enhancing the luminescence properties of these compounds (Cao *et al.*, 2020). In this context, multidentate N-donor heterocycles, particularly 3-(pyridin-2-yl)-1,2,4-triazole derivatives, are considered as effective building blocks for the construction of stable coordination architectures (Zhang *et al.*, 2021; Wang *et al.*, 2018*a*).





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Recently, we reported the synthesis and magnetochemical characterization of a series of copper(II) complexes based on 1-[(5*R*)-1,2,4-triazol-3-yl]methanamines (Petrenko *et al.*, 2026). In all cases, we observed coordination of the amino group to the metal center, resulting in the formation of a five-membered metallacycle. Here, we extend this approach to the more complex ligand 1-[3-(pyridin-2-yl)-1*H*-1,2,4-triazol-5-yl] methanamine (Vashchenko *et al.*, 2025), which contains two potential chelating sites, *i.e.* pyridyl–triazole and methyl-amino–triazole moieties.

Owing to the propensity of the pyridyl–triazole moiety to adopt chelating bidentate and bridging coordination modes (Pang *et al.*, 2017; Petrenko *et al.*, 2020; Petrenko *et al.*, 2023), the amino group may remain uninvolved in coordination. Nevertheless, its ability to form hydrogen bonds can give rise to an extended network of intermolecular interactions involving both the complex molecules and lattice water molecules. In this work, we report the synthesis, crystal structure and Hirshfeld surface analysis of the title compound, a new binuclear zinc(II) complex with 1-[3-(pyridin-2-yl)-1*H*-1,2,4-triazol-5-yl]methanamine.

2. Structural commentary

The title compound exhibits an ionic crystal structure, which is built up from centrosymmetric dinuclear $[Zn_2(HL)_4(H_2O)_2]^{4+}$ cations, SiF_6^{2-} anions and interstitial water molecules in a 1:2:4.8 ratio (Fig. 1 and Table 1). Each Zn^{II} ion is coordinated by five N atoms provided by three ligands and one O atom from a coordinated water molecule. The ZnN_5O coordination environment is best described as a distorted octahedron, as indicated by continuous shape measure (CShM) calculations performed with the program *SHAPE* (Version 2.1; Llunell *et al.*, 2013), which yielded the lowest value of 1.723 for an ideal octahedron (*OC*-6).

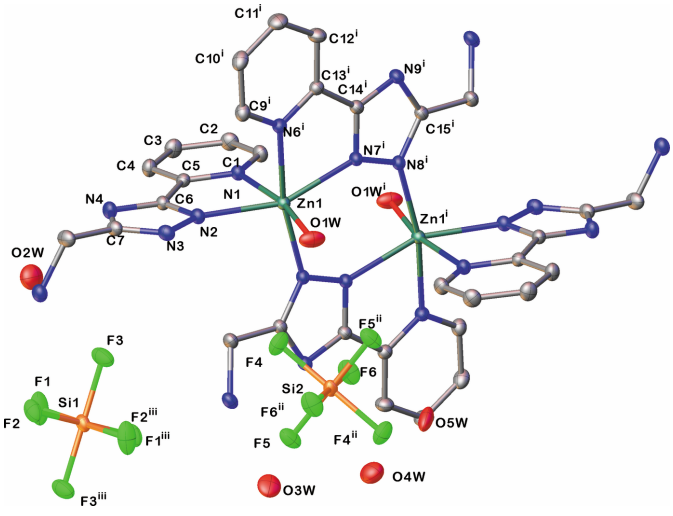


Figure 1
The molecular structure of $[Zn_2(HL)_4(H_2O)_2](SiF_6)_2{\cdot}4.8H_2O$. H atoms have been omitted for clarity.

Table 1
Selected geometric parameters (Å, °).

Zn1—O1*W*	2.1581 (18)	Zn1—N7^{i}	2.1669 (17)
Zn1—N1	2.2556 (18)	Zn1—N8	2.0943 (17)
Zn1—N2	2.1523 (17)	N7—N8	1.377 (2)
Zn1—N6^{i}	2.1907 (18)		
O1*W*—Zn1—N1	169.06 (8)	N8—Zn1—N2	100.42 (7)
O1*W*—Zn1—N6^{i}	85.67 (7)	N8—Zn1—N6^{i}	168.62 (7)
O1*W*—Zn1—N7^{i}	100.82 (8)	N8—Zn1—N7^{i}	96.08 (6)
N2—Zn1—O1*W*	94.68 (8)	C5—N1—Zn1	115.09 (13)
N2—Zn1—N1	74.80 (6)	C6—N2—Zn1	115.90 (13)
N2—Zn1—N6^{i}	89.24 (7)	C13—N6—Zn1^{i}	114.91 (13)
N2—Zn1—N7^{i}	157.79 (7)	C14—N7—Zn1^{i}	112.70 (13)
N6^{i}—Zn1—N1	97.00 (7)	N1—C5—C6	113.90 (18)
N7^{i}—Zn1—N1	90.12 (6)	N2—C6—C5	120.16 (18)
N7^{i}—Zn1—N6^{i}	76.29 (6)	N6—C13—C14	114.27 (18)
N8—Zn1—O1*W*	87.53 (7)	N7—C14—C13	120.53 (18)
N8—Zn1—N1	91.39 (7)		
Zn1—N1—C5—C6	4.3 (2)	N1—C5—C6—N2	−2.7 (3)
Zn1—N2—C6—C5	−0.4 (2)	N6—C13—C14—N7	2.7 (3)
Zn1^{i}—N6—C13—C14	6.5 (2)	C4—C5—C6—N4	−6.2 (3)
Zn1^{i}—N7—N8—Zn1	16.3 (3)	C12—C13—C14—N9	2.4 (3)
Zn1^{i}—N7—C14—C13	−10.3 (2)		

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Two ligands adopt a μ_2-bridging coordination mode, linking the Zn^{II} centres into a centrosymmetric dinuclear cation with a Zn···Zn separation of 4.2054 (3) Å, whereas the remaining two ligands act as terminal *N*,*N*′-chelating ligands. The Zn—N bond lengths fall in the range 2.0943 (17)–2.2556 (18) Å (Table 1), which is comparable with those reported for related dinuclear Zn^{II} complexes containing pyridyl–triazole ligands (Zhang *et al.*, 2021; Klingele *et al.*, 2007; Klingele *et al.*, 2006; Wang *et al.*, 2018*b*; Gusev *et al.*, 2011). The Zn—O bond distance of 2.1581 (18) Å is comparable with the corresponding Zn—O distances reported for related dinuclear Zn^{II} complexes, where oxygen coordination arises either from coordinated solvent molecules or from oxygen-donor ligand functionalities. These distances lie in the range 1.9228 (18)–2.1412 (18) Å (Zhang *et al.*, 2021; Klingele *et al.*, 2007; Klingele *et al.*, 2006; Wang *et al.*, 2018*b*; Gusev *et al.*, 2011).

The octahedral coordination environment is distorted, as evidenced by the *cis*-N/O—Zn—N angles ranging from 74.80 (6) to 100.82 (8)° and the *trans* angles ranging from 157.79 (7) to 169.06 (8)° (Table 1). The smallest *cis* angle corresponds to the bite angle of the terminal *N*,*N*′-chelating ligand, while the deviations of the remaining angles from the ideal values reflect the constraints associated with the bridging coordination mode of the μ_2-triazole ligands.

The five-membered ZnN_2C_2 chelate rings generated by coordination of the terminal and bridging ligands exhibit comparable internal geometries, as indicated by the similar internal bond angles of the metallacycles (Table 1). The absolute values of the torsion angles do not exceed 4.3 (2)° for the terminal-ligand chelate rings and 10.3 (2)° for the bridging-ligand chelate rings, confirming that both metallacycles are close to planar. The terminal chelate ring (Zn1/N1/C5/C6/N2) is the more planar of the two, with a maximum deviation of 0.0317 (19) Å from the least-squares plane (atom N1), whereas the corresponding metallacycle (Zn1/N6/C13/C14/

Table 2
Selected interplanar angles (°).

C1–C5/N1 and C6/N4/C7/N3/N2	4.41 (12)
C9–C13/N6 and C14/N9/C15/N8/N7	2.88 (9)
N2/C6/C5/N1/Zn1 and Zn1/N7/N8/Zn1/N7/N8	89.1 (4)
N6/C13/C14/N7/Zn1 and Zn1/N7/N8/Zn1/N7/N8	4.8 (4)

N7) involving the μ_2-bridging ligand displays a maximum deviation of 0.0804 (19) Å (atom N6).

The pyridyl and triazole rings of the ligands are nearly coplanar, forming interplanar angles of 4.41 (12) and 2.88 (9)° in the terminal and bridging ligands, respectively (Table 2). The corresponding torsion angles C4—C5—C6—N4 [6.2 (3)°] and N1—C5—C6—N2 [2.7 (3)°] in the terminal, and C12—C13—C14—N9 [2.4 (3)°] and N6—C13—C14—N7 [2.7 (3)°] in the bridging ligands indicate that both ligands adopt similar conformations, differing only slightly in the degree of twisting between the two heterocyclic rings (Table 2).

The five-membered metallacycle formed by the terminal *N*,*N*′-chelating ligand is nearly perpendicular to the six-membered Zn_2N_4 metallacycle. The dihedral angle between the least-squares planes of these metallacycles is 89.1 (4)° (Table 2). The six-membered metallacycle formed by the two Zn^{II} centres and the donor N atoms of the triazole rings of the two μ_2-bridging ligands is essentially planar, with the maximum deviation from the least-squares plane being 0.0733 (18) Å for atom N7. This metallacycle exhibits only a slight twist along the Zn1—N7—N8—Zn1 fragment, as reflected by the corresponding torsion angle of 16.3 (3)° (Table 2).

Table 3
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O3*W*^{ii}	0.81 (2)	2.01 (2)	2.764 (3)	157 (4)
O1*W*—H1*WB*···F4	0.85 (2)	2.09 (3)	2.844 (3)	149 (4)
O1*W*—H1*WB*···F6	0.85 (2)	2.61 (2)	3.383 (3)	153 (4)
O2*W*—H2*WA*···N4	0.85	2.10	2.941 (4)	172
O2*W*—H2*WB*···F1^{iii}	0.85	2.44	3.218 (5)	153
O2*W*—H2*WB*···F3	0.85	2.41	3.111 (4)	140
O3*W*—H3*WA*···O4*W*	0.84	2.16	3.002 (5)	177
O3*W*—H3*WB*···O4*W*^{iv}	0.84	2.15	2.932 (5)	157
O4*W*—H4*WA*···O2*W*^{v}	0.87	1.87	2.728 (5)	169
O4*W*—H4*WB*···F6	0.87	2.03	2.889 (4)	173
O5*W*—H5*WA*···F6	0.88	2.02	2.877 (14)	165
O5*W*—H5*WB*···N4^{v}	0.87	1.96	2.821 (13)	170
N5—H5*A*···F2^{iii}	0.87 (1)	2.40 (3)	2.977 (3)	124 (2)
N5—H5*A*···F3	0.87 (1)	1.96 (1)	2.829 (3)	171 (3)
N5—H5*B*···O4*W*^{vi}	0.87 (1)	2.31 (2)	3.123 (4)	156 (3)
N5—H5*C*···N3^{vii}	0.87 (1)	2.05 (2)	2.854 (3)	153 (3)
N10—H10*A*···O3*W*	0.87 (1)	2.10 (2)	2.915 (3)	155 (3)
N10—H10*B*···F1	0.88 (1)	1.96 (1)	2.831 (3)	174 (3)
N10—H10*B*···F2	0.88 (1)	2.43 (3)	2.876 (3)	112 (2)
N10—H10*C*···F5	0.88 (1)	1.92 (2)	2.785 (3)	167 (3)
N10—H10*C*···F6	0.88 (1)	2.58 (2)	3.227 (3)	131 (2)
C1—H1···F6^{i}	0.93	2.54	3.214 (3)	130
C2—H2···F5^{viii}	0.93	2.48	3.313 (3)	150
C8—H8*B*···F4^{vii}	0.97	2.48	2.993 (3)	113
C8—H8*B*···O5*W*^{vi}	0.97	2.62	3.139 (15)	114
C9—H9···F2^{ix}	0.93	2.61	3.216 (3)	123
C16—H16*A*···F4	0.97	2.47	3.165 (3)	129
C16—H16*A*···N2	0.97	2.68	3.183 (3)	113
C16—H16*B*···F3	0.97	2.46	3.140 (3)	127

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x-1, y, z$; (iii) $-x+2, -y, -z+2$; (iv) $-x+2, -y+1, -z+2$; (v) $x, y+1, z$; (vi) $x, y-1, z$; (vii) $-x+1, -y, -z+2$; (viii) $x, y, z-1$; (ix) $-x+2, -y+1, -z+1$.

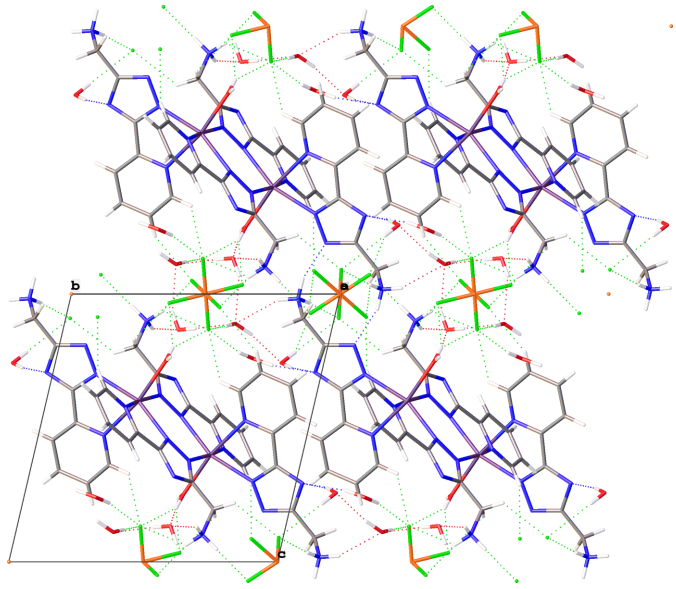


Figure 2
The crystal packing of $[Zn_2(HL)_4(H_2O)_2](SiF_6)_2{\cdot}4.8H_2O$, viewed down the *a* axis.

3. Supramolecular features

The crystal packing is governed by an extensive hydrogen-bonding network involving the complex cations, hexafluoridosilicate anions and water molecules (Table 3). The coordinated water molecule O1*W* acts as a hydrogen-bond donor towards a water molecule of crystallization [O1*W*—H1*WA*···O3*W*: O···O = 2.764 (3) Å] and towards F atoms of the $[SiF_6]^{2-}$ anion. The lattice water molecules participate both as donors and as acceptors, forming O—H···O contacts with one another, as well as O—H···N and O—H···F hydrogen bonds to the organic ligands and hexafluoridosilicate anions, respectively. Particularly short O—H···O and O—H···F contacts include O4*W*—H4*WA*···O2*W* [O···O = 2.728 (5) Å] and O4*W*—H4*WB*···F6 [O···F = 2.889 (4) Å].

The N—H groups of the aminomethyl substituents provide additional hydrogen-bond donors. They form N—H···F contacts with the $[SiF_6]^{2-}$ anions, including the nearly linear N5—H5*A*···F3 and N10—H10*B*···F1 interactions, with N···F separations of 2.829 (3) and 2.831 (3) Å, respectively, and N—H···F angles of 171 (3) and 174 (3)°, respectively. N—H···O and N—H···N hydrogen bonds further connect the ligand fragments with water molecules of crystallization and neighbouring complex cations. Thus, the $[SiF_6]^{2-}$ anions and water molecules act as important hydrogen-bonding linkers between the cationic coordination units, generating an extended supramolecular assembly. Weaker C—H···F and C—H···N contacts provide further consolidation of the crystal packing.

The crystal packing of $[Zn_2(HL)_4(H_2O)_2](SiF_6)_2{\cdot}4.8H_2O$ viewed down the *a* axis is illustrated in Fig. 2.

To gain further insight into the intermolecular interactions governing the crystal packing, a Hirshfeld surface analysis was performed using *CrystalExplorer21.5* (Spackman *et al.*, 2021). The Hirshfeld surface mapped over d_{norm} (Fig. 3) exhibits several intense red spots corresponding to close intermolecular contacts.

The two-dimensional fingerprint plots derived from the Hirshfeld surface are shown in Fig. 3 and indicate that the crystal packing is dominated by H···H contacts, which contribute 35.2% of the total Hirshfeld surface, reflecting the prevalence of van der Waals interactions. The second largest contribution arises from F···H/H···F contacts (28%), consistent with the O—H···F hydrogen-bonding network involving the coordinated/uncoordinated water molecules and the hexafluoridosilicate anions. C···H/H···C contacts account for 13.3% of the surface, and smaller contributions originate from N···H/H···N (8%), O···H/H···O (7.9%) and N···C/C···N (3.1%) contacts. The contribution from C···C contacts is 2.2%, suggesting only weak π–π stacking interactions between neighbouring aromatic rings. The remaining contact types, including O···C/C···O (1.3%), O···O (0.3%), F···C/C···F (0.3%), N···F/F···N (0.1%), N···N (0.1%), F···O/O···F (0.1%) and N···O/O···N (0.1%), each contribute only marginally to the Hirshfeld surface.

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 6.01, update of February 2026; Groom *et al.*, 2016) for dinuclear Zn^{II} complexes containing bridging ligands with a 3-(pyridin-2-yl)-1*H*-1,2,4-triazole framework similar to that of the title compound revealed five closely related structures,

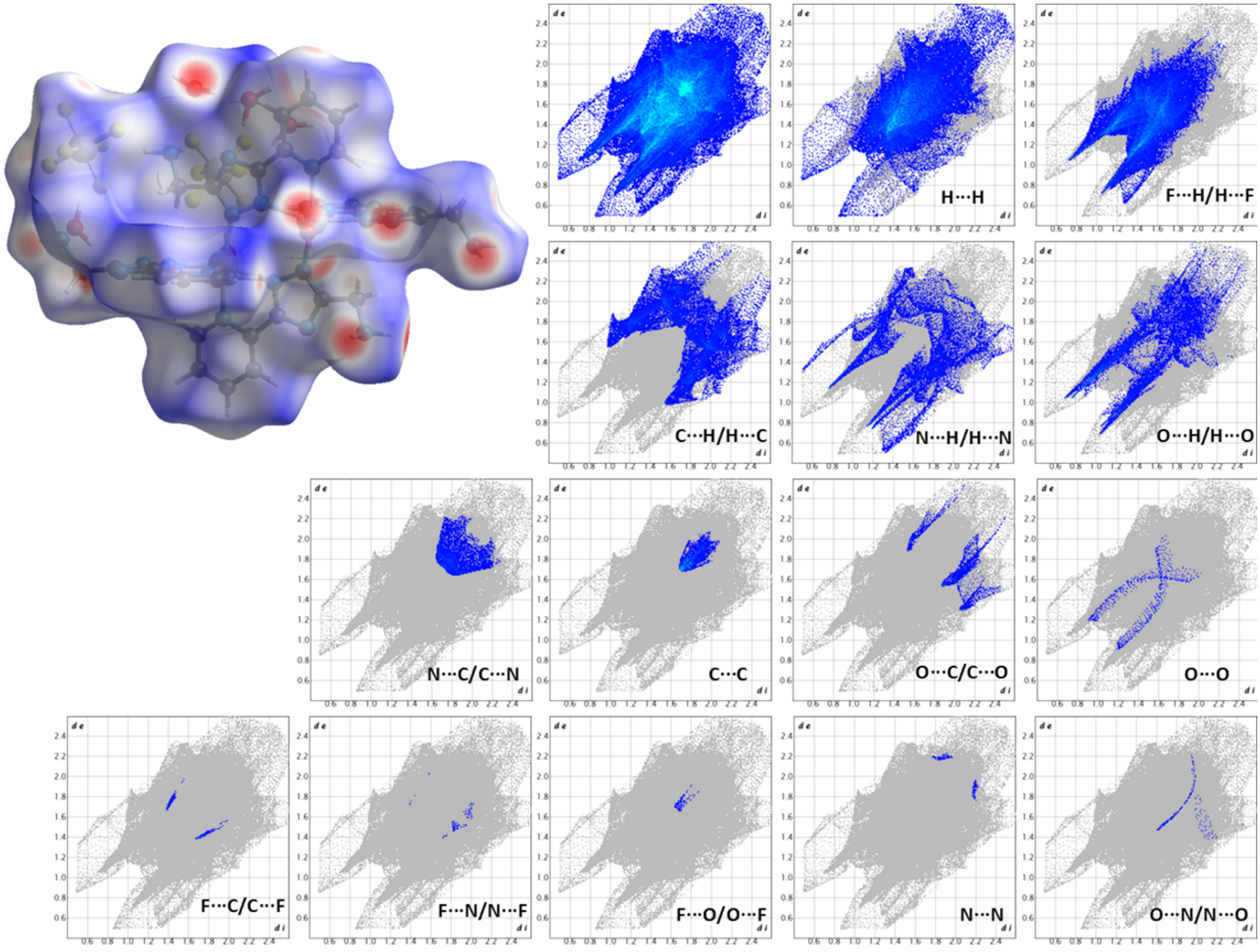


Figure 3
The Hirshfeld surface mapped over d_{norm}, with red, white and blue regions representing contacts shorter than, equal to and longer than the sum of the van der Waals radii, respectively, and the corresponding two-dimensional fingerprint plots showing all intermolecular contacts and their delineated contributions (blue regions) in $[Zn_2(HL)_4(H_2O)_2](SiF_6)_2{\cdot}4.8H_2O$. The relative contributions of individual contact types for the asymmetric unit are: H···H 35.2%, F···H/H···F 28%, C···H/H···C 13.3%, N···H/H···N 8%, O···H/H···O 7.9%, N···C/C···N 3.1%, C···C 2.2%, O···C/C···O 1.3%, O···O 0.3%, F···C/C···F 0.3%, N···F/F···N 0.1%, N···N 0.1%, F···O/O···F 0.1% and N···O/O···N 0.1%.

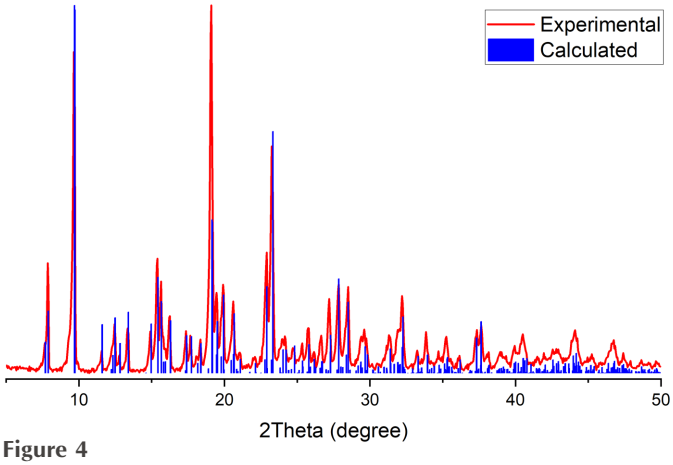


Figure 4
Experimental powder X-ray diffraction pattern (red) and calculated Bragg reflection positions (blue) of $[Zn_2(HL)_4(H_2O)_2](SiF_6)_2{\cdot}4.8H_2O$.

with CSD refcodes ASAYEB (Zhang *et al.*, 2021), JEYBOF (Klingele *et al.*, 2007), KEFGUY (Klingele *et al.*, 2006), MIKKEZ (Wang *et al.*, 2018*b*) and UZIDUD (Gusev *et al.*, 2011). In each of these compounds, two pyridyl–triazole ligands bridge two Zn^{II} centres to form dinuclear complexes. The title compound $[Zn_2(HL)_4(H_2O)_2](SiF_6)_2{\cdot}4.8H_2O$ is distinguished by the simultaneous presence of two μ_2-bridging ligands with two terminal *N*,*N*′-chelating ligands within the same molecule. The coordination modes of the pyridyl–triazole ligands vary among the related structures. In JEYBOF, KEFGUY and UZIDUD, each Zn^{II} centre is coordinated by two N atoms from each of two ligands, giving a symmetric *N*, *N*′-chelating environment. In contrast, ASAYEB and MIKKEZ exhibit an unsymmetrical coordination mode, in which one ligand coordinates through a single N atom, whereas the second ligand binds through two N atoms. The title compound differs from both coordination patterns, since each Zn^{II} centre is coordinated by five N atoms originating from three ligands. The compounds represented by ASAYEB, MIKKEZ and UZIDUD contain neutral coordination entities, whereas JEYBOF and KEFGUY comprise tetracationic complex cations, with perchlorate and tetrafluoridoborate

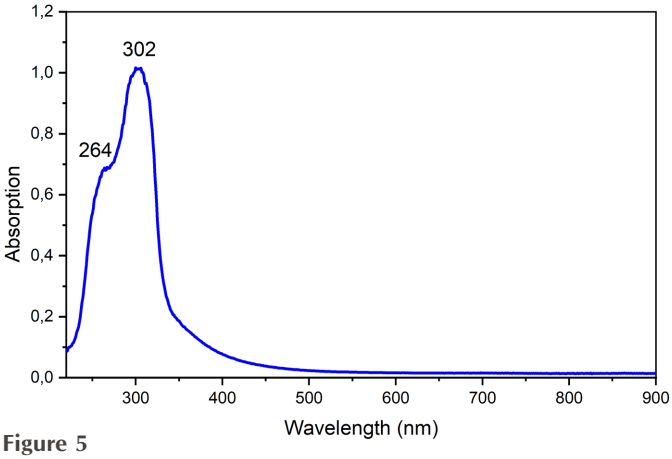


Figure 5
The solid-state UV–Vis absorption spectrum of $[Zn_2(HL)_4(H_2O)_2](SiF_6)_2{\cdot}4.8H_2O$ at room temperature.

Table 4
Experimental details.

Crystal data	
Chemical formula	$[Zn_2(C_8H_9N_5)_4(H_2O)_2](SF_6)_2{\cdot}4.8H_2O$
M_r	1238.23
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	300
a, b, c (Å)	9.1980 (2), 11.6301 (3), 11.7906 (3)
α, β, γ (°)	76.611 (2), 87.293 (2), 81.214 (2)
V (Å^3)	1212.51 (5)
Z	1
Radiation type	Cu $K\alpha$
μ (mm^{-1})	2.72
Crystal size (mm)	0.15 × 0.1 × 0.1
Data collection	
Diffractometer	Rigaku XtaLAB Synergy Dualflex diffractometer with a HyPix detector
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2024)
T_{min}, T_{max}	0.766, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14372, 4796, 4499
R_{int}	0.025
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.631
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.037, 0.108, 1.04
No. of reflections	4796
No. of parameters	380
No. of restraints	22
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.89, −0.35

Computer programs: *CrysAlis PRO* (Rigaku OD, 2024), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

counter-anions, respectively. In ASAYEB, the octahedral coordination sphere is completed by one coordinated water molecule, one coordinated methanol molecule and a donor O atom of the ligand substituent; one additional methanol molecule is present as a solvent molecule. In JEYBOF, each Zn^{II} centre is coordinated by two water molecules, whereas in KEFGUY, the remaining coordination sites are occupied by one water and one acetonitrile molecule. In MIKKEZ, the octahedral coordination sphere is completed by two coordinated water molecules and one nicotinate ligand. In contrast to the rest of the mentioned compounds, UZIDUD contains a five-coordinate Zn^{II} centre, in which the coordination sphere is completed by a donor atom of the ligand substituent, while one ethanol molecule is present as a solvent molecule. The title compound differs from all these analogues in that each Zn^{II} centre is coordinated by only one water molecule, with the remaining coordination sites occupied exclusively by neutral pyridyl–triazole ligands.

5. Synthesis and crystallization

[3-(Pyridin-2-yl)-1*H*-1,2,4-triazol-5-yl]methanamine (H*L*) was obtained according to the procedure described by Vashchenko *et al.* (2025).

A solution of 563 mg (0.78 mmol) of zinc hexafluorosilicate in 4 ml of water was added to a solution of 311 mg (1.78 mmol) of [3-(pyridin-2-yl)-1*H*-1,2,4-triazol-5-yl]methanamine in 4 ml of water. X-ray-quality colourless crystals of $[Zn_2(HL)_4(H_2O)_2](SiF_6)_2{\cdot}4.8H_2O$ were obtained by slow crystallization from the reaction mixture over one week (yield: 365 mg, 40.3%). IR data (in KBr, cm^{-1}): 3445, 3119, 2603, 1992, 1605, 1531, 1475, 1435, 1408, 1373, 1333, 1279, 1130, 1055, 1014, 960, 892, 749, 627, 532.

The phase purity of $[Zn_2(HL)_4(H_2O)_2](SiF_6)_2{\cdot}4.8H_2O$ was confirmed by comparing the observed and calculated powder X-ray diffraction patterns (Fig. 4). The PXRD pattern was acquired on a Shimadzu XRD-6000 diffractometer using Cu $K\alpha$ radiation over the 5–50° 2θ range with a step size of 0.05°.

The UV–Vis absorption spectrum of $[Zn_2(HL)_4(H_2O)_2](SiF_6)_2{\cdot}4.8H_2O$ was measured in diffuse reflectance mode using a Shimadzu UV-2600i spectrophotometer and a powdered microcrystalline sample at ambient temperature (Fig. 5). The absorption bands at 265 and 302 nm are attributed to intraligand π–π^* transitions.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4.

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References

Cao, Y., Zhang, Y., Gu, L., Qin, X., Li, H.-Y., Bian, H.-D. & Huang, F.-P. (2020). *New J. Chem.* **44**, 10681–10688.

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.

Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.

Gusev, A. N., Shul'gin, V. F., Konnic, O. V., Meshkova, S. B., Aleksandrov, G. G., Kiskin, M. A., Eremenko, I. L. & Linert, W. (2011). *Inorg. Chim. Acta* **376**, 509–514.

Klingele, M. H., Boyd, P. D. W., Moubaraki, B., Murray, K. S. & Brooker, S. (2006). *Eur. J. Inorg. Chem.* **2006**, 573–589.

Klingele, M. H., Noble, A., Boyd, P. D. W. & Brooker, S. (2007). *Polyhedron* **26**, 479–485.

Llunell, M., Casanova, D., Cirera, J., Alemany, P. & Alvarez, S. (2013). *SHAPE*. Barcelona, Spain.

Pang, X., Shu, C., Li, H., Bian, H., Liu, H. & Huang, F.-P. (2017). *Transition Met. Chem.* **42**, 533–542.

Petrenko, Y. P., Khomenko, D. M., Doroshchuk, R. O., Raspertova, I. V., Shova, S. & Lampeka, R. D. (2023). *Acta Cryst.* E**79**, 432–435.

Petrenko, Y. P., Khomenko, D. M., Doroshchuk, R. O., Shova, S., Novitchi, G., Piasta, K., Gumienna-Kontecka, E. & Lampeka, R. D. (2020). *Inorg. Chim. Acta* **500**, 119216.

Petrenko, Y. P., Khomenko, D. M., Doroshchuk, R. O., Vassilyeva, O. Y., Shova, S., Novitchi, G. & Lampeka, R. D. (2026). *Inorg. Chim. Acta* **602**, 123302.

Rigaku OD (2024). *CrysAlis PRO*. Rigaku Oxford Diffraction Ltd, Yarnton, Oxfordshire, England.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

Spackman, P. R., Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Jayatilaka, D. & Spackman, M. A. (2021). *J. Appl. Cryst.* **54**, 1006–1011.

Su, Q., Jiang, L., Li, Q., Zhang, J., Qin, L.-Q., Tan, M., Liang, H. & Qin, Q.-P. (2025). *Bioorg. Chem.* **166**, 109163.

Vashchenko, O. V., Ivanova, H. V., Bondarchuk, T. V., Doroshchuk, R. O., Raspertova, I. V., Rozhenko, A. B., Volochnyuk, D. M., Ryabukhin, S. V., Lampeka, R. D. & Khomenko, D. M. (2025). *Eur. J. Org. Chem.* **28**, e202500646.

Wang, X. R., Wang, X. Z., Li, Y., Du, J., Liu, S. X., Luo, Y., Huo, J. Z., Liu, Y. Y., Wu, X. X. & Ding, B. (2018*a*). *Z. Anorg. Allg. Chem.* **644**, 357–366.

Wang, Y.-F., Wang, L.-P., Wang, S.-P., Li, Y.-L. & Zhou, X.-L. (2018*b*). *Z. Anorg. Allg. Chem.* **644**, 1164–1171.

Zhang, X., Xing, N., Bai, F., Wan, L., Shan, H., Hou, Y., Xing, Y. & Shi, Z. (2013). *CrystEngComm* **15**, 9135–9147.

Zhang, Y., Li, Y.-H., Jiang, S.-B., Wang, S.-L., Qian, S.-S., Qin, J., Ma, J.-P. & Li, J. (2021). *J. Coord. Chem.* **74**, 1522–1533.

supporting information

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Synthesis, crystal structure and Hirshfeld surface analysis of a dinuclear zinc(II) complex with 1-[3-(pyridin-2-yl)-1*H*-1,2,4-triazol-5-yl]methanamine

Tetyana V. Bondarchuk, Mariia B. Struhatska, Dmytro M. Khomenko, Alexandra Bargan and Oleksandr V. Vaschenko

Computing details

Bis[*μ*-5-(azaniumylmethyl)-3-(pyridin-2-yl)-1*H*-1,2,4-triazol-1-ido]bis{aqua[5-(azaniumylmethyl)-3-(pyridin-2-yl)-1*H*-1,2,4-triazol-1-ido]zinc(II)} bis(hexafluoridosilicate) 4.8-hydrate

Crystal data

$[Zn_2(C_8H_9N_5)_4(H_2O)_2](SF_6)_2\cdot 4.8H_2O$
M_r = 1238.23
Triclinic, $P\overline{1}$
a = 9.1980 (2) Å
b = 11.6301 (3) Å
c = 11.7906 (3) Å
α = 76.611 (2)°
β = 87.293 (2)°
γ = 81.214 (2)°
V = 1212.51 (5) Å^3
Z = 1
$F(000)$ = 632
D_x = 1.696 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 10928 reflections
θ = 3.8–76.4°
μ = 2.72 mm^{-1}
T = 300 K
Prism, clear dark colourless
0.15 × 0.1 × 0.1 mm

Data collection

Rigaku XtaLAB Synergy Dualflex diffractometer with a HyPix detector
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2024)
T_{min} = 0.766, T_{max} = 1.000
14372 measured reflections
4796 independent reflections
4499 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 76.8°, θ_{min} = 4.0°
h = −11→11
k = −14→14
l = −14→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.108
S = 1.04
4796 reflections
380 parameters
22 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0659P)^2 + 0.7516P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.89 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}
Extinction correction: SHELXL2018 (Sheldrick, 2015*b*), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0016 (3)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Zn1	0.43245 (3)	0.34258 (2)	0.60085 (2)	0.02794 (12)	
Si1	1.000000	0.000000	1.000000	0.0352 (2)	
Si2	0.500000	0.500000	1.000000	0.0331 (2)	
F1	0.8962 (3)	0.09294 (18)	1.07193 (18)	0.0835 (7)	
F2	1.06214 (18)	0.11756 (14)	0.91383 (15)	0.0550 (4)	
F3	0.8593 (2)	0.01640 (18)	0.90929 (19)	0.0786 (7)	
F4	0.4744 (2)	0.37224 (15)	0.96651 (18)	0.0655 (5)	
F5	0.66812 (19)	0.43637 (17)	1.04985 (14)	0.0585 (4)	
F6	0.5731 (2)	0.54124 (17)	0.86720 (13)	0.0625 (5)	
O1W	0.3356 (2)	0.4088 (2)	0.74794 (18)	0.0549 (5)	
H1WA	0.250 (2)	0.423 (4)	0.764 (3)	0.082*	
H1WB	0.386 (3)	0.424 (4)	0.799 (3)	0.082*	
O2W	0.9029 (4)	−0.1582 (3)	0.7425 (3)	0.0740 (9)	0.75
H2WA	0.817037	−0.120957	0.725428	0.111*	0.75
H2WB	0.939170	−0.116960	0.781807	0.111*	0.75
O3W	1.0698 (3)	0.4300 (3)	0.8662 (3)	0.0665 (8)	0.75
H3WA	1.006901	0.489560	0.871103	0.100*	0.75
H3WB	1.103302	0.391757	0.930970	0.100*	0.75
O4W	0.8400 (4)	0.6366 (3)	0.8893 (3)	0.0730 (9)	0.75
H4WA	0.866261	0.703594	0.849679	0.110*	0.75
H4WB	0.764578	0.603369	0.880398	0.110*	0.75
O5W	0.7325 (15)	0.7334 (11)	0.7586 (16)	0.067 (4)	0.15
H5WA	0.674743	0.678709	0.779794	0.100*	0.15
H5WB	0.696632	0.808055	0.733663	0.100*	0.15
N1	0.5535 (2)	0.24347 (16)	0.47317 (15)	0.0294 (4)	
N2	0.4946 (2)	0.16270 (15)	0.69984 (15)	0.0296 (4)	
N3	0.4706 (2)	0.09658 (17)	0.80929 (15)	0.0335 (4)	
N4	0.6042 (2)	−0.02445 (17)	0.70680 (16)	0.0363 (4)	
N5	0.6631 (2)	−0.15231 (18)	0.98282 (17)	0.0378 (4)	
H5A	0.730 (3)	−0.105 (2)	0.966 (3)	0.045*	
H5B	0.708 (3)	−0.2229 (15)	0.978 (3)	0.045*	
H5C	0.647 (3)	−0.152 (3)	1.0565 (13)	0.045*	
N6	0.78621 (19)	0.70081 (16)	0.42228 (16)	0.0296 (4)	
N7	0.65809 (19)	0.51555 (15)	0.54254 (15)	0.0273 (4)	
N8	0.61912 (19)	0.41805 (15)	0.62223 (15)	0.0272 (3)	
N9	0.8292 (2)	0.45952 (16)	0.68110 (16)	0.0317 (4)	
N10	0.8147 (2)	0.30411 (19)	0.89896 (17)	0.0375 (4)	
H10A	0.896 (2)	0.331 (3)	0.871 (2)	0.045*	
H10B	0.833 (3)	0.2380 (17)	0.953 (2)	0.045*	

H10C	0.766 (3)	0.355 (2)	0.937 (2)	0.045*
C1	0.5859 (3)	0.2895 (2)	0.36169 (19)	0.0360 (5)
H1	0.547328	0.368366	0.328967	0.043*
C2	0.6741 (3)	0.2252 (2)	0.2931 (2)	0.0408 (5)
H2	0.696107	0.260732	0.216436	0.049*
C3	0.7292 (3)	0.1073 (2)	0.3402 (2)	0.0416 (5)
H3	0.787378	0.061843	0.295155	0.050*
C4	0.6966 (3)	0.0578 (2)	0.4550 (2)	0.0367 (5)
H4	0.731835	−0.021546	0.488648	0.044*
C5	0.6099 (2)	0.12924 (18)	0.51910 (18)	0.0282 (4)
C6	0.5724 (2)	0.08791 (18)	0.64243 (17)	0.0282 (4)
C7	0.5369 (3)	−0.0132 (2)	0.80884 (19)	0.0341 (5)
C8	0.5283 (3)	−0.1170 (2)	0.9097 (2)	0.0436 (6)
H8A	0.444766	−0.097330	0.958573	0.052*
H8B	0.510832	−0.184903	0.880290	0.052*
C9	0.8498 (3)	0.7896 (2)	0.3555 (2)	0.0358 (5)
H9	0.803146	0.834104	0.287671	0.043*
C10	0.9822 (3)	0.8177 (2)	0.3838 (2)	0.0424 (5)
H10	1.023030	0.880781	0.336630	0.051*
C11	1.0525 (3)	0.7503 (3)	0.4832 (3)	0.0468 (6)
H11	1.141183	0.767960	0.504388	0.056*
C12	0.9900 (3)	0.6562 (2)	0.5513 (2)	0.0407 (5)
H12	1.036538	0.608811	0.618016	0.049*
C13	0.8571 (2)	0.63434 (18)	0.51770 (18)	0.0289 (4)
C14	0.7822 (2)	0.53614 (18)	0.58198 (18)	0.0284 (4)
C15	0.7247 (2)	0.38854 (18)	0.70160 (18)	0.0283 (4)
C16	0.7297 (3)	0.2839 (2)	0.80353 (19)	0.0339 (5)
H16A	0.630416	0.272948	0.830655	0.041*
H16B	0.775424	0.211974	0.780083	0.041*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02818 (17)	0.02679 (17)	0.02729 (17)	−0.00577 (11)	−0.00294 (11)	−0.00133 (11)
Si1	0.0342 (4)	0.0307 (4)	0.0344 (4)	−0.0030 (3)	−0.0019 (3)	0.0048 (3)
Si2	0.0445 (5)	0.0284 (4)	0.0242 (4)	0.0000 (3)	−0.0027 (3)	−0.0045 (3)
F1	0.1137 (17)	0.0529 (11)	0.0654 (12)	0.0152 (11)	0.0309 (12)	−0.0001 (9)
F2	0.0491 (9)	0.0454 (8)	0.0579 (9)	−0.0101 (7)	0.0005 (7)	0.0157 (7)
F3	0.0779 (13)	0.0676 (12)	0.0792 (13)	−0.0308 (10)	−0.0412 (11)	0.0269 (10)
F4	0.0863 (13)	0.0427 (9)	0.0744 (12)	−0.0148 (9)	0.0031 (10)	−0.0245 (8)
F5	0.0530 (9)	0.0693 (11)	0.0474 (9)	0.0114 (8)	−0.0125 (7)	−0.0123 (8)
F6	0.0738 (11)	0.0711 (11)	0.0312 (8)	0.0001 (9)	0.0088 (7)	0.0027 (7)
O1W	0.0412 (10)	0.0880 (15)	0.0482 (11)	−0.0144 (10)	0.0057 (8)	−0.0391 (11)
O2W	0.0652 (19)	0.072 (2)	0.084 (2)	0.0042 (16)	0.0050 (16)	−0.0252 (17)
O3W	0.0256 (11)	0.0735 (19)	0.099 (2)	−0.0069 (12)	0.0062 (13)	−0.0181 (17)
O4W	0.076 (2)	0.068 (2)	0.079 (2)	−0.0271 (16)	−0.0060 (17)	−0.0148 (17)
O5W	0.046 (7)	0.028 (6)	0.127 (14)	−0.004 (5)	−0.001 (8)	−0.019 (7)
N1	0.0339 (9)	0.0270 (8)	0.0254 (8)	−0.0045 (7)	−0.0015 (7)	−0.0018 (7)

N2	0.0331 (9)	0.0289 (9)	0.0244 (8)	−0.0063 (7)	−0.0002 (7)	0.0001 (7)
N3	0.0349 (9)	0.0389 (10)	0.0243 (8)	−0.0098 (8)	0.0002 (7)	0.0002 (7)
N4	0.0468 (11)	0.0283 (9)	0.0299 (9)	−0.0048 (8)	−0.0029 (8)	0.0011 (7)
N5	0.0459 (11)	0.0330 (10)	0.0308 (9)	−0.0045 (8)	−0.0020 (8)	0.0002 (8)
N6	0.0284 (8)	0.0287 (9)	0.0309 (9)	−0.0064 (7)	−0.0018 (7)	−0.0034 (7)
N7	0.0281 (8)	0.0248 (8)	0.0273 (8)	−0.0054 (6)	−0.0033 (7)	−0.0005 (6)
N8	0.0282 (8)	0.0244 (8)	0.0273 (8)	−0.0042 (6)	−0.0018 (6)	−0.0016 (6)
N9	0.0305 (9)	0.0320 (9)	0.0302 (9)	−0.0047 (7)	−0.0060 (7)	−0.0011 (7)
N10	0.0388 (10)	0.0379 (10)	0.0316 (10)	0.0014 (8)	−0.0082 (8)	−0.0028 (8)
C1	0.0440 (12)	0.0318 (11)	0.0281 (10)	−0.0055 (9)	−0.0027 (9)	0.0015 (8)
C2	0.0499 (14)	0.0449 (13)	0.0258 (10)	−0.0103 (11)	0.0028 (9)	−0.0031 (9)
C3	0.0488 (14)	0.0407 (12)	0.0355 (12)	−0.0054 (10)	0.0067 (10)	−0.0112 (10)
C4	0.0440 (12)	0.0292 (10)	0.0349 (11)	−0.0026 (9)	0.0010 (9)	−0.0056 (9)
C5	0.0306 (10)	0.0263 (10)	0.0278 (10)	−0.0076 (8)	−0.0025 (8)	−0.0037 (8)
C6	0.0311 (10)	0.0256 (9)	0.0265 (10)	−0.0060 (8)	−0.0028 (8)	−0.0018 (8)
C7	0.0395 (12)	0.0330 (11)	0.0275 (10)	−0.0121 (9)	−0.0043 (8)	0.0028 (8)
C8	0.0520 (14)	0.0420 (13)	0.0331 (12)	−0.0190 (11)	−0.0073 (10)	0.0083 (10)
C9	0.0355 (11)	0.0307 (11)	0.0387 (12)	−0.0070 (9)	0.0033 (9)	−0.0019 (9)
C10	0.0362 (12)	0.0336 (12)	0.0564 (15)	−0.0124 (9)	0.0095 (11)	−0.0057 (10)
C11	0.0351 (12)	0.0513 (15)	0.0573 (15)	−0.0190 (11)	−0.0024 (11)	−0.0104 (12)
C12	0.0341 (11)	0.0473 (13)	0.0414 (12)	−0.0123 (10)	−0.0078 (9)	−0.0059 (10)
C13	0.0281 (10)	0.0289 (10)	0.0302 (10)	−0.0059 (8)	0.0004 (8)	−0.0068 (8)
C14	0.0272 (10)	0.0281 (10)	0.0290 (10)	−0.0035 (8)	−0.0034 (8)	−0.0044 (8)
C15	0.0282 (10)	0.0277 (10)	0.0274 (10)	−0.0022 (8)	−0.0024 (8)	−0.0040 (8)
C16	0.0390 (11)	0.0315 (11)	0.0285 (10)	−0.0044 (9)	−0.0062 (9)	−0.0007 (8)

Geometric parameters (Å, º)

Zn1—O1W	2.1581 (18)	N5—H5C	0.874 (13)
Zn1—N1	2.2556 (18)	N5—C8	1.493 (3)
Zn1—N2	2.1523 (17)	N6—C9	1.339 (3)
Zn1—N6^{i}	2.1907 (18)	N6—C13	1.342 (3)
Zn1—N7^{i}	2.1669 (17)	N7—N8	1.377 (2)
Zn1—N8	2.0943 (17)	N7—C14	1.327 (3)
Si1—F1^{ii}	1.6827 (19)	N8—C15	1.331 (3)
Si1—F1	1.6827 (19)	N9—C14	1.340 (3)
Si1—F2	1.6640 (14)	N9—C15	1.339 (3)
Si1—F2^{ii}	1.6640 (14)	N10—H10A	0.874 (13)
Si1—F3^{ii}	1.6781 (18)	N10—H10B	0.876 (13)
Si1—F3	1.6781 (18)	N10—H10C	0.881 (13)
Si2—F4	1.6754 (16)	N10—C16	1.482 (3)
Si2—F4^{iii}	1.6754 (16)	C1—H1	0.9300
Si2—F5^{iii}	1.6790 (16)	C1—C2	1.380 (3)
Si2—F5	1.6790 (16)	C2—H2	0.9300
Si2—F6	1.6690 (15)	C2—C3	1.381 (4)
Si2—F6^{iii}	1.6690 (15)	C3—H3	0.9300
O1W—H1WA	0.805 (17)	C3—C4	1.381 (3)
O1W—H1WB	0.845 (18)	C4—H4	0.9300

O2W—H2WA	0.8500	C4—C5	1.389 (3)
O2W—H2WB	0.8500	C5—C6	1.464 (3)
O3W—H3WA	0.8430	C7—C8	1.494 (3)
O3W—H3WB	0.8357	C8—H8A	0.9700
O4W—H4WA	0.8728	C8—H8B	0.9700
O4W—H4WB	0.8653	C9—H9	0.9300
O5W—H5WA	0.8752	C9—C10	1.382 (4)
O5W—H5WB	0.8678	C10—H10	0.9300
N1—C1	1.338 (3)	C10—C11	1.377 (4)
N1—C5	1.345 (3)	C11—H11	0.9300
N2—N3	1.368 (2)	C11—C12	1.383 (4)
N2—C6	1.328 (3)	C12—H12	0.9300
N3—C7	1.329 (3)	C12—C13	1.380 (3)
N4—C6	1.347 (3)	C13—C14	1.464 (3)
N4—C7	1.351 (3)	C15—C16	1.496 (3)
N5—H5A	0.874 (13)	C16—H16A	0.9700
N5—H5B	0.873 (13)	C16—H16B	0.9700

O1W—Zn1—N1	169.06 (8)	C13—N6—Zn1^{i}	114.91 (13)
O1W—Zn1—N6^{i}	85.67 (7)	N8—N7—Zn1^{i}	140.81 (13)
O1W—Zn1—N7^{i}	100.82 (8)	C14—N7—Zn1^{i}	112.70 (13)
N2—Zn1—O1W	94.68 (8)	C14—N7—N8	105.28 (16)
N2—Zn1—N1	74.80 (6)	N7—N8—Zn1	121.87 (13)
N2—Zn1—N6^{i}	89.24 (7)	C15—N8—Zn1	132.96 (14)
N2—Zn1—N7^{i}	157.79 (7)	C15—N8—N7	105.11 (16)
N6^{i}—Zn1—N1	97.00 (7)	C15—N9—C14	101.48 (17)
N7^{i}—Zn1—N1	90.12 (6)	H10A—N10—H10B	111 (3)
N7^{i}—Zn1—N6^{i}	76.29 (6)	H10A—N10—H10C	108 (3)
N8—Zn1—O1W	87.53 (7)	H10B—N10—H10C	103 (3)
N8—Zn1—N1	91.39 (7)	C16—N10—H10A	110 (2)
N8—Zn1—N2	100.42 (7)	C16—N10—H10B	110 (2)
N8—Zn1—N6^{i}	168.62 (7)	C16—N10—H10C	114 (2)
N8—Zn1—N7^{i}	96.08 (6)	N1—C1—H1	118.6
F1^{ii}—Si1—F1	180.00 (12)	N1—C1—C2	122.9 (2)
F2^{ii}—Si1—F1^{ii}	89.00 (9)	C2—C1—H1	118.6
F2—Si1—F1	89.00 (9)	C1—C2—H2	120.5
F2—Si1—F1^{ii}	91.00 (9)	C1—C2—C3	119.0 (2)
F2^{ii}—Si1—F1	91.00 (9)	C3—C2—H2	120.5
F2^{ii}—Si1—F2	180.0	C2—C3—H3	120.4
F2^{ii}—Si1—F3^{ii}	89.92 (8)	C2—C3—C4	119.1 (2)
F2^{ii}—Si1—F3	90.08 (8)	C4—C3—H3	120.4
F2—Si1—F3	89.92 (8)	C3—C4—H4	120.8
F2—Si1—F3^{ii}	90.08 (8)	C3—C4—C5	118.4 (2)
F3^{ii}—Si1—F1	91.20 (13)	C5—C4—H4	120.8
F3—Si1—F1^{ii}	91.20 (13)	N1—C5—C4	122.77 (19)
F3—Si1—F1	88.80 (13)	N1—C5—C6	113.90 (18)
F3^{ii}—Si1—F1^{ii}	88.80 (13)	C4—C5—C6	123.34 (19)
F3^{ii}—Si1—F3	180.00 (9)	N2—C6—N4	113.69 (18)

F4^{iii}—Si2—F4	180.0	N2—C6—C5	120.16 (18)
F4—Si2—F5	89.83 (10)	N4—C6—C5	126.08 (19)
F4^{iii}—Si2—F5	90.17 (10)	N3—C7—N4	114.32 (18)
F4—Si2—F5^{iii}	90.17 (10)	N3—C7—C8	122.7 (2)
F4^{iii}—Si2—F5^{iii}	89.83 (10)	N4—C7—C8	122.8 (2)
F5^{iii}—Si2—F5	180.0	N5—C8—C7	114.1 (2)
F6—Si2—F4	88.43 (10)	N5—C8—H8A	108.7
F6—Si2—F4^{iii}	91.57 (10)	N5—C8—H8B	108.7
F6^{iii}—Si2—F4^{iii}	88.43 (10)	C7—C8—H8A	108.7
F6^{iii}—Si2—F4	91.57 (10)	C7—C8—H8B	108.7
F6—Si2—F5	89.18 (9)	H8A—C8—H8B	107.6
F6—Si2—F5^{iii}	90.82 (9)	N6—C9—H9	118.8
F6^{iii}—Si2—F5	90.82 (9)	N6—C9—C10	122.4 (2)
F6^{iii}—Si2—F5^{iii}	89.18 (9)	C10—C9—H9	118.8
F6—Si2—F6^{iii}	180.0	C9—C10—H10	120.6
Zn1—O1W—H1WA	128 (2)	C11—C10—C9	118.7 (2)
Zn1—O1W—H1WB	123 (2)	C11—C10—H10	120.6
H1WA—O1W—H1WB	109 (3)	C10—C11—H11	120.3
H2WA—O2W—H2WB	104.5	C10—C11—C12	119.5 (2)
H3WA—O3W—H3WB	112.9	C12—C11—H11	120.3
H4WA—O4W—H4WB	129.4	C11—C12—H12	120.8
H5WA—O5W—H5WB	121.0	C13—C12—C11	118.4 (2)
C1—N1—Zn1	126.75 (15)	C13—C12—H12	120.8
C1—N1—C5	117.82 (19)	N6—C13—C12	122.7 (2)
C5—N1—Zn1	115.09 (13)	N6—C13—C14	114.27 (18)
N3—N2—Zn1	137.82 (14)	C12—C13—C14	123.1 (2)
C6—N2—Zn1	115.90 (13)	N7—C14—N9	114.09 (18)
C6—N2—N3	106.18 (17)	N7—C14—C13	120.53 (18)
C7—N3—N2	104.91 (17)	N9—C14—C13	125.37 (19)
C6—N4—C7	100.88 (18)	N8—C15—N9	114.03 (18)
H5A—N5—H5B	106 (3)	N8—C15—C16	123.58 (19)
H5A—N5—H5C	100 (3)	N9—C15—C16	122.38 (19)
H5B—N5—H5C	108 (3)	N10—C16—C15	109.84 (18)
C8—N5—H5A	116 (2)	N10—C16—H16A	109.7
C8—N5—H5B	112 (2)	N10—C16—H16B	109.7
C8—N5—H5C	114 (2)	C15—C16—H16A	109.7
C9—N6—Zn1^{i}	126.66 (15)	C15—C16—H16B	109.7
C9—N6—C13	118.31 (19)	H16A—C16—H16B	108.2

Zn1—N1—C1—C2	172.83 (18)	N8—C15—C16—N10	−155.2 (2)
Zn1—N1—C5—C4	−175.27 (17)	N9—C15—C16—N10	26.4 (3)
Zn1—N1—C5—C6	4.3 (2)	C1—N1—C5—C4	−1.5 (3)
Zn1—N2—N3—C7	176.15 (17)	C1—N1—C5—C6	178.13 (19)
Zn1—N2—C6—N4	−177.76 (15)	C1—C2—C3—C4	−1.1 (4)
Zn1—N2—C6—C5	−0.4 (2)	C2—C3—C4—C5	−0.4 (4)
Zn1^{i}—N6—C9—C10	173.26 (18)	C3—C4—C5—N1	1.7 (3)
Zn1^{i}—N6—C13—C12	−174.24 (18)	C3—C4—C5—C6	−177.8 (2)
Zn1^{i}—N6—C13—C14	6.5 (2)	C4—C5—C6—N2	176.9 (2)

Zn1^{i}—N7—N8—Zn1	16.3 (3)	C4—C5—C6—N4	−6.2 (3)
Zn1^{i}—N7—N8—C15	−166.12 (17)	C5—N1—C1—C2	−0.2 (3)
Zn1^{i}—N7—C14—N9	170.58 (14)	C6—N2—N3—C7	0.3 (2)
Zn1^{i}—N7—C14—C13	−10.3 (2)	C6—N4—C7—N3	−0.8 (3)
Zn1—N8—C15—N9	177.85 (14)	C6—N4—C7—C8	174.9 (2)
Zn1—N8—C15—C16	−0.7 (3)	C7—N4—C6—N2	1.0 (2)
N1—C1—C2—C3	1.5 (4)	C7—N4—C6—C5	−176.1 (2)
N1—C5—C6—N2	−2.7 (3)	C9—N6—C13—C12	2.0 (3)
N1—C5—C6—N4	174.2 (2)	C9—N6—C13—C14	−177.32 (19)
N2—N3—C7—N4	0.4 (3)	C9—C10—C11—C12	0.6 (4)
N2—N3—C7—C8	−175.4 (2)	C10—C11—C12—C13	−1.1 (4)
N3—N2—C6—N4	−0.8 (2)	C11—C12—C13—N6	−0.2 (4)
N3—N2—C6—C5	176.47 (18)	C11—C12—C13—C14	179.0 (2)
N3—C7—C8—N5	−102.4 (3)	C12—C13—C14—N7	−176.6 (2)
N4—C7—C8—N5	82.2 (3)	C12—C13—C14—N9	2.4 (3)
N6—C9—C10—C11	1.2 (4)	C13—N6—C9—C10	−2.5 (3)
N6—C13—C14—N7	2.7 (3)	C14—N7—N8—Zn1	−178.23 (13)
N6—C13—C14—N9	−178.3 (2)	C14—N7—N8—C15	−0.6 (2)
N7—N8—C15—N9	0.6 (2)	C14—N9—C15—N8	−0.3 (2)
N7—N8—C15—C16	−177.95 (19)	C14—N9—C15—C16	178.2 (2)
N8—N7—C14—N9	0.4 (2)	C15—N9—C14—N7	−0.1 (2)
N8—N7—C14—C13	179.53 (18)	C15—N9—C14—C13	−179.1 (2)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+2, −*y*, −*z*+2; (iii) −*x*+1, −*y*+1, −*z*+2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O3*W*^{iv}	0.81 (2)	2.01 (2)	2.764 (3)	157 (4)
O1*W*—H1*WB*···F4	0.85 (2)	2.09 (3)	2.844 (3)	149 (4)
O1*W*—H1*WB*···F6	0.85 (2)	2.61 (2)	3.383 (3)	153 (4)
O2*W*—H2*WA*···N4	0.85	2.10	2.941 (4)	172
O2*W*—H2*WB*···F1^{ii}	0.85	2.44	3.218 (5)	153
O2*W*—H2*WB*···F3	0.85	2.41	3.111 (4)	140
O3*W*—H3*WA*···O4*W*	0.84	2.16	3.002 (5)	177
O3*W*—H3*WB*···O4*W*^{v}	0.84	2.15	2.932 (5)	157
O4*W*—H4*WA*···O2*W*^{vi}	0.87	1.87	2.728 (5)	169
O4*W*—H4*WB*···F6	0.87	2.03	2.889 (4)	173
O5*W*—H5*WA*···F6	0.88	2.02	2.877 (14)	165
O5*W*—H5*WB*···N4^{vi}	0.87	1.96	2.821 (13)	170
N5—H5*A*···F2^{ii}	0.87 (1)	2.40 (3)	2.977 (3)	124 (2)
N5—H5*A*···F3	0.87 (1)	1.96 (1)	2.829 (3)	171 (3)
N5—H5*B*···O4*W*^{vii}	0.87 (1)	2.31 (2)	3.123 (4)	156 (3)
N5—H5*C*···N3^{viii}	0.87 (1)	2.05 (2)	2.854 (3)	153 (3)
N10—H10*A*···O3*W*	0.87 (1)	2.10 (2)	2.915 (3)	155 (3)
N10—H10*B*···F1	0.88 (1)	1.96 (1)	2.831 (3)	174 (3)
N10—H10*B*···F2	0.88 (1)	2.43 (3)	2.876 (3)	112 (2)
N10—H10*C*···F5	0.88 (1)	1.92 (2)	2.785 (3)	167 (3)

N10—H10*C*···F6	0.88 (1)	2.58 (2)	3.227 (3)	131 (2)
C1—H1···F6^{i}	0.93	2.54	3.214 (3)	130
C2—H2···F5^{ix}	0.93	2.48	3.313 (3)	150
C8—H8*B*···F4^{viii}	0.97	2.48	2.993 (3)	113
C8—H8*B*···O5*W*^{vii}	0.97	2.62	3.139 (15)	114
C9—H9···F2^{x}	0.93	2.61	3.216 (3)	123
C16—H16*A*···F4	0.97	2.47	3.165 (3)	129
C16—H16*A*···N2	0.97	2.68	3.183 (3)	113
C16—H16*B*···F3	0.97	2.46	3.140 (3)	127

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+2, −*y*, −*z*+2; (iv) *x*−1, *y*, *z*; (v) −*x*+2, −*y*+1, −*z*+2; (vi) *x*, *y*+1, *z*; (vii) *x*, *y*−1, *z*; (viii) −*x*+1, −*y*, −*z*+2; (ix) *x*, *y*, *z*−1; (x) −*x*+2, −*y*+1, −*z*+1.