Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

The crystal structure of tetrakis(5-phenyl-1*H*-imidazole-κN^3)zinc(II) dinitrate

Nomampondo Penelope Magwa*

University of South Africa, Department of Chemistry, Private Bag X6, Florida, Gauteng, 1710, South Africa. *Correspondence e-mail: magwanp@unisa.ac.za

Received 1 October 2025
Accepted 3 December 2025

Edited by S. P. Kelley, University of Missouri-Columbia, USA

Keywords: 5-phenyl-1*H*-imidazole; Zn-complex; crystal structure.

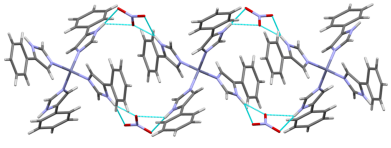
CCDC reference: 2433548

Supporting information: this article has supporting information at journals.iucr.org/e

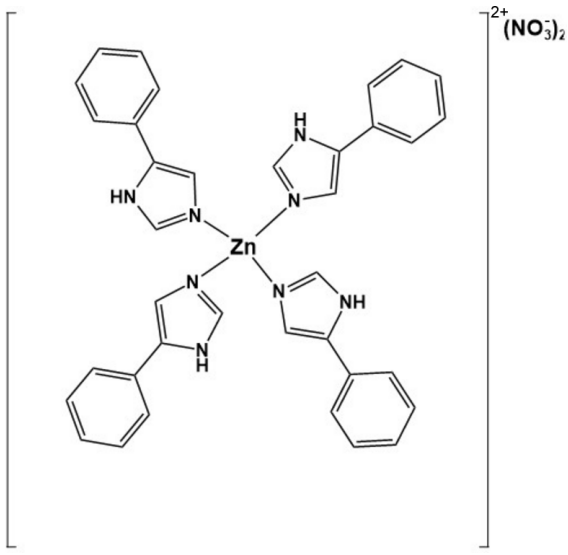
The title complex salt, $[Zn(C_9H_8N_2)_4](NO_3)_2$, features a central zinc(II) ion coordinated by four 5-phenylimidazole ligands, with two nitrate anions providing charge balance. It crystallizes in the monoclinic space group *C2/c*. In the crystal, the nitrate ions occupy the voids formed by the $[Zn(C_9H_8N_2)_4]^{2+}$ cations and function as counter-ions. The nitrate oxygen atoms participate in strong N—H···O hydrogen-bonding interactions. The crystal studied was refined as a two-component twin.

1. Chemical context

The 5-phenyl-1*H*-imidazole scaffold is an important framework in medicinal chemistry due to its versatility and biological significance. It significantly contributes to the creation of pharmacologically active molecules, particularly in the fields of HIV, anticancer, and antibacterial research (Abu Almaaty *et al.*, 2021; Rashamuse *et al.*, 2020, 2021; Roy *et al.*, 2005). The imidazole moiety is frequently included in a variety of medicinal drugs, and its pharmacokinetic and pharmacodynamic qualities are further improved by the addition of a phenyl group at the 5-position (Devi *et al.*, 2024; Blass *et al.*, 2000). 5-Phenyl-1*H*-imidazole is a structurally straightforward aromatic heterocycle composed of a five-membered imidazole ring with two non-adjacent nitrogen atoms substituted at the 5-position with a phenyl group. This basic structure has several functionalization sites, making it a promising starting point for drug discovery and synthetic modification. In addition to its biological value, imidazole derivatives, such as 5-phenyl-1*H*-imidazole, have shown great promise in coordination chemistry. These compounds readily form coordination complexes with a wide range of transition metals, including zinc, copper, ruthenium, and iron (Rashamuse *et al.*, 2023; Baranoff *et al.*, 2011; Magwa & Rashamuse, 2024; Bonomo *et al.*, 1988; Carver *et al.*, 2003; Li *et al.*, 2024). In metal complexes, the nitrogen atom in the imidazole ring works as a σ-donor ligand, typically binding through the sp^2-hybridized nitrogen atom (also known as the imine-type nitrogen at position 3 of the ring). This coordination stabilizes the metal center compared to its unligated or aqua-ligated state, and significantly affects the complex's redox potential, geometry, and chemical reactivity. These metal–imidazole complexes are important in bioinorganic chemistry because they frequently serve as models for metalloenzymes (Roy *et al.*, 2005). Enzymes such as carbonic anhydrase and cytochrome c oxidase rely on imidazole moieties for catalytic activity and electron transport, respectively (Roy *et al.*, 2005; Maneeta *et al.*, 2024). Thus, synthesized imidazole–metal complexes offer important insights into enzyme functions and are being investigated for therapeutic



uses including as imaging probes, anticancer medicines, and antibacterial compounds.



2. Structural commentary

The title compound crystallizes in the monoclinic space group *C*2/*c*, with the zinc(II) atom occupying a special position on a symmetry element. As a result, the molecule's intrinsic symmetry matches the crystallographic symmetry, so only a fraction of the molecule is present in the asymmetric unit. The zinc(II) atom is coordinated by four 5-phenyl-1*H*-imidazole ligands, forming a distorted tetrahedral geometry (Table 1, Fig. 1). This distortion is evident from the six N—Zn—N bond angles, which deviate slightly from the ideal tetrahedral angle of 109.5°. The Zn—N bond lengths are consistent, with symmetry-equivalent values averaged to 1.986 Å, confirming a relatively symmetrical coordination sphere. The nitrate anions act as counter-ions and exhibit slight distortions from an ideal trigonal planar geometry (Table 1). These deviations arise from hydrogen-bonding interactions with the imidazole ligands, which are discussed in the *Supramolecular features* section. Generally, the structural parameters and symmetry constraints define a stable, well-organized crystal structure, with the zinc center adopting a distorted tetrahedral coordination environment stabilized by both covalent and non-covalent interactions. These interactions arise from crystal packing and intermolecular forces, which slightly adjust bond angles and distances to optimize crystal stability. As a result, the coordination sphere deviates from an ideal tetrahedron, reflecting the combined influence of both strong covalent bonding and secondary non-covalent forces.

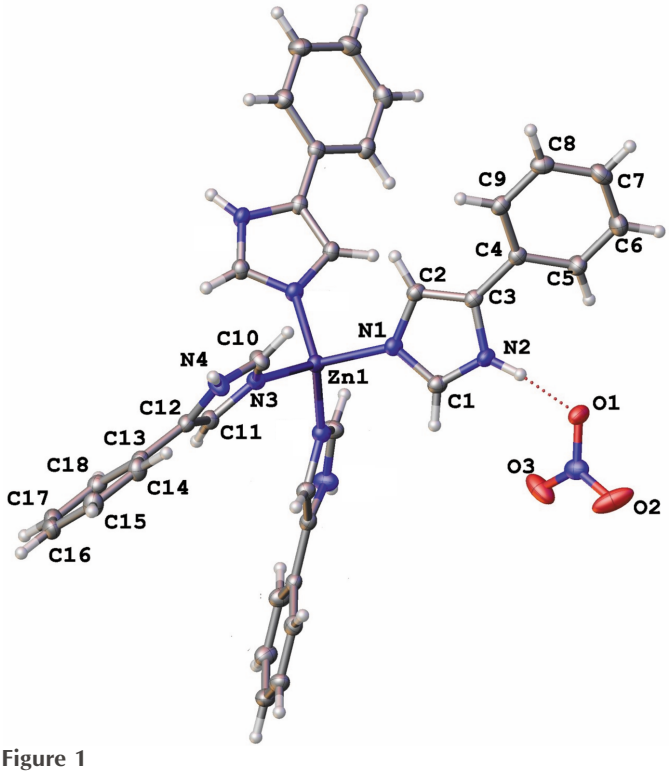


Figure 1
Displacement ellipsoid plot of the title compound showing the atom-numbering scheme and the interactions between the nitrate ion and the 5-phenyl-1*H*-imidazole ligand (dashed lines). Displacement ellipsoids are drawn at the 50% probability level. Unlabelled atoms are generated by the symmetry operation $-x+1, y, -z+\frac{1}{2}$.

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	1.9882 (11)	O2—N5	1.2295 (19)
Zn1—N3	1.9828 (11)	O3—N5	1.2585 (18)
O1—N5	1.2606 (16)		
$N1^{i}$—Zn1—N1	105.44 (6)	O2—N5—O1	119.84 (14)
N3—Zn1—$N1^{i}$	110.19 (4)	O2—N5—O3	123.65 (14)
N3—Zn1—N1	111.70 (4)	O3—N5—O1	116.51 (13)
N3—Zn1—$N3^{i}$	107.68 (7)		

Symmetry code: (i) $-x+1, y, -z+\frac{1}{2}$.

3. Supramolecular features

The molecular packing of the title compound is illustrated in Fig. 2, showing how the three-dimensional arrangement of $[Zn(C_9H_8N_2)_4]^{2+}$ cations and nitrate anions defines the crystal structure. The nitrate ions play an active role in shaping the packing by accepting strong N—H···O hydrogen bonds (Table 2) with hydrogen atoms from the imidazole moieties. Each nitrate anion accepts three hydrogen bonds from

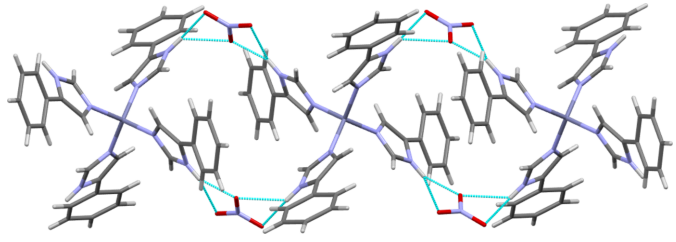


Figure 2
Packing diagram of the title compound showing the nitrate cations lying in the voids between the cationic complexes.

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O1	0.88	1.91	2.7425 (14)	156
N4—H4···O1^{ii}	0.88	2.30	2.9779 (16)	134
N4—H4···O3^{ii}	0.88	2.07	2.8326 (18)	145
C5—H5···O3^{iii}	0.95	2.46	3.3915 (19)	166
C6—H6···O2^{iv}	0.95	2.54	3.278 (2)	135

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

neighboring cations, while each cation interacts with two nitrate anions and several adjacent cations. In addition to hydrogen bonding, phenyl rings from adjacent cations exhibit notable π–π stacking and edge-to-face interactions, characterized by a parallel-displaced arrangement [centroid–centroid distance = 4.037 (2) Å, interplanar separation = 3.408 Å, slippage = 2.165 Å] and a T-shaped contact [centroid–centroid distance = 5.536 (2) Å, ring-normal angle = 69.9°, centroid-to-plane separations = 3.835 and 4.137 Å], highlighting non-covalent cation–cation contacts that contribute to the crystal cohesion. Together, these hydrogen bonds and aromatic interactions organize the crystal into a robust structure, integrating electrostatic forces, directional hydrogen bonding, and π–π stacking. to optimize the crystal stability.

4. Database survey

The title complex, represents a new addition to the family of zinc(II)–imidazole derivatives, a group known for their structural flexibility and diverse coordination behavior. Zinc(II) readily adopts various geometries, while imidazole ligands provide multiple coordination possibilities. A search of the Cambridge Structural Database (CSD, Version 5.45, March 2024 update; Groom *et al.*, 2016) and Google Scholar found no prior example of a complex with the same formulation, $[Zn(C_9H_8N_2)_4]^{2+}\cdot 2NO_3^-$, confirming its originality. Related zinc–imidazole complexes are rare but include $Zn(C_3H_4N_2)_4^{2+}$ (CCDC No. 639568; Huang *et al.*, 2007), $[Zn(dmit)_4][BF_4]_2$, and $[Zn(dmit)_4][NO_3]_2$ (CCDC Nos. 772715 and 772716; William *et al.*, 2010), helical frameworks $[Zn(bdt)]^{2+}$ (CCDC Nos. 772872 and 772873; Liu *et al.*, 2010), and $Zn(C_4H_6N_2)_4^{2+}$ (CDCC No. 861722; Reedijk *et al.*, 2012). Structural comparison with these reported systems shows that Zn—N bond lengths in tetrahedral Zn^{II} complexes generally range from 1.97–2.00 Å, consistent with the mean value of 1.986 Å in the present compound. Likewise, the observed N—Zn—N bond angles [105.44 (6)–111.70 (4)°] fall within the expected range of 104–113° reported for similar complexes in the CSD, confirming a slightly distorted tetrahedral environment. Such deviations from the ideal tetrahedral angle of 109.5° are common and have been attributed to steric effects of bulky substituents and hydrogen-bonding interactions (Huang *et al.*, 2007; William *et al.*, 2010; Reedijk *et al.*, 2012). In this complex, the distortion likely arises from the phenylimidazole ligands and nitrate-mediated hydrogen bonding, in agreement with established structural trends for imidazole-based Zn^{II} systems.

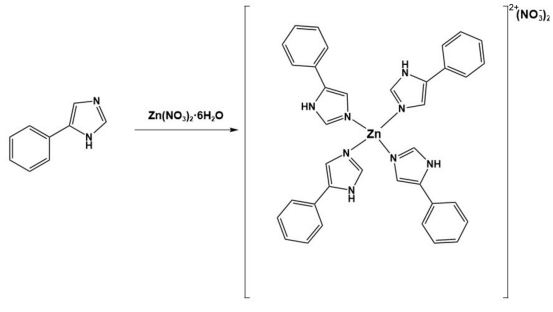
Table 3
Experimental details.

Crystal data	
Chemical formula	$[Zn(C_9H_8N_2)_4](NO_3)_2$
M_r	766.08
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	100
a, *b*, *c* (Å)	20.2757 (5), 8.5411 (2), 20.2328 (5)
β (°)	94.908 (1)
V (Å^3)	3491.00 (15)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.77
Crystal size (mm)	0.33 × 0.28 × 0.21
Data collection	
Diffractometer	Bruker D8 Venture Photon CCD area detector
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.676, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	37634, 4362, 3778
R_{int}	0.039
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.668
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.032, 0.083, 1.08
No. of reflections	4131
No. of parameters	240
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.58, −0.54

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *OLEX2.solve* (Bourhis *et al.*, 2015), *SHELXL2018/3* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

5. Synthesis and crystallization

To prepare the title compound, 0.14 g (0.485 mmol) of zinc nitrate hexahydrate were added to a stirred solution of 0.58 g (4 mmol) of 4-phenylimidazole in a solvent mixture of dichloromethane (DCM, 25 mL) and methanol (MeOH, 3 mL) in a round-bottom flask. The resulting slurry was stirred continuously for 5 h until a clear solution formed, after which the solution was filtered, and the filtrate was allowed to evaporate slowly at ambient temperatures (298–300 K). After 16 days, light-yellow crystals formed, which were collected by filtration and dried in air. The synthesis is shown in the scheme below.



6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All C-bound H were placed in

geometrically idealized positions and refined using the riding model, with isotropic displacement parameters set to 1.2 or 1.5 times those of the corresponding parent carbon atoms. The crystal studied was refined as a two-component twin, and an appropriate twin law was applied during the refinement process. A B-level PLAT910 alert indicates that low-angle reflections below θ_{min} = 3.92° were omitted. This exclusion is intentional because the reflections at such low angles were either partially obscured by the beamstop or detector gap or severely overloaded. The omission prevents systematic errors in intensity data without affecting the completeness of the dataset or the refinement stability.

Funding information

The author gratefully acknowledges the financial support provided by the College of Science, Engineering and Technology at the University of South Africa (UNISA), as well as the National Research Foundation (NRF) of South Africa through the Thuthuka funding programme (grant No. UID: 129744).

References

Abu Almaaty, A. H., Toson, E. E. M., El-Sayed, E. H., Tantawy, M. A. M., Fayad, E., Abu Ali, O. A. & Zaki, I. (2021). *Molecules* **26**, 1706.

Baranoff, E., Fantacci, S., De Angelis, F., Zhang, X., Scopelliti, R., Grätzel, M. & Nazeeruddin, Md. K. (2011). *Inorg. Chem.* **50**, 451–462.

Blass, B. E., Huang, C. T., Kawamoto, R. M., Li, M., Liu, S., Portlock, D. E., Rennells, W. M. & Simmons, M. (2000). *Bioorg. Med. Chem. Lett.* **10**, 1543–1545.

Bonomo, R. P., Riggi, F. & Di Bilio, A. J. (1988). *Inorg. Chem.* **27**, 2510–2512.

Bourhis, L. J., Dolomanov, O. V., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2015). *Acta Cryst.* A**71**, 59–75.

Bruker (2016). *APEX3* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Carver, G., Tregenna-Piggott, P. L. W., Barra, A.-L., Neels, A. & Stride, J. A. (2003). *Inorg. Chem.* **42**, 5771–5777.

Devi, M. M., Devi, K. S., Singh, O. M. & Singh, T. P. (2024). *Heterocycl. Commun.* **30**, 20220173.

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.

Huang, F., Song, W.-D. & Li, S.-D. (2007). *Acta Cryst.* E**63**, m388–m389.

Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.

Li, Z., Bhowmik, S., Sagresti, L., Brancato, G., Smith, M., Benson, D. E., Li, P. & Merz, K. M. Jr (2024). *J. Chem. Theory Comput.* **20**, 15, 6706–6716.

Liu, W.-T., Qu, Y.-C., Lin, Z.-J. & Tong, M.-L. (2010). *CrystEngComm* **12**, 3487–3489.

Magwa, N. P. & Rashamuse, T. J. (2024). *Acta Cryst.* E**80**, 1054–1058.

Rashamuse, T. J., Coyanis, E. M., Erasmus, R. & Magwa, N. P. (2023). *Int. J. Mol. Sci.* **24**, 12260.

Rashamuse, T. J., Fish, M. Q., Coyanis, E. M. & Bode, M. L. (2021). *Molecules* **26**, 6203.

Rashamuse, T. J., Njengele, Z., Coyanis, E. M., Sayed, Y., Mosebi, S. & Bode, M. L. (2020). *Eur. J. Med. Chem.* **190**, 112111.

Reedijk, J., van Albada, G. A., Limburg, B., Mutikainen, I. & Turpeinen, U. (2012). *Acta Cryst.* E**68**, m90.

Roy, K. & Leonard, T. J. (2005). *Bioorg. Med. Chem.* **13**, 2967–2973.

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

Williams, D. J., Arrowood, K. A., Bloodworth, L. M., Carmack, A. L., Gulla, D., Gray, M. W., Maasen, I., Rizvi, F., Rosenbaum, S. L., Gwaltney, K. P. & VanDerveer, D. (2010). *J. Chem. Crystallogr.* **40**, 1074–1077.

supporting information

Acta Cryst. (2026). E**82**, 99-102 [https://doi.org/10.1107/S2056989025010874]

The crystal structure of tetrakis(5-phenyl-1*H*-imidazole-κN^3)zinc(II) dinitrate

Nomampondo Penelope Magwa

Computing details

Tetrakis(5-phenyl-1*H*-imidazole-κN^3)zinc(II) dinitrate

Crystal data

$[Zn(C_9H_8N_2)_4](NO_3)_2$
M_r = 766.08
Monoclinic, *C*2/*c*
a = 20.2757 (5) Å
b = 8.5411 (2) Å
c = 20.2328 (5) Å
β = 94.908 (1)°
V = 3491.00 (15) Å^3
Z = 4
F(000) = 1584
D_x = 1.458 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 9886 reflections
θ = 3.9–28.3°
μ = 0.77 mm^{-1}
T = 100 K
Block, colourless
0.33 × 0.28 × 0.21 mm

Data collection

Bruker D8 Venture Photon CCD area detector diffractometer
Graphite monochromator
ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.676, T_{max} = 0.746
37634 measured reflections
4362 independent reflections
3778 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 28.3°, θ_{min} = 3.9°
h = −26→26
k = −11→11
l = −26→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.083
S = 1.08
4131 reflections
240 parameters
0 restraints
Primary atom site location: iterative
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0364P)^2 + 3.5607P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-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}
Zn1	0.500000	0.49768 (2)	0.250000	0.01768 (9)
N1	0.53202 (5)	0.63867 (13)	0.32410 (5)	0.0197 (2)
N2	0.59820 (5)	0.73921 (13)	0.40463 (5)	0.0200 (2)
H2	0.631233	0.748065	0.435560	0.024*
N3	0.42707 (6)	0.36069 (13)	0.27471 (5)	0.0200 (2)
N4	0.34930 (6)	0.27794 (14)	0.33445 (6)	0.0259 (3)
H4	0.319267	0.278378	0.363381	0.031*
C1	0.58505 (7)	0.61404 (16)	0.36617 (6)	0.0207 (3)
H1	0.610201	0.520057	0.368544	0.025*
C2	0.51038 (6)	0.78840 (15)	0.33734 (6)	0.0193 (2)
H2A	0.473079	0.838709	0.315000	0.023*
C3	0.55109 (6)	0.85247 (15)	0.38757 (6)	0.0180 (2)
C4	0.55155 (7)	1.00688 (14)	0.41913 (6)	0.0181 (2)
C5	0.61083 (7)	1.07279 (17)	0.44644 (7)	0.0243 (3)
H5	0.651257	1.017424	0.444524	0.029*
C6	0.61072 (8)	1.21885 (17)	0.47632 (8)	0.0295 (3)
H6	0.651080	1.262996	0.495073	0.035*
C7	0.55174 (8)	1.30109 (17)	0.47897 (8)	0.0291 (3)
H7	0.551861	1.401404	0.499269	0.035*
C8	0.49274 (7)	1.23615 (17)	0.45189 (7)	0.0255 (3)
H8	0.452460	1.292215	0.453632	0.031*
C9	0.49242 (6)	1.08976 (16)	0.42230 (6)	0.0211 (3)
H9	0.451869	1.045539	0.404097	0.025*
C10	0.38769 (7)	0.39837 (16)	0.32101 (7)	0.0243 (3)
H10	0.386876	0.497897	0.341889	0.029*
C11	0.41252 (6)	0.20659 (15)	0.25808 (6)	0.0198 (2)
H11	0.432820	0.147352	0.225633	0.024*
C12	0.36429 (6)	0.15292 (15)	0.29572 (6)	0.0190 (2)
C13	0.33328 (6)	−0.00064 (14)	0.30077 (7)	0.0186 (3)
C14	0.33421 (6)	−0.10875 (16)	0.24892 (7)	0.0218 (3)
H14	0.354879	−0.082393	0.210011	0.026*
C15	0.30492 (7)	−0.25450 (17)	0.25434 (7)	0.0252 (3)
H15	0.305487	−0.327515	0.218969	0.030*
C16	0.27481 (7)	−0.29434 (17)	0.31107 (7)	0.0262 (3)
H16	0.255042	−0.394519	0.314562	0.031*
C17	0.27360 (7)	−0.18784 (18)	0.36261 (7)	0.0276 (3)
H17	0.252828	−0.215062	0.401350	0.033*
C18	0.30266 (7)	−0.04139 (18)	0.35785 (7)	0.0242 (3)
H18	0.301760	0.031187	0.393345	0.029*
O1	0.67549 (5)	0.73031 (12)	0.52263 (5)	0.0244 (2)
O2	0.71165 (7)	0.51909 (14)	0.48003 (8)	0.0457 (4)
O3	0.74061 (6)	0.5820 (2)	0.58356 (6)	0.0526 (4)
N5	0.70964 (6)	0.60692 (15)	0.52796 (6)	0.0258 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.01953 (12)	0.01818 (12)	0.01528 (12)	0.000	0.00119 (8)	0.000
N1	0.0211 (5)	0.0212 (5)	0.0165 (5)	0.0007 (4)	0.0007 (4)	−0.0006 (4)
N2	0.0191 (5)	0.0229 (5)	0.0175 (5)	0.0024 (4)	−0.0015 (4)	−0.0007 (4)
N3	0.0213 (5)	0.0199 (5)	0.0190 (5)	0.0001 (4)	0.0016 (4)	0.0005 (4)
N4	0.0234 (6)	0.0241 (6)	0.0320 (6)	−0.0023 (4)	0.0123 (5)	−0.0067 (5)
C1	0.0220 (6)	0.0218 (6)	0.0182 (6)	0.0025 (5)	0.0013 (5)	0.0002 (5)
C2	0.0190 (6)	0.0220 (6)	0.0169 (6)	0.0023 (5)	0.0009 (4)	0.0007 (5)
C3	0.0172 (5)	0.0218 (6)	0.0153 (5)	0.0011 (5)	0.0028 (4)	0.0014 (5)
C4	0.0198 (6)	0.0205 (6)	0.0141 (5)	0.0000 (4)	0.0024 (4)	0.0016 (4)
C5	0.0200 (6)	0.0241 (7)	0.0287 (7)	−0.0002 (5)	0.0021 (5)	−0.0006 (5)
C6	0.0274 (7)	0.0246 (7)	0.0359 (8)	−0.0054 (6)	−0.0001 (6)	−0.0027 (6)
C7	0.0381 (8)	0.0195 (6)	0.0300 (7)	0.0001 (6)	0.0039 (6)	−0.0025 (5)
C8	0.0281 (7)	0.0257 (7)	0.0233 (6)	0.0072 (5)	0.0051 (5)	0.0017 (5)
C9	0.0200 (6)	0.0265 (7)	0.0169 (6)	0.0017 (5)	0.0012 (4)	0.0012 (5)
C10	0.0232 (6)	0.0202 (6)	0.0302 (7)	−0.0007 (5)	0.0062 (5)	−0.0043 (5)
C11	0.0207 (6)	0.0207 (6)	0.0181 (6)	−0.0005 (5)	0.0020 (5)	−0.0018 (5)
C12	0.0171 (5)	0.0206 (6)	0.0190 (6)	0.0014 (5)	0.0000 (4)	−0.0020 (5)
C13	0.0153 (6)	0.0199 (6)	0.0201 (6)	0.0004 (4)	−0.0004 (5)	0.0006 (5)
C14	0.0187 (6)	0.0237 (6)	0.0231 (6)	0.0024 (5)	0.0024 (5)	−0.0015 (5)
C15	0.0236 (6)	0.0226 (6)	0.0287 (7)	0.0006 (5)	−0.0009 (5)	−0.0059 (5)
C16	0.0253 (7)	0.0212 (6)	0.0311 (7)	−0.0039 (5)	−0.0038 (5)	0.0023 (6)
C17	0.0287 (7)	0.0310 (7)	0.0230 (7)	−0.0067 (6)	0.0013 (5)	0.0033 (6)
C18	0.0256 (7)	0.0267 (7)	0.0203 (6)	−0.0042 (5)	0.0022 (5)	−0.0021 (5)
O1	0.0228 (5)	0.0292 (5)	0.0207 (5)	0.0060 (4)	−0.0011 (4)	−0.0020 (4)
O2	0.0471 (8)	0.0277 (6)	0.0664 (9)	−0.0079 (5)	0.0281 (7)	−0.0178 (6)
O3	0.0389 (7)	0.0844 (11)	0.0365 (7)	0.0302 (7)	0.0154 (5)	0.0324 (7)
N5	0.0219 (5)	0.0271 (6)	0.0299 (6)	0.0007 (5)	0.0111 (5)	0.0059 (5)

Geometric parameters (Å, º)

Zn1—N1^{i}	1.9881 (11)	C7—H7	0.9500
Zn1—N1	1.9882 (11)	C7—C8	1.388 (2)
Zn1—N3^{i}	1.9829 (11)	C8—H8	0.9500
Zn1—N3	1.9828 (11)	C8—C9	1.386 (2)
N1—C1	1.3297 (17)	C9—H9	0.9500
N1—C2	1.3856 (17)	C10—H10	0.9500
N2—H2	0.8800	C11—H11	0.9500
N2—C1	1.3357 (17)	C11—C12	1.3689 (18)
N2—C3	1.3824 (16)	C12—C13	1.4618 (17)
N3—C10	1.3217 (18)	C13—C14	1.3990 (19)
N3—C11	1.3841 (17)	C13—C18	1.4012 (19)
N4—H4	0.8800	C14—H14	0.9500
N4—C10	1.3320 (18)	C14—C15	1.388 (2)
N4—C12	1.3739 (17)	C15—H15	0.9500
C1—H1	0.9500	C15—C16	1.388 (2)

C2—H2A	0.9500	C16—H16	0.9500
C2—C3	1.3675 (18)	C16—C17	1.386 (2)
C3—C4	1.4649 (18)	C17—H17	0.9500
C4—C5	1.3975 (19)	C17—C18	1.389 (2)
C4—C9	1.3985 (18)	C18—H18	0.9500
C5—H5	0.9500	O1—N5	1.2606 (16)
C5—C6	1.386 (2)	O2—N5	1.2295 (19)
C6—H6	0.9500	O3—N5	1.2585 (18)
C6—C7	1.392 (2)		

$N1^{i}$—Zn1—N1	105.44 (6)	C8—C7—H7	120.1
N3—Zn1—$N1^{i}$	110.19 (4)	C7—C8—H8	119.9
N3—Zn1—N1	111.70 (4)	C9—C8—C7	120.20 (13)
$N3^{i}$—Zn1—N1	110.18 (4)	C9—C8—H8	119.9
$N3^{i}$—Zn1—$N1^{i}$	111.70 (4)	C4—C9—H9	119.9
N3—Zn1—$N3^{i}$	107.68 (7)	C8—C9—C4	120.27 (13)
C1—N1—Zn1	125.51 (9)	C8—C9—H9	119.9
C1—N1—C2	105.92 (11)	N3—C10—N4	110.84 (12)
C2—N1—Zn1	128.06 (9)	N3—C10—H10	124.6
C1—N2—H2	125.8	N4—C10—H10	124.6
C1—N2—C3	108.39 (11)	N3—C11—H11	125.3
C3—N2—H2	125.8	C12—C11—N3	109.31 (11)
C10—N3—Zn1	122.94 (9)	C12—C11—H11	125.3
C10—N3—C11	105.94 (11)	N4—C12—C13	122.68 (12)
C11—N3—Zn1	130.38 (9)	C11—C12—N4	105.10 (11)
C10—N4—H4	125.6	C11—C12—C13	132.17 (12)
C10—N4—C12	108.79 (11)	C14—C13—C12	120.42 (12)
C12—N4—H4	125.6	C14—C13—C18	119.31 (12)
N1—C1—N2	110.88 (12)	C18—C13—C12	120.27 (12)
N1—C1—H1	124.6	C13—C14—H14	120.0
N2—C1—H1	124.6	C15—C14—C13	119.98 (12)
N1—C2—H2A	125.3	C15—C14—H14	120.0
C3—C2—N1	109.40 (11)	C14—C15—H15	119.8
C3—C2—H2A	125.3	C14—C15—C16	120.45 (13)
N2—C3—C4	122.87 (11)	C16—C15—H15	119.8
C2—C3—N2	105.41 (11)	C15—C16—H16	120.0
C2—C3—C4	131.70 (12)	C17—C16—C15	119.92 (13)
C5—C4—C3	120.55 (12)	C17—C16—H16	120.0
C5—C4—C9	119.31 (12)	C16—C17—H17	119.9
C9—C4—C3	120.14 (12)	C16—C17—C18	120.27 (13)
C4—C5—H5	119.9	C18—C17—H17	119.9
C6—C5—C4	120.10 (13)	C13—C18—H18	120.0
C6—C5—H5	119.9	C17—C18—C13	120.07 (13)
C5—C6—H6	119.9	C17—C18—H18	120.0
C5—C6—C7	120.28 (14)	O2—N5—O1	119.84 (14)
C7—C6—H6	119.9	O2—N5—O3	123.65 (14)
C6—C7—H7	120.1	O3—N5—O1	116.51 (13)
C8—C7—C6	119.83 (13)		

Zn1—N1—C1—N2	171.98 (9)	C4—C5—C6—C7	−0.4 (2)
Zn1—N1—C2—C3	−172.01 (9)	C5—C4—C9—C8	0.38 (19)
Zn1—N3—C10—N4	−171.23 (9)	C5—C6—C7—C8	0.3 (2)
Zn1—N3—C11—C12	169.66 (9)	C6—C7—C8—C9	0.1 (2)
N1—C2—C3—N2	0.22 (14)	C7—C8—C9—C4	−0.4 (2)
N1—C2—C3—C4	178.14 (12)	C9—C4—C5—C6	0.0 (2)
N2—C3—C4—C5	26.89 (19)	C10—N3—C11—C12	−0.57 (15)
N2—C3—C4—C9	−152.98 (12)	C10—N4—C12—C11	−1.02 (16)
N3—C11—C12—N4	0.97 (15)	C10—N4—C12—C13	176.80 (12)
N3—C11—C12—C13	−176.56 (13)	C11—N3—C10—N4	−0.09 (16)
N4—C12—C13—C14	160.74 (13)	C11—C12—C13—C14	−22.1 (2)
N4—C12—C13—C18	−19.7 (2)	C11—C12—C13—C18	157.50 (15)
C1—N1—C2—C3	0.08 (14)	C12—N4—C10—N3	0.71 (17)
C1—N2—C3—C2	−0.44 (14)	C12—C13—C14—C15	179.68 (12)
C1—N2—C3—C4	−178.59 (12)	C12—C13—C18—C17	−179.60 (13)
C2—N1—C1—N2	−0.37 (15)	C13—C14—C15—C16	−0.2 (2)
C2—C3—C4—C5	−150.72 (14)	C14—C13—C18—C17	0.0 (2)
C2—C3—C4—C9	29.4 (2)	C14—C15—C16—C17	0.3 (2)
C3—N2—C1—N1	0.52 (15)	C15—C16—C17—C18	−0.2 (2)
C3—C4—C5—C6	−179.86 (13)	C16—C17—C18—C13	0.1 (2)
C3—C4—C9—C8	−179.74 (12)	C18—C13—C14—C15	0.1 (2)

Symmetry code: (i) −*x*+1, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1	0.88	1.91	2.7425 (14)	156
N4—H4···O1^{ii}	0.88	2.30	2.9779 (16)	134
N4—H4···O3^{ii}	0.88	2.07	2.8326 (18)	145
C5—H5···O3^{iii}	0.95	2.46	3.3915 (19)	166
C6—H6···O2^{iv}	0.95	2.54	3.278 (2)	135

Symmetry codes: (ii) −*x*+1, −*y*+1, −*z*+1; (iii) −*x*+3/2, −*y*+3/2, −*z*+1; (iv) *x*, *y*+1, *z*.