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Crystal structure of poly[(μ_6-benzene-1,3,5-tricarboxylato)tris(1-methylpyrrolidin-2-one)nitratodizinc(II)]

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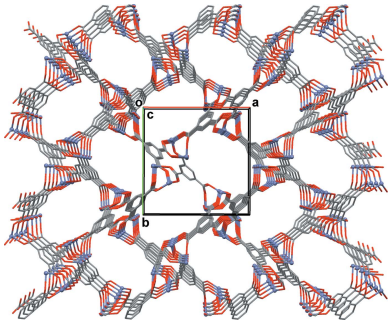
The asymmetric unit of the title compound, $[Zn_2(C_9H_3O_6)(NO_3)(C_5H_9NO)_3]_n$, **I**, consists of two different zinc(II) ions bridged by the carboxylate group of benzene-1,3,5-tricarboxylate (BTC^{3-}). The Zn1 center is tetra-coordinated by the carboxylate O atoms of three symmetrically equivalent BTC^{3-} anions and one nitrate O atom in a distorted tetrahedral geometry with $Zn-O_{carboxylate}$ bond lengths (average value 1.958 Å) slightly shorter than the $Zn-O_{nitrate}$ distance [2.013 (6) Å]. The Zn2 center is hexa-coordinated by three O atoms from the carboxylic groups of different BTC^{3-} linkers and three O atoms of 1-methylpyrrolidin-2-one (NMP) in a slightly distorted octahedral geometry with nearly equivalent Zn—O bond lengths (average values of 2.091 and 2.088 Å, respectively). Linking of the paddle-wheel dizinc building units by the three carboxylate groups of the BTC^{3-} molecule results in the formation of the three-dimensional coordination framework.

1. Chemical context

Metal–organic frameworks (MOFs), crystalline coordination polymers built up of metal-containing fragments (secondary building units, SBUs) joined by multidentate organic linkers, have been of continuous interest over the last few decades because of their potential for applications in different areas including gas storage, separation, catalysis, sensing *etc.* (Farrusseng, 2011; MacGillivray & Lukehart, 2014; Kaskel, 2016). Aromatic carboxylates are the most widely used bridging ligands (Rao *et al.*, 2004; Yoshinari & Konno, 2023) and benzene-1,3,5-tricarboxylic acid (H_3BTC), a potential 3-connected linker, is one of the most extensively studied.

Syntheses of Zn-based MOFs starting from the Zn^{II} inorganic salts and H_3BTC have been attempted many times, resulting in a large number of compounds, characterized by extreme variability of SBU types (di-, tri-, tetra- and higher nuclearity clusters) and network topologies, which reflects the flexibility of the coordination sphere inherent to the Zn^{II} ion. Among them, trigonal ('three-bladed') binuclear clusters with a paddle-wheel structure represent an important class of SBUs (Vagin *et al.*, 2007).

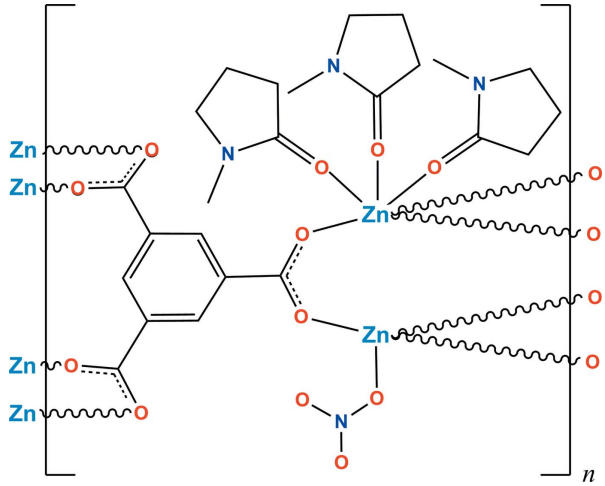
One of the first examples of MOFs with such an SBU is the complex $[Zn_2(BTC)(NO_3)(EtOH)_3]\cdot 2EtOH\cdot H_2O]_n$, called also MOF-4, which was prepared *via* room-temperature reaction in ethanol/thiethylamine. The Zn_2 units in this compound are joined with the BTC^{3-} bridges to form a porous network of **srs** topology ($P2_13$ space group) with a three-dimensional channel system filled with ethanol and water



molecules of crystallization (Yaghi *et al.*, 1997; Eddaoudi *et al.*, 2000). At the same time, solvothermal reactions of Zn^{II} salts and BTC^{3-} result in the formation of a MOF with a similar structure only in dimethylacetamide (DMA) (Hao *et al.*, 2012; Lou *et al.*, 2013; Wang *et al.*, 2021*a*), whereas the reaction in DMF, for example, leads to the Zn analogue of HKUST-1 (Feldblyum *et al.*, 2011). It seems, however, that solvent effects can be smoothed by the addition of serine as a template, resulting in a series of MOFs $[Zn_2(BTC)(NO_3)(Solv)_3]_n$ including different solvent molecules coordinated to the Zn ion (Oh *et al.*, 2013). All these compounds are usually treated as isostructural because of the identical **srs** framework topology, although the majority of them crystallize in the related orthorhombic subgroup $P2_12_12_1$.

Besides common amide solvents, several attempts have been documented that utilize *N*-methyl-2-pyrrolidone (NMP), which is widely used in industry and for nanomaterials processing (Basma *et al.*, 2018), in the MOF synthesis. Its use in Zn–BTC reactions led to different products depending on the conditions employed and some of them contain 'three-bladed' paddle-wheel SBUs (Ordonez *et al.*, 2014; Yuan *et al.*, 2019). However, compounds of the MOF-4 type {namely, $[Zn_2(BTC)(NO_3)(py)(NMP)_2]_n$} was obtained only with an NMP/pyridine mixture (Wang *et al.*, 2021*b*).

Whilst testing NMP as a possible reaction medium for the synthesis of MOFs, we have found that the reaction of zinc(II) nitrate with H_3BTC in pure NMP does not lead to the precipitation of any crystalline products, but the addition of a small amount of DMF results in the formation of the related compound poly[(μ_6-benzene-1,3,5-tricarboxylato)-tris(1-methylpyrrolidin-2-one)nitratodizinc(II)], $[Zn_2(BTC)(NO_3)(NMP)_3]_n$, **I**, whose structure is reported herein.



2. Structural commentary

The asymmetric unit of the title compound **I** is built of two zinc(II) ions bridged by the carboxylate group of the BTC^{3-} anion with an intermetallic Zn1···Zn2 distance of 3.6547 (9) Å (Fig. 1). Zn1 is additionally coordinated by the O atom of the nitrate anion, and Zn2 by the amide oxygen atoms of three NMP molecules. Two of these NMP molecules are disordered with the site occupancies of the major components being 0.620 (16) and 0.638 (16). The coordination of the carboxylate groups of two additional symmetry-related BTC^{3-} anions results in the formation of distorted tetrahedral and octahedral environments of the Zn1 and Zn2 ions, respectively.

Table 1
Selected bond lengths (Å).

Zn1—O1	1.956 (4)	Zn2—O4	2.097 (4)
Zn1—O3	1.943 (4)	Zn2—O6	2.086 (4)
Zn1—O5	1.960 (4)	Zn2—O1_1	2.100 (5)
Zn1—O10	2.013 (6)	Zn2—O1_3	2.042 (5)
Zn2—O2	2.086 (4)	Zn2—O1_4	2.094 (5)

The carboxylic groups in **I** are tilted slightly with respect to the benzene ring (the average angle between the corresponding mean planes is 6.7°) and the $C—O_{carboxylate}$ bond lengths (average value of 1.260 Å) are typical of bis-(monodentate) μ_2-COO^- groups with a high degree of delocalization. In spite of this, there is a considerable difference between the $Zn—O_{carboxylate}$ bond lengths in the tetrahedral and octahedral ions – these are shorter by *ca* 0.14 Å in the first case (average values of 1.953 and 2.090 Å, see Table 1). Interestingly, the distances from the octahedral Zn ion to the O atoms of the NMP molecules (average value 2.079 Å) are not too different from the $Zn2—O_{carboxylate}$ distances. At the same time, the binding of the nitrate anion to the tetrahedral Zn1 ion is obviously weaker than that of the carboxylate, as indicated by the Zn1—O10 distance of 2.013 (6) Å (Table 1).

The 'three-bladed' paddle-wheel Zn_2O_6 core in **I** represents a skewed elongated triangular bipyramid. This skewing is a source of chirality and can be characterized by dihedral

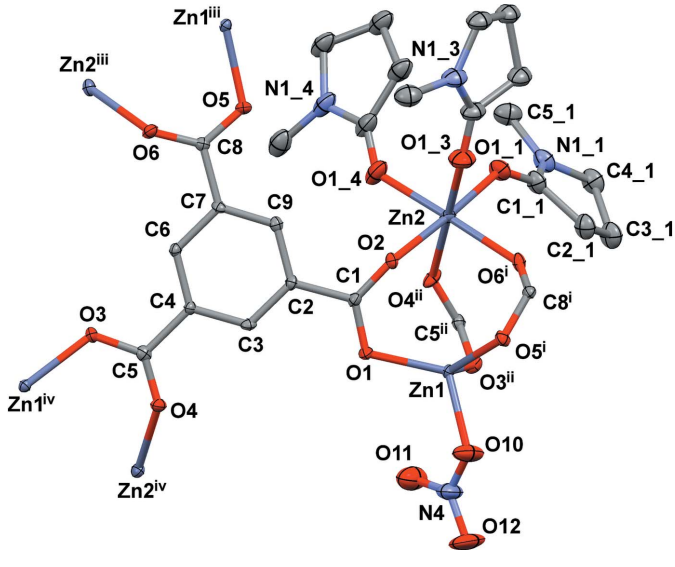


Figure 1
The extended asymmetric unit in **I** showing the atom-labeling scheme with displacement ellipsoids drawn at the 30% probability level. C-bound H atoms are omitted for clarity. Only the major occupancy components of disordered NMP molecules are shown. Symmetry codes: (i) $-x+\frac{1}{2}, -y+1, z+\frac{1}{2}$; (ii) $x+\frac{1}{2}, -y+\frac{1}{2}, -z+1$; (iii) $-x+\frac{1}{2}, -y+1, z-\frac{1}{2}$; (iv) $x-\frac{1}{2}, -y+\frac{1}{2}, -z+1$.

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

D—H···A	D—H	H···A	D···A	D—H···A
C5_1—H5A_1···O1^{i}	0.98	2.55	3.488 (10)	160
C4_2—H4A_2···O12^{ii}	0.99	2.24	3.12 (2)	147
C5_2—H5B_2···O6^{iii}	0.98	2.65	3.61 (2)	168
C2_3—H2A_3···O3^{iii}	0.99	2.48	3.472 (14)	177
C2_3—H2B_3···O1_1	0.99	2.58	3.335 (13)	133
C4_3—H4B_3···O12^{ii}	0.99	2.49	3.417 (17)	156
C2_4—H2B_4···O1_1	0.99	2.56	3.297 (15)	132
C4_4—H4A_4···O1^{ii}	0.99	2.58	3.564 (16)	170
C4_4—H4B_4···O12^{i}	0.99	2.47	3.448 (17)	169
C2_5—H2A_5···O10^{ii}	0.99	2.45	3.30 (2)	143
C4_5—H4A_5···O1^{ii}	0.99	2.56	3.34 (2)	135

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

skewing angles Zn1—On···On—Zn2 (s). In spite of the lack of strict symmetry, these angles are not too different in **I** and have an average value of 49.8°. It is worth noting that the tetrahedral Zn1 ion lies close to the plane of the carboxylic groups of BTC^{3-}, while the octahedral Zn2 ion exhibits a large deviation from this plane.

3. Supramolecular features

Linking of the 'three-bladed' paddle-wheel dizinc SBUs by BTC^{3-} units results in the formation of a three-dimensional covalent framework with **srs** topology. A detailed description of such a structure can be found in Yaghi *et al.* (1997). It is characterized by the presence of interconnected channels parallel to all three crystallographic axes (Fig. 2). However, the crystals of **I** as a whole are non-porous, because these channels are occupied by coordinated nitrate anions and NMP molecules, though the removal of the NMP molecules could lead to a highly porous material [solvent-accessible volume of 1820.8 Å^3 (63.4% of the unit-cell volume) as calculated by *PLATON* (Spek, 2020)]. Extensive C—H···O hydrogen bonding occurs (Table 2).

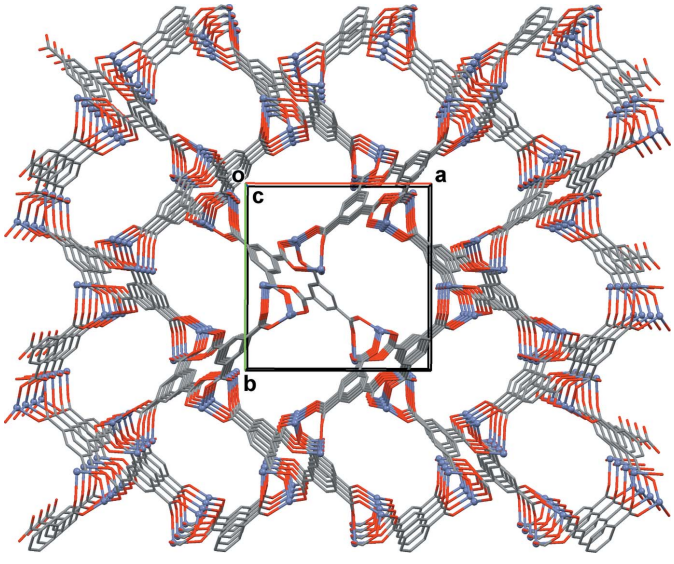


Figure 2
View of the framework structure in **I** down the *c*-axis direction. Coordinated nitrate anions and NMP molecules are not shown.

4. Database survey

A search of the Cambridge Structural Database (CSD, version 5.43, last update September 2022; Groom *et al.*, 2016) revealed nine structures of **srs**-type connectivity with the composition $[Zn_2(BTC)(NO_3)(Solv)_3]_n$, that differ in the nature of solvent molecules coordinated to the octahedral Zn^{II} ion. Two of them [refcodes RIZXUT (Solv = EtOH; Yaghi *et al.*, 1997) and SENWEP (Solv = DMF; Oh *et al.*, 2013)] crystallize in the cubic $P2_13$ space group, while the others belong to the orthorhombic $P2_12_12_1$ space group. In general, the coordination bond lengths in all these compounds are very similar and close to those observed in **I**. Interestingly, the Zn—O distances for the coordinated solvent molecules (in particular for EtOH and different amides) are practically the same, despite the different chemical nature of the donor atoms.

Nevertheless, these MOFs demonstrate considerable variations in the structure of the Zn_2O_6 core. The degree of skewing, as characterized by the averaged value of *s*, varies by *ca* 10°, and its increase correlates with the decrease of the unit-cell volume, as can be illustrated by comparison of structures RIZXUT (*s* = 39.4°) and SENWEP (*s* = 48.4°) possessing maximum and minimum values of 3194.71 and 2807.34 Å^3, respectively. The series as a whole demonstrates a rough correlation between these parameters. Compounds crystallizing in the $P2_12_12_1$ space group reveal asymmetry of the Zn_2O_6 core, which can be characterized by the difference between maximum and minimum values of skewing angles. This difference is the largest (*ca* 27°) for compounds containing coordinated DMA molecules [VEHJID (Hao *et al.*, 2012), VEHJID01 (Lou *et al.*, 2013), VEHJID02 (Wang *et al.*, 2021*a*), and SENWIT (Oh *et al.*, 2013)], while for structures with coordinated EtOH (SENWAL; Oh *et al.*, 2013), diethylformamide (SENWOZ; Oh *et al.*, 2013) and NMP/pyridine (ISIQOT; Wang *et al.*, 2021*b*), it does not exceed 11°, being minimum (4.6°) in **I**. Interestingly, increase of core asymmetry is accompanied by an increase in the difference between unit-cell lengths ($b-a$) from 0.104 Å in **I** to 2.009 Å in VEHJID02.

5. Synthesis and crystallization

All chemicals and solvents used in this work were purchased from Sigma–Aldrich and were used without further purification.

To prepare $[Zn_2(BTC)(NO_3)(NMP)_3]_n$, **I**, a solution of 200 mg (0.952 mmol) of H_3BTC in 1 ml of DMF was added to a solution of 610 mg (2.051 mmol) of $Zn(NO_3)_2{\cdot}6H_2O$ in 20 ml of NMP and the mixture was heated at *ca* 363 K for two days. In the course of heating, the gradual formation of a white crystalline precipitate occurred, accompanied by an intense dark-orange coloration of the solution. The precipitate was filtered off, washed with NMP and dried under vacuum. Yield: 483 mg (73%). Analysis calculated for $C_{24}H_{30}N_4O_{12}Zn_2$: C,

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Zn_2(C_9H_3O_6)(NO_3)(C_5H_9NO)_3]$
M_r	697.26
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	160
a, b, c (Å)	13.6870 (5), 13.7912 (5), 15.2165 (5)
V (Å^3)	2872.26 (17)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.74
Crystal size (mm)	0.2 × 0.2 × 0.15
Data collection	
Diffractometer	Rigaku Xcalibur Eos
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2021)
T_{min}, T_{max}	0.640, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18130, 6787, 5981
R_{int}	0.046
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.687
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.050, 0.116, 1.05
No. of reflections	6787
No. of parameters	494
No. of restraints	450
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.95, −0.54
Absolute structure	Flack x determined using 2151 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.003 (8)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2021), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2020), and *publCIF* (Westrip, 2010).

41.34; H, 4.34; N, 8.04%. Found: C, 41.22; H, 4.25; N, 7.92%. Single crystals suitable for X-ray diffraction analysis were picked from the sample.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The H atoms in **I** were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.95 (aromatic H atoms), 0.99 (methylene H atoms), and 0.98 Å (methyl H atoms), with U_{iso}(H) values of 1.2 (CH and CH_2 groups) or 1.5 (CH_3 groups) times those of the corresponding parent C atoms. Two of the NMP molecules are disordered with the site occupancies of the major components being 0.620 (16) and 0.638 (16). Disordered fragments were modeled using the RESI routine available in *SHELXL*.

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supporting information

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Crystal structure of poly[(μ_6-benzene-1,3,5-tricarboxylato)tris(1-methylpyrrolidin-2-one)nitratodizinc(II)]

Sergey P. Gavrish, Sergiu Shova and Yaroslaw D. Lampeka

Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2021); cell refinement: *CrysAlis PRO* (Rigaku OD, 2021); data reduction: *CrysAlis PRO* (Rigaku OD, 2021); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: *Mercury* (Macrae *et al.*, 2020); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Poly[(μ_6-benzene-1,3,5-tricarboxylato)tris(1-methylpyrrolidin-2-one)nitratodizinc(II)]

Crystal data

$[Zn_2(C_9H_3O_6)(NO_3)(C_5H_9NO)_3]$
$M_r = 697.26$
Orthorhombic, $P2_12_12_1$
$a = 13.6870$ (5) Å
$b = 13.7912$ (5) Å
$c = 15.2165$ (5) Å
$V = 2872.26$ (17) Å^3
$Z = 4$
$F(000) = 1432$
$D_x = 1.612$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6077 reflections
$\theta = 2.0$–$25.9°$
$\mu = 1.74$ mm^{-1}
$T = 160$ K
Irregular, clear light colourless
0.2 × 0.2 × 0.15 mm

Data collection

Rigaku Xcalibur Eos diffractometer
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2021)
$T_{min} = 0.640$, $T_{max} = 1.000$
18130 measured reflections
6787 independent reflections
5981 reflections with $I > 2\sigma(I)$
$R_{int} = 0.046$
$\theta_{max} = 29.2°$, $\theta_{min} = 2.0°$
$h = -18\rightarrow16$
$k = -18\rightarrow17$
$l = -20\rightarrow20$
10 standard reflections every 50 reflections
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.116$
$S = 1.05$
6787 reflections
494 parameters
450 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0475P)^2 + 3.9623P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.95$ e Å^{-3}
$\Delta\rho_{min} = -0.54$ e Å^{-3}
Absolute structure: Flack *x* determined using 2151 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.003 (8)

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	0.26242 (5)	0.29446 (5)	0.72606 (4)	0.01560 (16)	
Zn2	0.40511 (5)	0.45592 (5)	0.58535 (4)	0.02064 (17)	
O1	0.1740 (3)	0.3102 (3)	0.6260 (3)	0.0202 (9)	
O2	0.2533 (3)	0.4472 (3)	0.5943 (2)	0.0195 (8)	
O3	0.3789 (3)	0.2222 (3)	0.6939 (3)	0.0229 (10)	
O4	0.4112 (4)	0.3049 (3)	0.5705 (3)	0.0265 (10)	
O5	0.2878 (3)	0.4076 (3)	0.8006 (3)	0.0224 (10)	
O6	0.4200 (3)	0.4452 (3)	0.7215 (3)	0.0230 (9)	
O10	0.2034 (5)	0.2190 (4)	0.8261 (4)	0.0608 (19)	
O11	0.1951 (7)	0.1017 (5)	0.7347 (5)	0.084 (3)	
O12	0.1699 (8)	0.0761 (6)	0.8725 (5)	0.112 (4)	
N4	0.1905 (7)	0.1312 (6)	0.8116 (5)	0.062 (2)	
C1	0.1926 (4)	0.3820 (4)	0.5767 (4)	0.0190 (12)	
C2	0.1352 (4)	0.3889 (4)	0.4924 (4)	0.0176 (12)	
C3	0.0599 (4)	0.3249 (4)	0.4747 (4)	0.0179 (12)	
H3	0.043649	0.275756	0.515988	0.021*	
C4	0.5076 (4)	0.1675 (4)	0.6039 (4)	0.0165 (12)	
C5	0.4265 (5)	0.2377 (4)	0.6230 (4)	0.0205 (13)	
C6	0.5313 (5)	0.0964 (4)	0.6640 (4)	0.0171 (12)	
H6	0.495030	0.090692	0.716959	0.021*	
C7	0.3908 (4)	0.5321 (4)	0.8529 (4)	0.0169 (11)	
C8	0.3643 (4)	0.4570 (4)	0.7856 (4)	0.0170 (11)	
C9	0.3407 (4)	0.5405 (5)	0.9312 (4)	0.0184 (12)	
H9	0.288545	0.497058	0.943489	0.022*	
O1_1	0.5572 (3)	0.4623 (4)	0.5680 (3)	0.0424 (11)	
N1_1	0.7026 (4)	0.3919 (5)	0.5521 (4)	0.0431 (12)	
C1_1	0.6253 (4)	0.4181 (6)	0.5950 (4)	0.0412 (11)	
C2_1	0.6392 (6)	0.3816 (6)	0.6892 (5)	0.0461 (13)	
H2A_1	0.654201	0.435940	0.729435	0.055*	
H2B_1	0.579715	0.348012	0.710282	0.055*	
C3_1	0.7251 (6)	0.3114 (6)	0.6835 (5)	0.0512 (14)	
H3A_1	0.768756	0.318481	0.734951	0.061*	
H3B_1	0.702041	0.243433	0.680296	0.061*	
C4_1	0.7773 (5)	0.3402 (6)	0.5994 (5)	0.0495 (14)	
H4A_1	0.834152	0.382416	0.611853	0.059*	
H4B_1	0.799562	0.282478	0.566320	0.059*	
C5_1	0.7180 (7)	0.4199 (6)	0.4606 (5)	0.0534 (19)	
H5A_1	0.711556	0.362707	0.422809	0.080*	
H5B_1	0.783634	0.447384	0.453918	0.080*	

H5C_1	0.669223	0.468418	0.443581	0.080*	
O1_2	0.3924 (5)	0.6022 (4)	0.6028 (4)	0.0565 (13)	0.380 (9)
N1_2	0.4149 (11)	0.7633 (8)	0.5886 (15)	0.053 (2)	0.380 (9)
C1_2	0.3711 (12)	0.6810 (6)	0.5781 (15)	0.054 (2)	0.380 (9)
C2_2	0.2660 (11)	0.6917 (10)	0.5452 (15)	0.056 (2)	0.380 (9)
H2A_2	0.259279	0.671717	0.483043	0.067*	0.380 (9)
H2B_2	0.219348	0.654664	0.581900	0.067*	0.380 (9)
C3_2	0.2532 (12)	0.8009 (11)	0.557 (2)	0.056 (3)	0.380 (9)
H3A_2	0.217745	0.828544	0.505664	0.068*	0.380 (9)
H3B_2	0.215575	0.815071	0.610591	0.068*	0.380 (9)
C4_2	0.3549 (11)	0.8443 (10)	0.5628 (16)	0.055 (3)	0.380 (9)
H4A_2	0.376135	0.870798	0.505447	0.066*	0.380 (9)
H4B_2	0.357235	0.896507	0.607397	0.066*	0.380 (9)
C5_2	0.5189 (10)	0.7729 (16)	0.6082 (16)	0.055 (4)	0.380 (9)
H5A_2	0.542991	0.712415	0.634061	0.082*	0.380 (9)
H5B_2	0.528650	0.826252	0.649858	0.082*	0.380 (9)
H5C_2	0.554762	0.786566	0.553860	0.082*	0.380 (9)
O1_3	0.3924 (5)	0.6022 (4)	0.6028 (4)	0.0565 (13)	0.620 (9)
N1_3	0.3812 (7)	0.7644 (5)	0.5717 (9)	0.0484 (18)	0.620 (9)
C1_3	0.4215 (7)	0.6820 (5)	0.5899 (10)	0.0483 (16)	0.620 (9)
C2_3	0.5316 (7)	0.7011 (8)	0.5935 (9)	0.0495 (19)	0.620 (9)
H2A_3	0.554507	0.706489	0.655009	0.059*	0.620 (9)
H2B_3	0.568354	0.648763	0.563745	0.059*	0.620 (9)
C3_3	0.5435 (8)	0.7973 (8)	0.5450 (9)	0.050 (2)	0.620 (9)
H3A_3	0.597135	0.836311	0.570650	0.060*	0.620 (9)
H3B_3	0.556772	0.786696	0.481775	0.060*	0.620 (9)
C4_3	0.4453 (8)	0.8460 (7)	0.5588 (10)	0.051 (2)	0.620 (9)
H4A_3	0.446195	0.888724	0.611045	0.061*	0.620 (9)
H4B_3	0.425907	0.884348	0.506638	0.061*	0.620 (9)
C5_3	0.2756 (7)	0.7744 (11)	0.5609 (14)	0.057 (3)	0.620 (9)
H5A_3	0.260915	0.792627	0.500046	0.085*	0.620 (9)
H5B_3	0.251232	0.824646	0.600758	0.085*	0.620 (9)
H5C_3	0.243831	0.712505	0.574555	0.085*	0.620 (9)
O1_4	0.3920 (4)	0.4595 (5)	0.4483 (3)	0.0542 (13)	0.638 (16)
N1_4	0.4320 (8)	0.4834 (9)	0.3054 (5)	0.0533 (19)	0.638 (16)
C1_4	0.4316 (15)	0.4996 (11)	0.3892 (6)	0.0509 (17)	0.638 (16)
C2_4	0.4914 (11)	0.5930 (9)	0.3965 (7)	0.057 (2)	0.638 (16)
H2A_4	0.447709	0.649208	0.406292	0.068*	0.638 (16)
H2B_4	0.537630	0.588669	0.446379	0.068*	0.638 (16)
C3_4	0.5470 (11)	0.6048 (11)	0.3102 (7)	0.059 (2)	0.638 (16)
H3A_4	0.546572	0.673201	0.290540	0.071*	0.638 (16)
H3B_4	0.615468	0.582740	0.316310	0.071*	0.638 (16)
C4_4	0.4909 (10)	0.5407 (11)	0.2467 (7)	0.058 (2)	0.638 (16)
H4A_4	0.449879	0.579727	0.206480	0.070*	0.638 (16)
H4B_4	0.535579	0.499515	0.211755	0.070*	0.638 (16)
C5_4	0.3807 (11)	0.3999 (11)	0.2686 (9)	0.061 (3)	0.638 (16)
H5A_4	0.362782	0.355207	0.315976	0.092*	0.638 (16)
H5B_4	0.423380	0.366555	0.226621	0.092*	0.638 (16)

H5C_4	0.321455	0.421919	0.238366	0.092*	0.638 (16)
O1_5	0.3920 (4)	0.4595 (5)	0.4483 (3)	0.0542 (13)	0.362 (16)
N1_5	0.4502 (17)	0.4618 (11)	0.3094 (8)	0.056 (2)	0.362 (16)
C1_5	0.429 (3)	0.4963 (13)	0.3862 (11)	0.054 (2)	0.362 (16)
C2_5	0.447 (2)	0.6058 (11)	0.3844 (11)	0.056 (2)	0.362 (16)
H2A_5	0.385287	0.642731	0.388133	0.068*	0.362 (16)
H2B_5	0.491293	0.626390	0.432474	0.068*	0.362 (16)
C3_5	0.4954 (18)	0.6173 (14)	0.2946 (10)	0.058 (3)	0.362 (16)
H3A_5	0.475497	0.679185	0.266967	0.069*	0.362 (16)
H3B_5	0.567448	0.616531	0.300346	0.069*	0.362 (16)
C4_5	0.4609 (19)	0.5319 (13)	0.2399 (10)	0.057 (3)	0.362 (16)
H4A_5	0.398036	0.545410	0.210086	0.069*	0.362 (16)
H4B_5	0.510248	0.511644	0.196053	0.069*	0.362 (16)
C5_5	0.430 (2)	0.3623 (13)	0.2822 (18)	0.065 (4)	0.362 (16)
H5A_5	0.395470	0.328276	0.329510	0.097*	0.362 (16)
H5B_5	0.491603	0.328925	0.269647	0.097*	0.362 (16)
H5C_5	0.389197	0.362877	0.229282	0.097*	0.362 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0167 (3)	0.0170 (3)	0.0130 (3)	0.0003 (3)	−0.0002 (3)	−0.0002 (3)
Zn2	0.0199 (4)	0.0211 (3)	0.0209 (3)	−0.0001 (3)	0.0031 (3)	0.0048 (3)
O1	0.024 (2)	0.017 (2)	0.0198 (19)	−0.0012 (18)	−0.0040 (17)	0.0037 (18)
O2	0.015 (2)	0.022 (2)	0.0212 (18)	0.0008 (18)	−0.0023 (17)	−0.0016 (17)
O3	0.024 (2)	0.025 (2)	0.0192 (19)	0.0088 (19)	0.0059 (17)	−0.0007 (18)
O4	0.040 (3)	0.023 (2)	0.0173 (19)	0.014 (2)	0.0014 (19)	0.0014 (18)
O5	0.025 (2)	0.022 (2)	0.021 (2)	−0.0057 (18)	−0.0002 (17)	−0.0064 (18)
O6	0.019 (2)	0.030 (2)	0.0200 (19)	0.0014 (19)	−0.0018 (17)	−0.0100 (19)
O10	0.090 (5)	0.044 (4)	0.048 (3)	−0.021 (4)	0.029 (3)	0.002 (3)
O11	0.134 (8)	0.069 (5)	0.049 (4)	−0.038 (5)	0.012 (4)	−0.007 (4)
O12	0.210 (12)	0.072 (5)	0.053 (4)	−0.071 (6)	0.008 (5)	0.025 (4)
N4	0.087 (7)	0.049 (5)	0.049 (4)	−0.032 (5)	0.005 (4)	0.011 (4)
C1	0.019 (3)	0.022 (3)	0.017 (3)	0.002 (2)	−0.002 (2)	0.003 (3)
C2	0.017 (3)	0.018 (3)	0.017 (3)	0.003 (2)	−0.002 (2)	0.000 (2)
C3	0.023 (3)	0.011 (3)	0.019 (3)	−0.001 (2)	0.003 (2)	0.001 (2)
C4	0.020 (3)	0.017 (3)	0.013 (3)	0.002 (2)	0.000 (2)	−0.001 (2)
C5	0.022 (3)	0.020 (3)	0.020 (3)	0.000 (2)	−0.003 (2)	−0.005 (2)
C6	0.021 (3)	0.017 (3)	0.013 (3)	0.001 (2)	0.002 (2)	−0.001 (2)
C7	0.018 (3)	0.011 (3)	0.022 (3)	−0.001 (2)	−0.001 (2)	0.000 (2)
C8	0.018 (3)	0.016 (3)	0.018 (3)	0.000 (2)	−0.002 (2)	0.001 (2)
C9	0.018 (3)	0.019 (3)	0.018 (3)	0.001 (3)	0.000 (2)	0.004 (3)
O1_1	0.024 (2)	0.054 (3)	0.050 (3)	−0.001 (2)	0.006 (2)	0.004 (2)
N1_1	0.030 (2)	0.047 (3)	0.052 (2)	0.001 (2)	0.005 (2)	−0.008 (2)
C1_1	0.026 (2)	0.050 (3)	0.048 (2)	0.001 (2)	0.0017 (19)	−0.006 (2)
C2_1	0.032 (3)	0.058 (3)	0.049 (3)	0.006 (3)	0.000 (2)	−0.005 (3)
C3_1	0.034 (3)	0.062 (3)	0.058 (3)	0.008 (3)	−0.001 (2)	−0.004 (3)
C4_1	0.031 (3)	0.055 (3)	0.062 (3)	0.006 (2)	0.003 (2)	−0.008 (3)

C5_1	0.057 (5)	0.049 (4)	0.055 (3)	0.000 (4)	0.019 (3)	−0.004 (3)
O1_2	0.080 (3)	0.030 (2)	0.059 (3)	−0.010 (2)	0.002 (3)	0.005 (2)
N1_2	0.080 (5)	0.030 (3)	0.049 (5)	−0.006 (4)	−0.003 (5)	0.002 (4)
C1_2	0.079 (4)	0.031 (3)	0.051 (4)	−0.006 (3)	0.000 (4)	0.001 (3)
C2_2	0.080 (5)	0.035 (4)	0.052 (5)	−0.005 (4)	−0.002 (5)	0.000 (4)
C3_2	0.081 (5)	0.036 (4)	0.052 (5)	−0.003 (4)	−0.004 (5)	0.001 (5)
C4_2	0.081 (6)	0.032 (4)	0.050 (5)	−0.003 (4)	−0.004 (5)	0.001 (4)
C5_2	0.084 (6)	0.032 (7)	0.049 (8)	−0.008 (5)	−0.012 (7)	0.004 (7)
O1_3	0.080 (3)	0.030 (2)	0.059 (3)	−0.010 (2)	0.002 (3)	0.005 (2)
N1_3	0.069 (4)	0.028 (3)	0.048 (4)	−0.004 (3)	0.005 (4)	0.000 (3)
C1_3	0.070 (4)	0.028 (2)	0.047 (3)	−0.005 (3)	0.003 (3)	0.002 (3)
C2_3	0.069 (4)	0.032 (3)	0.048 (4)	−0.005 (3)	−0.002 (4)	0.002 (3)
C3_3	0.068 (4)	0.032 (3)	0.050 (4)	−0.008 (3)	0.001 (4)	0.003 (4)
C4_3	0.071 (4)	0.030 (3)	0.051 (4)	−0.005 (3)	0.004 (4)	0.003 (3)
C5_3	0.067 (4)	0.042 (6)	0.061 (7)	0.001 (4)	0.008 (6)	0.002 (6)
O1_4	0.038 (3)	0.090 (3)	0.035 (2)	0.010 (3)	0.004 (2)	0.023 (2)
N1_4	0.035 (4)	0.088 (4)	0.037 (3)	0.016 (3)	0.007 (3)	0.023 (3)
C1_4	0.033 (3)	0.083 (4)	0.036 (3)	0.014 (3)	0.005 (3)	0.021 (3)
C2_4	0.040 (4)	0.084 (4)	0.046 (3)	0.012 (3)	0.007 (3)	0.022 (3)
C3_4	0.043 (4)	0.088 (5)	0.047 (4)	0.011 (3)	0.007 (3)	0.026 (4)
C4_4	0.040 (4)	0.092 (5)	0.042 (3)	0.014 (4)	0.009 (3)	0.025 (3)
C5_4	0.046 (6)	0.096 (7)	0.042 (5)	0.010 (5)	0.004 (5)	0.011 (5)
O1_5	0.038 (3)	0.090 (3)	0.035 (2)	0.010 (3)	0.004 (2)	0.023 (2)
N1_5	0.037 (5)	0.091 (5)	0.038 (4)	0.006 (5)	0.001 (4)	0.022 (4)
C1_5	0.035 (4)	0.089 (4)	0.037 (3)	0.008 (4)	0.000 (3)	0.023 (4)
C2_5	0.037 (5)	0.090 (5)	0.042 (4)	0.007 (5)	−0.004 (4)	0.023 (4)
C3_5	0.037 (6)	0.093 (5)	0.043 (4)	0.005 (5)	−0.004 (4)	0.026 (4)
C4_5	0.037 (5)	0.095 (6)	0.040 (4)	0.006 (5)	−0.001 (4)	0.024 (4)
C5_5	0.049 (9)	0.092 (6)	0.053 (7)	0.002 (8)	−0.001 (8)	0.015 (5)

Geometric parameters (Å, º)

Zn1—O1	1.956 (4)	C3_2—H3A_2	0.9900
Zn1—O3	1.943 (4)	C3_2—H3B_2	0.9900
Zn1—O5	1.960 (4)	C3_2—C4_2	1.518 (8)
Zn1—O10	2.013 (6)	C4_2—H4A_2	0.9900
Zn2—O2	2.086 (4)	C4_2—H4B_2	0.9900
Zn2—O4	2.097 (4)	C5_2—H5A_2	0.9800
Zn2—O6	2.086 (4)	C5_2—H5B_2	0.9800
Zn2—O1_1	2.100 (5)	C5_2—H5C_2	0.9800
Zn2—O1_2	2.042 (5)	O1_3—C1_3	1.186 (6)
Zn2—O1_3	2.042 (5)	N1_3—C1_3	1.294 (6)
Zn2—O1_4	2.094 (5)	N1_3—C4_3	1.440 (7)
Zn2—O1_5	2.094 (5)	N1_3—C5_3	1.461 (8)
O1—C1	1.268 (7)	C1_3—C2_3	1.531 (8)
O2—C1	1.253 (7)	C2_3—H2A_3	0.9900
O3—C5	1.278 (7)	C2_3—H2B_3	0.9900
O4—C5	1.241 (7)	C2_3—C3_3	1.526 (8)

O5—C8	1.269 (7)	C3_3—H3A_3	0.9900
O6—C8	1.250 (7)	C3_3—H3B_3	0.9900
O10—N4	1.244 (9)	C3_3—C4_3	1.518 (8)
O11—N4	1.239 (10)	C4_3—H4A_3	0.9900
O12—N4	1.232 (10)	C4_3—H4B_3	0.9900
C1—C2	1.507 (8)	C5_3—H5A_3	0.9800
C2—C3	1.384 (8)	C5_3—H5B_3	0.9800
C2—C9^{i}	1.388 (9)	C5_3—H5C_3	0.9800
C3—H3	0.9500	O1_4—C1_4	1.186 (6)
C3—C4^{ii}	1.397 (8)	N1_4—C1_4	1.294 (6)
C4—C5	1.501 (8)	N1_4—C4_4	1.440 (7)
C4—C6	1.380 (8)	N1_4—C5_4	1.461 (8)
C6—H6	0.9500	C1_4—C2_4	1.531 (8)
C6—C7^{iii}	1.410 (8)	C2_4—H2A_4	0.9900
C7—C8	1.501 (8)	C2_4—H2B_4	0.9900
C7—C9	1.381 (8)	C2_4—C3_4	1.526 (8)
C9—H9	0.9500	C3_4—H3A_4	0.9900
O1_1—C1_1	1.187 (5)	C3_4—H3B_4	0.9900
N1_1—C1_1	1.295 (6)	C3_4—C4_4	1.518 (8)
N1_1—C4_1	1.440 (7)	C4_4—H4A_4	0.9900
N1_1—C5_1	1.460 (8)	C4_4—H4B_4	0.9900
C1_1—C2_1	1.531 (8)	C5_4—H5A_4	0.9800
C2_1—H2A_1	0.9900	C5_4—H5B_4	0.9800
C2_1—H2B_1	0.9900	C5_4—H5C_4	0.9800
C2_1—C3_1	1.526 (8)	O1_5—C1_5	1.186 (6)
C3_1—H3A_1	0.9900	N1_5—C1_5	1.294 (6)
C3_1—H3B_1	0.9900	N1_5—C4_5	1.440 (7)
C3_1—C4_1	1.518 (8)	N1_5—C5_5	1.461 (8)
C4_1—H4A_1	0.9900	C1_5—C2_5	1.531 (8)
C4_1—H4B_1	0.9900	C2_5—H2A_5	0.9900
C5_1—H5A_1	0.9800	C2_5—H2B_5	0.9900
C5_1—H5B_1	0.9800	C2_5—C3_5	1.526 (8)
C5_1—H5C_1	0.9800	C3_5—H3A_5	0.9900
O1_2—C1_2	1.186 (6)	C3_5—H3B_5	0.9900
N1_2—C1_2	1.294 (6)	C3_5—C4_5	1.518 (8)
N1_2—C4_2	1.440 (7)	C4_5—H4A_5	0.9900
N1_2—C5_2	1.460 (8)	C4_5—H4B_5	0.9900
C1_2—C2_2	1.531 (8)	C5_5—H5A_5	0.9800
C2_2—H2A_2	0.9900	C5_5—H5B_5	0.9800
C2_2—H2B_2	0.9900	C5_5—H5C_5	0.9800
C2_2—C3_2	1.526 (8)		

O1—Zn1—O5	118.14 (18)	C2_2—C3_2—H3A_2	110.3
O1—Zn1—O10	113.4 (3)	C2_2—C3_2—H3B_2	110.3
O3—Zn1—O1	111.59 (18)	H3A_2—C3_2—H3B_2	108.6
O3—Zn1—O5	114.10 (19)	C4_2—C3_2—C2_2	106.9 (12)
O3—Zn1—O10	104.8 (2)	C4_2—C3_2—H3A_2	110.3
O5—Zn1—O10	92.6 (2)	C4_2—C3_2—H3B_2	110.3

O2—Zn2—O4	89.36 (18)	N1_2—C4_2—C3_2	103.6 (12)
O2—Zn2—O6	91.63 (15)	N1_2—C4_2—H4A_2	111.0
O2—Zn2—O1_1	176.43 (18)	N1_2—C4_2—H4B_2	111.0
O2—Zn2—O1_4	88.92 (19)	C3_2—C4_2—H4A_2	111.0
O2—Zn2—O1_5	88.92 (19)	C3_2—C4_2—H4B_2	111.0
O4—Zn2—O1_1	89.4 (2)	H4A_2—C4_2—H4B_2	109.0
O6—Zn2—O4	91.85 (16)	N1_2—C5_2—H5A_2	109.5
O6—Zn2—O1_1	91.76 (18)	N1_2—C5_2—H5B_2	109.5
O6—Zn2—O1_4	177.2 (2)	N1_2—C5_2—H5C_2	109.5
O6—Zn2—O1_5	177.2 (2)	H5A_2—C5_2—H5B_2	109.5
O1_2—Zn2—O2	87.9 (2)	H5A_2—C5_2—H5C_2	109.5
O1_2—Zn2—O4	177.1 (2)	H5B_2—C5_2—H5C_2	109.5
O1_2—Zn2—O6	87.1 (2)	C1_3—O1_3—Zn2	150.1 (8)
O1_2—Zn2—O1_1	93.4 (3)	C1_3—N1_3—C4_3	117.1 (8)
O1_2—Zn2—O1_4	95.7 (3)	C1_3—N1_3—C5_3	121.9 (10)
O1_3—Zn2—O2	87.9 (2)	C4_3—N1_3—C5_3	121.0 (9)
O1_3—Zn2—O4	177.1 (2)	O1_3—C1_3—N1_3	135.0 (10)
O1_3—Zn2—O6	87.1 (2)	O1_3—C1_3—C2_3	119.0 (9)
O1_3—Zn2—O1_1	93.4 (3)	N1_3—C1_3—C2_3	106.0 (7)
O1_3—Zn2—O1_5	95.7 (3)	C1_3—C2_3—H2A_3	111.0
O1_4—Zn2—O4	85.4 (2)	C1_3—C2_3—H2B_3	111.0
O1_4—Zn2—O1_1	87.6 (2)	H2A_3—C2_3—H2B_3	109.0
O1_5—Zn2—O4	85.4 (2)	C3_3—C2_3—C1_3	103.8 (8)
O1_5—Zn2—O1_1	87.6 (2)	C3_3—C2_3—H2A_3	111.0
C1—O1—Zn1	115.0 (4)	C3_3—C2_3—H2B_3	111.0
C1—O2—Zn2	133.4 (4)	C2_3—C3_3—H3A_3	111.2
C5—O3—Zn1	123.1 (4)	C2_3—C3_3—H3B_3	111.2
C5—O4—Zn2	132.8 (4)	H3A_3—C3_3—H3B_3	109.1
C8—O5—Zn1	118.0 (4)	C4_3—C3_3—C2_3	102.9 (9)
C8—O6—Zn2	135.0 (4)	C4_3—C3_3—H3A_3	111.2
N4—O10—Zn1	115.2 (5)	C4_3—C3_3—H3B_3	111.2
O11—N4—O10	118.7 (7)	N1_3—C4_3—C3_3	102.3 (8)
O12—N4—O10	120.0 (8)	N1_3—C4_3—H4A_3	111.3
O12—N4—O11	121.3 (8)	N1_3—C4_3—H4B_3	111.3
O1—C1—C2	116.6 (5)	C3_3—C4_3—H4A_3	111.3
O2—C1—O1	124.5 (5)	C3_3—C4_3—H4B_3	111.3
O2—C1—C2	118.9 (5)	H4A_3—C4_3—H4B_3	109.2
C3—C2—C1	121.0 (5)	N1_3—C5_3—H5A_3	109.5
C3—C2—C9^{i}	119.6 (5)	N1_3—C5_3—H5B_3	109.5
C9^{i}—C2—C1	119.4 (5)	N1_3—C5_3—H5C_3	109.5
C2—C3—H3	120.0	H5A_3—C5_3—H5B_3	109.5
C2—C3—C4^{ii}	120.0 (5)	H5A_3—C5_3—H5C_3	109.5
C4^{ii}—C3—H3	120.0	H5B_3—C5_3—H5C_3	109.5
C3^{iv}—C4—C5	119.7 (5)	C1_4—O1_4—Zn2	136.6 (8)
C6—C4—C3^{iv}	120.0 (5)	C1_4—N1_4—C4_4	121.2 (9)
C6—C4—C5	120.2 (5)	C1_4—N1_4—C5_4	120.8 (10)
O3—C5—C4	115.7 (5)	C4_4—N1_4—C5_4	117.6 (9)
O4—C5—O3	125.5 (6)	O1_4—C1_4—N1_4	132.0 (11)

O4—C5—C4	118.8 (5)	O1_4—C1_4—C2_4	125.5 (9)
C4—C6—H6	119.9	N1_4—C1_4—C2_4	102.4 (7)
C4—C6—C7^{iii}	120.3 (5)	C1_4—C2_4—H2A_4	110.3
C7^{iii}—C6—H6	119.9	C1_4—C2_4—H2B_4	110.3
C6^{v}—C7—C8	119.5 (5)	H2A_4—C2_4—H2B_4	108.6
C9—C7—C6^{v}	118.7 (5)	C3_4—C2_4—C1_4	107.1 (8)
C9—C7—C8	121.7 (5)	C3_4—C2_4—H2A_4	110.3
O5—C8—C7	116.6 (5)	C3_4—C2_4—H2B_4	110.3
O6—C8—O5	125.0 (5)	C2_4—C3_4—H3A_4	111.1
O6—C8—C7	118.4 (5)	C2_4—C3_4—H3B_4	111.1
C2^{vi}—C9—H9	119.3	H3A_4—C3_4—H3B_4	109.0
C7—C9—C2^{vi}	121.3 (6)	C4_4—C3_4—C2_4	103.5 (9)
C7—C9—H9	119.3	C4_4—C3_4—H3A_4	111.1
C1_1—O1_1—Zn2	135.5 (5)	C4_4—C3_4—H3B_4	111.1
C1_1—N1_1—C4_1	117.8 (6)	N1_4—C4_4—C3_4	102.0 (8)
C1_1—N1_1—C5_1	121.7 (7)	N1_4—C4_4—H4A_4	111.4
C4_1—N1_1—C5_1	120.3 (6)	N1_4—C4_4—H4B_4	111.4
O1_1—C1_1—N1_1	127.6 (7)	C3_4—C4_4—H4A_4	111.4
O1_1—C1_1—C2_1	126.2 (6)	C3_4—C4_4—H4B_4	111.4
N1_1—C1_1—C2_1	106.2 (6)	H4A_4—C4_4—H4B_4	109.2
C1_1—C2_1—H2A_1	110.8	N1_4—C5_4—H5A_4	109.5
C1_1—C2_1—H2B_1	110.8	N1_4—C5_4—H5B_4	109.5
H2A_1—C2_1—H2B_1	108.9	N1_4—C5_4—H5C_4	109.5
C3_1—C2_1—C1_1	104.6 (6)	H5A_4—C5_4—H5B_4	109.5
C3_1—C2_1—H2A_1	110.8	H5A_4—C5_4—H5C_4	109.5
C3_1—C2_1—H2B_1	110.8	H5B_4—C5_4—H5C_4	109.5
C2_1—C3_1—H3A_1	110.9	C1_5—O1_5—Zn2	140.0 (15)
C2_1—C3_1—H3B_1	110.9	C1_5—N1_5—C4_5	116.1 (14)
H3A_1—C3_1—H3B_1	108.9	C1_5—N1_5—C5_5	124.0 (16)
C4_1—C3_1—C2_1	104.1 (6)	C4_5—N1_5—C5_5	116.2 (14)
C4_1—C3_1—H3A_1	110.9	O1_5—C1_5—N1_5	131.1 (14)
C4_1—C3_1—H3B_1	110.9	O1_5—C1_5—C2_5	120.4 (13)
N1_1—C4_1—C3_1	102.5 (6)	N1_5—C1_5—C2_5	108.1 (10)
N1_1—C4_1—H4A_1	111.3	C1_5—C2_5—H2A_5	111.6
N1_1—C4_1—H4B_1	111.3	C1_5—C2_5—H2B_5	111.6
C3_1—C4_1—H4A_1	111.3	H2A_5—C2_5—H2B_5	109.4
C3_1—C4_1—H4B_1	111.3	C3_5—C2_5—C1_5	100.9 (10)
H4A_1—C4_1—H4B_1	109.2	C3_5—C2_5—H2A_5	111.6
N1_1—C5_1—H5A_1	109.5	C3_5—C2_5—H2B_5	111.6
N1_1—C5_1—H5B_1	109.5	C2_5—C3_5—H3A_5	110.5
N1_1—C5_1—H5C_1	109.5	C2_5—C3_5—H3B_5	110.5
H5A_1—C5_1—H5B_1	109.5	H3A_5—C3_5—H3B_5	108.7
H5A_1—C5_1—H5C_1	109.5	C4_5—C3_5—C2_5	106.0 (13)
H5B_1—C5_1—H5C_1	109.5	C4_5—C3_5—H3A_5	110.5
C1_2—O1_2—Zn2	152.2 (11)	C4_5—C3_5—H3B_5	110.5
C1_2—N1_2—C4_2	112.5 (11)	N1_5—C4_5—C3_5	98.6 (12)
C1_2—N1_2—C5_2	123.8 (14)	N1_5—C4_5—H4A_5	112.1
C4_2—N1_2—C5_2	122.8 (13)	N1_5—C4_5—H4B_5	112.1

O1_2—C1_2—N1_2	130.6 (13)	C3_5—C4_5—H4A_5	112.1
O1_2—C1_2—C2_2	115.1 (11)	C3_5—C4_5—H4B_5	112.1
N1_2—C1_2—C2_2	113.0 (9)	H4A_5—C4_5—H4B_5	109.7
C1_2—C2_2—H2A_2	111.9	N1_5—C5_5—H5A_5	109.5
C1_2—C2_2—H2B_2	111.9	N1_5—C5_5—H5B_5	109.5
H2A_2—C2_2—H2B_2	109.6	N1_5—C5_5—H5C_5	109.5
C3_2—C2_2—C1_2	99.6 (10)	H5A_5—C5_5—H5B_5	109.5
C3_2—C2_2—H2A_2	111.9	H5A_5—C5_5—H5C_5	109.5
C3_2—C2_2—H2B_2	111.9	H5B_5—C5_5—H5C_5	109.5

Zn1—O1—C1—O2	−9.5 (8)	C2_1—C3_1—C4_1—N1_1	−20.5 (9)
Zn1—O1—C1—C2	171.9 (4)	C4_1—N1_1—C1_1—O1_1	178.6 (8)
Zn1—O3—C5—O4	7.1 (9)	C4_1—N1_1—C1_1—C2_1	−0.7 (10)
Zn1—O3—C5—C4	−173.2 (4)	C5_1—N1_1—C1_1—O1_1	3.4 (14)
Zn1—O5—C8—O6	7.6 (8)	C5_1—N1_1—C1_1—C2_1	−176.0 (8)
Zn1—O5—C8—C7	−169.7 (4)	C5_1—N1_1—C4_1—C3_1	−170.6 (7)
Zn1—O10—N4—O11	−14.6 (13)	O1_2—C1_2—C2_2—C3_2	158 (2)
Zn1—O10—N4—O12	168.2 (9)	N1_2—C1_2—C2_2—C3_2	−11 (3)
Zn2—O2—C1—O1	79.8 (8)	C1_2—N1_2—C4_2—C3_2	15 (3)
Zn2—O2—C1—C2	−101.7 (6)	C1_2—C2_2—C3_2—C4_2	19 (3)
Zn2—O4—C5—O3	55.3 (9)	C2_2—C3_2—C4_2—N1_2	−21 (3)
Zn2—O4—C5—C4	−124.4 (5)	C4_2—N1_2—C1_2—O1_2	−169 (2)
Zn2—O6—C8—O5	62.3 (9)	C4_2—N1_2—C1_2—C2_2	−3 (3)
Zn2—O6—C8—C7	−120.5 (5)	C5_2—N1_2—C1_2—O1_2	22 (5)
Zn2—O1_1—C1_1—N1_1	140.1 (7)	C5_2—N1_2—C1_2—C2_2	−172 (2)
Zn2—O1_1—C1_1—C2_1	−40.6 (13)	C5_2—N1_2—C4_2—C3_2	−176 (2)
Zn2—O1_2—C1_2—N1_2	−139 (2)	O1_3—C1_3—C2_3—C3_3	161.6 (13)
Zn2—O1_2—C1_2—C2_2	55 (4)	N1_3—C1_3—C2_3—C3_3	−18.1 (16)
Zn2—O1_3—C1_3—N1_3	138.3 (15)	C1_3—N1_3—C4_3—C3_3	16.4 (18)
Zn2—O1_3—C1_3—C2_3	−41 (3)	C1_3—C2_3—C3_3—C4_3	26.9 (14)
Zn2—O1_4—C1_4—N1_4	163.9 (16)	C2_3—C3_3—C4_3—N1_3	−25.8 (14)
Zn2—O1_4—C1_4—C2_4	−21 (3)	C4_3—N1_3—C1_3—O1_3	−178.5 (17)
Zn2—O1_5—C1_5—N1_5	139 (3)	C4_3—N1_3—C1_3—C2_3	1.1 (18)
Zn2—O1_5—C1_5—C2_5	−50 (5)	C5_3—N1_3—C1_3—O1_3	−1 (3)
O1—C1—C2—C3	5.9 (8)	C5_3—N1_3—C1_3—C2_3	178.6 (15)
O1—C1—C2—C9^{i}	−173.0 (5)	C5_3—N1_3—C4_3—C3_3	−161.1 (15)
O2—C1—C2—C3	−172.7 (5)	O1_4—C1_4—C2_4—C3_4	167.2 (19)
O2—C1—C2—C9^{i}	8.4 (9)	N1_4—C1_4—C2_4—C3_4	−17 (2)
C1—C2—C3—C4^{ii}	−179.9 (5)	C1_4—N1_4—C4_4—C3_4	5 (2)
C3^{iv}—C4—C5—O3	176.1 (5)	C1_4—C2_4—C3_4—C4_4	19.6 (17)
C3^{iv}—C4—C5—O4	−4.1 (9)	C2_4—C3_4—C4_4—N1_4	−14.7 (15)
C3^{iv}—C4—C6—C7^{iii}	1.0 (9)	C4_4—N1_4—C1_4—O1_4	−177 (2)
C5—C4—C6—C7^{iii}	−178.3 (5)	C4_4—N1_4—C1_4—C2_4	7 (2)
C6—C4—C5—O3	−4.5 (8)	C5_4—N1_4—C1_4—O1_4	−3 (4)
C6—C4—C5—O4	175.2 (6)	C5_4—N1_4—C1_4—C2_4	−179.1 (13)
C6^{v}—C7—C8—O5	−173.3 (5)	C5_4—N1_4—C4_4—C3_4	−168.8 (12)
C6^{v}—C7—C8—O6	9.2 (8)	O1_5—C1_5—C2_5—C3_5	179 (3)
C6^{v}—C7—C9—C2^{vi}	0.7 (9)	N1_5—C1_5—C2_5—C3_5	−8 (3)

C8—C7—C9—C2^{vi}	−179.1 (5)	C1_5—N1_5—C4_5—C3_5	29 (3)
C9^{i}—C2—C3—C4^{ii}	−1.0 (9)	C1_5—C2_5—C3_5—C4_5	25 (3)
C9—C7—C8—O5	6.5 (8)	C2_5—C3_5—C4_5—N1_5	−31 (2)
C9—C7—C8—O6	−171.0 (5)	C4_5—N1_5—C1_5—O1_5	158 (4)
O1_1—C1_1—C2_1—C3_1	167.6 (8)	C4_5—N1_5—C1_5—C2_5	−14 (4)
N1_1—C1_1—C2_1—C3_1	−13.0 (9)	C5_5—N1_5—C1_5—O1_5	0 (6)
C1_1—N1_1—C4_1—C3_1	14.1 (10)	C5_5—N1_5—C1_5—C2_5	−172 (2)
C1_1—C2_1—C3_1—C4_1	20.7 (9)	C5_5—N1_5—C4_5—C3_5	−172 (2)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2_1—H2*B*_1···O6	0.99	2.57	3.163 (8)	119
C5_1—H5*A*_1···O1^{iv}	0.98	2.55	3.488 (10)	160
C5_1—H5*A*_1···O11^{iv}	0.98	2.46	3.003 (11)	115
C4_2—H4*A*_2···O12^{i}	0.99	2.24	3.12 (2)	147
C5_2—H5*B*_2···O6^{v}	0.98	2.65	3.61 (2)	168
C2_3—H2*A*_3···O3^{v}	0.99	2.48	3.472 (14)	177
C2_3—H2*B*_3···O1_1	0.99	2.58	3.335 (13)	133
C4_3—H4*B*_3···O12^{i}	0.99	2.49	3.417 (17)	156
C2_4—H2*B*_4···O1_1	0.99	2.56	3.297 (15)	132
C4_4—H4*A*_4···O1^{i}	0.99	2.58	3.564 (16)	170
C4_4—H4*B*_4···O12^{iv}	0.99	2.47	3.448 (17)	169
C2_5—H2*A*_5···O10^{i}	0.99	2.45	3.30 (2)	143
C4_5—H4*A*_5···O1^{i}	0.99	2.56	3.34 (2)	135

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

Selected bond lengths (Å).

Zn1—O1	1.956 (4)	Zn2—O2	2.086 (4)
Zn1—O3i	1.943 (4)	Zn2—O4i	2.097 (4)
Zn1—O5ii	1.960 (4)	Zn2—O6ii	2.086 (4)
Zn1—O10	2.013 (6)	Zn2—O1_1	2.100 (5)
		Zn2—O1_3	2.042 (5)
		Zn2—O1_4	2.094 (5)

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