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Crystal structure of *catena*-poly[[[bis(3-oxo-1,3-diphenylprop-1-enolato-κ^2O,O')zinc(II)]-μ_2-tris[4-(pyridin-3-yl)phenyl]amine-$\kappa^2N:N'$] tetrahydrofuran monosolvate]

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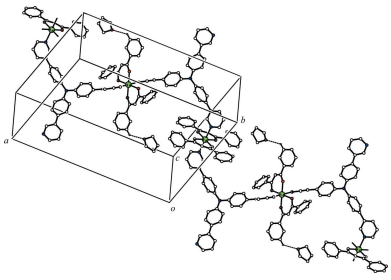
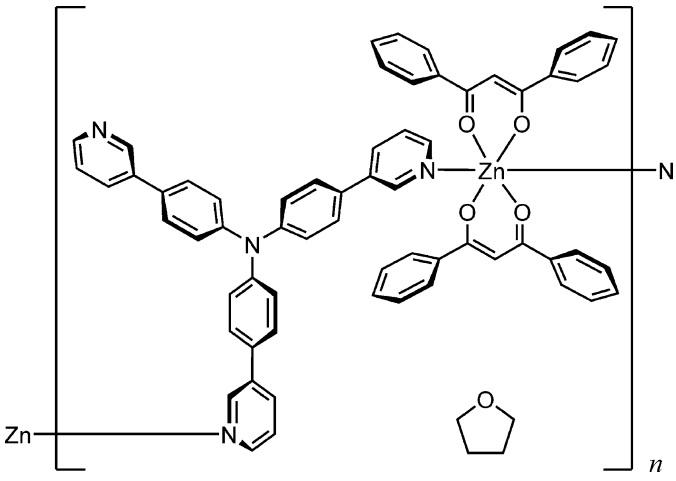
The reaction of bis(3-oxo-1,3-diphenylprop-1-enolato-κ^2O,O')zinc(II), [Zn(dbm)$_2$], with tris[4-(pyridin-3-yl)phenyl]amine (T3PyA) in tetrahydrofuran (THF) afforded the title crystalline coordination polymer, $\{[Zn(C_{15}H_{11}O_2)_2(C_{33}H_{24}N_4)]\cdot C_4H_8O\}_n$. The asymmetric unit contains two independent halves of Zn(dbm)$_2$, one T3PyA and one THF. Each Zn^{II} atom is located on an inversion centre and adopts an elongated octahedral coordination geometry, ligated by four O atoms of two dbm ligands in equatorial positions and by two N atoms of pyridine moieties from two different bridging T3PyA ligands in axial positions. The crystal packing shows a one-dimensional polymer chain in which the two pyridyl groups of the T3PyA ligand bridge two independent Zn atoms of Zn(dbm)$_2$. In the crystal, the coordination polymer chains are linked *via* C—H$\cdots\pi$ interactions into a sheet structure parallel to (010). The sheets are cross-linked *via* further C—H$\cdots\pi$ interactions into a three-dimensional network. The solvate THF molecule shows disorder over two sets of atomic sites having occupancies of 0.631 (7) and 0.369 (7).

1. Chemical context

The structure of coordination polymers generated from the self-assembly of metal ions and bridging organic ligands depends on the molecular structures of the ligands and the coordination geometries of the metal ions. The pyridyl-group-terminated spacer ligands with coordinating ability and optical or electronic functionalities have been widely used to construct a variety of coordination polymers with designable structures and attractive potential applications in material science (Robin & Fromm, 2006; Allendorf *et al.*, 2009; Stavila *et al.*, 2014). Triphenylamine-based structures are some of the most important moieties and electron-donating groups in organic electronic materials, *e.g.* organic or organic–inorganic hybrid light-emitting diodes and solar cells, because of their electroactivity, photoactivity and chemical stability (Shirota & Kageyama, 2007; Mahmood, 2016; Agarwala & Kabra, 2017). One of the pyridyl-group-terminated triphenylamine derivatives, tris[4-(pyridin-3-yl)phenyl]amine (T3PyA), was firstly synthesized by Hu *et al.* (2013) as a pH-sensitive fluorophore. Recently, its Pd^{II} complex was also reported (Wang *et al.*, 2016). We report herein on the crystal structure of the title coordination polymer composed of an *exo*-tridentate tripyridyl-type ligand, a β-diketonato ligand and a closed-shell Zn^{II} atom as the building blocks.





2. Structural commentary

The asymmetric unit of the title coordination polymer is composed of two unique halves of the bis(3-oxo-1,3-diphenylprop-1-enolato-κ^2O,O')zinc(II) [Zn(dbm)$_2$] moiety, one T3PyA ligand bridging the Zn atoms in a μ_2-κ^2 mode and one tetrahydrofuran (THF) solvate molecule (Fig. 1). Each Zn atom is located on an inversion centre and adopts an elongated octahedral coordination geometry, ligated by four O atoms of bidentate β-diketonato dbm ligands in equatorial positions and by two N atoms of pyridine moieties from two different bridging T3PyA ligands in axial positions. The equatorial Zn—O bond lengths [2.0440 (17)–2.0629 (18) Å] are shorter than the axial Zn—N bond lengths [Zn1—N9 = 2.199 (2) Å and Zn2—N10 = 2.238 (2) Å]. In the two independent Zn(dbm)$_2$ moieties, the bond lengths and angles are similar, but a difference in the dihedral angles between the mean planes of the benzene rings in dbm is observed [56.19 (16)° between the C12–C17 and C21–C26 rings in the moiety containing Zn1, and 30.68 (14)° between the C27–C32 and C36–C41 rings in the moiety containing Zn2]. The bridging T3PyA ligand has three pyridyl N atoms (N9, N10 and N11). Atoms N9 and N10 each coordinate to two different Zn atoms, while atom N11 does not interact with the surrounding atoms. The central N atom (N8) of T3PyA shows no pyramidalization, with a displacement of 0.052 (2) Å from the plane of the bonded C atoms (C42, C48 and C54) in the benzene rings. The dihedral angles between the mean planes of the benzene and pyridine rings in T3PyA are 47.56 (13), 33.60 (13) and 26.35 (15)°, respectively, between the C42–C47 and N9/C60–C64 rings, the C48–C53 and N10/C65–C69 rings, and the C54–C59 and N11/C70–C74 rings.

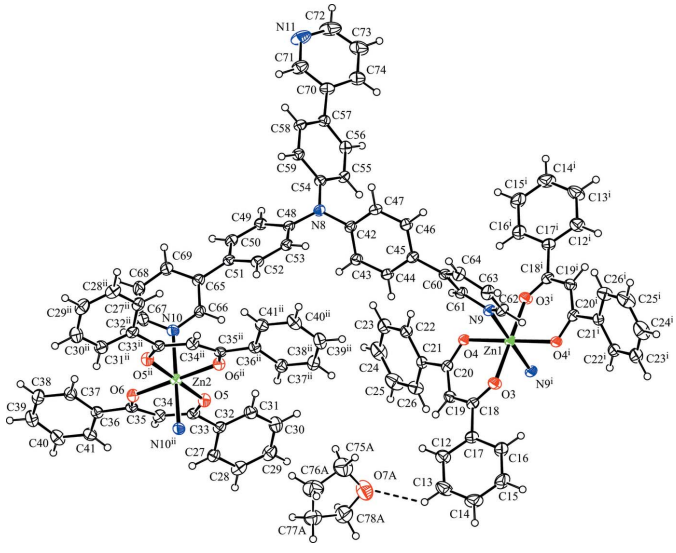


Figure 1
The molecular structure of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by spheres of arbitrary radius. The intermolecular C—H···O hydrogen bond is shown as a dashed line. The minor component of the disordered THF molecule has been omitted for clarity. [Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $-x, -y+1, -z+1$.]

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of the N10/C65–C69, C54–C59, C36–C41 and N11/C70–C74 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13···O7*A*	0.95	2.47	3.197 (7)	134
C40—H40···*Cg*1^{i}	0.95	2.74	3.594 (3)	150
C43—H43···*Cg*2^{ii}	0.95	2.78	3.572 (3)	142
C68—H68···*Cg*3^{iii}	0.95	2.65	3.513 (3)	152
C75*B*—H75*C*···*Cg*4^{ii}	0.99	2.78	3.649 (17)	146

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

3. Supramolecular features

In the crystal, the two independent Zn(dbm)$_2$ moieties and the bridging T3PyA ligand form a zigzag one-dimensional coordination polymer along [101] (Fig. 2). There is a C—H···O

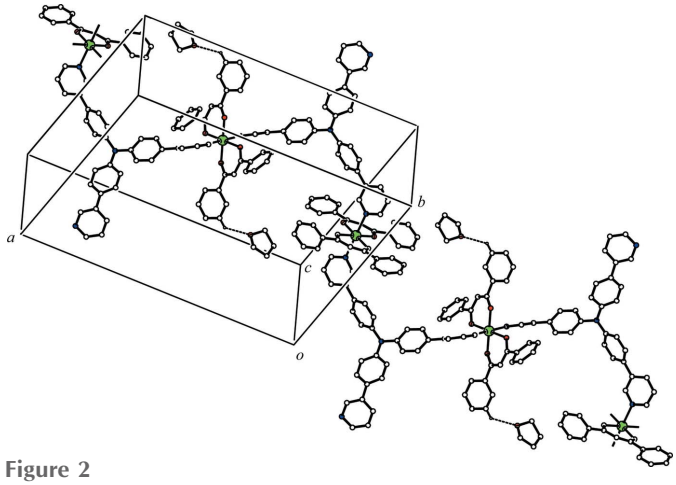


Figure 2
A packing diagram of the title compound, showing a zigzag one-dimensional coordination polymer and solvate THF molecules with the major disordered component. The C—H···O hydrogen bonds are shown as dashed lines. H atoms not involved in the interactions have been omitted for clarity.

hydrogen bond between the coordination polymer and the major disorder component of the solvate THF molecule (C13—H13···O7*A*, Table 1), while a C—H···π interaction is observed between the minor disorder component of the solvate THF molecule and the coordination polymer (C75*B*—H75*C*···*Cg*4^{ii}; *Cg*4 is the centroid of the N11/C70–C74 ring; symmetry code as in Table 1). The coordination polymer chains related by translation along the *c* axis are linked *via* a C—H···π interaction (C40—H40···*Cg*1^{i}; *Cg*1 is the centroid of the N10/C65–C69 ring; symmetry code as in Table 1) into a network sheet parallel to (010) (Fig. 3). In addition, the coordination polymer chains related by a *c*-glide plane are linked *via* C—H···π interactions (C43—H43···*Cg*2^{ii} and C68—H68···*Cg*3^{iii}; *Cg*2 and *Cg*3 are the centroids of the C54–C59 and C36–C41 rings, respectively; symmetry codes as in Table 1) (Fig. 4). The sheets parallel to (010) are cross-linked *via* these C—H···π interactions into a three-dimensional network.

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.40, update February 2019; Groom *et al.*, 2016) of the compound containing T3PyA yielded only one hit (AXUBIG; Wang *et al.*, 2016), a trinuclear palladium(II) complex with the exo-tridentate ligand bridging three palladium(II) atoms, namely, μ_3-tris[4-(pyridin-3-yl)phenyl]amine-*N*,*N*′,*N*″-tris-{[1,3-bis(2,6-diisopropylphenyl)-2,3-dihydro-1*H*-imidazol-2-ylidene]dichloropalladium(II)} ethyl acetate solvate trihydrate. A search for compounds containing tris[4-(pyridin-4-yl)phenyl]amine (T4PyA), pseudo D_3-symmetric structural isomers of T3PyA, gave 51 hits (48 compounds), including 46 hits for metal complexes (nine, twelve, eleven, seven, three, three and one hits for Zn, Co, Cd, Cu, Ni, Ag and Mn complexes, respectively). Focusing on the coordination number of T4PyA, it featured in 20 hits for the *exo*-tridentate ligand, 24 hits for the *exo*-bidentate ligand, one hit for the monodentate ligand and another hit containing both the *exo*-bidentate and the monodentate ligand. A search for the Zn(dbm)$_2$ moiety gave 34 hits (32 compounds). Limiting the search for a pyridine-coordinated Zn(dbm)$_2$ moiety gave 15 hits. Seven of these compounds are bipyridyl-ligand-bridged polymeric structures, for example, *catena*-bis(3-oxo-1,3-diphenylprop-1-enolato)-(μ_2-4,4′-bipyridyl)zinc(II) (AQIQIA; Soldatov *et al.*, 2003). In this complex, the Zn^{II} atom is ligated by the two N atoms of the 4,4′-bipyridyl ligand and the four O atoms of two β-diketonate anions, hence the Zn^{II} atom is *trans*-N_2O_4 six-coordinate, similar to that in the title compound.

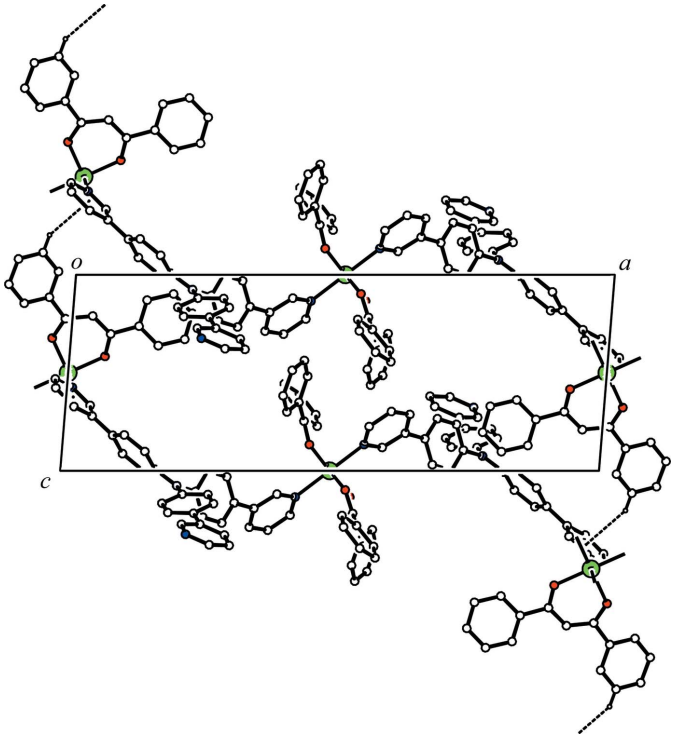


Figure 3
A packing diagram of the title compound viewed along the *b* axis, showing the network sheet structure. The C—H···π interactions between the coordination polymer chains related by translation along the *c* axis are shown as dashed lines. H atoms not involved in the interactions and all components of the disordered THF molecule have been omitted for clarity.

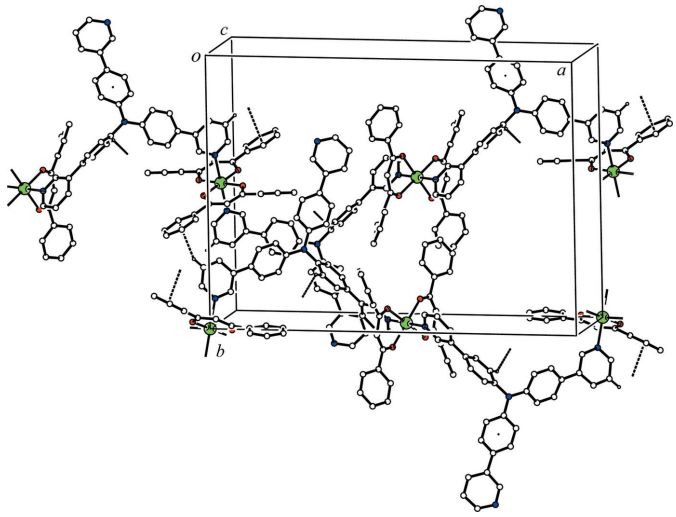


Figure 4
A packing diagram of the title compound, showing the network structure between the coordination polymer chains related by a *c*-glide plane. The C—H···π interactions are shown as dashed lines. H atoms not involved in the interactions and all components of the disordered THF molecule have been omitted for clarity.

5. Synthesis and crystallization

T3PyA was prepared by a modification of the reported Suzuki–Miyaura reaction of pyridine boronic esters (Billingsley & Buchwald, 2007). 3-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)pyridine (820 mg, 4.0 mmol), tris(4-iodophenyl)amine (623 mg, 1.0 mmol), tetrakis(triphenylphosphine)palladium(0) (23 mg, 0.02 mmol), K_3PO_4 (freshly ground, 1.27 g, 6.0 mmol) and 1-butanol (7.5 ml) were placed

in a 30 mL round-bottom flask. After the solution was purged with nitrogen for 15 min, it was heated at 398 K under nitrogen for 48 h. The solvent was removed under vacuum and the residue was redissolved in ethyl acetate. The organic layer was washed three times with water. The organic layer was then dried over Na_2SO_4 and the solvent evaporated to yield a pale-white crude product. The crude product was purified by column chromatography on silica gel [EtOAc/MeOH = 10/1 (*v*/*v*) as eluent] to yield the pure product as a white solid (375 mg, 0.79 mmol, 79%). $Zn(dbm)_2$ was prepared according to literature methods (Soldatov *et al.*, 2001). Single crystals of $\{[Zn(dbm)_2(T3PyA)]\cdot THF\}_n$ were grown by slow evaporation from a THF solution, prepared by filtering a dispersion containing 32 mg of T3PyA and 40 mg of $Zn(dbm)_2$ in 12 ml of THF. Colourless crystals suitable for X-ray diffraction were obtained after 2–3 weeks.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Hydrogen atoms were placed in geometrically calculated positions (C—H = 0.93–0.99 Å) and refined as part of a riding model with $U_{iso}(H) = 1.2U_{eq}$ (C). The solvate THF molecule is disordered over two sets of sites with refined occupancies of 0.631 (7) and 0.369 (7). *EADP* constraints and *SAME* restraints were used to model this disordered molecule. A small number of reflections affected by the beam stop and one outlier ($\bar{3}11$) were omitted from the refinement.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Zn(C_{15}H_{11}O_2)_2(C_{33}H_{24}N_4)]\cdot C_4H_8O$
M_r	1060.53
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	193
a, b, c (Å)	27.2823 (14), 19.7693 (12), 9.9674 (5)
β (°)	94.614 (7)
V (Å^3)	5358.5 (5)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.52
Crystal size (mm)	0.20 × 0.20 × 0.10
Data collection	
Diffractometer	Rigaku R-AXIS RAPID
Absorption correction	Multi-scan (*ABSCOR*; Higashi, 1995)
T_{min}, T_{max}	0.669, 0.950
No. of measured, independent and observed [$F^2 > 2.0\sigma(F^2)$] reflections	51154, 12244, 8421
R_{int}	0.083
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.058, 0.128, 1.04
No. of reflections	12244
No. of parameters	713
No. of restraints	10
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.51, −0.55

Computer programs: *RAPID-AUTO* (Rigaku, 2006), *SIR92* (Altomare *et al.*, 1993), *SHELXL2014* (Sheldrick, 2015), *PLATON* (Spek, 2009) and *CrystalStructure* (Rigaku, 2016).

Acknowledgements

We thank Professor Takahiko Kojima (University of Tsukuba) for fruitful discussions and assistance with the X-ray crystallographic experiments. We also thank Dr Masashi Saitoh (Osaka Research Institute of Industrial Science and Technology) for his helpful advice.

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supporting information

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Crystal structure of *catena*-poly[[[bis(3-oxo-1,3-diphenylprop-1-enolato-κ^2O,O')zinc(II)]-μ_2-tris[4-(pyridin-3-yl)phenyl]amine-$\kappa^2N:N'$] tetrahydrofuran monosolvate]

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Computing details

Data collection: *RAPID-AUTO* (Rigaku, 2006); cell refinement: *RAPID-AUTO* (Rigaku, 2006); data reduction: *RAPID-AUTO* (Rigaku, 2006); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *CrystalStructure* (Rigaku, 2016).

catena-Poly[[[bis(3-oxo-1,3-diphenylprop-1-enolato-κ^2O,O')zinc(II)]-μ_2-tris[4-(pyridin-3-yl)phenyl]amine-$\kappa^2N:N'$] tetrahydrofuran monosolvate]

Crystal data

$[Zn(C_{15}H_{11}O_2)_2(C_{33}H_{24}N_4)]\cdot C_4H_8O$
$M_r = 1060.53$
Monoclinic, $P2_1/c$
$a = 27.2823$ (14) Å
$b = 19.7693$ (12) Å
$c = 9.9674$ (5) Å
$\beta = 94.614$ (7)°
$V = 5358.5$ (5) Å^3
$Z = 4$
$F(000) = 2216.00$
$D_x = 1.315$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å
Cell parameters from 32853 reflections
$\theta = 3.0$–$27.5°$
$\mu = 0.52$ mm^{-1}
$T = 193$ K
Block, colorless
0.20 × 0.20 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Detector resolution: 10.000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
$T_{min} = 0.669$, $T_{max} = 0.950$
51154 measured reflections
12244 independent reflections
8421 reflections with $F^2 > 2.0\sigma(F^2)$
$R_{int} = 0.083$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
$h = -35\rightarrow33$
$k = -25\rightarrow25$
$l = -12\rightarrow12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.128$
$S = 1.04$
12244 reflections
713 parameters
10 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0403P)^2 + 4.506P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.51$ e Å^{-3}
$\Delta\rho_{min} = -0.55$ 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.

Refinement. Refinement was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating R-factor (gt).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Zn1	0.5000	0.5000	1.0000	0.02737 (11)	
Zn2	0.0000	0.5000	0.5000	0.02745 (11)	
O3	0.46823 (7)	0.41755 (9)	0.90263 (18)	0.0343 (4)	
O4	0.45865 (7)	0.56001 (9)	0.86625 (17)	0.0307 (4)	
O5	0.06591 (7)	0.50291 (10)	0.41611 (18)	0.0329 (4)	
O6	−0.03477 (7)	0.53567 (9)	0.32255 (18)	0.0304 (4)	
N8	0.21836 (8)	0.75706 (11)	1.0755 (2)	0.0303 (5)	
N9	0.43981 (8)	0.50191 (11)	1.1341 (2)	0.0302 (5)	
N10	0.00979 (8)	0.60638 (11)	0.5743 (2)	0.0308 (5)	
N11	0.24217 (12)	1.13638 (14)	1.3238 (3)	0.0608 (9)	
C12	0.40705 (12)	0.33603 (15)	0.6141 (3)	0.0412 (7)	
H12	0.3861	0.3717	0.5807	0.049*	
C13	0.40264 (14)	0.27253 (17)	0.5561 (3)	0.0517 (9)	
H13	0.3790	0.2649	0.4824	0.062*	
C14	0.43237 (13)	0.22048 (16)	0.6048 (4)	0.0535 (9)	
H14	0.4299	0.1772	0.5634	0.064*	
C15	0.46578 (13)	0.23118 (16)	0.7136 (4)	0.0526 (9)	
H15	0.4858	0.1949	0.7487	0.063*	
C16	0.47034 (11)	0.29448 (15)	0.7719 (3)	0.0413 (7)	
H16	0.4932	0.3014	0.8477	0.050*	
C17	0.44182 (10)	0.34795 (13)	0.7208 (3)	0.0310 (6)	
C18	0.45079 (10)	0.41676 (14)	0.7820 (3)	0.0304 (6)	
C19	0.44048 (10)	0.47457 (14)	0.7012 (3)	0.0314 (6)	
H19	0.4296	0.4675	0.6093	0.038*	
C20	0.44503 (9)	0.54118 (13)	0.7465 (3)	0.0274 (6)	
C21	0.43292 (9)	0.59851 (13)	0.6508 (3)	0.0264 (6)	
C22	0.41197 (10)	0.65671 (14)	0.6995 (3)	0.0328 (6)	
H22	0.4040	0.6584	0.7905	0.039*	
C23	0.40258 (12)	0.71197 (15)	0.6173 (3)	0.0441 (8)	
H23	0.3871	0.7509	0.6505	0.053*	
C24	0.41568 (14)	0.71056 (18)	0.4867 (4)	0.0576 (10)	
H24	0.4101	0.7491	0.4306	0.069*	
C25	0.43677 (14)	0.65346 (18)	0.4373 (3)	0.0541 (9)	

H25	0.4457	0.6528	0.3471	0.065*
C26	0.44509 (11)	0.59711 (16)	0.5176 (3)	0.0384 (7)
H26	0.4591	0.5575	0.4823	0.046*
C27	0.13575 (10)	0.51169 (13)	0.1293 (3)	0.0322 (6)
H27	0.1099	0.5097	0.0597	0.039*
C28	0.18406 (11)	0.50517 (15)	0.0978 (3)	0.0389 (7)
H28	0.1911	0.4978	0.0072	0.047*
C29	0.22161 (11)	0.50935 (16)	0.1968 (4)	0.0449 (8)
H29	0.2547	0.5051	0.1749	0.054*
C30	0.21144 (11)	0.51977 (18)	0.3292 (4)	0.0480 (8)
H30	0.2376	0.5236	0.3978	0.058*
C31	0.16317 (10)	0.52457 (15)	0.3615 (3)	0.0374 (7)
H31	0.1563	0.5303	0.4527	0.045*
C32	0.12475 (10)	0.52116 (13)	0.2621 (3)	0.0284 (6)
C33	0.07303 (10)	0.52595 (13)	0.3015 (3)	0.0279 (6)
C34	0.03721 (10)	0.55579 (14)	0.2102 (3)	0.0304 (6)
H34	0.0486	0.5761	0.1320	0.037*
C35	−0.01330 (9)	0.55847 (13)	0.2236 (3)	0.0263 (6)
C36	−0.04605 (10)	0.59145 (13)	0.1145 (3)	0.0283 (6)
C37	−0.09199 (10)	0.61582 (15)	0.1451 (3)	0.0346 (6)
H37	−0.1020	0.6103	0.2336	0.042*
C38	−0.12305 (11)	0.64781 (15)	0.0484 (3)	0.0412 (7)
H38	−0.1540	0.6643	0.0711	0.049*
C39	−0.10916 (11)	0.65585 (16)	−0.0810 (3)	0.0439 (8)
H39	−0.1302	0.6784	−0.1470	0.053*
C40	−0.06450 (12)	0.63083 (16)	−0.1134 (3)	0.0420 (7)
H40	−0.0551	0.6353	−0.2027	0.050*
C41	−0.03314 (10)	0.59917 (14)	−0.0170 (3)	0.0339 (6)
H41	−0.0024	0.5825	−0.0408	0.041*
C42	0.25467 (9)	0.70554 (13)	1.1048 (3)	0.0277 (6)
C43	0.27359 (10)	0.66926 (14)	1.0018 (3)	0.0308 (6)
H43	0.2615	0.6770	0.9111	0.037*
C44	0.31018 (10)	0.62179 (14)	1.0312 (3)	0.0301 (6)
H44	0.3236	0.5981	0.9597	0.036*
C45	0.32775 (9)	0.60808 (13)	1.1632 (3)	0.0268 (6)
C46	0.30764 (10)	0.64398 (14)	1.2660 (3)	0.0310 (6)
H46	0.3188	0.6353	1.3571	0.037*
C47	0.27148 (10)	0.69210 (14)	1.2365 (3)	0.0301 (6)
H47	0.2581	0.7161	1.3076	0.036*
C48	0.17551 (9)	0.74194 (13)	0.9924 (3)	0.0258 (5)
C49	0.15424 (10)	0.78918 (13)	0.9014 (3)	0.0299 (6)
H49	0.1680	0.8332	0.8976	0.036*
C50	0.11354 (10)	0.77273 (13)	0.8170 (3)	0.0307 (6)
H50	0.0997	0.8058	0.7559	0.037*
C51	0.09207 (9)	0.70849 (13)	0.8189 (3)	0.0266 (6)
C52	0.11303 (9)	0.66233 (13)	0.9123 (3)	0.0288 (6)
H52	0.0990	0.6185	0.9170	0.035*
C53	0.15362 (10)	0.67833 (13)	0.9983 (3)	0.0286 (6)

H53	0.1667	0.6459	1.0617	0.034*	
C54	0.22980 (9)	0.82375 (13)	1.1193 (3)	0.0267 (6)	
C55	0.27766 (9)	0.84818 (13)	1.1208 (3)	0.0287 (6)	
H55	0.3027	0.8203	1.0893	0.034*	
C56	0.28929 (10)	0.91228 (14)	1.1673 (3)	0.0300 (6)	
H56	0.3222	0.9280	1.1662	0.036*	
C57	0.25386 (10)	0.95476 (13)	1.2162 (3)	0.0281 (6)	
C58	0.20597 (10)	0.92973 (13)	1.2127 (3)	0.0302 (6)	
H58	0.1809	0.9576	1.2439	0.036*	
C59	0.19376 (10)	0.86593 (14)	1.1655 (3)	0.0295 (6)	
H59	0.1607	0.8506	1.1643	0.035*	
C60	0.36486 (9)	0.55430 (13)	1.1920 (3)	0.0265 (6)	
C61	0.40591 (10)	0.55061 (13)	1.1191 (3)	0.0290 (6)	
H61	0.4102	0.5849	1.0544	0.035*	
C62	0.43328 (11)	0.45340 (14)	1.2257 (3)	0.0338 (6)	
H62	0.4569	0.4181	1.2373	0.041*	
C63	0.39405 (11)	0.45289 (15)	1.3029 (3)	0.0381 (7)	
H63	0.3905	0.4177	1.3663	0.046*	
C64	0.35945 (10)	0.50436 (15)	1.2875 (3)	0.0346 (6)	
H64	0.3324	0.5054	1.3418	0.041*	
C65	0.05086 (10)	0.69018 (13)	0.7199 (3)	0.0294 (6)	
C66	0.04572 (9)	0.62529 (13)	0.6664 (3)	0.0289 (6)	
H66	0.0692	0.5922	0.6972	0.035*	
C67	−0.02290 (11)	0.65327 (15)	0.5312 (3)	0.0383 (7)	
H67	−0.0488	0.6408	0.4665	0.046*	
C68	−0.02076 (12)	0.71905 (16)	0.5767 (3)	0.0450 (8)	
H68	−0.0444	0.7512	0.5424	0.054*	
C69	0.01594 (11)	0.73772 (15)	0.6722 (3)	0.0392 (7)	
H69	0.0175	0.7828	0.7056	0.047*	
C70	0.26721 (11)	1.02246 (14)	1.2723 (3)	0.0339 (6)	
C71	0.23316 (13)	1.07453 (16)	1.2725 (3)	0.0464 (8)	
H71	0.2009	1.0657	1.2332	0.056*	
C72	0.28771 (15)	1.14791 (19)	1.3772 (4)	0.0627 (11)	
H72	0.2950	1.1912	1.4152	0.075*	
C73	0.32479 (14)	1.10082 (18)	1.3806 (4)	0.0545 (9)	
H73	0.3569	1.1117	1.4184	0.065*	
C74	0.31441 (12)	1.03756 (16)	1.3278 (3)	0.0418 (7)	
H74	0.3395	1.0042	1.3294	0.050*	
O7A	0.30876 (19)	0.3309 (4)	0.3809 (5)	0.0718 (15)	0.631 (7)
C75A	0.2656 (4)	0.3526 (8)	0.4433 (8)	0.071 (2)	0.631 (7)
H75A	0.2644	0.4026	0.4491	0.085*	0.631 (7)
H75B	0.2651	0.3335	0.5350	0.085*	0.631 (7)
C76A	0.2224 (4)	0.3257 (8)	0.3513 (9)	0.071 (2)	0.631 (7)
H76A	0.2103	0.2824	0.3859	0.085*	0.631 (7)
H76B	0.1949	0.3587	0.3443	0.085*	0.631 (7)
C77A	0.2426 (3)	0.3159 (7)	0.2184 (9)	0.064 (2)	0.631 (7)
H77A	0.2273	0.3479	0.1511	0.076*	0.631 (7)
H77B	0.2366	0.2692	0.1854	0.076*	0.631 (7)

C78A	0.2966 (4)	0.3293 (12)	0.2427 (12)	0.072 (3)	0.631 (7)
H78A	0.3154	0.2932	0.2010	0.087*	0.631 (7)
H78B	0.3049	0.3731	0.2020	0.087*	0.631 (7)
O7B	0.3004 (4)	0.3737 (6)	0.3829 (10)	0.0718 (15)	0.369 (7)
C75B	0.2723 (7)	0.3464 (15)	0.4837 (14)	0.071 (2)	0.369 (7)
H75C	0.2667	0.3807	0.5533	0.085*	0.369 (7)
H75D	0.2890	0.3067	0.5274	0.085*	0.369 (7)
C76B	0.2240 (7)	0.3260 (16)	0.4069 (17)	0.071 (2)	0.369 (7)
H76C	0.2128	0.2816	0.4389	0.085*	0.369 (7)
H76D	0.1982	0.3601	0.4196	0.085*	0.369 (7)
C77B	0.2343 (7)	0.3219 (14)	0.2619 (18)	0.064 (2)	0.369 (7)
H77C	0.2140	0.3549	0.2071	0.076*	0.369 (7)
H77D	0.2276	0.2759	0.2257	0.076*	0.369 (7)
C78B	0.2879 (8)	0.339 (2)	0.263 (2)	0.072 (3)	0.369 (7)
H78C	0.3077	0.2970	0.2592	0.087*	0.369 (7)
H78D	0.2940	0.3674	0.1845	0.087*	0.369 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0355 (2)	0.0210 (2)	0.0252 (2)	0.00777 (19)	−0.00072 (18)	−0.00111 (18)
Zn2	0.0287 (2)	0.0261 (2)	0.0277 (2)	−0.00193 (19)	0.00256 (18)	0.00102 (19)
O3	0.0497 (12)	0.0221 (10)	0.0298 (10)	0.0016 (9)	−0.0045 (9)	0.0008 (8)
O4	0.0418 (11)	0.0241 (10)	0.0253 (9)	0.0101 (8)	−0.0045 (8)	−0.0023 (8)
O5	0.0307 (9)	0.0352 (11)	0.0329 (10)	−0.0002 (9)	0.0039 (8)	0.0035 (9)
O6	0.0299 (10)	0.0306 (11)	0.0306 (10)	−0.0008 (8)	0.0020 (8)	0.0031 (8)
N8	0.0307 (12)	0.0192 (11)	0.0399 (13)	0.0023 (9)	−0.0033 (10)	−0.0039 (10)
N9	0.0360 (12)	0.0222 (11)	0.0322 (11)	0.0076 (10)	0.0006 (10)	−0.0010 (10)
N10	0.0322 (12)	0.0273 (12)	0.0323 (12)	−0.0003 (10)	−0.0010 (10)	−0.0013 (10)
N11	0.067 (2)	0.0284 (15)	0.090 (2)	−0.0033 (14)	0.0235 (18)	−0.0145 (15)
C12	0.0544 (19)	0.0268 (16)	0.0416 (17)	−0.0041 (14)	−0.0021 (15)	0.0012 (13)
C13	0.073 (2)	0.0350 (18)	0.0444 (18)	−0.0114 (17)	−0.0111 (18)	−0.0035 (15)
C14	0.071 (2)	0.0231 (16)	0.066 (2)	−0.0053 (16)	0.004 (2)	−0.0109 (16)
C15	0.053 (2)	0.0221 (16)	0.081 (3)	0.0039 (14)	−0.0039 (19)	−0.0039 (16)
C16	0.0415 (17)	0.0243 (15)	0.0567 (19)	−0.0017 (13)	−0.0043 (15)	−0.0005 (14)
C17	0.0374 (15)	0.0202 (13)	0.0356 (15)	−0.0025 (11)	0.0043 (13)	0.0009 (11)
C18	0.0338 (14)	0.0231 (14)	0.0342 (15)	0.0035 (11)	0.0025 (12)	−0.0015 (11)
C19	0.0411 (16)	0.0254 (14)	0.0266 (13)	0.0020 (12)	−0.0038 (12)	0.0004 (11)
C20	0.0274 (13)	0.0245 (14)	0.0305 (14)	0.0025 (11)	0.0034 (12)	0.0017 (11)
C21	0.0262 (13)	0.0228 (13)	0.0295 (13)	−0.0024 (11)	−0.0016 (11)	0.0023 (11)
C22	0.0366 (15)	0.0253 (15)	0.0355 (15)	0.0009 (12)	−0.0028 (13)	0.0019 (12)
C23	0.0529 (19)	0.0234 (16)	0.053 (2)	0.0018 (14)	−0.0120 (16)	0.0046 (14)
C24	0.081 (3)	0.0334 (19)	0.055 (2)	−0.0125 (18)	−0.0185 (19)	0.0205 (16)
C25	0.081 (3)	0.049 (2)	0.0326 (16)	−0.0166 (19)	0.0001 (17)	0.0128 (15)
C26	0.0490 (18)	0.0347 (17)	0.0319 (15)	−0.0063 (14)	0.0062 (14)	0.0018 (13)
C27	0.0342 (14)	0.0247 (15)	0.0379 (15)	0.0009 (11)	0.0036 (13)	0.0044 (11)
C28	0.0400 (16)	0.0296 (16)	0.0489 (17)	−0.0017 (13)	0.0153 (14)	0.0032 (14)
C29	0.0298 (15)	0.0380 (19)	0.068 (2)	−0.0031 (13)	0.0109 (15)	0.0005 (16)

C30	0.0321 (16)	0.055 (2)	0.056 (2)	−0.0032 (14)	−0.0022 (15)	−0.0050 (16)
C31	0.0328 (15)	0.0380 (16)	0.0413 (16)	−0.0035 (13)	0.0032 (13)	−0.0050 (13)
C32	0.0307 (14)	0.0156 (12)	0.0391 (15)	−0.0025 (10)	0.0049 (12)	−0.0001 (11)
C33	0.0295 (13)	0.0178 (12)	0.0368 (15)	−0.0039 (11)	0.0051 (12)	−0.0026 (11)
C34	0.0327 (14)	0.0256 (14)	0.0334 (14)	−0.0008 (11)	0.0054 (12)	0.0033 (12)
C35	0.0320 (14)	0.0167 (13)	0.0300 (13)	−0.0020 (11)	0.0006 (12)	−0.0043 (10)
C36	0.0295 (14)	0.0232 (14)	0.0318 (14)	−0.0053 (11)	0.0012 (12)	−0.0001 (11)
C37	0.0314 (14)	0.0339 (16)	0.0383 (16)	−0.0019 (12)	0.0017 (13)	−0.0002 (13)
C38	0.0332 (15)	0.0336 (17)	0.0556 (19)	0.0014 (13)	−0.0032 (14)	0.0022 (15)
C39	0.0430 (18)	0.0367 (18)	0.0492 (19)	−0.0061 (14)	−0.0122 (15)	0.0082 (15)
C40	0.0480 (18)	0.0399 (18)	0.0367 (16)	−0.0104 (15)	−0.0043 (14)	0.0057 (14)
C41	0.0343 (15)	0.0317 (16)	0.0355 (15)	−0.0058 (12)	0.0014 (13)	−0.0025 (12)
C42	0.0265 (13)	0.0207 (13)	0.0361 (14)	0.0010 (11)	0.0034 (12)	−0.0017 (11)
C43	0.0388 (15)	0.0255 (14)	0.0277 (13)	0.0045 (12)	0.0005 (12)	0.0008 (11)
C44	0.0340 (14)	0.0279 (14)	0.0287 (14)	0.0034 (12)	0.0051 (12)	−0.0032 (11)
C45	0.0279 (13)	0.0227 (13)	0.0304 (14)	0.0008 (11)	0.0056 (11)	0.0013 (11)
C46	0.0369 (15)	0.0292 (15)	0.0271 (14)	0.0040 (12)	0.0038 (12)	0.0019 (11)
C47	0.0337 (14)	0.0272 (15)	0.0299 (14)	0.0033 (12)	0.0064 (12)	−0.0047 (11)
C48	0.0262 (13)	0.0212 (13)	0.0302 (13)	0.0013 (10)	0.0030 (11)	−0.0031 (11)
C49	0.0310 (14)	0.0212 (14)	0.0374 (15)	−0.0029 (11)	0.0015 (12)	−0.0013 (11)
C50	0.0348 (15)	0.0221 (14)	0.0353 (15)	0.0035 (11)	0.0033 (12)	0.0022 (11)
C51	0.0292 (13)	0.0200 (13)	0.0310 (14)	0.0008 (11)	0.0040 (12)	−0.0025 (11)
C52	0.0314 (14)	0.0201 (13)	0.0353 (14)	−0.0024 (11)	0.0049 (12)	−0.0002 (11)
C53	0.0325 (14)	0.0215 (13)	0.0316 (14)	0.0030 (11)	0.0020 (12)	0.0006 (11)
C54	0.0301 (13)	0.0211 (13)	0.0286 (13)	0.0002 (11)	0.0007 (11)	−0.0005 (11)
C55	0.0285 (13)	0.0243 (14)	0.0337 (14)	0.0040 (11)	0.0046 (12)	−0.0004 (11)
C56	0.0280 (13)	0.0277 (14)	0.0341 (14)	−0.0045 (11)	0.0022 (12)	0.0050 (12)
C57	0.0334 (14)	0.0225 (13)	0.0284 (13)	−0.0005 (11)	0.0026 (12)	0.0011 (11)
C58	0.0323 (14)	0.0246 (14)	0.0339 (14)	0.0021 (11)	0.0050 (12)	−0.0044 (11)
C59	0.0268 (13)	0.0284 (15)	0.0337 (14)	−0.0006 (11)	0.0053 (12)	−0.0018 (12)
C60	0.0313 (14)	0.0205 (13)	0.0275 (13)	0.0018 (11)	0.0016 (11)	−0.0017 (11)
C61	0.0376 (15)	0.0209 (13)	0.0284 (13)	0.0053 (11)	0.0022 (12)	0.0022 (11)
C62	0.0401 (16)	0.0202 (14)	0.0405 (16)	0.0057 (12)	0.0001 (14)	0.0024 (12)
C63	0.0456 (17)	0.0266 (15)	0.0420 (16)	0.0023 (13)	0.0023 (14)	0.0117 (13)
C64	0.0341 (14)	0.0344 (16)	0.0357 (14)	0.0010 (13)	0.0059 (12)	0.0054 (13)
C65	0.0300 (14)	0.0244 (14)	0.0337 (14)	−0.0002 (11)	0.0034 (12)	0.0008 (11)
C66	0.0272 (13)	0.0219 (13)	0.0373 (15)	0.0023 (11)	−0.0001 (12)	−0.0001 (11)
C67	0.0368 (16)	0.0352 (17)	0.0406 (16)	0.0012 (13)	−0.0108 (13)	0.0003 (13)
C68	0.0470 (18)	0.0313 (17)	0.0537 (19)	0.0099 (14)	−0.0152 (16)	−0.0001 (14)
C69	0.0416 (16)	0.0251 (15)	0.0491 (18)	0.0034 (13)	−0.0075 (14)	−0.0033 (13)
C70	0.0418 (16)	0.0258 (14)	0.0351 (15)	−0.0057 (12)	0.0084 (13)	−0.0010 (12)
C71	0.0488 (18)	0.0295 (17)	0.062 (2)	−0.0036 (14)	0.0134 (17)	−0.0065 (15)
C72	0.076 (3)	0.037 (2)	0.079 (3)	−0.0200 (19)	0.024 (2)	−0.0221 (19)
C73	0.058 (2)	0.044 (2)	0.062 (2)	−0.0194 (17)	0.0076 (18)	−0.0151 (17)
C74	0.0472 (18)	0.0316 (17)	0.0469 (18)	−0.0088 (14)	0.0066 (15)	−0.0037 (14)
O7A	0.065 (2)	0.092 (5)	0.057 (2)	−0.002 (3)	−0.0053 (19)	0.006 (3)
C75A	0.098 (5)	0.070 (4)	0.045 (5)	0.005 (4)	0.003 (5)	0.015 (5)
C76A	0.072 (3)	0.078 (4)	0.066 (8)	−0.009 (3)	0.023 (5)	−0.012 (8)

C77A	0.064 (5)	0.057 (4)	0.069 (7)	0.002 (3)	0.005 (4)	−0.013 (5)
C78A	0.070 (5)	0.080 (8)	0.067 (5)	0.015 (6)	0.007 (3)	−0.005 (4)
O7B	0.065 (2)	0.092 (5)	0.057 (2)	−0.002 (3)	−0.0053 (19)	0.006 (3)
C75B	0.098 (5)	0.070 (4)	0.045 (5)	0.005 (4)	0.003 (5)	0.015 (5)
C76B	0.072 (3)	0.078 (4)	0.066 (8)	−0.009 (3)	0.023 (5)	−0.012 (8)
C77B	0.064 (5)	0.057 (4)	0.069 (7)	0.002 (3)	0.005 (4)	−0.013 (5)
C78B	0.070 (5)	0.080 (8)	0.067 (5)	0.015 (6)	0.007 (3)	−0.005 (4)

Geometric parameters (Å, º)

Zn1—O3^{i}	2.0528 (19)	C43—C44	1.384 (4)
Zn1—O3	2.0529 (19)	C43—H43	0.9500
Zn1—O4	2.0531 (18)	C44—C45	1.390 (4)
Zn1—O4^{i}	2.0531 (18)	C44—H44	0.9500
Zn1—N9^{i}	2.199 (2)	C45—C46	1.395 (3)
Zn1—N9	2.199 (2)	C45—C60	1.480 (4)
Zn2—O5	2.0440 (17)	C46—C47	1.385 (4)
Zn2—O5^{ii}	2.0440 (17)	C46—H46	0.9500
Zn2—O6^{ii}	2.0628 (18)	C47—H47	0.9500
Zn2—O6	2.0629 (18)	C48—C53	1.395 (4)
Zn2—N10	2.238 (2)	C48—C49	1.396 (4)
Zn2—N10^{ii}	2.238 (2)	C49—C50	1.377 (4)
O3—C18	1.257 (3)	C49—H49	0.9500
O4—C20	1.276 (3)	C50—C51	1.399 (4)
O5—C33	1.260 (3)	C50—H50	0.9500
O6—C35	1.270 (3)	C51—C52	1.393 (4)
N8—C48	1.409 (3)	C51—C65	1.480 (4)
N8—C54	1.416 (3)	C52—C53	1.381 (4)
N8—C42	1.434 (3)	C52—H52	0.9500
N9—C61	1.335 (3)	C53—H53	0.9500
N9—C62	1.346 (3)	C54—C55	1.391 (4)
N10—C67	1.333 (4)	C54—C59	1.395 (4)
N10—C66	1.341 (3)	C55—C56	1.378 (4)
N11—C72	1.331 (5)	C55—H55	0.9500
N11—C71	1.340 (4)	C56—C57	1.397 (4)
C12—C13	1.383 (4)	C56—H56	0.9500
C12—C17	1.387 (4)	C57—C58	1.395 (4)
C12—H12	0.9500	C57—C70	1.485 (4)
C13—C14	1.374 (5)	C58—C59	1.378 (4)
C13—H13	0.9500	C58—H58	0.9500
C14—C15	1.376 (5)	C59—H59	0.9500
C14—H14	0.9500	C60—C61	1.385 (4)
C15—C16	1.381 (4)	C60—C64	1.388 (4)
C15—H15	0.9500	C61—H61	0.9500
C16—C17	1.385 (4)	C62—C63	1.367 (4)
C16—H16	0.9500	C62—H62	0.9500
C17—C18	1.503 (4)	C63—C64	1.388 (4)
C18—C19	1.413 (4)	C63—H63	0.9500

C19—C20	1.395 (4)	C64—H64	0.9500
C19—H19	0.9500	C65—C66	1.392 (4)
C20—C21	1.501 (4)	C65—C69	1.394 (4)
C21—C22	1.390 (4)	C66—H66	0.9500
C21—C26	1.395 (4)	C67—C68	1.377 (4)
C22—C23	1.377 (4)	C67—H67	0.9500
C22—H22	0.9500	C68—C69	1.376 (4)
C23—C24	1.377 (5)	C68—H68	0.9500
C23—H23	0.9500	C69—H69	0.9500
C24—C25	1.376 (5)	C70—C71	1.387 (4)
C24—H24	0.9500	C70—C74	1.393 (4)
C25—C26	1.380 (4)	C71—H71	0.9500
C25—H25	0.9500	C72—C73	1.373 (5)
C26—H26	0.9500	C72—H72	0.9500
C27—C28	1.385 (4)	C73—C74	1.377 (4)
C27—C32	1.394 (4)	C73—H73	0.9500
C27—H27	0.9500	C74—H74	0.9500
C28—C29	1.366 (4)	O7A—C78A	1.391 (12)
C28—H28	0.9500	O7A—C75A	1.441 (11)
C29—C30	1.386 (5)	C75A—C76A	1.529 (9)
C29—H29	0.9500	C75A—H75A	0.9900
C30—C31	1.384 (4)	C75A—H75B	0.9900
C30—H30	0.9500	C76A—C77A	1.489 (8)
C31—C32	1.385 (4)	C76A—H76A	0.9900
C31—H31	0.9500	C76A—H76B	0.9900
C32—C33	1.498 (4)	C77A—C78A	1.496 (9)
C33—C34	1.410 (4)	C77A—H77A	0.9900
C34—C35	1.396 (4)	C77A—H77B	0.9900
C34—H34	0.9500	C78A—H78A	0.9900
C35—C36	1.500 (4)	C78A—H78B	0.9900
C36—C41	1.392 (4)	O7B—C78B	1.399 (15)
C36—C37	1.399 (4)	O7B—C75B	1.418 (14)
C37—C38	1.384 (4)	C75B—C76B	1.525 (14)
C37—H37	0.9500	C75B—H75C	0.9900
C38—C39	1.383 (4)	C75B—H75D	0.9900
C38—H38	0.9500	C76B—C77B	1.496 (13)
C39—C40	1.377 (4)	C76B—H76C	0.9900
C39—H39	0.9500	C76B—H76D	0.9900
C40—C41	1.384 (4)	C77B—C78B	1.500 (14)
C40—H40	0.9500	C77B—H77C	0.9900
C41—H41	0.9500	C77B—H77D	0.9900
C42—C47	1.381 (4)	C78B—H78C	0.9900
C42—C43	1.386 (4)	C78B—H78D	0.9900

O3^{i}—Zn1—O3	180.0	C45—C44—H44	119.3
O3^{i}—Zn1—O4	92.14 (8)	C44—C45—C46	118.0 (2)
O3—Zn1—O4	87.87 (8)	C44—C45—C60	120.1 (2)
O3^{i}—Zn1—O4^{i}	87.86 (8)	C46—C45—C60	121.8 (2)

O3—Zn1—O4^{i}	92.14 (8)	C47—C46—C45	120.6 (2)
O4—Zn1—O4^{i}	180.0	C47—C46—H46	119.7
O3^{i}—Zn1—N9^{i}	89.62 (8)	C45—C46—H46	119.7
O3—Zn1—N9^{i}	90.38 (8)	C42—C47—C46	120.7 (2)
O4—Zn1—N9^{i}	90.77 (8)	C42—C47—H47	119.7
O4^{i}—Zn1—N9^{i}	89.23 (8)	C46—C47—H47	119.7
O3^{i}—Zn1—N9	90.38 (8)	C53—C48—C49	118.2 (2)
O3—Zn1—N9	89.62 (8)	C53—C48—N8	120.3 (2)
O4—Zn1—N9	89.23 (8)	C49—C48—N8	121.5 (2)
O4^{i}—Zn1—N9	90.77 (8)	C50—C49—C48	120.8 (2)
N9^{i}—Zn1—N9	180.00 (7)	C50—C49—H49	119.6
O5—Zn2—O5^{ii}	180.0	C48—C49—H49	119.6
O5—Zn2—O6^{ii}	90.08 (7)	C49—C50—C51	121.6 (3)
O5^{ii}—Zn2—O6^{ii}	89.92 (7)	C49—C50—H50	119.2
O5—Zn2—O6	89.92 (7)	C51—C50—H50	119.2
O5^{ii}—Zn2—O6	90.08 (7)	C52—C51—C50	117.0 (2)
O6^{ii}—Zn2—O6	180.0	C52—C51—C65	122.3 (2)
O5—Zn2—N10	91.34 (8)	C50—C51—C65	120.6 (2)
O5^{ii}—Zn2—N10	88.66 (8)	C53—C52—C51	122.0 (2)
O6^{ii}—Zn2—N10	90.18 (8)	C53—C52—H52	119.0
O6—Zn2—N10	89.82 (8)	C51—C52—H52	119.0
O5—Zn2—N10^{ii}	88.66 (8)	C52—C53—C48	120.3 (2)
O5^{ii}—Zn2—N10^{ii}	91.34 (8)	C52—C53—H53	119.8
O6^{ii}—Zn2—N10^{ii}	89.82 (8)	C48—C53—H53	119.8
O6—Zn2—N10^{ii}	90.18 (8)	C55—C54—C59	118.3 (2)
N10—Zn2—N10^{ii}	180.0	C55—C54—N8	120.7 (2)
C18—O3—Zn1	125.10 (17)	C59—C54—N8	121.0 (2)
C20—O4—Zn1	122.82 (16)	C56—C55—C54	120.9 (2)
C33—O5—Zn2	125.89 (18)	C56—C55—H55	119.6
C35—O6—Zn2	125.35 (17)	C54—C55—H55	119.6
C48—N8—C54	122.0 (2)	C55—C56—C57	121.5 (2)
C48—N8—C42	119.7 (2)	C55—C56—H56	119.2
C54—N8—C42	117.8 (2)	C57—C56—H56	119.2
C61—N9—C62	117.5 (2)	C58—C57—C56	116.8 (2)
C61—N9—Zn1	119.27 (18)	C58—C57—C70	122.0 (2)
C62—N9—Zn1	123.11 (18)	C56—C57—C70	121.2 (2)
C67—N10—C66	117.4 (2)	C59—C58—C57	122.2 (2)
C67—N10—Zn2	119.21 (19)	C59—C58—H58	118.9
C66—N10—Zn2	123.32 (18)	C57—C58—H58	118.9
C72—N11—C71	116.5 (3)	C58—C59—C54	120.2 (2)
C13—C12—C17	120.4 (3)	C58—C59—H59	119.9
C13—C12—H12	119.8	C54—C59—H59	119.9
C17—C12—H12	119.8	C61—C60—C64	117.2 (2)
C14—C13—C12	120.2 (3)	C61—C60—C45	120.3 (2)
C14—C13—H13	119.9	C64—C60—C45	122.4 (2)
C12—C13—H13	119.9	N9—C61—C60	124.2 (2)
C13—C14—C15	119.9 (3)	N9—C61—H61	117.9
C13—C14—H14	120.1	C60—C61—H61	117.9

C15—C14—H14	120.1	N9—C62—C63	122.7 (3)
C14—C15—C16	120.2 (3)	N9—C62—H62	118.7
C14—C15—H15	119.9	C63—C62—H62	118.7
C16—C15—H15	119.9	C62—C63—C64	119.2 (3)
C15—C16—C17	120.5 (3)	C62—C63—H63	120.4
C15—C16—H16	119.7	C64—C63—H63	120.4
C17—C16—H16	119.7	C60—C64—C63	119.2 (2)
C16—C17—C12	118.8 (3)	C60—C64—H64	120.4
C16—C17—C18	118.2 (3)	C63—C64—H64	120.4
C12—C17—C18	123.0 (3)	C66—C65—C69	116.5 (3)
O3—C18—C19	125.3 (3)	C66—C65—C51	121.9 (2)
O3—C18—C17	115.9 (2)	C69—C65—C51	121.6 (2)
C19—C18—C17	118.8 (2)	N10—C66—C65	124.4 (2)
C20—C19—C18	124.8 (2)	N10—C66—H66	117.8
C20—C19—H19	117.6	C65—C66—H66	117.8
C18—C19—H19	117.6	N10—C67—C68	122.8 (3)
O4—C20—C19	126.1 (2)	N10—C67—H67	118.6
O4—C20—C21	114.0 (2)	C68—C67—H67	118.6
C19—C20—C21	119.9 (2)	C69—C68—C67	119.4 (3)
C22—C21—C26	119.0 (3)	C69—C68—H68	120.3
C22—C21—C20	118.6 (2)	C67—C68—H68	120.3
C26—C21—C20	122.2 (2)	C68—C69—C65	119.6 (3)
C23—C22—C21	120.7 (3)	C68—C69—H69	120.2
C23—C22—H22	119.6	C65—C69—H69	120.2
C21—C22—H22	119.6	C71—C70—C74	116.0 (3)
C22—C23—C24	119.7 (3)	C71—C70—C57	121.7 (3)
C22—C23—H23	120.1	C74—C70—C57	122.3 (3)
C24—C23—H23	120.1	N11—C71—C70	125.1 (3)
C25—C24—C23	120.2 (3)	N11—C71—H71	117.4
C25—C24—H24	119.9	C70—C71—H71	117.4
C23—C24—H24	119.9	N11—C72—C73	123.7 (3)
C24—C25—C26	120.6 (3)	N11—C72—H72	118.1
C24—C25—H25	119.7	C73—C72—H72	118.1
C26—C25—H25	119.7	C72—C73—C74	118.5 (3)
C25—C26—C21	119.7 (3)	C72—C73—H73	120.7
C25—C26—H26	120.1	C74—C73—H73	120.7
C21—C26—H26	120.1	C73—C74—C70	120.1 (3)
C28—C27—C32	120.6 (3)	C73—C74—H74	119.9
C28—C27—H27	119.7	C70—C74—H74	119.9
C32—C27—H27	119.7	C78A—O7A—C75A	107.2 (7)
C29—C28—C27	120.2 (3)	O7A—C75A—C76A	104.8 (8)
C29—C28—H28	119.9	O7A—C75A—H75A	110.8
C27—C28—H28	119.9	C76A—C75A—H75A	110.8
C28—C29—C30	120.0 (3)	O7A—C75A—H75B	110.8
C28—C29—H29	120.0	C76A—C75A—H75B	110.8
C30—C29—H29	120.0	H75A—C75A—H75B	108.9
C31—C30—C29	119.9 (3)	C77A—C76A—C75A	104.7 (6)
C31—C30—H30	120.0	C77A—C76A—H76A	110.8

C29—C30—H30	120.0	C75A—C76A—H76A	110.8
C30—C31—C32	120.7 (3)	C77A—C76A—H76B	110.8
C30—C31—H31	119.7	C75A—C76A—H76B	110.8
C32—C31—H31	119.7	H76A—C76A—H76B	108.9
C31—C32—C27	118.5 (2)	C76A—C77A—C78A	105.3 (7)
C31—C32—C33	119.0 (2)	C76A—C77A—H77A	110.7
C27—C32—C33	122.5 (3)	C78A—C77A—H77A	110.7
O5—C33—C34	125.9 (2)	C76A—C77A—H77B	110.7
O5—C33—C32	115.6 (2)	C78A—C77A—H77B	110.7
C34—C33—C32	118.4 (2)	H77A—C77A—H77B	108.8
C35—C34—C33	126.4 (2)	O7A—C78A—C77A	108.5 (8)
C35—C34—H34	116.8	O7A—C78A—H78A	110.0
C33—C34—H34	116.8	C77A—C78A—H78A	110.0
O6—C35—C34	125.5 (2)	O7A—C78A—H78B	110.0
O6—C35—C36	115.6 (2)	C77A—C78A—H78B	110.0
C34—C35—C36	118.9 (2)	H78A—C78A—H78B	108.4
C41—C36—C37	117.8 (3)	C78B—O7B—C75B	108.0 (16)
C41—C36—C35	123.3 (2)	O7B—C75B—C76B	103.9 (11)
C37—C36—C35	118.9 (2)	O7B—C75B—H75C	111.0
C38—C37—C36	121.0 (3)	C76B—C75B—H75C	111.0
C38—C37—H37	119.5	O7B—C75B—H75D	111.0
C36—C37—H37	119.5	C76B—C75B—H75D	111.0
C39—C38—C37	120.3 (3)	H75C—C75B—H75D	109.0
C39—C38—H38	119.9	C77B—C76B—C75B	106.1 (11)
C37—C38—H38	119.9	C77B—C76B—H76C	110.5
C40—C39—C38	119.4 (3)	C75B—C76B—H76C	110.5
C40—C39—H39	120.3	C77B—C76B—H76D	110.5
C38—C39—H39	120.3	C75B—C76B—H76D	110.5
C39—C40—C41	120.6 (3)	H76C—C76B—H76D	108.7
C39—C40—H40	119.7	C76B—C77B—C78B	103.9 (12)
C41—C40—H40	119.7	C76B—C77B—H77C	111.0
C40—C41—C36	121.0 (3)	C78B—C77B—H77C	111.0
C40—C41—H41	119.5	C76B—C77B—H77D	111.0
C36—C41—H41	119.5	C78B—C77B—H77D	111.0
C47—C42—C43	119.3 (2)	H77C—C77B—H77D	109.0
C47—C42—N8	120.1 (2)	O7B—C78B—C77B	106.7 (12)
C43—C42—N8	120.6 (2)	O7B—C78B—H78C	110.4
C44—C43—C42	120.0 (3)	C77B—C78B—H78C	110.4
C44—C43—H43	120.0	O7B—C78B—H78D	110.4
C42—C43—H43	120.0	C77B—C78B—H78D	110.4
C43—C44—C45	121.4 (2)	H78C—C78B—H78D	108.6
C43—C44—H44	119.3		

C17—C12—C13—C14	0.7 (5)	C54—N8—C48—C53	−151.5 (2)
C12—C13—C14—C15	1.6 (5)	C42—N8—C48—C53	35.9 (3)
C13—C14—C15—C16	−1.6 (5)	C54—N8—C48—C49	29.4 (4)
C14—C15—C16—C17	−0.7 (5)	C42—N8—C48—C49	−143.2 (2)
C15—C16—C17—C12	3.0 (4)	C53—C48—C49—C50	−1.8 (4)

C15—C16—C17—C18	−175.8 (3)	N8—C48—C49—C50	177.3 (2)
C13—C12—C17—C16	−3.0 (4)	C48—C49—C50—C51	−0.1 (4)
C13—C12—C17—C18	175.7 (3)	C49—C50—C51—C52	1.4 (4)
Zn1—O3—C18—C19	−14.1 (4)	C49—C50—C51—C65	−175.0 (2)
Zn1—O3—C18—C17	164.23 (17)	C50—C51—C52—C53	−0.9 (4)
C16—C17—C18—O3	−26.9 (4)	C65—C51—C52—C53	175.5 (2)
C12—C17—C18—O3	154.4 (3)	C51—C52—C53—C48	−0.9 (4)
C16—C17—C18—C19	151.6 (3)	C49—C48—C53—C52	2.3 (4)
C12—C17—C18—C19	−27.1 (4)	N8—C48—C53—C52	−176.8 (2)
O3—C18—C19—C20	−4.6 (5)	C48—N8—C54—C55	−138.1 (3)
C17—C18—C19—C20	177.1 (3)	C42—N8—C54—C55	34.6 (4)
Zn1—O4—C20—C19	22.9 (4)	C48—N8—C54—C59	43.6 (4)
Zn1—O4—C20—C21	−157.62 (16)	C42—N8—C54—C59	−143.6 (3)
C18—C19—C20—O4	−0.5 (5)	C59—C54—C55—C56	0.3 (4)
C18—C19—C20—C21	−180.0 (2)	N8—C54—C55—C56	−177.9 (2)
O4—C20—C21—C22	−33.9 (3)	C54—C55—C56—C57	0.8 (4)
C19—C20—C21—C22	145.6 (3)	C55—C56—C57—C58	−1.4 (4)
O4—C20—C21—C26	141.5 (3)	C55—C56—C57—C70	177.0 (3)
C19—C20—C21—C26	−39.0 (4)	C56—C57—C58—C59	0.9 (4)
C26—C21—C22—C23	1.0 (4)	C70—C57—C58—C59	−177.5 (3)
C20—C21—C22—C23	176.6 (3)	C57—C58—C59—C54	0.2 (4)
C21—C22—C23—C24	−2.3 (5)	C55—C54—C59—C58	−0.8 (4)
C22—C23—C24—C25	1.9 (5)	N8—C54—C59—C58	177.4 (2)
C23—C24—C25—C26	−0.1 (6)	C44—C45—C60—C61	47.1 (4)
C24—C25—C26—C21	−1.3 (5)	C46—C45—C60—C61	−136.1 (3)
C22—C21—C26—C25	0.8 (4)	C44—C45—C60—C64	−130.2 (3)
C20—C21—C26—C25	−174.6 (3)	C46—C45—C60—C64	46.6 (4)
C32—C27—C28—C29	−1.3 (4)	C62—N9—C61—C60	0.2 (4)
C27—C28—C29—C30	0.3 (5)	Zn1—N9—C61—C60	175.8 (2)
C28—C29—C30—C31	1.3 (5)	C64—C60—C61—N9	0.9 (4)
C29—C30—C31—C32	−2.0 (5)	C45—C60—C61—N9	−176.6 (3)
C30—C31—C32—C27	1.0 (4)	C61—N9—C62—C63	−0.5 (4)
C30—C31—C32—C33	179.5 (3)	Zn1—N9—C62—C63	−175.9 (2)
C28—C27—C32—C31	0.6 (4)	N9—C62—C63—C64	−0.3 (5)
C28—C27—C32—C33	−177.7 (2)	C61—C60—C64—C63	−1.7 (4)
Zn2—O5—C33—C34	1.8 (4)	C45—C60—C64—C63	175.7 (3)
Zn2—O5—C33—C32	−178.96 (16)	C62—C63—C64—C60	1.5 (4)
C31—C32—C33—O5	−30.8 (4)	C52—C51—C65—C66	−32.2 (4)
C27—C32—C33—O5	147.5 (3)	C50—C51—C65—C66	144.0 (3)
C31—C32—C33—C34	148.5 (3)	C52—C51—C65—C69	149.8 (3)
C27—C32—C33—C34	−33.1 (4)	C50—C51—C65—C69	−34.0 (4)
O5—C33—C34—C35	−7.6 (5)	C67—N10—C66—C65	0.3 (4)
C32—C33—C34—C35	173.1 (2)	Zn2—N10—C66—C65	−176.1 (2)
Zn2—O6—C35—C34	8.4 (4)	C69—C65—C66—N10	−0.3 (4)
Zn2—O6—C35—C36	−170.81 (16)	C51—C65—C66—N10	−178.4 (2)
C33—C34—C35—O6	1.9 (4)	C66—N10—C67—C68	0.4 (4)
C33—C34—C35—C36	−178.9 (3)	Zn2—N10—C67—C68	177.0 (2)
O6—C35—C36—C41	−158.3 (3)	N10—C67—C68—C69	−1.2 (5)

C34—C35—C36—C41	22.5 (4)	C67—C68—C69—C65	1.1 (5)
O6—C35—C36—C37	21.6 (3)	C66—C65—C69—C68	−0.4 (4)
C34—C35—C36—C37	−157.6 (3)	C51—C65—C69—C68	177.7 (3)
C41—C36—C37—C38	−1.4 (4)	C58—C57—C70—C71	−27.2 (4)
C35—C36—C37—C38	178.7 (3)	C56—C57—C70—C71	154.5 (3)
C36—C37—C38—C39	0.4 (5)	C58—C57—C70—C74	152.7 (3)
C37—C38—C39—C40	1.0 (5)	C56—C57—C70—C74	−25.6 (4)
C38—C39—C40—C41	−1.4 (5)	C72—N11—C71—C70	0.7 (5)
C39—C40—C41—C36	0.4 (4)	C74—C70—C71—N11	−1.5 (5)
C37—C36—C41—C40	1.0 (4)	C57—C70—C71—N11	178.5 (3)
C35—C36—C41—C40	−179.1 (3)	C71—N11—C72—C73	0.7 (6)
C48—N8—C42—C47	−128.3 (3)	N11—C72—C73—C74	−1.1 (6)
C54—N8—C42—C47	58.8 (3)	C72—C73—C74—C70	0.2 (5)
C48—N8—C42—C43	52.4 (3)	C71—C70—C74—C73	1.0 (4)
C54—N8—C42—C43	−120.5 (3)	C57—C70—C74—C73	−179.0 (3)
C47—C42—C43—C44	−2.2 (4)	C78A—O7A—C75A—C76A	31.5 (15)
N8—C42—C43—C44	177.1 (2)	O7A—C75A—C76A—C77A	−22.7 (14)
C42—C43—C44—C45	1.7 (4)	C75A—C76A—C77A—C78A	6.4 (17)
C43—C44—C45—C46	−0.4 (4)	C75A—O7A—C78A—C77A	−28.1 (18)
C43—C44—C45—C60	176.5 (2)	C76A—C77A—C78A—O7A	12.8 (19)
C44—C45—C46—C47	−0.4 (4)	C78B—O7B—C75B—C76B	−33 (3)
C60—C45—C46—C47	−177.3 (3)	O7B—C75B—C76B—C77B	19 (3)
C43—C42—C47—C46	1.4 (4)	C75B—C76B—C77B—C78B	1 (3)
N8—C42—C47—C46	−178.0 (2)	C75B—O7B—C78B—C77B	35 (3)
C45—C46—C47—C42	−0.1 (4)	C76B—C77B—C78B—O7B	−21 (4)

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

Hydrogen-bond geometry (Å, º)

*Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of the N10/C65–C69, C54–C59, C36–C41 and N11/C70–C74 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···O7*A*	0.95	2.47	3.197 (7)	134
C40—H40···*Cg*1^{iii}	0.95	2.74	3.594 (3)	150
C43—H43···*Cg*2^{iv}	0.95	2.78	3.572 (3)	142
C68—H68···*Cg*3^{v}	0.95	2.65	3.513 (3)	152
C75*B*—H75*C*···*Cg*4^{iv}	0.99	2.78	3.649 (17)	146

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