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Bis[μ-2-hydroxy-*N*′-(4-hydroxy-2-oxidobenzylidene)benzohydrazide]-bis[pyridinezinc(II)] dimethylformamide disolvate

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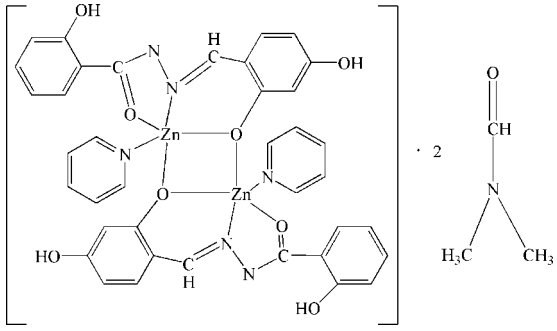
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.005 Å; R factor = 0.048; wR factor = 0.130; data-to-parameter ratio = 17.3.

Reaction of 2,4-dihydroxybenzaldehye salicylhydrazide (L) with $Zn(OAc)_2\cdot 2H_2O$ in a mixed solvent of pyridine and *N*,*N*-dimethylformamide (DMF) resulted in the formation of the title complex, $[Zn_2(C_{14}H_{10}N_2O_4)_2(C_5H_5N)_2]\cdot 2C_3H_7NO$. The asymmetric unit contains one complete neutral zinc complex and one-half of a second complex with crystallographic inversion symmetry, together with three DMF solvent molecules. The Zn atoms, all having the same coordination geometry, are coordinated by three O atoms and two N atoms in a distorted tetragonal–pyramidal geometry, with phenolate O atoms acting as bridges between the Zn atoms.

Related literature

For chemically related materials arising from metal–Schiff base compounds which contain Zn coordinated by N and O atoms, see: Hu *et al.* (2005, 2006). For details of the preparation of the Schiff base, see: Liu *et al.* (2001). For related literature, see: Ando *et al.* (2004); Maurya *et al.* (2005); Schurig *et al.* (1980); Siddall *et al.* (1983).



Experimental

Crystal data

$[Zn_2(C_{14}H_{10}N_2O_4)_2(C_5H_5N)_2]\cdot 2C_3H_7NO$
M_r = 975.61
Monoclinic, $P2_1/c$
a = 24.5015 (16) Å
b = 10.3868 (7) Å
c = 28.8550 (18) Å
β = 113.127 (1)°
V = 6753.2 (8) Å^3
Z = 6
Mo $K\alpha$ radiation
μ = 1.13 mm^{-1}
T = 292 (2) K
0.20 × 0.16 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.805, T_{max} = 0.895
45215 measured reflections
15421 independent reflections
9826 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.130
S = 1.01
15421 reflections
889 parameters
8 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N7—Zn3	2.042 (2)	N6—Zn2	2.051 (2)
N9—Zn3	2.064 (2)	O2—Zn2	1.9976 (17)
O10—Zn3	2.0798 (18)	O2—Zn1	2.0859 (17)
O11—Zn3	2.0316 (18)	O3—Zn1	2.0388 (18)
N1—Zn1	2.033 (2)	O6—Zn1	1.9834 (18)
N3—Zn2	2.045 (2)	O6—Zn2	2.1035 (17)
N5—Zn1	2.056 (2)	O7—Zn2	2.0372 (18)
O6—Zn1—N1	145.01 (9)	O2—Zn2—N3	137.52 (9)
O6—Zn1—O3	105.16 (8)	O7—Zn2—N3	77.84 (8)
N1—Zn1—O3	77.87 (8)	O10^{i}—Zn3—O11	105.13 (8)
O6—Zn1—O2	79.55 (7)	O10^{i}—Zn3—N7	142.28 (9)
N1—Zn1—O2	86.86 (8)	O10^{i}—Zn3—O10	78.66 (7)
O3—Zn1—O2	159.26 (8)	O10^{i}—Zn3—Zn3^{i}	40.37 (5)
O2—Zn2—O7	106.32 (7)	O11—Zn3—Zn3^{i}	141.28 (6)

Symmetry code: (i) $-x, -y+2, -z+2$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···N2	0.80 (5)	1.89 (3)	2.595 (3)	147 (5)
O12—H12···N8	0.82 (3)	1.94 (4)	2.575 (3)	134 (5)
O8—H8···N4	0.87 (3)	1.77 (4)	2.546 (3)	147 (5)

Symmetry codes: .

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2000); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2107).

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supplementary materials

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Bis[μ-2-hydroxy-*N*'-(4-hydroxy-2-oxidobenzylidene)benzohydrazide]bis[pyridinezinc(II)] dimethylformamide disolvate

J.-S. Huang and M.-T. Li

Comment

Studies of Schiff bases and their metal compounds are of current interest owing to their wide range of applications as biocides and homogeneous catalysts in the industry, antitumor activities and structural elucidation (Schurig *et al.*, 1980; Siddall *et al.*, 1983, Ando *et al.*, 2004; Maurya *et al.*, 2005). We report here the crystal structure of such a Zn(II) Schiff base compound, (I) $[Zn_2(L)_2(py)_2]\cdot 2DMF$, (*L* is 2,4-dihydroxybenzaldehyde salicylhydrazide, py is pyridine and DMF is *N*,*N*-dimethylformamide).

The molecular structure of (I) is shown in Fig.1. The crystal structure of the title complex consists of neutral binuclear Zn(II) dimers and solvent DMF molecules. Selected bond lengths and angles are given in Table 1. There are crystallographically independent zinc(II) centers with identical coordination geometry within the asymmetric unit of the title complex. All Zn(II) atoms are coordinated by three O atoms and two N atoms, in a distorted tetragonal-pyramidal geometry, due to the different distances of Zn—O and Zn—N. Three O atoms and one N atom from *L* ligands are located in the basal plane of the distorted square pyramid, and the apical position is occupied by an N atom belonging to a pyridine molecule. The Zn atoms are displaced by 0.4519 (3), 0.045 (3) and 0.4810 (3) Å, respectively, for Zn1, Zn2 and Zn3 out of the basal planes. Pairs of zinc atoms are bridged by two phenolate O atoms, to give a neutral dimer containing a planar Zn_2O_2 ring. It is interesting that the plane constructed by Zn1, Zn2, O2 and O6 is asymmetric because of the slight differences in coordination bonds and angles; however, the other dinuclear complex containing Zn3 has exact inversion symmetry. The distances of Zn—N and Zn—O (Table 1) are in agreement with the complex $[Zn_2(dhaash)_2(py)_4]$ (H_2dhaash is 2,4-dihydroxy-5-acetylacetophenone-N-salicylhydrazone; Zn—N, 2.0818 (19), 2.255 (2) and 2.234 (2) Å; Zn—O, 2.234 (2), 2.0511 (17) and 2.085 (17) Å) (Hu *et al.*, 2006). The Zn···Zn distances are 3.147 (2) and 3.149 (2) Å for Zn1···Zn2 and Zn3····Zn3a (a: $-x$, $-y$, $-z$), respectively, which are comparable with those of the complex $[Zn_2(dhaash)_2(py)_4]$.

The ligand *L*, acting in a tridentate mode through the imide N, phenolate O and carbonyl O, forms two five/six-membered chelate rings. The dihedral angle of the pyridine molecules coordinated to Zn1 and Zn2 is 48.88 (18)°, whereas it is exactly zero by symmetry in the Zn3 complex.

Although DMF molecules are uncoordinated to metal atoms, they play an important role in stabilizing the crystal structure of the title complex. O—H···N hydrogen bonds are formed by the phenolic hydroxyl groups and N atoms belonging to DMF molecules.

Experimental

2,4-Dihydroxybenzaldehyde salicylhydrazide was prepared by a standard method reported in the literature (Liu *et al.*, 2001). To a solution of 2,4-dihydroxybenzaldehyde salicylhydrazide (0.136 g, 0.5 mmol) in DMF (10 ml) was added $Zn(OAc)_2\cdot 2H_2O$ (0.110 g, 1 mmol) dissolved in pyridine (5 ml). The mixture was stirred for 5 h at 323 K. After filtering, the

yellow solution was allowed to stand at room temperature. Well shaped yellow block-like crystals were obtained by slow evaporation of the solvent at room temperature after seven days.

Refinement

All H atoms were initially located in a difference Fourier map. The hydroxyl H atoms were then refined with the distance restraint O—H = 0.83 (3) Å and with U_{iso}(H) = 1.5U_{eq}(O). All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances of 0.93–0.96 Å and U_{iso}(H) = 1.2U_{eq}(C) [U_{iso}(H) = 1.5U_{eq}(C) for methyl groups].

Figures

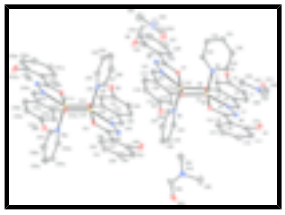

Fig. 1. Molecular structure of the title complex, showing labelling of the non-H atoms and 20% probability ellipsoids.

Bis[μ-2-hydroxy-*N*'-(4-hydroxy-2- oxidobenzylidene)benzohydrazide]bis[pyridinezinc(II)] dimethylformamide disolvate

Crystal data

$[Zn_2(C_{14}H_{10}N_2O_4)_2(C_5H_5N)_2]\cdot 2C_3H_7NO$	F_{000} = 3024
M_r = 975.61	D_x = 1.439 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P2ybc	Cell parameters from 8439 reflections
a = 24.5015 (16) Å	θ = 2.2–24.1º
b = 10.3868 (7) Å	μ = 1.13 mm^{-1}
c = 28.8550 (18) Å	T = 292 (2) K
β = 113.127 (1)º	Block, yellow
V = 6753.2 (8) Å^3	0.20 × 0.16 × 0.10 mm
Z = 6	

Data collection

Bruker SMART CCD area-detector diffractometer	15421 independent reflections
Radiation source: fine-focus sealed tube	9826 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.042
T = 292(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 0.9º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	h = −31→31

T_{min} = 0.805, T_{max} = 0.895
45215 measured reflections
k = −13→13
l = −37→33

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.130
S = 1.01
15421 reflections
889 parameters
8 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0567P)^2 + 0.3991P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.019
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}
Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C39	−0.13981 (15)	1.1389 (3)	0.83565 (12)	0.0698 (10)
H39	−0.1424	1.1270	0.8029	0.084*
C40	−0.18049 (15)	1.2164 (3)	0.84285 (12)	0.0716 (10)
H40	−0.2098	1.2571	0.8157	0.086*
C41	−0.17738 (13)	1.2335 (3)	0.89139 (12)	0.0570 (8)
C42	−0.13180 (12)	1.1765 (3)	0.93168 (11)	0.0498 (7)
H42	−0.1293	1.1915	0.9642	0.060*
C43	−0.09024 (12)	1.0985 (3)	0.92473 (10)	0.0425 (6)
C44	−0.09424 (13)	1.0761 (3)	0.87489 (11)	0.0511 (7)
C45	−0.05620 (13)	0.9916 (3)	0.86169 (11)	0.0555 (8)
H45	−0.0621	0.9880	0.8279	0.067*
C46	0.05520 (12)	0.7705 (3)	0.90646 (11)	0.0465 (7)
C47	0.09223 (13)	0.6838 (3)	0.89027 (12)	0.0538 (8)
C48	0.08175 (17)	0.6626 (4)	0.83995 (15)	0.0757 (11)

C49	0.1161 (2)	0.5736 (4)	0.82740 (17)	0.0942 (13)
H49	0.1081	0.5570	0.7937	0.113*
C50	0.16137 (19)	0.5107 (4)	0.86387 (19)	0.0927 (14)
H50	0.1841	0.4519	0.8549	0.111*
C51	0.17375 (17)	0.5333 (4)	0.91381 (17)	0.0871 (12)
H51	0.2052	0.4916	0.9388	0.105*
C52	0.13887 (15)	0.6184 (3)	0.92632 (14)	0.0710 (10)
H52	0.1469	0.6326	0.9602	0.085*
C53	−0.10147 (16)	0.7683 (4)	0.97847 (14)	0.0773 (11)
H53	−0.1066	0.8520	0.9874	0.093*
C54	−0.14351 (18)	0.6781 (5)	0.97527 (17)	0.0975 (14)
H54	−0.1765	0.7007	0.9819	0.117*
C55	−0.13668 (19)	0.5562 (4)	0.96245 (16)	0.0903 (13)
H55	−0.1640	0.4928	0.9612	0.108*
C56	−0.08934 (19)	0.5283 (4)	0.95149 (15)	0.0885 (12)
H56	−0.0844	0.4458	0.9413	0.106*
C57	−0.04889 (15)	0.6221 (3)	0.95547 (14)	0.0680 (10)
H57	−0.0163	0.6012	0.9481	0.082*
N7	−0.01495 (10)	0.9209 (2)	0.89227 (9)	0.0465 (6)
N8	0.01622 (11)	0.8430 (3)	0.87155 (9)	0.0524 (6)
N9	−0.05371 (10)	0.7414 (2)	0.96935 (9)	0.0475 (6)
O10	−0.04673 (8)	1.04600 (18)	0.96459 (7)	0.0463 (5)
O11	0.06377 (8)	0.77032 (19)	0.95335 (7)	0.0522 (5)
C1	0.53682 (14)	1.1453 (3)	0.50955 (12)	0.0604 (9)
H1A	0.5347	1.1337	0.4769	0.072*
C2	0.49826 (13)	1.2285 (3)	0.51657 (11)	0.0568 (8)
H2	0.4711	1.2738	0.4895	0.068*
C3	0.50004 (12)	1.2449 (3)	0.56487 (11)	0.0458 (7)
C4	0.54248 (11)	1.1813 (3)	0.60507 (10)	0.0419 (6)
H4A	0.5441	1.1954	0.6374	0.050*
C5	0.58279 (11)	1.0970 (2)	0.59834 (10)	0.0377 (6)
C6	0.57988 (12)	1.0755 (3)	0.54859 (10)	0.0429 (7)
C7	0.61585 (13)	0.9864 (3)	0.53544 (11)	0.0490 (7)
H7	0.6098	0.9824	0.5016	0.059*
C8	0.72613 (12)	0.7633 (3)	0.57867 (12)	0.0445 (7)
C9	0.76086 (13)	0.6715 (3)	0.56169 (12)	0.0514 (8)
C10	0.74549 (16)	0.6407 (3)	0.51100 (14)	0.0641 (9)
C11	0.77854 (19)	0.5498 (4)	0.49796 (16)	0.0834 (12)
H11	0.7677	0.5275	0.4643	0.100*
C12	0.82691 (19)	0.4927 (4)	0.53409 (19)	0.0898 (13)
H12A	0.8487	0.4322	0.5248	0.108*
C13	0.84336 (16)	0.5242 (4)	0.58397 (17)	0.0851 (12)
H13	0.8766	0.4863	0.6084	0.102*
C14	0.81059 (14)	0.6118 (3)	0.59757 (14)	0.0668 (10)
H14	0.8217	0.6319	0.6315	0.080*
C15	0.79873 (16)	0.8112 (4)	0.83424 (13)	0.0778 (11)
H15A	0.7970	0.8095	0.8659	0.093*
C16	0.84181 (16)	0.7417 (4)	0.82722 (14)	0.0776 (11)
H16	0.8681	0.6919	0.8532	0.093*

C17	0.84613 (13)	0.7458 (3)	0.78087 (13)	0.0593 (9)
C18	0.80483 (12)	0.8150 (3)	0.74174 (11)	0.0506 (7)
H18	0.8072	0.8146	0.7104	0.061*
C19	0.76020 (12)	0.8844 (3)	0.74804 (11)	0.0431 (7)
C20	0.75654 (13)	0.8857 (3)	0.79604 (11)	0.0538 (8)
C21	0.71601 (14)	0.9616 (3)	0.80886 (11)	0.0609 (9)
H21	0.7176	0.9529	0.8415	0.073*
C22	0.60709 (12)	1.1883 (3)	0.76932 (11)	0.0453 (7)
C23	0.56973 (13)	1.2669 (3)	0.78813 (12)	0.0547 (8)
C24	0.57610 (17)	1.2643 (4)	0.83837 (15)	0.0786 (11)
C25	0.5423 (2)	1.3450 (5)	0.85447 (17)	0.1076 (16)
H25	0.5474	1.3445	0.8881	0.129*
C26	0.5015 (2)	1.4254 (5)	0.8213 (2)	0.1072 (17)
H26	0.4789	1.4791	0.8326	0.129*
C27	0.49319 (19)	1.4278 (4)	0.7711 (2)	0.0972 (15)
H27	0.4651	1.4821	0.7484	0.117*
C28	0.52743 (15)	1.3481 (3)	0.75535 (15)	0.0718 (10)
H28	0.5219	1.3488	0.7216	0.086*
C29	0.60496 (14)	0.6467 (3)	0.61160 (12)	0.0590 (8)
H29	0.6175	0.6513	0.5851	0.071*
C30	0.56612 (17)	0.5516 (4)	0.61068 (14)	0.0794 (11)
H30	0.5524	0.4937	0.5840	0.095*
C31	0.54776 (17)	0.5426 (4)	0.64922 (15)	0.0826 (12)
H31	0.5208	0.4796	0.6492	0.099*
C32	0.56997 (17)	0.6286 (4)	0.68808 (14)	0.0822 (12)
H32	0.5590	0.6233	0.7154	0.099*
C33	0.60830 (14)	0.7221 (3)	0.68643 (12)	0.0630 (9)
H33	0.6228	0.7805	0.7129	0.076*
C34	0.76581 (14)	1.2361 (3)	0.69807 (12)	0.0622 (9)
H34	0.7751	1.1533	0.6913	0.075*
C35	0.80319 (17)	1.3359 (4)	0.69887 (15)	0.0842 (12)
H35	0.8371	1.3202	0.6928	0.101*
C36	0.79015 (19)	1.4575 (4)	0.70864 (15)	0.0866 (12)
H36	0.8147	1.5262	0.7091	0.104*
C37	0.74053 (19)	1.4763 (4)	0.71765 (15)	0.0882 (12)
H37	0.7307	1.5584	0.7246	0.106*
C38	0.70497 (15)	1.3735 (3)	0.71641 (13)	0.0666 (9)
H38	0.6710	1.3879	0.7227	0.080*
C58	0.69475 (18)	0.2615 (4)	0.49964 (16)	0.0981 (14)
H58A	0.7361	0.2826	0.5113	0.147*
H58B	0.6775	0.2619	0.4635	0.147*
H58C	0.6904	0.1776	0.5117	0.147*
C59	0.68097 (18)	0.3602 (4)	0.57223 (14)	0.0984 (14)
H59A	0.6457	0.3637	0.5791	0.148*
H59B	0.7048	0.4352	0.5860	0.148*
H59C	0.7032	0.2844	0.5873	0.148*
C60	0.62674 (15)	0.4399 (4)	0.48899 (13)	0.0661 (9)
H60	0.6189	0.4349	0.4548	0.079*
C61	0.6792 (2)	0.5286 (5)	0.90595 (19)	0.1362 (19)

H61A	0.7166	0.5631	0.9285	0.204*
H61B	0.6834	0.4381	0.9014	0.204*
H61C	0.6500	0.5417	0.9200	0.204*
C62	0.6224 (2)	0.7033 (5)	0.8490 (2)	0.146 (2)
H62A	0.6108	0.7308	0.8147	0.219*
H62B	0.6432	0.7719	0.8713	0.219*
H62C	0.5878	0.6808	0.8550	0.219*
C63	0.6769 (2)	0.5424 (6)	0.82513 (19)	0.1182 (18)
H63	0.6635	0.5845	0.7942	0.142*
C64	0.0345 (2)	0.2513 (5)	0.82233 (19)	0.1297 (19)
H64A	0.0745	0.2781	0.8294	0.195*
H64B	0.0126	0.2478	0.7865	0.195*
H64C	0.0349	0.1676	0.8366	0.195*
C65	0.0269 (2)	0.3277 (5)	0.89926 (18)	0.145 (2)
H65A	0.0108	0.3965	0.9123	0.217*
H65B	0.0694	0.3307	0.9146	0.217*
H65C	0.0133	0.2467	0.9068	0.217*
C66	−0.0273 (2)	0.4296 (5)	0.8205 (2)	0.124 (2)
H66	−0.0382	0.4350	0.7859	0.149*
N1	0.65551 (10)	0.9115 (2)	0.56540 (9)	0.0430 (5)
N2	0.68481 (10)	0.8309 (2)	0.54383 (9)	0.0501 (6)
N3	0.67750 (10)	1.0409 (2)	0.77984 (8)	0.0461 (6)
N4	0.64395 (11)	1.1071 (2)	0.80141 (9)	0.0539 (7)
N5	0.62581 (9)	0.7330 (2)	0.64829 (9)	0.0439 (6)
N6	0.71668 (10)	1.2541 (2)	0.70666 (8)	0.0449 (6)
N10	0.66478 (12)	0.3565 (3)	0.51865 (11)	0.0645 (7)
N11	0.66080 (16)	0.5928 (4)	0.85816 (14)	0.0903 (10)
N12	0.00686 (15)	0.3419 (4)	0.84401 (14)	0.0911 (10)
O1	0.46196 (9)	1.3230 (2)	0.57503 (8)	0.0603 (6)
H1	0.4395 (14)	1.354 (4)	0.5493 (11)	0.090*
O2	0.62409 (7)	1.03809 (17)	0.63830 (6)	0.0414 (4)
O3	0.73819 (8)	0.77002 (19)	0.62614 (7)	0.0532 (5)
O4	0.69857 (14)	0.6951 (3)	0.47371 (10)	0.0908 (9)
H4	0.6820 (19)	0.742 (4)	0.4860 (16)	0.136*
O5	0.88845 (10)	0.6825 (3)	0.77117 (10)	0.0828 (8)
H5	0.9114 (16)	0.639 (4)	0.7946 (13)	0.124*
O6	0.72031 (8)	0.94960 (17)	0.70896 (7)	0.0433 (4)
O7	0.60160 (8)	1.20387 (19)	0.72382 (7)	0.0511 (5)
O8	0.61562 (15)	1.1868 (4)	0.87241 (10)	0.1209 (12)
H8	0.631 (2)	1.137 (4)	0.8569 (19)	0.181*
O9	−0.21681 (11)	1.3052 (3)	0.90247 (10)	0.0839 (8)
H9	−0.2375 (18)	1.337 (5)	0.8795 (13)	0.126*
O12	0.03810 (15)	0.7243 (4)	0.80240 (11)	0.1214 (13)
H12	0.024 (2)	0.788 (4)	0.810 (2)	0.182*
O13	0.60078 (11)	0.5232 (2)	0.50210 (9)	0.0738 (7)
O14	0.70709 (14)	0.4477 (3)	0.82828 (11)	0.1173 (11)
O15	−0.04849 (13)	0.5139 (3)	0.84213 (12)	0.1122 (11)
Zn1	0.677430 (13)	0.88007 (3)	0.640099 (12)	0.03916 (10)
Zn2	0.664039 (13)	1.10261 (3)	0.708892 (12)	0.04011 (10)

Zn3	0.003714 (13)	0.88356 (3)	0.966433 (11)	0.04081 (10)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C39	0.078 (2)	0.078 (3)	0.0405 (19)	0.025 (2)	0.0094 (17)	0.0031 (17)
C40	0.069 (2)	0.074 (3)	0.046 (2)	0.0267 (19)	−0.0050 (17)	0.0024 (18)
C41	0.0477 (18)	0.053 (2)	0.056 (2)	0.0091 (15)	0.0060 (15)	−0.0066 (16)
C42	0.0517 (17)	0.0462 (18)	0.0450 (18)	0.0069 (14)	0.0118 (14)	0.0010 (14)
C43	0.0438 (16)	0.0358 (16)	0.0390 (16)	−0.0019 (12)	0.0065 (13)	0.0002 (12)
C44	0.0525 (18)	0.0536 (19)	0.0381 (17)	0.0060 (15)	0.0081 (14)	0.0013 (14)
C45	0.059 (2)	0.064 (2)	0.0388 (18)	0.0065 (16)	0.0145 (15)	0.0012 (15)
C46	0.0431 (16)	0.0508 (19)	0.0489 (19)	−0.0057 (14)	0.0217 (14)	−0.0049 (15)
C47	0.0515 (18)	0.056 (2)	0.061 (2)	−0.0023 (15)	0.0298 (16)	−0.0071 (16)
C48	0.078 (3)	0.092 (3)	0.069 (3)	0.011 (2)	0.041 (2)	−0.009 (2)
C49	0.106 (3)	0.113 (4)	0.084 (3)	0.016 (3)	0.060 (3)	−0.018 (3)
C50	0.094 (3)	0.085 (3)	0.123 (4)	0.019 (2)	0.068 (3)	−0.014 (3)
C51	0.082 (3)	0.077 (3)	0.107 (4)	0.028 (2)	0.043 (3)	−0.001 (2)
C52	0.069 (2)	0.075 (3)	0.073 (3)	0.0154 (19)	0.034 (2)	−0.0070 (19)
C53	0.084 (3)	0.064 (2)	0.106 (3)	−0.008 (2)	0.061 (2)	−0.004 (2)
C54	0.087 (3)	0.094 (3)	0.138 (4)	−0.017 (3)	0.073 (3)	0.002 (3)
C55	0.089 (3)	0.077 (3)	0.103 (3)	−0.030 (2)	0.036 (3)	0.014 (3)
C56	0.100 (3)	0.053 (2)	0.115 (4)	−0.018 (2)	0.045 (3)	−0.003 (2)
C57	0.069 (2)	0.047 (2)	0.090 (3)	−0.0024 (17)	0.033 (2)	−0.0021 (18)
N7	0.0459 (14)	0.0533 (16)	0.0402 (14)	0.0043 (12)	0.0170 (11)	0.0018 (11)
N8	0.0542 (15)	0.0627 (17)	0.0439 (15)	0.0068 (13)	0.0231 (12)	−0.0006 (13)
N9	0.0519 (15)	0.0430 (15)	0.0475 (15)	0.0005 (11)	0.0194 (12)	0.0043 (11)
O10	0.0495 (11)	0.0439 (12)	0.0356 (11)	0.0111 (9)	0.0061 (9)	−0.0006 (9)
O11	0.0513 (12)	0.0610 (14)	0.0449 (12)	0.0116 (10)	0.0194 (10)	−0.0014 (10)
C1	0.072 (2)	0.065 (2)	0.0403 (19)	0.0176 (18)	0.0169 (16)	0.0099 (15)
C2	0.060 (2)	0.054 (2)	0.0438 (19)	0.0164 (16)	0.0065 (15)	0.0118 (15)
C3	0.0413 (16)	0.0352 (16)	0.053 (2)	0.0025 (13)	0.0103 (14)	0.0017 (13)
C4	0.0441 (16)	0.0389 (16)	0.0393 (16)	0.0009 (13)	0.0127 (13)	0.0016 (12)
C5	0.0372 (14)	0.0325 (15)	0.0386 (16)	−0.0024 (12)	0.0098 (12)	0.0035 (12)
C6	0.0458 (16)	0.0429 (17)	0.0382 (16)	0.0038 (13)	0.0144 (13)	0.0019 (13)
C7	0.0606 (19)	0.0505 (19)	0.0377 (17)	0.0024 (15)	0.0212 (14)	0.0018 (14)
C8	0.0426 (16)	0.0444 (17)	0.0528 (19)	−0.0047 (13)	0.0253 (15)	−0.0027 (14)
C9	0.0582 (19)	0.0411 (17)	0.068 (2)	−0.0009 (14)	0.0394 (17)	−0.0036 (15)
C10	0.083 (2)	0.057 (2)	0.069 (3)	0.0070 (18)	0.048 (2)	0.0037 (18)
C11	0.112 (3)	0.073 (3)	0.094 (3)	0.013 (2)	0.071 (3)	−0.007 (2)
C12	0.100 (3)	0.070 (3)	0.131 (4)	0.022 (2)	0.080 (3)	−0.002 (3)
C13	0.071 (2)	0.073 (3)	0.119 (4)	0.026 (2)	0.046 (2)	−0.004 (2)
C14	0.0539 (19)	0.065 (2)	0.085 (3)	0.0096 (17)	0.0322 (19)	−0.0060 (19)
C15	0.088 (3)	0.088 (3)	0.047 (2)	0.038 (2)	0.0156 (19)	0.0174 (19)
C16	0.075 (2)	0.076 (3)	0.060 (2)	0.033 (2)	0.0018 (19)	0.0125 (19)
C17	0.0439 (18)	0.053 (2)	0.062 (2)	0.0103 (15)	0.0012 (16)	−0.0030 (16)
C18	0.0464 (17)	0.0456 (18)	0.0511 (19)	0.0068 (14)	0.0098 (14)	−0.0001 (14)
C19	0.0404 (15)	0.0342 (16)	0.0433 (17)	−0.0003 (12)	0.0043 (13)	−0.0012 (13)

C20	0.0540 (18)	0.056 (2)	0.0410 (18)	0.0122 (15)	0.0072 (14)	0.0077 (15)
C21	0.070 (2)	0.073 (2)	0.0372 (18)	0.0171 (18)	0.0182 (16)	0.0092 (16)
C22	0.0432 (16)	0.0481 (18)	0.0450 (18)	−0.0017 (13)	0.0178 (14)	−0.0061 (14)
C23	0.0546 (19)	0.056 (2)	0.060 (2)	−0.0039 (15)	0.0286 (16)	−0.0128 (16)
C24	0.072 (2)	0.104 (3)	0.064 (3)	0.007 (2)	0.031 (2)	−0.023 (2)
C25	0.095 (3)	0.155 (5)	0.086 (3)	0.008 (3)	0.049 (3)	−0.051 (3)
C26	0.092 (3)	0.098 (4)	0.158 (5)	−0.001 (3)	0.077 (4)	−0.050 (3)
C27	0.095 (3)	0.072 (3)	0.150 (5)	0.025 (2)	0.075 (3)	0.005 (3)
C28	0.071 (2)	0.061 (2)	0.097 (3)	0.0165 (19)	0.048 (2)	0.010 (2)
C29	0.075 (2)	0.054 (2)	0.048 (2)	−0.0143 (17)	0.0242 (17)	−0.0028 (16)
C30	0.102 (3)	0.068 (3)	0.065 (3)	−0.037 (2)	0.030 (2)	−0.0117 (19)
C31	0.093 (3)	0.075 (3)	0.083 (3)	−0.039 (2)	0.037 (2)	0.000 (2)
C32	0.097 (3)	0.093 (3)	0.073 (3)	−0.026 (2)	0.052 (2)	0.001 (2)
C33	0.070 (2)	0.067 (2)	0.059 (2)	−0.0104 (18)	0.0332 (18)	−0.0059 (17)
C34	0.066 (2)	0.056 (2)	0.071 (2)	−0.0017 (17)	0.0347 (19)	0.0000 (17)
C35	0.074 (3)	0.085 (3)	0.106 (3)	−0.016 (2)	0.049 (2)	0.000 (2)
C36	0.097 (3)	0.064 (3)	0.100 (3)	−0.032 (2)	0.040 (3)	−0.004 (2)
C37	0.101 (3)	0.051 (2)	0.112 (4)	−0.012 (2)	0.041 (3)	−0.007 (2)
C38	0.071 (2)	0.048 (2)	0.079 (3)	−0.0020 (17)	0.0283 (19)	−0.0031 (17)
C58	0.094 (3)	0.076 (3)	0.118 (4)	0.025 (2)	0.035 (3)	0.010 (3)
C59	0.112 (3)	0.093 (3)	0.058 (3)	−0.005 (3)	−0.001 (2)	0.019 (2)
C60	0.076 (2)	0.068 (2)	0.046 (2)	0.010 (2)	0.0149 (18)	0.0052 (18)
C61	0.171 (5)	0.119 (5)	0.125 (5)	0.002 (4)	0.066 (4)	−0.005 (4)
C62	0.142 (5)	0.111 (4)	0.144 (5)	0.058 (4)	0.011 (4)	−0.018 (4)
C63	0.115 (4)	0.139 (5)	0.077 (4)	0.042 (4)	0.012 (3)	0.024 (3)
C64	0.133 (4)	0.123 (4)	0.119 (4)	0.038 (4)	0.034 (3)	−0.009 (3)
C65	0.166 (5)	0.143 (5)	0.091 (4)	−0.009 (4)	0.013 (4)	0.008 (3)
C66	0.089 (3)	0.101 (4)	0.145 (5)	0.031 (3)	0.006 (3)	0.042 (4)
N1	0.0468 (13)	0.0421 (14)	0.0449 (14)	0.0029 (11)	0.0232 (11)	0.0018 (11)
N2	0.0594 (15)	0.0505 (16)	0.0481 (16)	0.0091 (12)	0.0295 (13)	0.0003 (12)
N3	0.0466 (14)	0.0521 (15)	0.0382 (14)	0.0085 (12)	0.0150 (11)	0.0024 (11)
N4	0.0570 (15)	0.0653 (18)	0.0401 (15)	0.0127 (13)	0.0200 (12)	−0.0004 (13)
N5	0.0471 (14)	0.0404 (14)	0.0437 (15)	−0.0006 (11)	0.0170 (11)	0.0027 (11)
N6	0.0482 (14)	0.0399 (14)	0.0420 (14)	−0.0011 (11)	0.0128 (11)	0.0012 (11)
N10	0.0677 (18)	0.0538 (18)	0.0618 (19)	0.0052 (14)	0.0144 (15)	0.0086 (14)
N11	0.098 (3)	0.095 (3)	0.066 (2)	0.011 (2)	0.021 (2)	−0.008 (2)
N12	0.086 (2)	0.096 (3)	0.077 (3)	0.005 (2)	0.016 (2)	−0.011 (2)
O1	0.0512 (13)	0.0585 (15)	0.0624 (16)	0.0203 (11)	0.0130 (11)	0.0047 (12)
O2	0.0432 (10)	0.0404 (11)	0.0338 (11)	0.0093 (8)	0.0079 (8)	−0.0003 (8)
O3	0.0485 (12)	0.0605 (14)	0.0508 (13)	0.0150 (10)	0.0198 (10)	−0.0031 (10)
O4	0.122 (2)	0.100 (2)	0.0624 (18)	0.0381 (18)	0.0494 (16)	0.0043 (15)
O5	0.0574 (15)	0.087 (2)	0.087 (2)	0.0349 (13)	0.0100 (14)	0.0024 (15)
O6	0.0454 (11)	0.0380 (11)	0.0386 (11)	0.0100 (9)	0.0081 (9)	0.0008 (8)
O7	0.0523 (12)	0.0583 (13)	0.0440 (13)	0.0140 (10)	0.0205 (10)	0.0033 (10)
O8	0.126 (3)	0.192 (4)	0.0504 (18)	0.060 (2)	0.0415 (17)	0.005 (2)
O9	0.0729 (18)	0.090 (2)	0.0721 (19)	0.0392 (15)	0.0107 (14)	−0.0042 (15)
O12	0.126 (3)	0.185 (4)	0.0566 (18)	0.073 (2)	0.0401 (17)	0.004 (2)
O13	0.0861 (17)	0.0692 (17)	0.0656 (16)	0.0234 (14)	0.0293 (13)	0.0055 (13)
O14	0.115 (2)	0.134 (3)	0.090 (2)	0.061 (2)	0.0260 (18)	0.020 (2)

O15	0.095 (2)	0.101 (3)	0.137 (3)	0.0457 (19)	0.042 (2)	0.028 (2)
Zn1	0.04099 (18)	0.03685 (19)	0.0397 (2)	0.00210 (14)	0.01589 (14)	−0.00053 (14)
Zn2	0.04315 (18)	0.03859 (19)	0.03748 (19)	0.00409 (14)	0.01463 (14)	0.00014 (14)
Zn3	0.04396 (19)	0.0392 (2)	0.03812 (19)	0.00194 (14)	0.01485 (14)	−0.00090 (14)

Geometric parameters (Å, °)

C39—C40	1.359 (4)	C22—N4	1.315 (4)
C39—C44	1.401 (4)	C22—C23	1.480 (4)
C39—H39	0.930	C23—C28	1.382 (4)
C40—C41	1.384 (4)	C23—C24	1.396 (4)
C40—H40	0.930	C24—O8	1.343 (5)
C41—O9	1.354 (4)	C24—C25	1.380 (5)
C41—C42	1.389 (4)	C25—C26	1.364 (6)
C42—C43	1.376 (4)	C25—H25	0.930
C42—H42	0.930	C26—C27	1.383 (6)
C43—O10	1.339 (3)	C26—H26	0.930
C43—C44	1.422 (4)	C27—C28	1.376 (5)
C44—C45	1.436 (4)	C27—H27	0.930
C45—N7	1.280 (3)	C28—H28	0.930
C45—H45	0.930	C29—N5	1.327 (4)
C46—O11	1.285 (3)	C29—C30	1.364 (4)
C46—N8	1.319 (4)	C29—H29	0.930
C46—C47	1.478 (4)	C30—C31	1.357 (5)
C47—C52	1.384 (4)	C30—H30	0.930
C47—C48	1.389 (4)	C31—C32	1.368 (5)
C48—O12	1.348 (5)	C31—H31	0.930
C48—C49	1.391 (5)	C32—C33	1.365 (4)
C49—C50	1.359 (6)	C32—H32	0.930
C49—H49	0.930	C33—N5	1.334 (3)
C50—C51	1.371 (5)	C33—H33	0.930
C50—H50	0.930	C34—N6	1.334 (3)
C51—C52	1.373 (4)	C34—C35	1.378 (4)
C51—H51	0.930	C34—H34	0.930
C52—H52	0.930	C35—C36	1.359 (5)
C53—N9	1.326 (4)	C35—H35	0.930
C53—C54	1.368 (5)	C36—C37	1.354 (5)
C53—H53	0.930	C36—H36	0.930
C54—C55	1.348 (6)	C37—C38	1.370 (5)
C54—H54	0.930	C37—H37	0.930
C55—C56	1.348 (5)	C38—N6	1.328 (4)
C55—H55	0.930	C38—H38	0.930
C56—C57	1.362 (5)	C58—N10	1.459 (4)
C56—H56	0.930	C58—H58A	0.960
C57—N9	1.322 (4)	C58—H58B	0.960
C57—H57	0.930	C58—H58C	0.960
N7—N8	1.398 (3)	C59—N10	1.438 (4)
N7—Zn3	2.042 (2)	C59—H59A	0.960
N9—Zn3	2.064 (2)	C59—H59B	0.960

O10—Zn3^{i}	1.9900 (18)	C59—H59C	0.960
O10—Zn3	2.0798 (18)	C60—O13	1.219 (4)
O11—Zn3	2.0316 (18)	C60—N10	1.313 (4)
C1—C2	1.353 (4)	C60—H60	0.930
C1—C6	1.405 (4)	C61—N11	1.435 (5)
C1—H1A	0.930	C61—H61A	0.960
C2—C3	1.388 (4)	C61—H61B	0.960
C2—H2	0.930	C61—H61C	0.960
C3—O1	1.353 (3)	C62—N11	1.441 (5)
C3—C4	1.384 (4)	C62—H62A	0.960
C4—C5	1.390 (3)	C62—H62B	0.960
C4—H4A	0.930	C62—H62C	0.960
C5—O2	1.346 (3)	C63—O14	1.213 (5)
C5—C6	1.427 (4)	C63—N11	1.278 (5)
C6—C7	1.428 (4)	C63—H63	0.930
C7—N1	1.279 (3)	C64—N12	1.439 (5)
C7—H7	0.930	C64—H64A	0.960
C8—O3	1.285 (3)	C64—H64B	0.960
C8—N2	1.315 (4)	C64—H64C	0.960
C8—C9	1.483 (4)	C65—N12	1.480 (5)
C9—C10	1.397 (4)	C65—H65A	0.960
C9—C14	1.397 (4)	C65—H65B	0.960
C10—O4	1.351 (4)	C65—H65C	0.960
C10—C11	1.389 (4)	C66—N12	1.243 (5)
C11—C12	1.368 (5)	C66—O15	1.296 (6)
C11—H11	0.930	C66—H66	0.930
C12—C13	1.373 (5)	N1—N2	1.398 (3)
C12—H12A	0.930	N1—Zn1	2.033 (2)
C13—C14	1.369 (4)	N3—N4	1.392 (3)
C13—H13	0.930	N3—Zn2	2.045 (2)
C14—H14	0.930	N5—Zn1	2.056 (2)
C15—C16	1.358 (4)	N6—Zn2	2.051 (2)
C15—C20	1.410 (4)	O1—H1	0.80 (2)
C15—H15A	0.930	O2—Zn2	1.9976 (17)
C16—C17	1.383 (5)	O2—Zn1	2.0859 (17)
C16—H16	0.930	O3—Zn1	2.0388 (18)
C17—O5	1.346 (4)	O4—H4	0.80 (5)
C17—C18	1.385 (4)	O5—H5	0.82 (5)
C18—C19	1.380 (4)	O6—Zn1	1.9834 (18)
C18—H18	0.930	O6—Zn2	2.1035 (17)
C19—O6	1.349 (3)	O7—Zn2	2.0372 (18)
C19—C20	1.423 (4)	O8—H8	0.87 (3)
C20—C21	1.426 (4)	O9—H9	0.73 (3)
C21—N3	1.284 (4)	O12—H12	0.82 (3)
C21—H21	0.930	Zn3—O10^{i}	1.9900 (18)
C22—O7	1.276 (3)	Zn3—Zn3^{i}	3.1486 (6)
C40—C39—C44	123.5 (3)	C27—C28—H28	118.9
C40—C39—H39	118.2	C23—C28—H28	118.9

C44—C39—H39	118.2	N5—C29—C30	123.5 (3)
C39—C40—C41	118.6 (3)	N5—C29—H29	118.3
C39—C40—H40	120.7	C30—C29—H29	118.3
C41—C40—H40	120.7	C31—C30—C29	119.1 (3)
O9—C41—C40	123.3 (3)	C31—C30—H30	120.4
O9—C41—C42	116.8 (3)	C29—C30—H30	120.4
C40—C41—C42	119.9 (3)	C30—C31—C32	118.3 (3)
C43—C42—C41	121.8 (3)	C30—C31—H31	120.9
C43—C42—H42	119.1	C32—C31—H31	120.9
C41—C42—H42	119.1	C33—C32—C31	119.6 (3)
O10—C43—C42	120.0 (3)	C33—C32—H32	120.2
O10—C43—C44	121.2 (3)	C31—C32—H32	120.2
C42—C43—C44	118.9 (3)	N5—C33—C32	122.5 (3)
C39—C44—C43	117.2 (3)	N5—C33—H33	118.7
C39—C44—C45	117.7 (3)	C32—C33—H33	118.7
C43—C44—C45	125.1 (3)	N6—C34—C35	122.3 (3)
N7—C45—C44	125.9 (3)	N6—C34—H34	118.9
N7—C45—H45	117.0	C35—C34—H34	118.9
C44—C45—H45	117.0	C36—C35—C34	119.6 (4)
O11—C46—N8	125.1 (3)	C36—C35—H35	120.2
O11—C46—C47	117.7 (3)	C34—C35—H35	120.2
N8—C46—C47	117.2 (3)	C37—C36—C35	118.4 (4)
C52—C47—C48	117.8 (3)	C37—C36—H36	120.8
C52—C47—C46	119.3 (3)	C35—C36—H36	120.8
C48—C47—C46	122.9 (3)	C36—C37—C38	119.5 (4)
O12—C48—C47	121.8 (3)	C36—C37—H37	120.3
O12—C48—C49	118.5 (4)	C38—C37—H37	120.3
C47—C48—C49	119.7 (4)	N6—C38—C37	123.1 (3)
C50—C49—C48	120.7 (4)	N6—C38—H38	118.5
C50—C49—H49	119.6	C37—C38—H38	118.5
C48—C49—H49	119.6	N10—C58—H58A	109.5
C49—C50—C51	120.6 (4)	N10—C58—H58B	109.5
C49—C50—H50	119.7	H58A—C58—H58B	109.5
C51—C50—H50	119.7	N10—C58—H58C	109.5
C50—C51—C52	118.9 (4)	H58A—C58—H58C	109.5
C50—C51—H51	120.6	H58B—C58—H58C	109.5
C52—C51—H51	120.6	N10—C59—H59A	109.5
C51—C52—C47	122.3 (4)	N10—C59—H59B	109.5
C51—C52—H52	118.9	H59A—C59—H59B	109.5
C47—C52—H52	118.9	N10—C59—H59C	109.5
N9—C53—C54	122.8 (4)	H59A—C59—H59C	109.5
N9—C53—H53	118.6	H59B—C59—H59C	109.5
C54—C53—H53	118.6	O13—C60—N10	126.1 (3)
C55—C54—C53	119.4 (4)	O13—C60—H60	116.9
C55—C54—H54	120.3	N10—C60—H60	116.9
C53—C54—H54	120.3	N11—C61—H61A	109.5
C54—C55—C56	118.5 (4)	N11—C61—H61B	109.5
C54—C55—H55	120.7	H61A—C61—H61B	109.5
C56—C55—H55	120.7	N11—C61—H61C	109.5

C55—C56—C57	119.4 (4)	H61A—C61—H61C	109.5
C55—C56—H56	120.3	H61B—C61—H61C	109.5
C57—C56—H56	120.3	N11—C62—H62A	109.5
N9—C57—C56	123.2 (3)	N11—C62—H62B	109.5
N9—C57—H57	118.4	H62A—C62—H62B	109.5
C56—C57—H57	118.4	N11—C62—H62C	109.5
C45—N7—N8	117.0 (2)	H62A—C62—H62C	109.5
C45—N7—Zn3	128.5 (2)	H62B—C62—H62C	109.5
N8—N7—Zn3	113.79 (17)	O14—C63—N11	129.3 (5)
C46—N8—N7	110.9 (2)	O14—C63—H63	115.3
C57—N9—C53	116.6 (3)	N11—C63—H63	115.3
C57—N9—Zn3	121.0 (2)	N12—C64—H64A	109.5
C53—N9—Zn3	121.8 (2)	N12—C64—H64B	109.5
C43—O10—$Zn3^{i}$	129.77 (17)	H64A—C64—H64B	109.5
C43—O10—Zn3	128.08 (17)	N12—C64—H64C	109.5
$Zn3^{i}$—O10—Zn3	101.34 (7)	H64A—C64—H64C	109.5
C46—O11—Zn3	111.35 (17)	H64B—C64—H64C	109.5
C2—C1—C6	123.9 (3)	N12—C65—H65A	109.5
C2—C1—H1A	118.0	N12—C65—H65B	109.5
C6—C1—H1A	118.0	H65A—C65—H65B	109.5
C1—C2—C3	118.7 (3)	N12—C65—H65C	109.5
C1—C2—H2	120.6	H65A—C65—H65C	109.5
C3—C2—H2	120.6	H65B—C65—H65C	109.5
O1—C3—C4	117.4 (3)	N12—C66—O15	122.9 (5)
O1—C3—C2	122.6 (3)	N12—C66—H66	118.5
C4—C3—C2	120.0 (3)	O15—C66—H66	118.5
C3—C4—C5	121.7 (3)	C7—N1—N2	116.7 (2)
C3—C4—H4A	119.2	C7—N1—Zn1	128.9 (2)
C5—C4—H4A	119.2	N2—N1—Zn1	114.07 (17)
O2—C5—C4	120.2 (2)	C8—N2—N1	110.8 (2)
O2—C5—C6	121.0 (2)	C21—N3—N4	115.9 (2)
C4—C5—C6	118.8 (2)	C21—N3—Zn2	130.0 (2)
C1—C6—C5	116.8 (3)	N4—N3—Zn2	113.66 (17)
C1—C6—C7	118.0 (3)	C22—N4—N3	111.4 (2)
C5—C6—C7	125.2 (3)	C29—N5—C33	117.0 (3)
N1—C7—C6	126.8 (3)	C29—N5—Zn1	118.2 (2)
N1—C7—H7	116.6	C33—N5—Zn1	124.7 (2)
C6—C7—H7	116.6	C38—N6—C34	117.1 (3)
O3—C8—N2	124.9 (3)	C38—N6—Zn2	121.2 (2)
O3—C8—C9	117.7 (3)	C34—N6—Zn2	121.5 (2)
N2—C8—C9	117.4 (3)	C60—N10—C59	120.5 (3)
C10—C9—C14	118.2 (3)	C60—N10—C58	122.3 (3)
C10—C9—C8	122.6 (3)	C59—N10—C58	117.1 (3)
C14—C9—C8	119.2 (3)	C63—N11—C61	117.0 (4)
O4—C10—C11	118.2 (3)	C63—N11—C62	124.1 (4)
O4—C10—C9	122.2 (3)	C61—N11—C62	118.8 (4)
C11—C10—C9	119.6 (4)	C66—N12—C64	125.0 (5)
C12—C11—C10	120.7 (4)	C66—N12—C65	121.9 (5)

C12—C11—H11	119.6	C64—N12—C65	112.9 (4)
C10—C11—H11	119.6	C3—O1—H1	109 (3)
C11—C12—C13	120.3 (4)	C5—O2—Zn2	128.58 (16)
C11—C12—H12A	119.8	C5—O2—Zn1	129.18 (16)
C13—C12—H12A	119.8	Zn2—O2—Zn1	100.80 (7)
C14—C13—C12	119.7 (4)	C8—O3—Zn1	111.17 (17)
C14—C13—H13	120.2	C10—O4—H4	109 (3)
C12—C13—H13	120.2	C17—O5—H5	115 (3)
C13—C14—C9	121.5 (4)	C19—O6—Zn1	125.41 (17)
C13—C14—H14	119.3	C19—O6—Zn2	129.76 (17)
C9—C14—H14	119.3	Zn1—O6—Zn2	100.66 (7)
C16—C15—C20	123.3 (3)	C22—O7—Zn2	111.57 (17)
C16—C15—H15A	118.3	C24—O8—H8	109 (4)
C20—C15—H15A	118.3	C41—O9—H9	110 (4)
C15—C16—C17	119.2 (3)	C48—O12—H12	117 (4)
C15—C16—H16	120.4	O6—Zn1—N1	145.01 (9)
C17—C16—H16	120.4	O6—Zn1—O3	105.16 (8)
O5—C17—C16	122.9 (3)	N1—Zn1—O3	77.87 (8)
O5—C17—C18	117.4 (3)	O6—Zn1—N5	105.26 (8)
C16—C17—C18	119.7 (3)	N1—Zn1—N5	108.85 (9)
C19—C18—C17	121.8 (3)	O3—Zn1—N5	97.82 (9)
C19—C18—H18	119.1	O6—Zn1—O2	79.55 (7)
C17—C18—H18	119.1	N1—Zn1—O2	86.86 (8)
O6—C19—C18	120.2 (3)	O3—Zn1—O2	159.26 (8)
O6—C19—C20	120.5 (2)	N5—Zn1—O2	100.37 (8)
C18—C19—C20	119.3 (3)	O2—Zn2—O7	106.32 (7)
C15—C20—C19	116.7 (3)	O2—Zn2—N3	137.52 (9)
C15—C20—C21	118.2 (3)	O7—Zn2—N3	77.84 (8)
C19—C20—C21	125.0 (3)	O2—Zn2—N6	106.71 (8)
N3—C21—C20	126.4 (3)	O7—Zn2—N6	98.30 (9)
N3—C21—H21	116.8	N3—Zn2—N6	114.57 (9)
C20—C21—H21	116.8	O2—Zn2—O6	78.81 (7)
O7—C22—N4	124.9 (3)	O7—Zn2—O6	159.44 (8)
O7—C22—C23	118.5 (3)	N3—Zn2—O6	85.08 (8)
N4—C22—C23	116.6 (3)	N6—Zn2—O6	99.18 (8)
C28—C23—C24	118.1 (3)	$O10^{i}$—Zn3—O11	105.13 (8)
C28—C23—C22	119.4 (3)	$O10^{i}$—Zn3—N7	142.28 (9)
C24—C23—C22	122.5 (3)	O11—Zn3—N7	78.21 (8)
O8—C24—C25	118.2 (4)	$O10^{i}$—Zn3—N9	108.91 (9)
O8—C24—C23	121.7 (3)	O11—Zn3—N9	98.54 (9)
C25—C24—C23	120.0 (4)	N7—Zn3—N9	107.63 (9)
C26—C25—C24	120.5 (4)	$O10^{i}$—Zn3—O10	78.66 (7)
C26—C25—H25	119.8	O11—Zn3—O10	158.66 (8)
C24—C25—H25	119.8	N7—Zn3—O10	86.15 (8)
C25—C26—C27	120.8 (4)	N9—Zn3—O10	99.99 (9)
C25—C26—H26	119.6	$O10^{i}$—Zn3—$Zn3^{i}$	40.37 (5)
C27—C26—H26	119.6	O11—Zn3—$Zn3^{i}$	141.28 (6)

C28—C27—C26	118.5 (4)	N7—Zn3—Zn3^{i}	117.10 (7)
C28—C27—H27	120.8	N9—Zn3—Zn3^{i}	108.63 (7)
C26—C27—H27	120.8	O10—Zn3—Zn3^{i}	38.29 (5)
C27—C28—C23	122.1 (4)		
C44—C39—C40—C41	−0.7 (6)	C30—C29—N5—Zn1	−174.0 (3)
C39—C40—C41—O9	−177.8 (4)	C32—C33—N5—C29	−1.0 (5)
C39—C40—C41—C42	2.8 (5)	C32—C33—N5—Zn1	174.4 (3)
O9—C41—C42—C43	178.1 (3)	C37—C38—N6—C34	0.3 (5)
C40—C41—C42—C43	−2.5 (5)	C37—C38—N6—Zn2	176.8 (3)
C41—C42—C43—O10	179.6 (3)	C35—C34—N6—C38	−0.3 (5)
C41—C42—C43—C44	0.1 (4)	C35—C34—N6—Zn2	−176.8 (3)
C40—C39—C44—C43	−1.6 (5)	O13—C60—N10—C59	−2.1 (6)
C40—C39—C44—C45	176.8 (3)	O13—C60—N10—C58	−178.7 (4)
O10—C43—C44—C39	−177.5 (3)	O14—C63—N11—C61	−1.6 (9)
C42—C43—C44—C39	1.9 (4)	O14—C63—N11—C62	−177.2 (5)
O10—C43—C44—C45	4.2 (5)	O15—C66—N12—C64	−175.8 (5)
C42—C43—C44—C45	−176.4 (3)	O15—C66—N12—C65	−0.8 (8)
C39—C44—C45—N7	−175.4 (3)	C4—C5—O2—Zn2	−31.3 (3)
C43—C44—C45—N7	2.9 (5)	C6—C5—O2—Zn2	148.0 (2)
O11—C46—C47—C52	−7.7 (4)	C4—C5—O2—Zn1	165.08 (18)
N8—C46—C47—C52	171.6 (3)	C6—C5—O2—Zn1	−15.6 (3)
O11—C46—C47—C48	171.0 (3)	N2—C8—O3—Zn1	8.1 (3)
N8—C46—C47—C48	−9.6 (5)	C9—C8—O3—Zn1	−171.20 (19)
C52—C47—C48—O12	−178.6 (4)	C18—C19—O6—Zn1	47.2 (3)
C46—C47—C48—O12	2.6 (6)	C20—C19—O6—Zn1	−132.4 (2)
C52—C47—C48—C49	2.8 (5)	C18—C19—O6—Zn2	−160.4 (2)
C46—C47—C48—C49	−176.0 (3)	C20—C19—O6—Zn2	20.1 (4)
O12—C48—C49—C50	178.8 (4)	N4—C22—O7—Zn2	−6.8 (4)
C47—C48—C49—C50	−2.5 (7)	C23—C22—O7—Zn2	173.0 (2)
C48—C49—C50—C51	0.4 (7)	C19—O6—Zn1—N1	−129.2 (2)
C49—C50—C51—C52	1.4 (7)	Zn2—O6—Zn1—N1	72.01 (15)
C50—C51—C52—C47	−1.1 (6)	C19—O6—Zn1—O3	−38.8 (2)
C48—C47—C52—C51	−1.0 (5)	Zn2—O6—Zn1—O3	162.43 (8)
C46—C47—C52—C51	177.8 (3)	C19—O6—Zn1—N5	63.9 (2)
N9—C53—C54—C55	0.2 (7)	Zn2—O6—Zn1—N5	−94.86 (9)
C53—C54—C55—C56	−2.2 (7)	C19—O6—Zn1—O2	162.0 (2)
C54—C55—C56—C57	2.4 (7)	Zn2—O6—Zn1—O2	3.15 (7)
C55—C56—C57—N9	−0.5 (6)	C7—N1—Zn1—O6	−77.5 (3)
C44—C45—N7—N8	178.6 (3)	N2—N1—Zn1—O6	108.6 (2)
C44—C45—N7—Zn3	9.3 (5)	C7—N1—Zn1—O3	−176.7 (3)
O11—C46—N8—N7	0.1 (4)	N2—N1—Zn1—O3	9.48 (17)
C47—C46—N8—N7	−179.2 (2)	C7—N1—Zn1—N5	89.1 (3)
C45—N7—N8—C46	−176.8 (3)	N2—N1—Zn1—N5	−84.75 (18)
Zn3—N7—N8—C46	−5.9 (3)	C7—N1—Zn1—O2	−10.8 (3)
C56—C57—N9—C53	−1.5 (5)	N2—N1—Zn1—O2	175.36 (18)
C56—C57—N9—Zn3	−172.7 (3)	C8—O3—Zn1—O6	−153.15 (18)
C54—C53—N9—C57	1.7 (5)	C8—O3—Zn1—N1	−9.06 (18)
C54—C53—N9—Zn3	172.8 (3)	C8—O3—Zn1—N5	98.64 (19)

C42—C43—O10—Zn3^{i}	−34.3 (4)	C8—O3—Zn1—O2	−52.5 (3)
C44—C43—O10—Zn3^{i}	145.2 (2)	C29—N5—Zn1—O6	−161.7 (2)
C42—C43—O10—Zn3	158.0 (2)	C33—N5—Zn1—O6	22.9 (3)
C44—C43—O10—Zn3	−22.6 (4)	C29—N5—Zn1—N1	26.2 (2)
N8—C46—O11—Zn3	5.7 (4)	C33—N5—Zn1—N1	−149.2 (2)
C47—C46—O11—Zn3	−174.9 (2)	C29—N5—Zn1—O3	−53.6 (2)
C6—C1—C2—C3	−1.3 (5)	C33—N5—Zn1—O3	131.0 (2)
C1—C2—C3—O1	−177.9 (3)	C29—N5—Zn1—O2	116.4 (2)
C1—C2—C3—C4	2.9 (5)	C33—N5—Zn1—O2	−59.0 (2)
O1—C3—C4—C5	178.7 (2)	C5—O2—Zn1—O6	163.7 (2)
C2—C3—C4—C5	−2.2 (4)	Zn2—O2—Zn1—O6	−3.32 (7)
C3—C4—C5—O2	179.0 (2)	C5—O2—Zn1—N1	16.1 (2)
C3—C4—C5—C6	−0.3 (4)	Zn2—O2—Zn1—N1	−150.93 (9)
C2—C1—C6—C5	−1.1 (5)	C5—O2—Zn1—O3	58.4 (3)
C2—C1—C6—C7	177.1 (3)	Zn2—O2—Zn1—O3	−108.6 (2)
O2—C5—C6—C1	−177.5 (3)	C5—O2—Zn1—N5	−92.5 (2)
C4—C5—C6—C1	1.9 (4)	Zn2—O2—Zn1—N5	100.47 (9)
O2—C5—C6—C7	4.5 (4)	C5—O2—Zn2—O7	36.5 (2)
C4—C5—C6—C7	−176.2 (3)	Zn1—O2—Zn2—O7	−156.34 (8)
C1—C6—C7—N1	−177.2 (3)	C5—O2—Zn2—N3	126.2 (2)
C5—C6—C7—N1	0.8 (5)	Zn1—O2—Zn2—N3	−66.64 (13)
O3—C8—C9—C10	169.4 (3)	C5—O2—Zn2—N6	−67.7 (2)
N2—C8—C9—C10	−10.0 (4)	Zn1—O2—Zn2—N6	99.47 (9)
O3—C8—C9—C14	−9.9 (4)	C5—O2—Zn2—O6	−164.0 (2)
N2—C8—C9—C14	170.8 (3)	Zn1—O2—Zn2—O6	3.14 (7)
C14—C9—C10—O4	−179.1 (3)	C22—O7—Zn2—O2	143.21 (19)
C8—C9—C10—O4	1.6 (5)	C22—O7—Zn2—N3	6.90 (19)
C14—C9—C10—C11	2.0 (5)	C22—O7—Zn2—N6	−106.58 (19)
C8—C9—C10—C11	−177.3 (3)	C22—O7—Zn2—O6	41.4 (3)
O4—C10—C11—C12	179.3 (4)	C21—N3—Zn2—O2	80.7 (3)
C9—C10—C11—C12	−1.8 (6)	N4—N3—Zn2—O2	−107.6 (2)
C10—C11—C12—C13	0.3 (6)	C21—N3—Zn2—O7	−178.3 (3)
C11—C12—C13—C14	1.0 (6)	N4—N3—Zn2—O7	−6.61 (18)
C12—C13—C14—C9	−0.8 (6)	C21—N3—Zn2—N6	−84.6 (3)
C10—C9—C14—C13	−0.7 (5)	N4—N3—Zn2—N6	87.1 (2)
C8—C9—C14—C13	178.5 (3)	C21—N3—Zn2—O6	13.2 (3)
C20—C15—C16—C17	1.8 (6)	N4—N3—Zn2—O6	−175.09 (19)
C15—C16—C17—O5	178.2 (3)	C38—N6—Zn2—O2	113.0 (2)
C15—C16—C17—C18	−3.3 (5)	C34—N6—Zn2—O2	−70.7 (2)
O5—C17—C18—C19	−179.1 (3)	C38—N6—Zn2—O7	3.1 (2)
C16—C17—C18—C19	2.3 (5)	C34—N6—Zn2—O7	179.4 (2)
C17—C18—C19—O6	−179.3 (3)	C38—N6—Zn2—N3	−77.3 (3)
C17—C18—C19—C20	0.3 (4)	C34—N6—Zn2—N3	99.1 (2)
C16—C15—C20—C19	0.8 (6)	C38—N6—Zn2—O6	−166.0 (2)
C16—C15—C20—C21	−175.7 (4)	C34—N6—Zn2—O6	10.3 (2)
O6—C19—C20—C15	177.8 (3)	C19—O6—Zn2—O2	−160.8 (2)
C18—C19—C20—C15	−1.8 (4)	Zn1—O6—Zn2—O2	−3.30 (7)
O6—C19—C20—C21	−6.0 (5)	C19—O6—Zn2—O7	−54.0 (3)

C18—C19—C20—C21	174.4 (3)	Zn1—O6—Zn2—O7	103.4 (2)
C15—C20—C21—N3	175.3 (3)	C19—O6—Zn2—N3	−20.3 (2)
C19—C20—C21—N3	−0.9 (6)	Zn1—O6—Zn2—N3	137.20 (10)
O7—C22—C23—C28	4.3 (4)	C19—O6—Zn2—N6	93.9 (2)
N4—C22—C23—C28	−175.9 (3)	Zn1—O6—Zn2—N6	−108.66 (9)
O7—C22—C23—C24	−174.5 (3)	C46—O11—Zn3—O10^{i}	−147.80 (18)
N4—C22—C23—C24	5.3 (5)	C46—O11—Zn3—N7	−6.48 (19)
C28—C23—C24—O8	179.1 (4)	C46—O11—Zn3—N9	99.87 (19)
C22—C23—C24—O8	−2.1 (6)	C46—O11—Zn3—O10	−50.2 (3)
C28—C23—C24—C25	−2.4 (6)	C46—O11—Zn3—Zn3^{i}	−125.41 (17)
C22—C23—C24—C25	176.4 (4)	C45—N7—Zn3—O10^{i}	−84.1 (3)
O8—C24—C25—C26	−179.9 (4)	N8—N7—Zn3—O10^{i}	106.4 (2)
C23—C24—C25—C26	1.6 (7)	C45—N7—Zn3—O11	176.4 (3)
C24—C25—C26—C27	−0.1 (8)	N8—N7—Zn3—O11	6.82 (18)
C25—C26—C27—C28	−0.5 (7)	C45—N7—Zn3—N9	81.0 (3)
C26—C27—C28—C23	−0.4 (6)	N8—N7—Zn3—N9	−88.50 (19)
C24—C23—C28—C27	1.9 (5)	C45—N7—Zn3—O10	−18.2 (3)
C22—C23—C28—C27	−177.0 (3)	N8—N7—Zn3—O10	172.22 (19)
N5—C29—C30—C31	−0.6 (6)	C45—N7—Zn3—Zn3^{i}	−41.6 (3)
C29—C30—C31—C32	−1.1 (6)	N8—N7—Zn3—Zn3^{i}	148.87 (16)
C30—C31—C32—C33	1.7 (6)	C57—N9—Zn3—O10^{i}	−120.0 (2)
C31—C32—C33—N5	−0.7 (6)	C53—N9—Zn3—O10^{i}	69.3 (3)
N6—C34—C35—C36	−0.1 (6)	C57—N9—Zn3—O11	−10.7 (3)
C34—C35—C36—C37	0.4 (6)	C53—N9—Zn3—O11	178.6 (3)
C35—C36—C37—C38	−0.4 (6)	C57—N9—Zn3—N7	69.5 (3)
C36—C37—C38—N6	0.0 (6)	C53—N9—Zn3—N7	−101.2 (3)
C6—C7—N1—N2	179.2 (3)	C57—N9—Zn3—O10	158.7 (2)
C6—C7—N1—Zn1	5.5 (5)	C53—N9—Zn3—O10	−12.0 (3)
O3—C8—N2—N1	0.0 (4)	C57—N9—Zn3—Zn3^{i}	−162.7 (2)
C9—C8—N2—N1	179.2 (2)	C53—N9—Zn3—Zn3^{i}	26.5 (3)
C7—N1—N2—C8	177.1 (2)	C43—O10—Zn3—O10^{i}	170.4 (3)
Zn1—N1—N2—C8	−8.2 (3)	Zn3^{i}—O10—Zn3—O10^{i}	0.0
C20—C21—N3—N4	−178.2 (3)	C43—O10—Zn3—O11	67.8 (3)
C20—C21—N3—Zn2	−6.6 (5)	Zn3^{i}—O10—Zn3—O11	−102.6 (2)
O7—C22—N4—N3	1.1 (4)	C43—O10—Zn3—N7	25.1 (2)
C23—C22—N4—N3	−178.7 (2)	Zn3^{i}—O10—Zn3—N7	−145.29 (10)
C21—N3—N4—C22	178.2 (3)	C43—O10—Zn3—N9	−82.1 (2)
Zn2—N3—N4—C22	5.2 (3)	Zn3^{i}—O10—Zn3—N9	107.47 (9)
C30—C29—N5—C33	1.7 (5)	C43—O10—Zn3—Zn3^{i}	170.4 (3)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4···N2	0.80 (5)	1.89 (3)	2.595 (3)	147 (5)
O12—H12···N8	0.82 (3)	1.94 (4)	2.575 (3)	134 (5)

O8—H8···N4	0.87 (3)	1.77 (4)	2.546 (3)	147 (5)

Fig. 1