Title

Crystal structure of poly[[[μ4-5-(9H-carbazol-9-yl)isophthalato][μ3-5-(9H-carbazol-9-yl)isophthalato]bis(dimethylformamide)(methanol)dizinc] dimethylformamide monosolvate]

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Crystal structure of poly[[[μ_4-5-(9*H*-carbazol-9-yl)isophthalato][μ_3-5-(9*H*-carbazol-9-yl)isophthalato]bis(dimethylformamide)(methanol)dizinc] dimethylformamide monosolvate]

Liubov M. Lifshits,[a] Charles Campana[b] and Jeremy K. Klosterman[a]*

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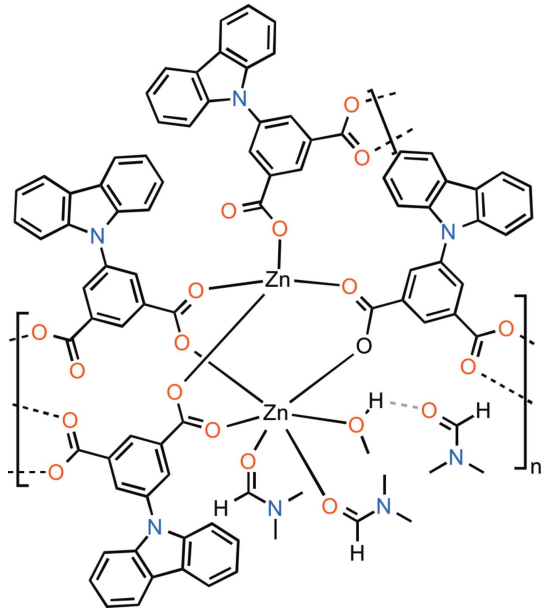
The structure of the polymeric title compound, {[Zn_2-($C_{20}H_{11}NO_4$)$_2$(C_3H_7NO)$_2$(CH_3OH)]·C_3H_7NO}$_n$, comprises carbazolylisophthalate moieties connecting dimetallic tetracarboxylate zinc secondary building units (SBUs) parallel to [100] and [010], leading to a layer-like arrangement parallel to (001). Each SBU consists of two Zn atoms in slightly distorted tetrahedral and octahedral coordination environments [Zn···Zn = 3.5953 (6) Å]. Three carboxylate groups bridge the two Zn atoms in a μ_2-*O*:*O*′ mode, whereas the fourth coordinates through a single carboxylate O atom (μ_1-*O*). The O atoms of two dimethylformamide (DMF) and one methanol molecule complete the Zn coordination spheres. The methanol ligand interacts with the noncoordinating DMF molecule *via* an O—H···O hydrogen bond of medium strength. Carbazoles between the layers interdigitate through weak C—H···π interactions to form a laminar solid stacked along [010]. Two kinds of C—H···π interactions are present, both with a distance of 2.64 Å, between the H atoms and the centroids, and a third C—H···π interaction, where the aromatic H atom is located above the carbazole N-atom lone pair (H···N = 2.89 Å). Several C—H···O interactions occur between the coordinating DMF molecule, the DMF solvent molecule, and ligating carboxylate O atoms.

Keywords: crystal structure; zinc; metal–organic framework; laminar solids.

CCDC reference: 1408495

1. Related literature

For solid-state emission behavior and intermolecular packing interactions for a closely related compound where methanol is replaced by ethanol, see: Lifshits *et al.* (2015). This compound and the title compound are solvatomorphs with identical space groups and comparable lattice parameters. Except for the identity of the coordinating solvent, *viz.* MeOH *versus* EtOH, the other structural components are the same.



2. Experimental

2.1. Crystal data

$[Zn_2(C_{20}H_{11}NO_4)_2(C_3H_7NO)_2(CH_3OH)]\cdot C_3H_7NO$
M_r = 1040.66
Orthorhombic, $P2_12_12_1$
a = 10.2867 (4) Å
b = 17.0328 (7) Å
c = 26.8808 (11) Å
V = 4709.8 (3) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 1.84 mm^{-1}
T = 100 K
0.40 × 0.22 × 0.22 mm

2.2. Data collection

Bruker D8 Venture CMOS diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2015)
T_{min} = 0.53, T_{max} = 0.68
41928 measured reflections
8611 independent reflections
8561 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.019
$wR(F^2)$ = 0.045
S = 1.08
8611 reflections
629 parameters
546 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Absolute structure: Flack x determined using 3716 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al*, 2013)
Absolute structure parameter: 0.005 (3)

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

*Cg*1, *Cg*3, *Cg*4 and *Cg*6 are the centroids of the N1/C1/C6/C7/C12, C1–C6, C7–C12 and C21–C26 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O12—H12*O*···O11	0.76	1.93	2.696 (2)	174
C42—H42*B*···O11^{i}	0.98	2.52	3.327 (3)	139
C43—H43···O10	0.95	2.44	3.028 (3)	120
C46—H46···O5	0.95	2.39	2.995 (2)	121
C47—H47*B*···O3^{ii}	0.98	2.61	3.417 (3)	140
C47—H47*C*···O9^{iii}	0.98	2.65	3.608 (3)	165
C2—H2···*Cg*6^{iv}	0.95	2.64	3.517 (2)	153
C10—H10···*Cg*3^{v}	0.95	2.64	3.418 (2)	139
C44—H44*B*···*Cg*4^{vi}	0.98	2.91	3.596 (2)	128
C45—H45*B*···*Cg*1^{vi}	0.98	2.85	3.411 (2)	117

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

Data collection: *APEX3* (Bruker, 2015); cell refinement: *SAINT* (Bruker, 2015); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ShelXle* (Hübschle *et al.*, 2011); software used to prepare material for publication: *APEX3*.

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: WM5180).

References

Bruker (2015). *APEX3*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Hübschle, C. B., Sheldrick, G. M. & Dittrich, B. (2011). *J. Appl. Cryst.* **44**, 1281–1284.
Lifshits, L. M., Noll, B. C. & Klosterman, J. K. (2015). *Chem. Commun.* **51**, 11603–11606.
Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.

supporting information

Acta Cryst. (2015). E**71**, m152–m153 [doi:10.1107/S2056989015013961]

Crystal structure of poly[[[μ_4-5-(9*H*-carbazol-9-yl)isophthalato][μ_3-5-(9*H*-carbazol-9-yl)isophthalato]bis(dimethylformamide)(methanol)dizinc] dimethylformamide monosolvate]

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S1. Synthesis and crystallization

The title compound was prepared in an analogous manner to Zn Cbz - EtOH (Lifshits *et al.*, 2015). Single crystals were obtained by the solvothermal reaction of 5-(9*H*-carbazol-9-yl)-isophthalic acid and zinc nitrate in DMF/MeOH at room temperature overnight.

S2. Refinement

All H-atom positions were located from difference maps, then refined with isotropic temperature factors. Subsequently, positional restraints were added for all hydrogen atoms and U_{iso} values for hydrogen atoms were restrained to $1.2U_{eq}$ of the attached atom.

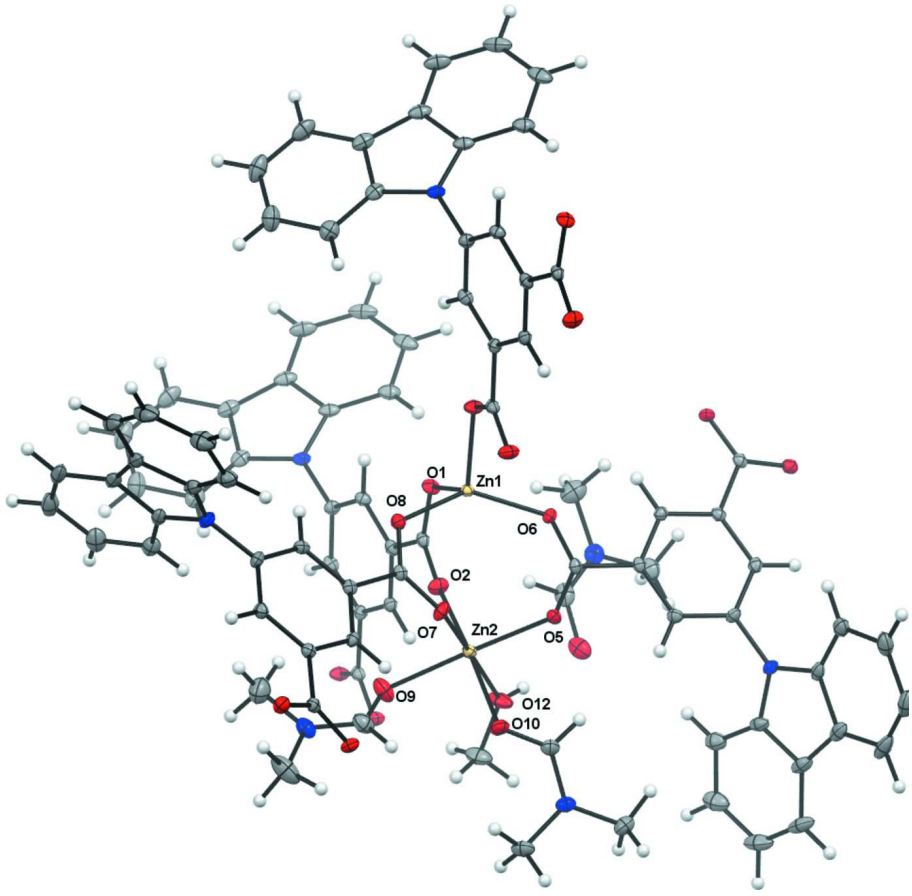

Figure 1

Part of the title structure showing the dimetallic Zn secondary building unit with displacement ellipsoids drawn at the 50% probability level.

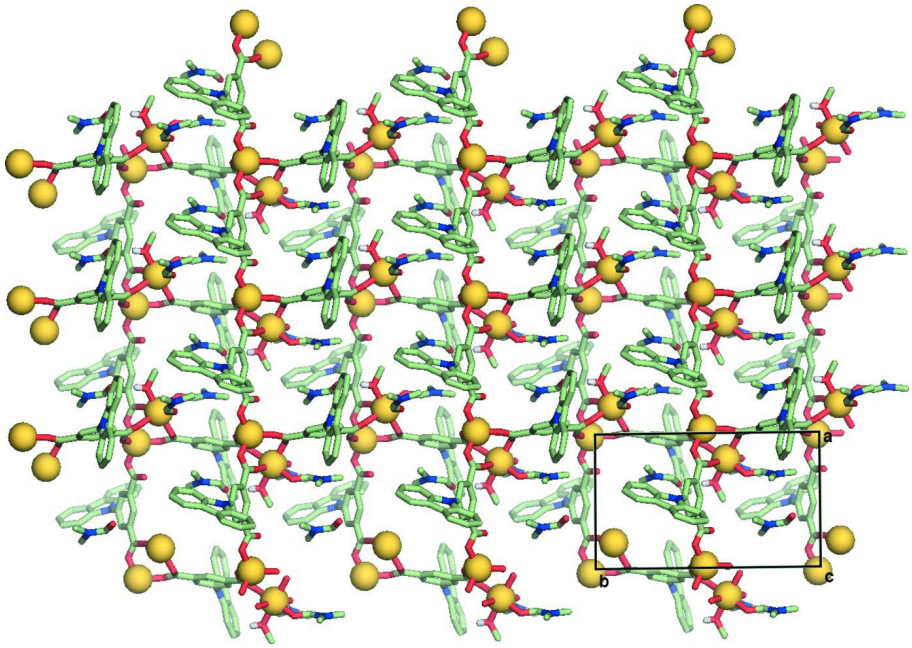

Figure 2

Crystal structure of the title complex in a projection down [001]. Colour code: light green: C, dark blue: N, red: O, white: H, yellow spheres: Zn.

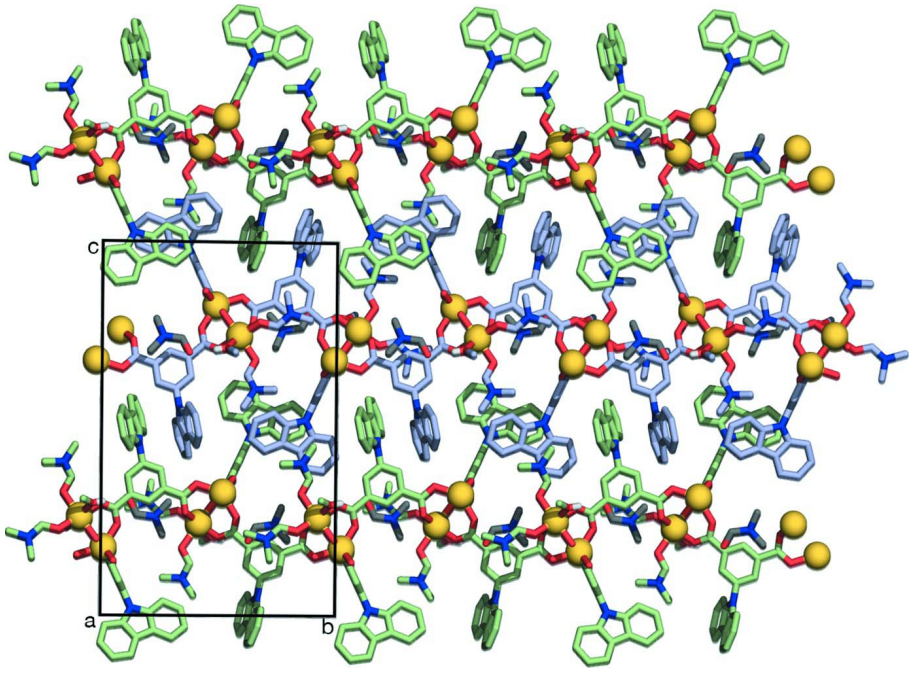

Figure 3

Crystal structure of the title complex in a projection down [100] showing the layer-like arrangement of the Zn secondary building units and the carbazole moieties parallel to (001), and the interdigitation of carbazoles to form stacked layers along [010]. Colour code as in Fig. 2.

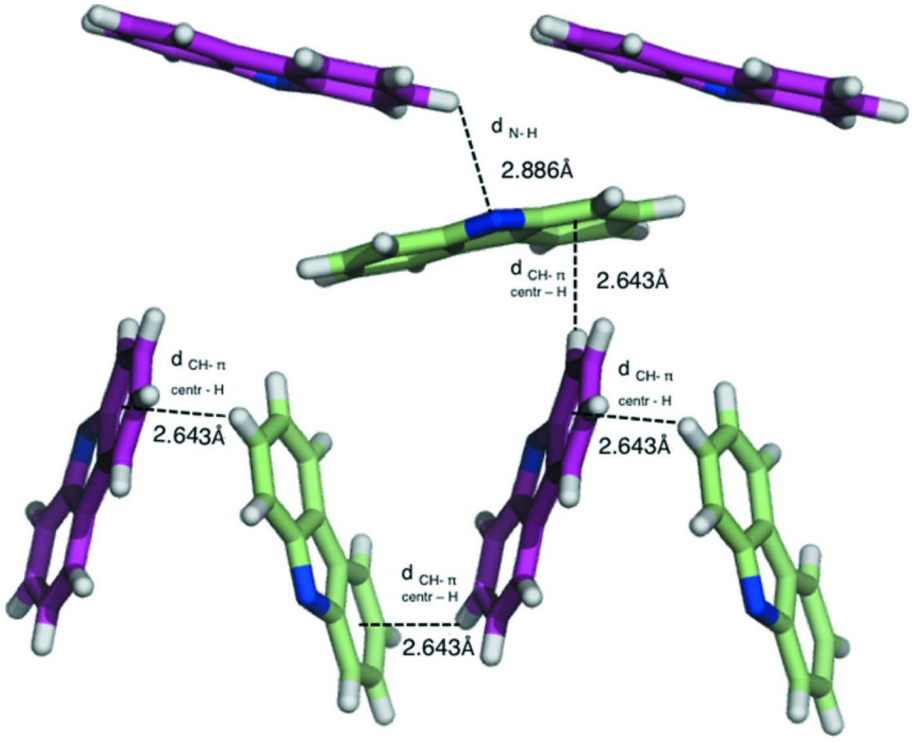

Figure 4

C—H···π interactions between carbazole moieties in the title structure.

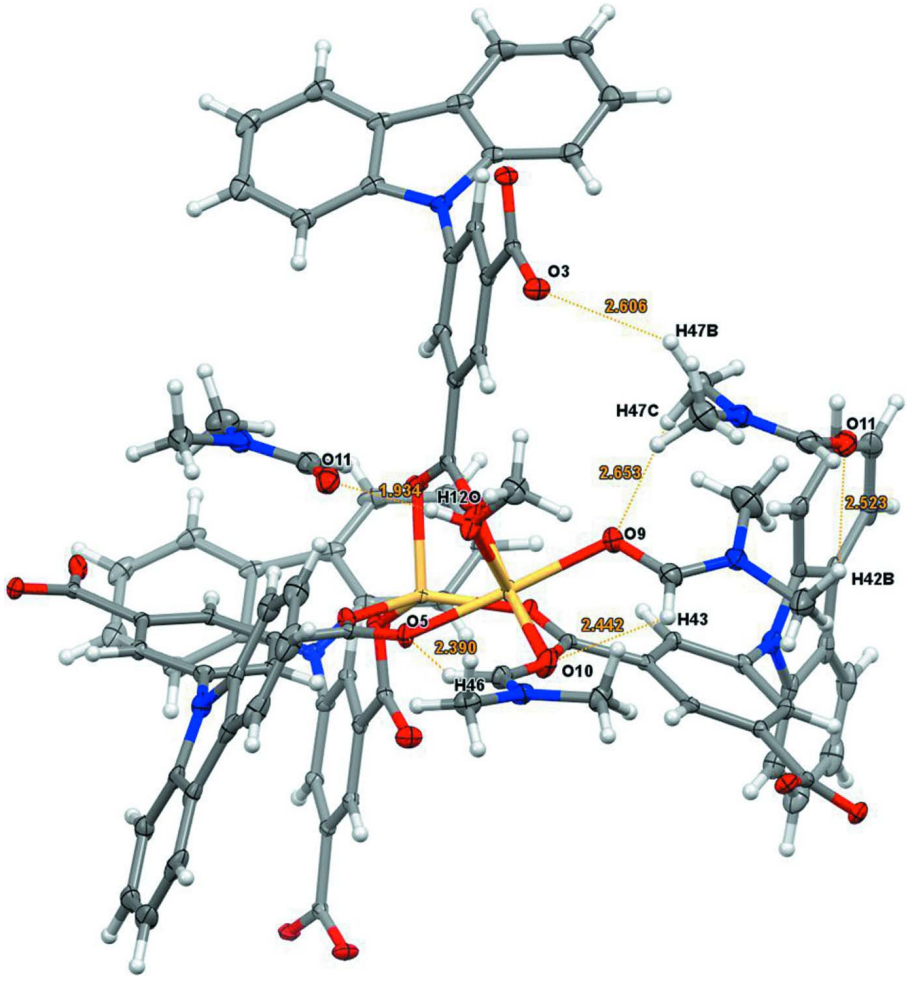

Figure 5

C—H···O interactions between the coordinating DMF molecule, the DMF solvate molecule, and ligating carboxylate oxygen atoms.

Poly[[[μ_4-5-(9*H*-carbazol-9-yl)isophthalato][μ_3-5-(9*H*-carbazol-9-yl)isophthalato]bis(dimethylformamide)(methanol)dizinc] dimethylformamide monosolvate]

Crystal data

$[Zn_2(C_{20}H_{11}NO_4)_2(C_3H_7NO)_2(CH_3OH)]\cdot C_3H_7NO$
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Orthorhombic, $P2_12_12_1$
a = 10.2867 (4) Å
b = 17.0328 (7) Å
c = 26.8808 (11) Å
V = 4709.8 (3) Å^3
Z = 4
$F(000)$ = 2152

D_x = 1.468 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9734 reflections
θ = 5.4–68.3°
μ = 1.84 mm^{-1}
T = 100 K
Prism, clear colourless
0.40 × 0.22 × 0.22 mm

Data collection

Bruker D8 Venture CMOS diffractometer
Radiation source: ImuS micro-focus source with QUAZAR optics
Mirrors monochromator
ω– and φ–scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2015)
T_{min} = 0.53, T_{max} = 0.68
41928 measured reflections
8611 independent reflections
8561 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 68.2°, θ_{min} = 3.1°
h = −12→11
k = −20→20
l = −31→32

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.019
$wR(F^2)$ = 0.045
S = 1.08
8611 reflections
629 parameters
546 restraints
0 constraints
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0221P)^2 + 1.2023P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Absolute structure: Flack x determined using 3716 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al*, 2013)
Absolute structure parameter: 0.005 (3)

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.

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

	x	y	z	U_{iso}*/U_{eq}
Zn1	0.52406 (2)	0.98187 (2)	0.67608 (2)	0.00831 (6)
Zn2	0.30186 (2)	1.08249 (2)	0.75728 (2)	0.01117 (6)
N1	1.01341 (16)	0.86300 (9)	0.51641 (6)	0.0129 (3)
C1	0.95145 (19)	0.89610 (12)	0.47539 (7)	0.0146 (4)
C2	0.9057 (2)	0.97254 (13)	0.46907 (8)	0.0180 (4)
H2	0.9108	1.0102	0.4951	0.022*
C3	0.8523 (2)	0.99110 (14)	0.42298 (8)	0.0248 (5)
H3	0.8192	1.0425	0.4176	0.03*
C4	0.8461 (2)	0.93588 (15)	0.38421 (8)	0.0277 (5)
H4	0.8103	0.9506	0.353	0.033*
C5	0.8915 (2)	0.86053 (15)	0.39113 (8)	0.0247 (5)
H5	0.8872	0.8233	0.3648	0.03*
C6	0.9441 (2)	0.83924 (13)	0.43731 (8)	0.0177 (4)
C7	0.99990 (19)	0.76781 (12)	0.45673 (8)	0.0171 (4)
C8	1.0156 (2)	0.69190 (13)	0.43782 (8)	0.0221 (4)
H8	0.9852	0.679	0.4055	0.027*
C9	1.0761 (2)	0.63599 (13)	0.46707 (9)	0.0238 (5)
H9	1.0863	0.5841	0.4547	0.029*
C10	1.1228 (2)	0.65440 (13)	0.51475 (9)	0.0223 (5)

H10	1.1652	0.6151	0.5339	0.027*
C11	1.1076 (2)	0.72951 (13)	0.53442 (8)	0.0178 (4)
H11	1.1396	0.7423	0.5666	0.021*
C12	1.04404 (19)	0.78507 (12)	0.50537 (7)	0.0150 (4)
C13	1.0189 (2)	0.89772 (10)	0.56479 (7)	0.0119 (4)
C14	1.13827 (19)	0.91247 (11)	0.58751 (7)	0.0119 (4)
H14	1.2173	0.8991	0.5713	0.014*
C15	1.13966 (19)	0.94734 (11)	0.63455 (7)	0.0115 (4)
C16	1.0238 (2)	0.96674 (10)	0.65848 (7)	0.0113 (3)
H16	1.0258	0.9911	0.6903	0.014*
C17	0.90537 (19)	0.95048 (11)	0.63589 (7)	0.0107 (4)
C18	0.90292 (19)	0.91604 (11)	0.58874 (7)	0.0117 (4)
H18	0.8222	0.9052	0.573	0.014*
C19	1.26733 (18)	0.96743 (10)	0.65857 (7)	0.0112 (4)
O1	1.36949 (13)	0.93922 (8)	0.63956 (5)	0.0135 (3)
O2	1.26507 (14)	1.01114 (9)	0.69596 (5)	0.0166 (3)
C20	0.77903 (18)	0.97111 (11)	0.66134 (7)	0.0118 (4)
O3	0.77960 (14)	1.01396 (9)	0.69850 (5)	0.0174 (3)
O4	0.67727 (13)	0.94091 (8)	0.64176 (5)	0.0145 (3)
N2	0.39399 (18)	0.83315 (10)	0.95005 (6)	0.0147 (3)
C21	0.4863 (2)	0.83442 (11)	0.98791 (7)	0.0155 (4)
C22	0.6179 (2)	0.81631 (12)	0.98552 (8)	0.0188 (4)
H22	0.6558	0.7959	0.956	0.023*
C23	0.6920 (3)	0.82912 (12)	1.02792 (8)	0.0245 (5)
H23	0.7825	0.8181	1.0272	0.029*
C24	0.6360 (3)	0.85803 (13)	1.07181 (8)	0.0270 (5)
H24	0.689	0.8669	1.1002	0.032*
C25	0.5048 (3)	0.87372 (12)	1.07420 (8)	0.0264 (5)
H25	0.4673	0.8919	1.1044	0.032*
C26	0.4265 (2)	0.86281 (12)	1.03187 (8)	0.0190 (4)
C27	0.2928 (2)	0.87905 (11)	1.01955 (8)	0.0197 (4)
C28	0.1854 (3)	0.90598 (12)	1.04676 (8)	0.0265 (5)
H28	0.1933	0.917	1.0813	0.032*
C29	0.0688 (3)	0.91627 (14)	1.02287 (10)	0.0302 (5)
H29	−0.0041	0.9346	1.0411	0.036*
C30	0.0554 (2)	0.90011 (13)	0.97173 (10)	0.0281 (5)
H30	−0.0264	0.9081	0.9561	0.034*
C31	0.1596 (2)	0.87272 (12)	0.94368 (8)	0.0212 (4)
H31	0.1509	0.8617	0.9092	0.025*
C32	0.2771 (2)	0.86227 (11)	0.96842 (8)	0.0167 (4)
C33	0.4234 (2)	0.81833 (11)	0.89901 (7)	0.0124 (4)
C34	0.42478 (19)	0.88080 (11)	0.86558 (7)	0.0121 (4)
H34	0.4032	0.9322	0.8765	0.015*
C35	0.45792 (18)	0.86756 (11)	0.81612 (7)	0.0109 (4)
C36	0.48732 (19)	0.79181 (11)	0.79992 (7)	0.0106 (4)
H36	0.5115	0.7829	0.7663	0.013*
C37	0.48112 (19)	0.72937 (10)	0.83313 (7)	0.0107 (3)
C38	0.45010 (18)	0.74252 (11)	0.88311 (7)	0.0118 (4)

H38	0.4474	0.7	0.9059	0.014*
C39	0.45579 (18)	0.93481 (11)	0.77969 (7)	0.0106 (4)
O5	0.39906 (14)	0.99586 (8)	0.79345 (5)	0.0146 (3)
O6	0.51058 (13)	0.92271 (7)	0.73846 (5)	0.0134 (3)
C40	0.50276 (18)	0.64683 (11)	0.81456 (7)	0.0107 (4)
O7	0.53555 (15)	0.63806 (8)	0.77011 (5)	0.0153 (3)
O8	0.48208 (14)	0.59232 (7)	0.84533 (5)	0.0131 (3)
N3	0.18493 (18)	1.29637 (10)	0.69906 (7)	0.0203 (4)
C41	0.1585 (3)	1.28253 (18)	0.64698 (9)	0.0359 (6)
H41A	0.1585	1.2259	0.6405	0.043*
H41B	0.2258	1.3078	0.6267	0.043*
H41C	0.0733	1.3045	0.6384	0.043*
C42	0.1993 (3)	1.37942 (14)	0.71429 (12)	0.0368 (6)
H42A	0.2282	1.3818	0.749	0.044*
H42B	0.1156	1.4063	0.711	0.044*
H42C	0.2638	1.4051	0.693	0.044*
C43	0.2047 (2)	1.23963 (13)	0.73133 (9)	0.0231 (4)
H43	0.2304	1.2537	0.7641	0.028*
O9	0.19190 (17)	1.16868 (9)	0.72161 (6)	0.0249 (3)
N4	0.23401 (18)	1.14908 (10)	0.90142 (6)	0.0165 (4)
C44	0.1897 (2)	1.23038 (12)	0.90000 (8)	0.0212 (4)
H44A	0.2421	1.2599	0.876	0.025*
H44B	0.1991	1.2539	0.9331	0.025*
H44C	0.0982	1.2319	0.89	0.025*
C45	0.2081 (2)	1.10314 (13)	0.94622 (7)	0.0206 (4)
H45A	0.1143	1.0943	0.9494	0.025*
H45B	0.2396	1.1318	0.9754	0.025*
H45C	0.2529	1.0525	0.9439	0.025*
C46	0.2883 (2)	1.11725 (12)	0.86199 (7)	0.0170 (4)
H46	0.317	1.0644	0.8644	0.02*
O10	0.30448 (16)	1.15212 (8)	0.82162 (5)	0.0193 (3)
N5	0.18348 (18)	0.76557 (10)	0.75996 (7)	0.0198 (4)
C47	0.1482 (2)	0.70971 (13)	0.79858 (9)	0.0228 (5)
H47A	0.1474	0.7363	0.8309	0.027*
H47B	0.2117	0.6668	0.7992	0.027*
H47C	0.0616	0.6884	0.7916	0.027*
C48	0.2438 (3)	0.73480 (16)	0.71458 (9)	0.0299 (5)
H48A	0.2654	0.7784	0.6923	0.036*
H48B	0.183	0.6992	0.6978	0.036*
H48C	0.3232	0.7062	0.7232	0.036*
C49	0.1679 (2)	0.84238 (13)	0.76636 (8)	0.0218 (4)
H49	0.1952	0.876	0.7402	0.026*
O11	0.12041 (16)	0.87346 (9)	0.80389 (6)	0.0238 (3)
C50	0.0105 (2)	1.06679 (13)	0.80194 (9)	0.0265 (5)
H50A	0.0221	1.1239	0.8027	0.032*
H50B	−0.0201	1.0487	0.8345	0.032*
H50C	−0.0536	1.053	0.7764	0.032*
O12	0.13112 (15)	1.03020 (9)	0.79064 (6)	0.0238 (3)

H12O	0.1229	0.9862	0.7954	0.029*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.00790 (11)	0.00827 (11)	0.00877 (11)	0.00017 (9)	0.00090 (9)	0.00012 (9)
Zn2	0.01339 (12)	0.00866 (11)	0.01146 (12)	0.00126 (9)	0.00188 (9)	−0.00029 (9)
N1	0.0120 (8)	0.0150 (7)	0.0118 (7)	0.0003 (6)	0.0004 (6)	−0.0050 (6)
C1	0.0096 (9)	0.0205 (10)	0.0136 (9)	−0.0038 (7)	0.0005 (7)	−0.0014 (7)
C2	0.0167 (10)	0.0191 (10)	0.0184 (10)	−0.0045 (8)	−0.0014 (8)	−0.0004 (8)
C3	0.0262 (12)	0.0244 (11)	0.0238 (11)	−0.0048 (9)	−0.0047 (9)	0.0069 (9)
C4	0.0296 (13)	0.0364 (13)	0.0172 (11)	−0.0084 (10)	−0.0071 (9)	0.0048 (9)
C5	0.0254 (12)	0.0343 (12)	0.0143 (10)	−0.0077 (10)	−0.0024 (9)	−0.0064 (9)
C6	0.0140 (10)	0.0240 (10)	0.0149 (9)	−0.0051 (8)	0.0017 (7)	−0.0052 (8)
C7	0.0112 (10)	0.0222 (10)	0.0178 (9)	−0.0035 (8)	0.0034 (7)	−0.0074 (8)
C8	0.0193 (11)	0.0234 (10)	0.0236 (10)	−0.0057 (9)	0.0057 (9)	−0.0122 (8)
C9	0.0197 (11)	0.0186 (10)	0.0331 (12)	−0.0035 (9)	0.0119 (9)	−0.0110 (9)
C10	0.0139 (10)	0.0188 (10)	0.0342 (12)	0.0015 (8)	0.0079 (9)	−0.0025 (9)
C11	0.0120 (9)	0.0200 (10)	0.0214 (10)	0.0001 (8)	0.0025 (8)	−0.0047 (8)
C12	0.0103 (9)	0.0174 (9)	0.0174 (9)	−0.0020 (7)	0.0042 (7)	−0.0055 (7)
C13	0.0128 (9)	0.0111 (8)	0.0119 (8)	−0.0007 (7)	−0.0006 (7)	−0.0014 (7)
C14	0.0100 (9)	0.0117 (9)	0.0140 (9)	0.0002 (7)	0.0009 (7)	−0.0005 (7)
C15	0.0113 (9)	0.0091 (8)	0.0141 (9)	−0.0005 (7)	0.0000 (7)	0.0017 (7)
C16	0.0138 (9)	0.0095 (8)	0.0106 (8)	−0.0002 (7)	0.0010 (7)	0.0008 (6)
C17	0.0112 (9)	0.0090 (8)	0.0118 (9)	−0.0002 (7)	0.0016 (7)	0.0017 (7)
C18	0.0092 (9)	0.0107 (8)	0.0152 (9)	−0.0007 (7)	−0.0014 (7)	0.0009 (7)
C19	0.0106 (9)	0.0104 (9)	0.0127 (9)	−0.0005 (7)	0.0001 (7)	0.0032 (7)
O1	0.0084 (7)	0.0156 (7)	0.0166 (7)	0.0000 (5)	−0.0013 (5)	−0.0023 (5)
O2	0.0141 (7)	0.0206 (7)	0.0151 (7)	−0.0022 (6)	−0.0027 (5)	−0.0063 (6)
C20	0.0109 (9)	0.0104 (8)	0.0140 (9)	0.0015 (7)	0.0021 (7)	0.0032 (7)
O3	0.0146 (7)	0.0222 (7)	0.0155 (7)	0.0014 (6)	0.0021 (5)	−0.0068 (6)
O4	0.0099 (7)	0.0173 (7)	0.0163 (7)	0.0003 (5)	0.0016 (5)	−0.0037 (5)
N2	0.0219 (9)	0.0129 (8)	0.0092 (8)	0.0017 (7)	0.0028 (7)	−0.0004 (6)
C21	0.0284 (11)	0.0080 (8)	0.0100 (8)	−0.0010 (8)	−0.0010 (8)	0.0009 (7)
C22	0.0277 (12)	0.0129 (9)	0.0157 (10)	0.0024 (8)	−0.0009 (8)	0.0016 (8)
C23	0.0364 (13)	0.0148 (9)	0.0221 (11)	0.0026 (10)	−0.0090 (10)	0.0031 (8)
C24	0.0468 (15)	0.0184 (10)	0.0159 (10)	−0.0035 (10)	−0.0105 (10)	0.0022 (8)
C25	0.0545 (17)	0.0136 (9)	0.0110 (9)	−0.0080 (10)	0.0022 (10)	−0.0012 (7)
C26	0.0357 (12)	0.0091 (9)	0.0122 (9)	−0.0044 (8)	0.0049 (8)	0.0001 (7)
C27	0.0348 (12)	0.0099 (9)	0.0145 (9)	−0.0059 (9)	0.0092 (9)	−0.0029 (7)
C28	0.0403 (14)	0.0167 (10)	0.0226 (11)	−0.0058 (10)	0.0180 (10)	−0.0065 (8)
C29	0.0340 (13)	0.0191 (10)	0.0376 (13)	−0.0027 (10)	0.0224 (11)	−0.0056 (10)
C30	0.0239 (12)	0.0215 (11)	0.0388 (13)	0.0007 (9)	0.0104 (10)	−0.0011 (10)
C31	0.0243 (11)	0.0159 (10)	0.0233 (11)	−0.0007 (8)	0.0063 (9)	−0.0007 (8)
C32	0.0251 (11)	0.0085 (8)	0.0165 (10)	−0.0006 (8)	0.0090 (8)	−0.0009 (7)
C33	0.0147 (9)	0.0145 (9)	0.0079 (8)	0.0004 (8)	0.0004 (7)	−0.0019 (7)
C34	0.0130 (9)	0.0104 (9)	0.0131 (9)	0.0005 (7)	0.0009 (7)	−0.0013 (7)
C35	0.0099 (9)	0.0112 (8)	0.0117 (9)	0.0000 (7)	−0.0011 (7)	0.0009 (7)

C36	0.0095 (9)	0.0133 (8)	0.0091 (8)	0.0007 (7)	−0.0007 (7)	−0.0009 (7)
C37	0.0088 (8)	0.0113 (8)	0.0119 (8)	0.0009 (7)	−0.0009 (7)	−0.0007 (7)
C38	0.0117 (9)	0.0117 (9)	0.0119 (9)	−0.0007 (7)	0.0007 (7)	0.0022 (7)
C39	0.0098 (9)	0.0110 (9)	0.0110 (8)	−0.0005 (7)	−0.0022 (7)	0.0007 (7)
O5	0.0215 (7)	0.0096 (6)	0.0127 (6)	0.0037 (5)	0.0014 (5)	0.0006 (5)
O6	0.0155 (7)	0.0140 (6)	0.0106 (6)	0.0024 (5)	0.0033 (5)	0.0030 (5)
C40	0.0085 (9)	0.0117 (8)	0.0120 (9)	0.0009 (7)	−0.0018 (7)	−0.0006 (7)
O7	0.0211 (7)	0.0141 (6)	0.0107 (6)	0.0067 (6)	0.0010 (6)	−0.0020 (5)
O8	0.0160 (7)	0.0097 (6)	0.0136 (6)	0.0005 (5)	0.0011 (5)	−0.0010 (5)
N3	0.0154 (9)	0.0186 (8)	0.0270 (9)	0.0020 (7)	−0.0017 (7)	0.0010 (7)
C41	0.0376 (15)	0.0446 (15)	0.0256 (12)	0.0053 (12)	−0.0028 (10)	0.0056 (11)
C42	0.0266 (13)	0.0203 (11)	0.0634 (18)	0.0022 (10)	−0.0086 (13)	−0.0019 (11)
C43	0.0193 (10)	0.0224 (10)	0.0276 (11)	0.0038 (9)	−0.0044 (9)	−0.0020 (9)
O9	0.0241 (8)	0.0159 (7)	0.0349 (8)	0.0039 (6)	−0.0082 (7)	0.0007 (6)
N4	0.0170 (9)	0.0172 (8)	0.0152 (8)	−0.0004 (7)	0.0013 (7)	−0.0041 (7)
C44	0.0235 (11)	0.0173 (10)	0.0229 (10)	0.0020 (9)	0.0041 (9)	−0.0065 (8)
C45	0.0227 (11)	0.0245 (10)	0.0146 (10)	−0.0006 (9)	0.0028 (8)	−0.0007 (8)
C46	0.0201 (10)	0.0151 (9)	0.0156 (10)	0.0021 (8)	0.0006 (8)	−0.0024 (7)
O10	0.0295 (8)	0.0143 (6)	0.0142 (6)	0.0018 (6)	0.0048 (7)	−0.0035 (5)
N5	0.0182 (9)	0.0209 (8)	0.0202 (8)	−0.0020 (7)	−0.0010 (7)	0.0009 (7)
C47	0.0216 (11)	0.0207 (10)	0.0260 (11)	−0.0009 (9)	−0.0006 (9)	0.0025 (9)
C48	0.0301 (13)	0.0351 (13)	0.0247 (12)	−0.0039 (11)	0.0027 (10)	−0.0041 (10)
C49	0.0163 (10)	0.0234 (10)	0.0257 (11)	−0.0037 (8)	−0.0019 (8)	0.0057 (9)
O11	0.0189 (8)	0.0186 (7)	0.0339 (9)	−0.0006 (6)	0.0013 (7)	0.0009 (6)
C50	0.0168 (11)	0.0255 (11)	0.0374 (12)	0.0029 (9)	0.0072 (9)	−0.0048 (9)
O12	0.0192 (8)	0.0142 (7)	0.0381 (9)	0.0015 (6)	0.0150 (7)	0.0019 (6)

Geometric parameters (Å, º)

Zn1—O4	1.9548 (14)	C27—C28	1.402 (3)
Zn1—O6	1.9614 (13)	C27—C32	1.413 (3)
Zn1—O8^{i}	1.9683 (13)	C28—C29	1.372 (4)
Zn1—O1^{ii}	2.0047 (14)	C28—H28	0.95
Zn2—O5	2.0303 (14)	C29—C30	1.409 (4)
Zn2—O7^{i}	2.0580 (14)	C29—H29	0.95
Zn2—O2^{ii}	2.0826 (14)	C30—C31	1.391 (3)
Zn2—O9	2.0867 (15)	C30—H30	0.95
Zn2—O10	2.0974 (14)	C31—C32	1.391 (3)
Zn2—O12	2.1638 (15)	C31—H31	0.95
N1—C1	1.393 (3)	C33—C38	1.388 (3)
N1—C12	1.396 (3)	C33—C34	1.393 (3)
N1—C13	1.430 (2)	C34—C35	1.391 (3)
C1—C2	1.395 (3)	C34—H34	0.95
C1—C6	1.411 (3)	C35—C36	1.395 (3)
C2—C3	1.392 (3)	C35—C39	1.507 (3)
C2—H2	0.95	C36—C37	1.390 (3)
C3—C4	1.405 (3)	C36—H36	0.95
C3—H3	0.95	C37—C38	1.399 (3)

C4—C5	1.378 (4)	C37—C40	1.508 (2)
C4—H4	0.95	C38—H38	0.95
C5—C6	1.402 (3)	C39—O5	1.248 (2)
C5—H5	0.95	C39—O6	1.260 (2)
C6—C7	1.443 (3)	C40—O7	1.250 (2)
C7—C8	1.399 (3)	C40—O8	1.262 (2)
C7—C12	1.415 (3)	O7—Zn2^{iv}	2.0580 (14)
C8—C9	1.383 (4)	O8—Zn1^{iv}	1.9683 (13)
C8—H8	0.95	N3—C43	1.315 (3)
C9—C10	1.404 (3)	N3—C41	1.445 (3)
C9—H9	0.95	N3—C42	1.480 (3)
C10—C11	1.393 (3)	C41—H41A	0.98
C10—H10	0.95	C41—H41B	0.98
C11—C12	1.390 (3)	C41—H41C	0.98
C11—H11	0.95	C42—H42A	0.98
C13—C18	1.391 (3)	C42—H42B	0.98
C13—C14	1.395 (3)	C42—H42C	0.98
C14—C15	1.397 (3)	C43—O9	1.243 (3)
C14—H14	0.95	C43—H43	0.95
C15—C16	1.395 (3)	N4—C46	1.315 (3)
C15—C19	1.503 (3)	N4—C44	1.458 (3)
C16—C17	1.389 (3)	N4—C45	1.461 (3)
C16—H16	0.95	C44—H44A	0.98
C17—C18	1.397 (3)	C44—H44B	0.98
C17—C20	1.510 (3)	C44—H44C	0.98
C18—H18	0.95	C45—H45A	0.98
C19—O2	1.251 (2)	C45—H45B	0.98
C19—O1	1.263 (2)	C45—H45C	0.98
O1—Zn1^{iii}	2.0047 (14)	C46—O10	1.248 (3)
O2—Zn2^{iii}	2.0825 (14)	C46—H46	0.95
C20—O3	1.237 (2)	N5—C49	1.329 (3)
C20—O4	1.279 (2)	N5—C47	1.454 (3)
N2—C32	1.391 (3)	N5—C48	1.465 (3)
N2—C21	1.392 (3)	C47—H47A	0.98
N2—C33	1.427 (2)	C47—H47B	0.98
C21—C22	1.390 (3)	C47—H47C	0.98
C21—C26	1.417 (3)	C48—H48A	0.98
C22—C23	1.388 (3)	C48—H48B	0.98
C22—H22	0.95	C48—H48C	0.98
C23—C24	1.402 (4)	C49—O11	1.240 (3)
C23—H23	0.95	C49—H49	0.95
C24—C25	1.377 (4)	C50—O12	1.421 (3)
C24—H24	0.95	C50—H50A	0.98
C25—C26	1.406 (3)	C50—H50B	0.98
C25—H25	0.95	C50—H50C	0.98
C26—C27	1.442 (4)	O12—H12O	0.7642
O4—Zn1—O6	106.09 (6)	C32—C27—C26	107.09 (19)

O4—Zn1—O8^{i}	103.24 (6)	C29—C28—C27	119.1 (2)
O6—Zn1—O8^{i}	137.62 (5)	C29—C28—H28	120.4
O4—Zn1—O1^{ii}	106.21 (5)	C27—C28—H28	120.4
O6—Zn1—O1^{ii}	100.16 (6)	C28—C29—C30	121.2 (2)
O8^{i}—Zn1—O1^{ii}	100.24 (6)	C28—C29—H29	119.4
O5—Zn2—O7^{i}	96.05 (6)	C30—C29—H29	119.4
O5—Zn2—O2^{ii}	92.55 (6)	C31—C30—C29	121.3 (2)
O7^{i}—Zn2—O2^{ii}	97.64 (5)	C31—C30—H30	119.4
O5—Zn2—O9	176.68 (7)	C29—C30—H30	119.4
O7^{i}—Zn2—O9	87.28 (6)	C30—C31—C32	116.9 (2)
O2^{ii}—Zn2—O9	87.04 (6)	C30—C31—H31	121.5
O5—Zn2—O10	90.56 (6)	C32—C31—H31	121.5
O7^{i}—Zn2—O10	91.40 (6)	C31—C32—N2	128.81 (18)
O2^{ii}—Zn2—O10	170.07 (6)	C31—C32—C27	122.6 (2)
O9—Zn2—O10	89.32 (6)	N2—C32—C27	108.6 (2)
O5—Zn2—O12	84.38 (6)	C38—C33—C34	120.68 (17)
O7^{i}—Zn2—O12	175.73 (6)	C38—C33—N2	120.16 (17)
O2^{ii}—Zn2—O12	86.58 (6)	C34—C33—N2	119.16 (17)
O9—Zn2—O12	92.30 (7)	C35—C34—C33	119.69 (17)
O10—Zn2—O12	84.34 (6)	C35—C34—H34	120.2
C1—N1—C12	108.65 (16)	C33—C34—H34	120.2
C1—N1—C13	124.80 (16)	C34—C35—C36	120.11 (17)
C12—N1—C13	125.29 (16)	C34—C35—C39	119.62 (17)
N1—C1—C2	128.95 (18)	C36—C35—C39	120.21 (16)
N1—C1—C6	108.73 (18)	C37—C36—C35	119.81 (16)
C2—C1—C6	122.29 (19)	C37—C36—H36	120.1
C3—C2—C1	117.0 (2)	C35—C36—H36	120.1
C3—C2—H2	121.5	C36—C37—C38	120.32 (16)
C1—C2—H2	121.5	C36—C37—C40	119.59 (16)
C2—C3—C4	121.7 (2)	C38—C37—C40	120.05 (16)
C2—C3—H3	119.1	C33—C38—C37	119.33 (17)
C4—C3—H3	119.1	C33—C38—H38	120.3
C5—C4—C3	120.5 (2)	C37—C38—H38	120.3
C5—C4—H4	119.7	O5—C39—O6	127.29 (17)
C3—C4—H4	119.7	O5—C39—C35	116.57 (16)
C4—C5—C6	119.4 (2)	O6—C39—C35	116.14 (16)
C4—C5—H5	120.3	C39—O5—Zn2	133.92 (12)
C6—C5—H5	120.3	C39—O6—Zn1	134.38 (12)
C5—C6—C1	119.1 (2)	O7—C40—O8	125.74 (17)
C5—C6—C7	133.8 (2)	O7—C40—C37	117.86 (16)
C1—C6—C7	107.15 (18)	O8—C40—C37	116.36 (15)
C8—C7—C12	119.4 (2)	C40—O7—Zn2^{iv}	128.02 (12)
C8—C7—C6	133.9 (2)	C40—O8—Zn1^{iv}	121.14 (12)
C12—C7—C6	106.67 (17)	C43—N3—C41	123.3 (2)
C9—C8—C7	118.8 (2)	C43—N3—C42	120.3 (2)
C9—C8—H8	120.6	C41—N3—C42	116.3 (2)
C7—C8—H8	120.6	N3—C41—H41A	109.5
C8—C9—C10	121.3 (2)	N3—C41—H41B	109.5

C8—C9—H9	119.4	H41A—C41—H41B	109.5
C10—C9—H9	119.4	N3—C41—H41C	109.5
C11—C10—C9	120.9 (2)	H41A—C41—H41C	109.5
C11—C10—H10	119.6	H41B—C41—H41C	109.5
C9—C10—H10	119.6	N3—C42—H42A	109.5
C12—C11—C10	117.7 (2)	N3—C42—H42B	109.5
C12—C11—H11	121.2	H42A—C42—H42B	109.5
C10—C11—H11	121.2	N3—C42—H42C	109.5
C11—C12—N1	129.34 (18)	H42A—C42—H42C	109.5
C11—C12—C7	121.91 (19)	H42B—C42—H42C	109.5
N1—C12—C7	108.75 (18)	O9—C43—N3	124.0 (2)
C18—C13—C14	120.81 (16)	O9—C43—H43	118.0
C18—C13—N1	118.69 (17)	N3—C43—H43	118.0
C14—C13—N1	120.50 (18)	C43—O9—Zn2	121.99 (15)
C13—C14—C15	118.82 (18)	C46—N4—C44	120.20 (18)
C13—C14—H14	120.6	C46—N4—C45	121.41 (17)
C15—C14—H14	120.6	C44—N4—C45	118.25 (17)
C16—C15—C14	120.63 (18)	N4—C44—H44A	109.5
C16—C15—C19	119.67 (17)	N4—C44—H44B	109.5
C14—C15—C19	119.64 (17)	H44A—C44—H44B	109.5
C17—C16—C15	120.06 (17)	N4—C44—H44C	109.5
C17—C16—H16	120.0	H44A—C44—H44C	109.5
C15—C16—H16	120.0	H44B—C44—H44C	109.5
C16—C17—C18	119.76 (18)	N4—C45—H45A	109.5
C16—C17—C20	120.68 (16)	N4—C45—H45B	109.5
C18—C17—C20	119.55 (17)	H45A—C45—H45B	109.5
C13—C18—C17	119.91 (17)	N4—C45—H45C	109.5
C13—C18—H18	120.0	H45A—C45—H45C	109.5
C17—C18—H18	120.0	H45B—C45—H45C	109.5
O2—C19—O1	124.52 (17)	O10—C46—N4	124.13 (19)
O2—C19—C15	117.67 (17)	O10—C46—H46	117.9
O1—C19—C15	117.81 (16)	N4—C46—H46	117.9
C19—O1—Zn1^{iii}	108.90 (12)	C46—O10—Zn2	116.49 (12)
C19—O2—Zn2^{iii}	168.46 (13)	C49—N5—C47	121.42 (19)
O3—C20—O4	124.97 (17)	C49—N5—C48	120.73 (19)
O3—C20—C17	119.93 (17)	C47—N5—C48	117.77 (18)
O4—C20—C17	115.10 (16)	N5—C47—H47A	109.5
C20—O4—Zn1	108.79 (12)	N5—C47—H47B	109.5
C32—N2—C21	108.95 (16)	H47A—C47—H47B	109.5
C32—N2—C33	125.96 (17)	N5—C47—H47C	109.5
C21—N2—C33	124.11 (18)	H47A—C47—H47C	109.5
C22—C21—N2	128.86 (18)	H47B—C47—H47C	109.5
C22—C21—C26	122.47 (19)	N5—C48—H48A	109.5
N2—C21—C26	108.58 (19)	N5—C48—H48B	109.5
C23—C22—C21	117.5 (2)	H48A—C48—H48B	109.5
C23—C22—H22	121.2	N5—C48—H48C	109.5
C21—C22—H22	121.2	H48A—C48—H48C	109.5
C22—C23—C24	121.3 (2)	H48B—C48—H48C	109.5

C22—C23—H23	119.3	O11—C49—N5	125.0 (2)
C24—C23—H23	119.3	O11—C49—H49	117.5
C25—C24—C23	120.7 (2)	N5—C49—H49	117.5
C25—C24—H24	119.7	O12—C50—H50A	109.5
C23—C24—H24	119.7	O12—C50—H50B	109.5
C24—C25—C26	119.8 (2)	H50A—C50—H50B	109.5
C24—C25—H25	120.1	O12—C50—H50C	109.5
C26—C25—H25	120.1	H50A—C50—H50C	109.5
C25—C26—C21	118.1 (2)	H50B—C50—H50C	109.5
C25—C26—C27	135.0 (2)	C50—O12—Zn2	128.06 (13)
C21—C26—C27	106.75 (18)	C50—O12—H12O	107.3
C28—C27—C32	118.9 (2)	Zn2—O12—H12O	124.2
C28—C27—C26	134.0 (2)		

C12—N1—C1—C2	−178.7 (2)	C26—C21—C22—C23	−1.8 (3)
C13—N1—C1—C2	13.6 (3)	C21—C22—C23—C24	1.0 (3)
C12—N1—C1—C6	−1.0 (2)	C22—C23—C24—C25	0.8 (3)
C13—N1—C1—C6	−168.66 (18)	C23—C24—C25—C26	−1.8 (3)
N1—C1—C2—C3	177.2 (2)	C24—C25—C26—C21	1.0 (3)
C6—C1—C2—C3	−0.4 (3)	C24—C25—C26—C27	−173.6 (2)
C1—C2—C3—C4	−0.8 (3)	C22—C21—C26—C25	0.8 (3)
C2—C3—C4—C5	1.0 (4)	N2—C21—C26—C25	−175.98 (17)
C3—C4—C5—C6	0.0 (4)	C22—C21—C26—C27	176.83 (18)
C4—C5—C6—C1	−1.2 (3)	N2—C21—C26—C27	0.0 (2)
C4—C5—C6—C7	−179.4 (2)	C25—C26—C27—C28	−6.7 (4)
N1—C1—C6—C5	−176.59 (19)	C21—C26—C27—C28	178.2 (2)
C2—C1—C6—C5	1.4 (3)	C25—C26—C27—C32	173.3 (2)
N1—C1—C6—C7	2.1 (2)	C21—C26—C27—C32	−1.7 (2)
C2—C1—C6—C7	−179.99 (18)	C32—C27—C28—C29	−0.9 (3)
C5—C6—C7—C8	−4.4 (4)	C26—C27—C28—C29	179.2 (2)
C1—C6—C7—C8	177.2 (2)	C27—C28—C29—C30	0.1 (3)
C5—C6—C7—C12	176.0 (2)	C28—C29—C30—C31	0.4 (4)
C1—C6—C7—C12	−2.4 (2)	C29—C30—C31—C32	−0.1 (3)
C12—C7—C8—C9	−1.1 (3)	C30—C31—C32—N2	177.3 (2)
C6—C7—C8—C9	179.4 (2)	C30—C31—C32—C27	−0.7 (3)
C7—C8—C9—C10	−0.7 (3)	C21—N2—C32—C31	179.0 (2)
C8—C9—C10—C11	1.0 (3)	C33—N2—C32—C31	10.0 (3)
C9—C10—C11—C12	0.5 (3)	C21—N2—C32—C27	−2.8 (2)
C10—C11—C12—N1	178.3 (2)	C33—N2—C32—C27	−171.78 (18)
C10—C11—C12—C7	−2.3 (3)	C28—C27—C32—C31	1.2 (3)
C1—N1—C12—C11	178.9 (2)	C26—C27—C32—C31	−178.88 (19)
C13—N1—C12—C11	−13.4 (3)	C28—C27—C32—N2	−177.18 (18)
C1—N1—C12—C7	−0.6 (2)	C26—C27—C32—N2	2.8 (2)
C13—N1—C12—C7	167.07 (18)	C32—N2—C33—C38	−117.0 (2)
C8—C7—C12—C11	2.6 (3)	C21—N2—C33—C38	75.7 (3)
C6—C7—C12—C11	−177.73 (19)	C32—N2—C33—C34	63.0 (3)
C8—C7—C12—N1	−177.81 (18)	C21—N2—C33—C34	−104.4 (2)
C6—C7—C12—N1	1.8 (2)	C38—C33—C34—C35	−2.4 (3)

C1—N1—C13—C18	57.1 (3)	N2—C33—C34—C35	177.66 (18)
C12—N1—C13—C18	−108.6 (2)	C33—C34—C35—C36	1.1 (3)
C1—N1—C13—C14	−123.2 (2)	C33—C34—C35—C39	178.31 (17)
C12—N1—C13—C14	71.1 (3)	C34—C35—C36—C37	1.2 (3)
C18—C13—C14—C15	−1.1 (3)	C39—C35—C36—C37	−175.98 (17)
N1—C13—C14—C15	179.23 (17)	C35—C36—C37—C38	−2.3 (3)
C13—C14—C15—C16	0.3 (3)	C35—C36—C37—C40	175.25 (17)
C13—C14—C15—C19	−176.94 (17)	C34—C33—C38—C37	1.2 (3)
C14—C15—C16—C17	0.9 (3)	N2—C33—C38—C37	−178.79 (18)
C19—C15—C16—C17	178.11 (17)	C36—C37—C38—C33	1.1 (3)
C15—C16—C17—C18	−1.2 (3)	C40—C37—C38—C33	−176.43 (17)
C15—C16—C17—C20	179.98 (17)	C34—C35—C39—O5	−14.1 (3)
C14—C13—C18—C17	0.7 (3)	C36—C35—C39—O5	163.01 (18)
N1—C13—C18—C17	−179.58 (17)	C34—C35—C39—O6	166.52 (18)
C16—C17—C18—C13	0.4 (3)	C36—C35—C39—O6	−16.3 (3)
C20—C17—C18—C13	179.24 (17)	O6—C39—O5—Zn2	28.8 (3)
C16—C15—C19—O2	−10.1 (3)	C35—C39—O5—Zn2	−150.43 (14)
C14—C15—C19—O2	167.10 (17)	O5—C39—O6—Zn1	−6.2 (3)
C16—C15—C19—O1	170.02 (17)	C35—C39—O6—Zn1	173.02 (12)
C14—C15—C19—O1	−12.7 (3)	C36—C37—C40—O7	5.3 (3)
O2—C19—O1—Zn1^{iii}	−3.8 (2)	C38—C37—C40—O7	−177.10 (17)
C15—C19—O1—Zn1^{iii}	175.98 (13)	C36—C37—C40—O8	−172.62 (17)
O1—C19—O2—Zn2^{iii}	3.9 (8)	C38—C37—C40—O8	4.9 (3)
C15—C19—O2—Zn2^{iii}	−175.9 (6)	O8—C40—O7—Zn2^{iv}	−59.3 (3)
C16—C17—C20—O3	11.8 (3)	C37—C40—O7—Zn2^{iv}	122.99 (16)
C18—C17—C20—O3	−166.93 (17)	O7—C40—O8—Zn1^{iv}	−8.6 (3)
C16—C17—C20—O4	−167.72 (17)	C37—C40—O8—Zn1^{iv}	169.16 (12)
C18—C17—C20—O4	13.5 (2)	C41—N3—C43—O9	−6.4 (4)
O3—C20—O4—Zn1	5.5 (2)	C42—N3—C43—O9	178.5 (2)
C17—C20—O4—Zn1	−174.97 (12)	N3—C43—O9—Zn2	149.88 (19)
C32—N2—C21—C22	−174.83 (19)	C44—N4—C46—O10	−0.8 (3)
C33—N2—C21—C22	−5.6 (3)	C45—N4—C46—O10	174.8 (2)
C32—N2—C21—C26	1.7 (2)	N4—C46—O10—Zn2	−150.09 (18)
C33—N2—C21—C26	170.93 (17)	C47—N5—C49—O11	−1.9 (3)
N2—C21—C22—C23	174.29 (19)	C48—N5—C49—O11	−178.5 (2)

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

Hydrogen-bond geometry (Å, º)

Cg1, Cg3, Cg4 and Cg6 are the centroids of the N1/C1/C6/C7/C12, C1–C6, C7–C12 and C21–C26 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O12—H12*O*···O11	0.76	1.93	2.696 (2)	174
C42—H42*B*···O11^{v}	0.98	2.52	3.327 (3)	139
C43—H43···O10	0.95	2.44	3.028 (3)	120
C46—H46···O5	0.95	2.39	2.995 (2)	121
C47—H47*B*···O3^{iv}	0.98	2.61	3.417 (3)	140
C47—H47*C*···O9^{vi}	0.98	2.65	3.608 (3)	165

C2—H2···*Cg*6^{vii}	0.95	2.64	3.517 (2)	153
C10—H10···*Cg*3^{viii}	0.95	2.64	3.418 (2)	139
C44—H44*B*···*Cg*4^{ix}	0.98	2.91	3.596 (2)	128
C45—H45*B*···*Cg*1^{ix}	0.98	2.85	3.411 (2)	117

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