Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diaquabis(2-bromobenzoato-κO)bis-(*N*,*N*-diethylnicotinamide-κN^1)zinc(II)

Tuncer Hökelek,[a] Hakan Dal,[b] Barış Tercan,[c] F. Elif Özbek[d] and Hacali Necefoğlu[d]*

[a]Hacettepe University, Department of Physics, 06800 Beytepe, Ankara, Turkey, [b]Anadolu University, Faculty of Science, Department of Chemistry, 26470 Yenibağlar, Eskişehir, Turkey, [c]Karabük University, Department of Physics, 78050 Karabük, Turkey, and [d]Kafkas University, Department of Chemistry, 63100 Kars, Turkey
Correspondence e-mail: merzifon@hacettepe.edu.tr

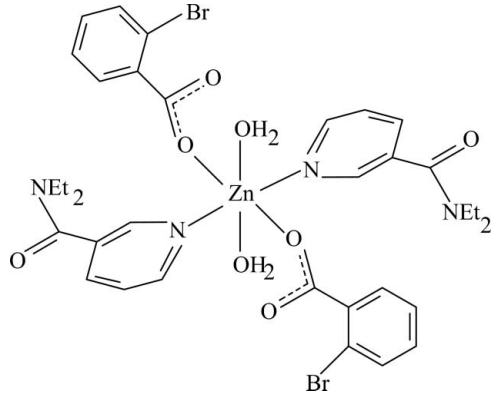
Received 27 March 2009; accepted 31 March 2009

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.029; wR factor = 0.073; data-to-parameter ratio = 19.7.

In the centrosymmetric title complex, $[Zn(C_7H_4BrO_2)_2(C_{10}H_{14}N_2O)_2(H_2O)_2]$, the Zn^{II} atom is located on an inversion center. The asymmetric unit contains one 2-bromobenzoate (BB), one diethylnicotinamide (DENA) ligand and one coordinating water molecule. The four O atoms in the equatorial plane around the Zn atom form a slightly distorted square-planar arrangement, while the slightly distorted octahedral coordination is completed by the two N atoms of the DENA ligands in the axial positions. The dihedral angle between the carboxyl group and the adjacent benzene ring is 85.51 (12)°, while the pyridine and benzene rings are oriented at a dihedral angle of 44.07 (6)°. In the crystal structure, O—H···O hydrogen bonds link the molecules into infinite chains.

Related literature

For general backgroud, see: Antolini *et al.* (1982); Bigoli *et al.* (1972); Nadzhafov *et al.* (1981); Shnulin *et al.* (1981). For related structures, see: Hökelek *et al.* (1995, 1997, 2007 2008); (Hökelek & Necefoğlu (1996, 1997, 2007).



Experimental

Crystal data

$[Zn(C_7H_4BrO_2)_2(C_{10}H_{14}N_2O)_2(H_2O)_2]$
M_r = 857.91
Monoclinic, $P2_1/n$
a = 13.0037 (2) Å
b = 10.3387 (2) Å
c = 14.9365 (3) Å
β = 114.180 (1)°
V = 1831.90 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.91 mm^{-1}
T = 100 K
0.40 × 0.30 × 0.23 mm

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.368, T_{max} = 0.517
16722 measured reflections
4566 independent reflections
3769 reflections with $I > 2\sigma(I)$
R_{int} = 0.072

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.073
S = 0.98
4566 reflections
232 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—O1	2.0600 (12)	Zn1—N1	2.1962 (14)
Zn1—O4	2.1269 (12)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H41···O3^{i}	0.88 (2)	1.88 (2)	2.7518 (18)	168 (3)
O4—H42···O2^{ii}	0.87 (2)	1.81 (2)	2.640 (2)	158 (2)

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors are indebted to Anadolu University and the Medicinal Plants and Medicine Research Centre of Anadolu University, Eskişehir, Turkey, for the use of the X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2502).

References

Antolini, L., Battaglia, L. P., Corradi, A. B., Marcotrigiano, G., Menabue, L., Pellacani, G. C. & Saladini, M. (1982). *Inorg. Chem.* **21**, 1391–1395.
Bigoli, F., Braibanti, A., Pellinghelli, M. A. & Tiripicchio, A. (1972). *Acta Cryst.* B**28**, 962–966.
Bruker (2005). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Hökelek, T., Budak, K. & Necefoğlu, H. (1997). *Acta Cryst.* C**53**, 1049–1051.
Hökelek, T., Çaylak, N. & Necefoğlu, H. (2007). *Acta Cryst.* E**63**, m2561–m2562.
Hökelek, T., Çaylak, N. & Necefoğlu, H. (2008). *Acta Cryst.* E**64**, m505–m506.
Hökelek, T. & Necefoğlu, H. (1996). *Acta Cryst.* C**52**, 1128–1131.
Hökelek, T. & Necefoğlu, H. (1997). *Acta Cryst.* C**53**, 187–189.
Hökelek, T. & Necefoğlu, H. (2007). *Acta Cryst.* E**63**, m821–m823.
Hökelek, T., Necefoğlu, H. & Balcı, M. (1995). *Acta Cryst.* C**51**, 2020–2023.
Nadzhafov, G. N., Shnulin, A. N. & Mamedov, Kh. S. (1981). *Zh. Strukt. Khim.* **22**, 124–128.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Shnulin, A. N., Nadzhafov, G. N., Amiraslanov, I. R., Usubaliev, B. T. & Mamedov, Kh. S. (1981). *Koord. Khim.* **7**, 1409–1416.

supplementary materials

Acta Cryst. (2009). E**65**, m481-m482 [**doi:10.1107/S160053680901191X**]

Diaquabis(2-bromobenzoato-κO)bis(*N*,*N*-diethylnicotinamide-κN^1)zinc(II)

T. Hökelek, H. Dal, B. Tercan, F. E. Özbek and H. Necefoglu

Comment

Transition metal complexes with biochemically active ligands frequently show interesting physical and/or chemical properties, as a result they may find applications in biological systems (Antolini *et al.*, 1982). The structural functions and coordination relationships of the arylcarboxylate ion in transition metal complexes of benzoic acid derivatives change depending on the nature and position of the substituent groups on the benzene ring, the nature of the additional ligand molecule or solvent, and the medium of the synthesis (Nadzhafov *et al.*, 1981; Shnulin *et al.*, 1981). The nicotinic acid derivative *N*,*N*-diethylnicotinamide (DENA) is an important respiratory stimulant (Bigoli *et al.*, 1972).

The structure determination of the title compound, (I), a zinc complex with two 2-bromobenzoate (BB), two diethylnicotinamide (DENA) ligands and two water molecules, was undertaken in order to determine the properties of the ligands and also to compare the results obtained with those reported previously.

Compound (I) is a monomeric complex, with the Zn atom on a centre of symmetry. It contains two BB, two DENA ligands and two water molecules (Fig. 1). All ligands are monodentate. The four O atoms (O1, O4, and the symmetry-related atoms, O1', O4') in the equatorial plane around the Zn atom form a slightly distorted square-planar arrangement, while the slightly distorted octahedral coordination is completed by the two N atoms of the DENA ligands (N1, N1') in the axial positions (Table 1 and Fig. 1).

The near equality of the C1—O1 [1.263 (2) Å] and C1—O2 [1.240 (2) Å] bonds in the carboxylate group indicates a delocalized bonding arrangement, rather than localized single and double bonds, and may be compared with the corresponding distances: 1.256 (6) and 1.245 (6) Å in $[Mn(DENA)_2(C_7H_4ClO_2)_2(H_2O)_2]$ (Hökelek *et al.*, 2008), 1.265 (6) and 1.275 (6) Å in $[Mn(C_9H_{10}NO_2)_2(H_2O)_4].2(H_2O)$ (Hökelek & Necefoğlu, 2007), 1.260 (4) and 1.252 (4) Å in $[Zn(DENA)_2(C_7H_4FO_2)_2(H_2O)_2]$ (Hökelek *et al.*, 2007), 1.259 (9) and 1.273 (9) Å in $Cu_2(DENA)_2(C_6H_5COO)_4$ (Hökelek *et al.*, 1995), 1.279 (4) and 1.246 (4) Å in $[Zn_2(DENA)_2(C_7H_5O_3)_4].2H_2O$ (Hökelek & Necefoğlu, 1996), 1.251 (6) and 1.254 (7) Å in $[Co(DENA)_2(C_7H_5O_3)_2(H_2O)_2]$ (Hökelek & Necefoğlu, 1997) and 1.278 (3) and 1.246 (3) Å in $[Cu(DENA)_2(C_7H_4NO_4)_2(H_2O)_2]$ (Hökelek *et al.*, 1997). In (I), the average Zn—O bond length is 2.0935 (12) Å and the Zn atom is displaced out of the least-squares plane of the carboxylate group (O1/C1/O2) by 0.332 (1) Å. The dihedral angle between the planar carboxylate group and the benzene ring A (C2—C7) is 85.51 (12)°, while that between rings A and B (N1/C8—C12) is 44.07 (6)°.

In the crystal structure, intermolecular O—H···O hydrogen bonds (Table 2) link the molecules into infinite chains, in which they may be effective in the stabilization of the structure.

Experimental

The title compound was prepared by the reaction of $ZnSO_4.H_2O$ (0.89 g, 5 mmol) in H_2O (20 ml) and DENA (1.78 g, 10 mmol) in H_2O (20 ml) with sodium 2-bromobenzoate (2.23 g, 10 mmol) in H_2O (50 ml). The mixture was filtered and set aside to crystallize at ambient temperature for 3 d, giving colorless single crystals.

Refinement

H atoms of water molecule were located in difference Fourier maps and refined isotropically, with restrains of O4—H41 = 0.885 (16) and O4—H42 = 0.869 (15) Å and H41—O4—H42 = 106 (2)°. The remaining H atoms were positioned geometrically with C—H = 0.93, 0.97 and 0.96 Å, for aromatic, methylene and methyl H atoms and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C)$, where $x = 1.5$ for methyl H and $x = 1.2$ for all other H atoms.

Figures

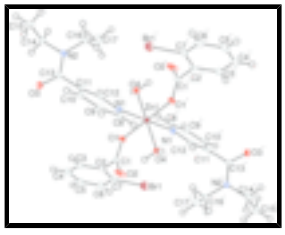


Fig. 1. The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Primed atoms are generated by the symmetry operator (1 - *x*, -*y*, -*z*).

Diaquabis(2-bromobenzoato-κ*O*)bis(*N*,*N*- diethylnicotinamide-κN^1)zinc(II)

Crystal data

$[Zn(C_7H_4BrO_2)_2(C_{10}H_{14}N_2O)_2(H_2O)_2]$	$F_{000} = 872$
$M_r = 857.91$	$D_x = 1.555$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 8223 reflections
$a = 13.0037$ (2) Å	$\theta = 2.5$–28.3º
$b = 10.3387$ (2) Å	$\mu = 2.91$ mm^{-1}
$c = 14.9365$ (3) Å	$T = 100$ K
$\beta = 114.180$ (1)º	Block, colorless
$V = 1831.90$ (6) Å^3	0.40 × 0.30 × 0.23 mm
$Z = 2$	

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer	4566 independent reflections
Radiation source: fine-focus sealed tube	3769 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.072$

T = 100 K	θ_{max} = 28.3º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Bruker, 2005)	h = −17→17
T_{min} = 0.368, T_{max} = 0.517	k = −13→12
16722 measured reflections	l = −15→19

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.029	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.073	$w = 1/[\sigma^2(F_o^2) + (0.0392P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.98	$(\Delta/\sigma)_{max} < 0.001$
4566 reflections	$\Delta\rho_{max}$ = 1.13 e Å^{-3}
232 parameters	$\Delta\rho_{min}$ = −0.53 e Å^{-3}
3 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}
Zn1	0.5000	0.0000	0.0000	0.00901 (8)
Br1	0.179310 (15)	0.14083 (2)	0.071591 (15)	0.02340 (7)
O1	0.46937 (9)	0.05066 (12)	0.12022 (9)	0.0132 (3)
O2	0.36846 (12)	−0.11814 (12)	0.13299 (11)	0.0250 (3)
H41	0.609 (2)	0.2335 (18)	0.0563 (19)	0.054*
H42	0.621 (2)	0.165 (2)	−0.0200 (14)	0.051 (8)*
O3	0.93267 (10)	−0.11602 (12)	0.39616 (9)	0.0145 (3)
O4	0.61756 (10)	0.15513 (11)	0.03656 (10)	0.0124 (3)
N1	0.64061 (11)	−0.12404 (13)	0.09229 (11)	0.0112 (3)
N2	0.98312 (12)	0.00393 (14)	0.29399 (11)	0.0144 (3)

C1	0.40861 (14)	−0.00793 (16)	0.15495 (13)	0.0126 (4)
C2	0.38508 (14)	0.06826 (17)	0.23084 (14)	0.0136 (4)
C3	0.46126 (15)	0.06990 (19)	0.32819 (14)	0.0195 (4)
H3	0.5255	0.0185	0.3482	0.023*
C4	0.44314 (17)	0.14731 (19)	0.39657 (16)	0.0239 (5)
H4	0.4946	0.1468	0.4619	0.029*
C5	0.34836 (17)	0.22509 (19)	0.36715 (15)	0.0239 (4)
H5	0.3375	0.2789	0.4124	0.029*
C6	0.26950 (16)	0.22321 (19)	0.27050 (15)	0.0221 (4)
H6	0.2050	0.2742	0.2507	0.026*
C7	0.28856 (15)	0.14373 (17)	0.20386 (15)	0.0166 (4)
C8	0.64246 (14)	−0.25181 (17)	0.07850 (14)	0.0136 (4)
H8	0.5822	−0.2893	0.0269	0.016*
C9	0.73019 (14)	−0.33078 (18)	0.13771 (14)	0.0145 (4)
H9	0.7280	−0.4193	0.1260	0.017*
C10	0.82084 (13)	−0.27652 (17)	0.21415 (13)	0.0129 (4)
H10	0.8799	−0.3276	0.2559	0.016*
C11	0.82133 (14)	−0.14260 (16)	0.22691 (13)	0.0118 (4)
C12	0.72970 (13)	−0.07125 (17)	0.16538 (13)	0.0120 (3)
H12	0.7299	0.0176	0.1752	0.014*
C13	0.91743 (13)	−0.08274 (16)	0.31181 (13)	0.0113 (3)
C14	1.08066 (14)	0.05572 (17)	0.37778 (14)	0.0157 (4)
H14A	1.0630	0.0598	0.4348	0.019*
H14B	1.0963	0.1429	0.3629	0.019*
C15	1.18465 (15)	−0.0281 (2)	0.40103 (15)	0.0227 (4)
H15A	1.2466	0.0073	0.4564	0.034*
H15B	1.2035	−0.0302	0.3452	0.034*
H15C	1.1694	−0.1144	0.4161	0.034*
C16	0.97478 (16)	0.0395 (2)	0.19646 (15)	0.0239 (4)
H16A	0.9254	−0.0213	0.1487	0.029*
H16B	1.0488	0.0327	0.1956	0.029*
C17	0.93007 (18)	0.1756 (2)	0.16644 (18)	0.0343 (6)
H17A	0.9327	0.1967	0.1048	0.051*
H17B	0.9756	0.2359	0.2156	0.051*
H17C	0.8536	0.1804	0.1599	0.051*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.00857 (13)	0.01000 (15)	0.00909 (15)	−0.00008 (10)	0.00427 (11)	−0.00017 (11)
Br1	0.02151 (11)	0.02979 (13)	0.01957 (12)	0.00542 (8)	0.00908 (9)	0.00255 (8)
O1	0.0148 (6)	0.0149 (6)	0.0135 (6)	−0.0024 (5)	0.0094 (5)	−0.0013 (5)
O2	0.0432 (9)	0.0140 (7)	0.0321 (9)	−0.0092 (6)	0.0300 (7)	−0.0064 (6)
O3	0.0162 (6)	0.0137 (6)	0.0112 (7)	−0.0013 (5)	0.0031 (5)	0.0008 (5)
O4	0.0138 (6)	0.0103 (6)	0.0138 (7)	−0.0008 (5)	0.0064 (5)	−0.0003 (5)
N1	0.0114 (7)	0.0109 (7)	0.0119 (8)	0.0006 (5)	0.0054 (6)	0.0000 (6)
N2	0.0141 (7)	0.0173 (8)	0.0114 (8)	−0.0032 (6)	0.0048 (6)	0.0002 (6)
C1	0.0138 (8)	0.0127 (9)	0.0131 (9)	0.0033 (6)	0.0074 (7)	0.0011 (7)

C2	0.0171 (8)	0.0109 (9)	0.0183 (9)	−0.0041 (7)	0.0128 (7)	−0.0020 (7)
C3	0.0174 (9)	0.0224 (11)	0.0205 (10)	−0.0018 (7)	0.0098 (8)	−0.0032 (8)
C4	0.0260 (10)	0.0318 (12)	0.0173 (10)	−0.0096 (8)	0.0123 (9)	−0.0067 (9)
C5	0.0349 (11)	0.0232 (11)	0.0243 (11)	−0.0068 (8)	0.0229 (9)	−0.0092 (9)
C6	0.0267 (10)	0.0206 (10)	0.0276 (11)	0.0011 (8)	0.0200 (9)	−0.0029 (9)
C7	0.0191 (9)	0.0187 (10)	0.0149 (9)	−0.0017 (7)	0.0102 (8)	0.0000 (8)
C8	0.0114 (8)	0.0157 (9)	0.0135 (9)	−0.0022 (6)	0.0050 (7)	−0.0013 (7)
C9	0.0171 (8)	0.0099 (8)	0.0172 (10)	0.0005 (7)	0.0076 (7)	0.0000 (7)
C10	0.0125 (8)	0.0143 (9)	0.0123 (9)	0.0026 (6)	0.0054 (7)	0.0023 (7)
C11	0.0119 (8)	0.0138 (9)	0.0107 (9)	−0.0016 (6)	0.0056 (7)	−0.0002 (7)
C12	0.0142 (8)	0.0114 (9)	0.0114 (9)	−0.0001 (6)	0.0063 (7)	−0.0002 (7)
C13	0.0097 (8)	0.0090 (8)	0.0132 (9)	0.0033 (6)	0.0026 (7)	0.0006 (7)
C14	0.0166 (8)	0.0152 (9)	0.0135 (9)	−0.0051 (7)	0.0043 (7)	−0.0023 (8)
C15	0.0175 (9)	0.0282 (11)	0.0213 (11)	−0.0017 (8)	0.0069 (8)	0.0031 (9)
C16	0.0200 (9)	0.0365 (12)	0.0147 (10)	−0.0114 (8)	0.0066 (8)	0.0017 (9)
C17	0.0270 (11)	0.0413 (14)	0.0281 (13)	−0.0069 (10)	0.0046 (10)	0.0191 (11)

Geometric parameters (Å, °)

Zn1—O1^{i}	2.0600 (12)	C6—H6	0.9300
Zn1—O1	2.0600 (12)	C7—C2	1.390 (2)
Zn1—O4	2.1269 (12)	C7—C6	1.389 (3)
Zn1—N1	2.1962 (14)	C8—C9	1.387 (2)
Zn1—O4^{i}	2.1269 (12)	C8—H8	0.9300
Zn1—N1^{i}	2.1962 (14)	C9—H9	0.9300
Br1—C7	1.903 (2)	C10—C9	1.380 (2)
O1—C1	1.263 (2)	C10—H10	0.9300
O2—C1	1.240 (2)	C11—C10	1.397 (2)
O3—C13	1.241 (2)	C11—C12	1.383 (2)
O4—Zn1	2.1269 (12)	C11—C13	1.502 (2)
O4—H41	0.885 (16)	C12—H12	0.9300
O4—H42	0.869 (15)	C13—N2	1.338 (2)
N1—Zn1	2.1962 (14)	C14—C15	1.522 (2)
N1—C8	1.339 (2)	C14—H14A	0.9700
N1—C12	1.340 (2)	C14—H14B	0.9700
N2—C14	1.470 (2)	C15—H15A	0.9600
N2—C16	1.463 (2)	C15—H15B	0.9600
C2—C1	1.511 (2)	C15—H15C	0.9600
C2—C3	1.384 (3)	C16—C17	1.518 (3)
C3—H3	0.9300	C16—H16A	0.9700
C4—C3	1.391 (3)	C16—H16B	0.9700
C4—C5	1.384 (3)	C17—H17A	0.9600
C4—H4	0.9300	C17—H17B	0.9600
C5—H5	0.9300	C17—H17C	0.9600
C6—C5	1.387 (3)		
O1^{i}—Zn1—O1	180.00 (5)	C6—C7—Br1	118.47 (14)
O1^{i}—Zn1—O4^{i}	87.69 (5)	C6—C7—C2	121.96 (19)
O1—Zn1—O4^{i}	92.31 (5)	N1—C8—C9	123.00 (16)

O1^{i}—Zn1—O4	92.31 (5)	N1—C8—H8	118.5
O1—Zn1—O4	87.69 (5)	C9—C8—H8	118.5
O4^{i}—Zn1—O4	180.00 (7)	C8—C9—H9	120.4
O1^{i}—Zn1—N1^{i}	90.56 (5)	C10—C9—C8	119.27 (17)
O1—Zn1—N1^{i}	89.44 (5)	C10—C9—H9	120.4
O1^{i}—Zn1—N1	89.44 (5)	C9—C10—C11	118.05 (16)
O1—Zn1—N1	90.56 (5)	C9—C10—H10	121.0
O4^{i}—Zn1—N1^{i}	87.31 (5)	C11—C10—H10	121.0
O4—Zn1—N1^{i}	92.69 (5)	C10—C11—C13	118.64 (15)
O4^{i}—Zn1—N1	92.69 (5)	C12—C11—C10	118.91 (16)
O4—Zn1—N1	87.31 (5)	C12—C11—C13	122.28 (15)
N1^{i}—Zn1—N1	180.00 (14)	N1—C12—C11	123.12 (16)
C1—O1—Zn1	127.79 (11)	N1—C12—H12	118.4
Zn1—O4—H41	126.9 (17)	C11—C12—H12	118.4
Zn1—O4—H42	98.8 (17)	O3—C13—N2	122.56 (16)
H42—O4—H41	106 (2)	O3—C13—C11	118.34 (15)
C8—N1—Zn1	122.85 (11)	N2—C13—C11	119.10 (16)
C8—N1—C12	117.59 (15)	N2—C14—C15	111.29 (15)
C12—N1—Zn1	119.56 (11)	N2—C14—H14A	109.4
C13—N2—C14	118.24 (15)	N2—C14—H14B	109.4
C13—N2—C16	125.02 (15)	C15—C14—H14A	109.4
C16—N2—C14	116.24 (14)	C15—C14—H14B	109.4
O1—C1—C2	114.26 (15)	H14A—C14—H14B	108.0
O2—C1—O1	126.75 (16)	C14—C15—H15A	109.5
O2—C1—C2	118.99 (15)	C14—C15—H15B	109.5
C3—C2—C1	121.12 (16)	C14—C15—H15C	109.5
C3—C2—C7	118.06 (17)	H15A—C15—H15B	109.5
C7—C2—C1	120.76 (17)	H15A—C15—H15C	109.5
C2—C3—C4	120.98 (18)	H15B—C15—H15C	109.5
C2—C3—H3	119.5	N2—C16—C17	112.98 (18)
C4—C3—H3	119.5	N2—C16—H16A	109.0
C3—C4—H4	120.1	N2—C16—H16B	109.0
C5—C4—C3	119.8 (2)	C17—C16—H16A	109.0
C5—C4—H4	120.1	C17—C16—H16B	109.0
C4—C5—C6	120.33 (18)	H16A—C16—H16B	107.8
C4—C5—H5	119.8	C16—C17—H17A	109.5
C6—C5—H5	119.8	C16—C17—H17B	109.5
C5—C6—C7	118.77 (18)	C16—C17—H17C	109.5
C5—C6—H6	120.6	H17A—C17—H17B	109.5
C7—C6—H6	120.6	H17A—C17—H17C	109.5
C2—C7—Br1	119.57 (14)	H17B—C17—H17C	109.5
O4^{i}—Zn1—O1—C1	5.89 (14)	C1—C2—C3—C4	175.41 (16)
O4—Zn1—O1—C1	−174.11 (14)	C7—C2—C3—C4	−1.6 (3)
N1^{i}—Zn1—O1—C1	93.18 (14)	C5—C4—C3—C2	−0.7 (3)
N1—Zn1—O1—C1	−86.82 (14)	C3—C4—C5—C6	2.1 (3)
Zn1—O1—C1—O2	11.8 (3)	C7—C6—C5—C4	−1.1 (3)

Zn1—O1—C1—C2	−168.33 (11)	Br1—C7—C2—C1	4.8 (2)
C8—N1—Zn1—O1^{i}	−61.43 (14)	Br1—C7—C2—C3	−178.23 (13)
C8—N1—Zn1—O1	118.57 (14)	C6—C7—C2—C1	−174.44 (16)
C8—N1—Zn1—O4^{i}	26.23 (14)	C6—C7—C2—C3	2.6 (3)
C8—N1—Zn1—O4	−153.77 (14)	Br1—C7—C6—C5	179.54 (14)
C12—N1—Zn1—O1^{i}	117.92 (13)	C2—C7—C6—C5	−1.2 (3)
C12—N1—Zn1—O1	−62.08 (13)	N1—C8—C9—C10	−0.6 (3)
C12—N1—Zn1—O4^{i}	−154.42 (13)	C11—C10—C9—C8	−1.6 (3)
C12—N1—Zn1—O4	25.58 (13)	C12—C11—C10—C9	2.5 (3)
Zn1—N1—C8—C9	−178.82 (13)	C13—C11—C10—C9	177.93 (16)
C12—N1—C8—C9	1.8 (3)	C10—C11—C12—N1	−1.3 (3)
Zn1—N1—C12—C11	179.78 (13)	C13—C11—C12—N1	−176.57 (16)
C8—N1—C12—C11	−0.8 (2)	C10—C11—C13—O3	−61.1 (2)
C13—N2—C14—C15	88.7 (2)	C10—C11—C13—N2	118.94 (18)
C16—N2—C14—C15	−83.6 (2)	C12—C11—C13—O3	114.20 (19)
C13—N2—C16—C17	109.9 (2)	C12—C11—C13—N2	−65.8 (2)
C14—N2—C16—C17	−78.4 (2)	O3—C13—N2—C14	3.5 (2)
C3—C2—C1—O1	−83.7 (2)	O3—C13—N2—C16	175.04 (17)
C3—C2—C1—O2	96.2 (2)	C11—C13—N2—C14	−176.49 (14)
C7—C2—C1—O1	93.2 (2)	C11—C13—N2—C16	−4.9 (3)
C7—C2—C1—O2	−86.9 (2)		

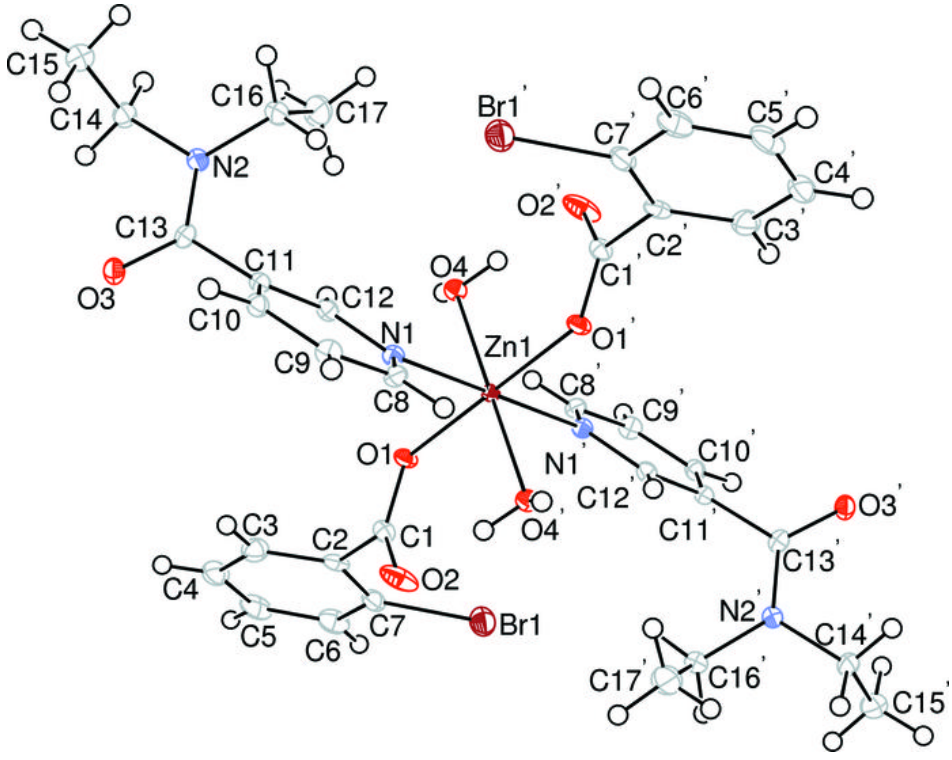
Symmetry codes: (i) −*x*+1, −*y*, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H41···O3^{ii}	0.88 (2)	1.88 (2)	2.7518 (18)	168 (3)
O4—H42···O2^{i}	0.87 (2)	1.81 (2)	2.640 (2)	158 (2)

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

Fig. 1


C15
C14
N2
C16
C17
C13
O3
C11
C12
C10
C9
N1
C8
O1
Zn1
O4
O2'
C1'
C2'
Br1'
C7'
C6'
C5'
C4'
C3'
O1'
C8'
C9'
N1'
C10'
C12'
C11'
O3'
C13'
N2'
C14'
C15'
C16'
C17'
O4'
C3
C2
C1
O2
C4
C5
C6
C7
Br1