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Tetraaquabis(2-methoxybenzaldehyde isonicotinoylhydrazone)zinc dinitrate

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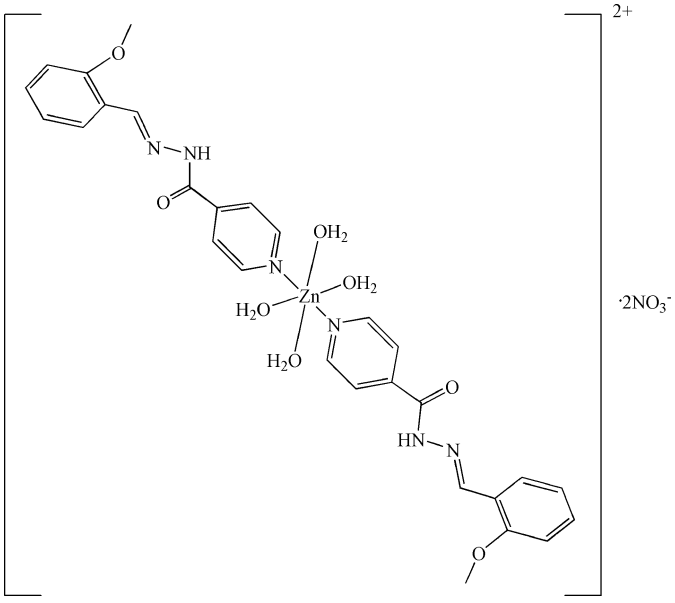
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.041; wR factor = 0.101; data-to-parameter ratio = 15.7.

In the title complex, $[Zn(C_{14}H_{13}N_3O_2)_2(H_2O)_4](NO_3)_2$, the Zn atom is located on a center of symmetry. The Zn—O bond distances are 2.0816 (19) and 2.1356 (18) Å, and the Zn—N bond distance is 2.166 (2) Å. The coordination polyhedron is a slightly distorted octahedron. The crystal structure is stabilized by O—H(coordinated water)···O(NO_3^- or carbonyl O) and N—H(imine)···O(NO_3^-) hydrogen bonds, forming a three-dimensional network.

Related literature

For compounds containing isonicotinoylhydrazone ligands, see: Bu *et al.* (2000); Fu *et al.* (2007); Ge *et al.* (2006). For discussion of Zn—N and Zn—O distances, see: Quirós *et al.* (1991); Ryu *et al.* (2005); Sun *et al.* (2007); Uçar *et al.* (2006); Zhu *et al.* (2003).



Experimental

Crystal data

$[Zn(C_{14}H_{13}N_3O_2)_2(H_2O)_4](NO_3)_2$
M_r = 772.02
Monoclinic, $P2_1/n$
a = 7.970 (4) Å
b = 17.647 (9) Å
c = 11.838 (4) Å
β = 99.062 (16)°
V = 1644.2 (13) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.83 mm^{-1}
T = 293 (2) K
0.20 × 0.15 × 0.12 mm

Data collection

Rigaku Weissenberg IP diffractometer
Absorption correction: multi-scan (*TEXRAY*; Molecular Structure Corporation, 1999)
T_{min} = 0.853, T_{max} = 0.912
14941 measured reflections
3665 independent reflections
2955 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.101
S = 1.05
3665 reflections
233 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O6—H61···O3	0.89	1.87	2.720 (3)	159
N2—H21···O5^{i}	0.86	2.19	3.022 (3)	162
O6—H62···O3^{ii}	0.83	2.00	2.811 (3)	165
O7—H71···O4^{iii}	0.87	2.24	3.014 (3)	148
O7—H72···O1^{iv}	0.81	2.01	2.788 (3)	159

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

Data collection: *TEXRAY* (Molecular Structure Corporation, 1999); cell refinement: *TEXRAY*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEX* (McArdle, 1995); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2055).

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supplementary materials

Acta Cryst. (2007). E**63**, m3004-m3005 [**doi:10.1107/S1600536807057236**]

Tetraaquabis(2-methoxybenzaldehyde isonicotinoylhydrazone)zinc dinitrate

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Comment

There has been considerable interests in the design and syntheses of transition metal complexes with isonicotinoylhydrazone ligands, owing to that there are multi–dimensional structure or extended multi–dimensional structures in these complexes (Bu *et al.*, 2000; Fu *et al*., 2007; Ge *et al.*, 2006). As a continued study in these complexes, herein we report the synthesis and crystal structure of complex $[Zn(C_{14}H_{13}N_3O_2)_2(H_2O)_4]\cdot(NO_3)_2$, (**I**), where $C_{14}H_{13}N_3O_2$ is 2–methoxybenzaldehyde isonicotinoylhydrazonate (*L*).

The complex $[Cd(L)_2(H_2O)_4]\cdot(NO_3)_2$ (**II**) has been reported (Fu *et al.*, 2007). The title complex **I** (Fig. 1) and the reported complex **II** form an isomorphous pair. These two complexes show similar molecular configurations and structure parameters. In **I**, the Zn atom placed on the center of symmetry. The Zn—O bond distances are 2.0816 (19) and 2.1356 (18)Å for Zn1—O6 and Zn1—O7, respectively. This difference between Zn—O(water) bonds in same compound is 0.054 (2) Å. It is normal among the values reported by Quirós *et al.*, 1991; Ryu *et al.*, 2005; Zhu *et al.*, 2003. While the length of 2.166 (2)Å in Zn1—N1 is in agreement with the values reported by Sun *et al.*, 2007 and Uçar *et al.*, 2006. Therefore, the coordination environment of metal centre displays a slightly distorted octahedron (Fig. 1). The dihedral angle between the phenyl and pyridine ring is 21.5 (1)°, which is little bigger than 18.8 (2)° in **II**.

The crystal structure is stabilized by hydrogen bonds, and confers a three dimensional network as complex **II**. Every two neighboring complex molecules in complex **I** are linked by O7—H72···O1^{iv} hydrogen bonds, forming a sheet along *bc* plane (Fig. 2). And these sheets were connected along *a* axis into a three dimensional supramolecule *via* the O6—H61···O3, O6—H62···O(3)^{iii}, O7^{i}—H71^{i}···O4 and N2^{ii}—H21^{ii}···O5 hydrogen bonds (Fig. 3) (symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $x+1/2, -y+1/2, z-1/2$; (iii) $-x, -y, -z+1$; (iv) $x-1/2, -y+1/2, z-1/2$).

Experimental

Ligand *L* was prepared according Fu *et al.*, 2007. The zinc nitrate hexahydrate (59 mg, 0.2 mmol) and *L* (51 mg, 0.2 mmol) were mixed and dissolved in 10 ml me thanol. After stirring for an hour, the solution was filtered. Slow evaporation from the solution afforded yellow crystals suitable for *X*–ray diffraction.

Refinement

The H atoms in water molecules were located in different Fourier maps, and then allowed to ride on the oxygen atoms with $U_{iso} = 1.5U_{eq}(O)$. The other H atoms were placed in idealized positions and treated as riding with d(C—H) = 0.93 Å, $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic, d(C—H) = 0.96 Å, $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl and d(N—H) = 0.86 Å, $U_{iso}(H) = 1.2U_{eq}(N)$ for the imine group.

Figures

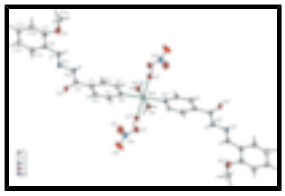


Fig. 1. A view of the title complex, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are presented as a spheres of arbitrary radius. Symmetry code: (i), −*x* + 1, −*y*, −*z* + 1.

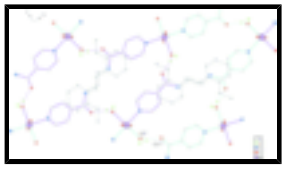


Fig. 2. The two–dimentional structure of **I** in the *bc* plane. Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted for clarity. Symmetry code: (iv) *x* − 1/2, −*y* + 1/2, *z* − 1/2.

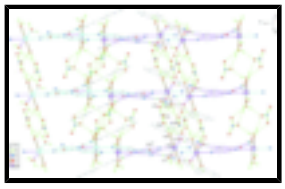


Fig. 3. The three–dimentional structure of **I**. Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted for clarity. Symmetry codes: (i) −*x* + 1, −*y*, −*z* + 1; (ii) *x* + 1/2, −*y* + 1/2, *z* − 1/2; (iii) −*x*, −*y*, −*z* + 1; (iv) *x* − 1/2, −*y* + 1/2, *z* − 1/2).

Tetraaquabis(2-methoxybenzaldehyde isonicotinoylhydrazone)zinc dinitrate

Crystal data

$[Zn(C_{14}H_{13}N_3O_2)_2(H_2O)_4](NO_3)_2$	F_{000} = 800
M_r = 772.02	D_x = 1.559 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 14941 reflections
a = 7.970 (4) Å	θ = 3.1–27.5º
b = 17.647 (9) Å	μ = 0.83 mm^{-1}
c = 11.838 (4) Å	*T* = 293 (2) K
β = 99.062 (16)º	Prism, yellow
V = 1644.2 (13) Å^3	0.20 × 0.15 × 0.12 mm
Z = 2	

Data collection

Rigaku Weissenberg IP diffractometer	2955 reflections with $I > 2\sigma(I)$
Radiation source: Fine–focus sealed tube	R_{int} = 0.053
Monochromator: Graphite	θ_{max} = 27.5º
T = 293(2) K	θ_{min} = 3.1º
φ–scan	*h* = −8→10
Absorption correction: Empirical (TEXRAY; Molecular Structure Corporation, 1999)	*k* = −22→22
T_{min} = 0.853, T_{max} = 0.912	*l* = −15→15
14941 measured reflections	Standard reflections: None
3665 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: Difmap
Least-squares matrix: Full	Hydrogen site location: Geom
$R[F^2 > 2\sigma(F^2)] = 0.041$	H-atom parameters constrained
$wR(F^2) = 0.101$	$w = 1/[\sigma^2(F_o^2) + (0.0413P)^2 + 1.115P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} < 0.001$
3665 reflections	$\Delta\rho_{max} = 0.45$ e Å^{-3}
233 parameters	$\Delta\rho_{min} = -0.49$ e Å^{-3}
Primary atom site location: Direct	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 $F^2 > 2\sigma(F^2)$ 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	0.5000	0.02783 (11)
N1	0.5422 (2)	0.11807 (10)	0.54594 (15)	0.0297 (4)
N2	0.6791 (3)	0.39700 (10)	0.53791 (16)	0.0391 (5)
H21	0.6215	0.3849	0.4728	0.047*
N3	0.7507 (3)	0.46831 (11)	0.55469 (17)	0.0407 (5)
N4	0.1088 (3)	0.09550 (13)	0.71546 (18)	0.0460 (5)
O1	0.7721 (3)	0.36189 (9)	0.72069 (14)	0.0500 (5)
O2	0.6753 (4)	0.59321 (12)	0.27438 (18)	0.0836 (9)
O3	0.0344 (3)	0.07244 (13)	0.62089 (17)	0.0603 (6)
O4	0.2662 (3)	0.09405 (17)	0.7342 (2)	0.0822 (8)
O5	0.0287 (3)	0.11849 (15)	0.78818 (17)	0.0775 (8)
O6	0.2392 (2)	0.01951 (10)	0.47521 (16)	0.0432 (4)
H61	0.1961	0.0371	0.5349	0.065*
H62	0.1652	−0.0061	0.4356	0.065*
O7	0.4919 (2)	0.02614 (10)	0.32308 (14)	0.0415 (4)
H71	0.5698	0.0062	0.2889	0.062*
H72	0.4224	0.0505	0.2806	0.062*
C1	0.4726 (3)	0.17490 (13)	0.47888 (19)	0.0368 (5)
H1	0.3919	0.1632	0.4156	0.044*

C2	0.5161 (3)	0.25000 (13)	0.49998 (19)	0.0372 (5)
H2	0.4658	0.2878	0.4513	0.045*
C3	0.6351 (3)	0.26846 (12)	0.59417 (18)	0.0309 (5)
C4	0.7015 (3)	0.21004 (13)	0.66525 (19)	0.0360 (5)
H4	0.7786	0.2203	0.7310	0.043*
C5	0.6527 (3)	0.13666 (12)	0.63803 (19)	0.0347 (5)
H5	0.6993	0.0981	0.6865	0.042*
C6	0.7003 (3)	0.34722 (12)	0.62393 (18)	0.0345 (5)
C7	0.7243 (4)	0.51018 (13)	0.4674 (2)	0.0429 (6)
H7	0.6562	0.4923	0.4018	0.051*
C8	0.7972 (3)	0.58583 (13)	0.4663 (2)	0.0387 (5)
C9	0.7676 (4)	0.62883 (14)	0.3661 (2)	0.0457 (6)
C10	0.8338 (4)	0.70137 (15)	0.3637 (3)	0.0544 (7)
H10	0.8120	0.7305	0.2975	0.065*
C11	0.9317 (4)	0.72970 (16)	0.4601 (3)	0.0584 (8)
H11	0.9745	0.7787	0.4594	0.070*
C12	0.9675 (4)	0.68698 (16)	0.5574 (3)	0.0619 (8)
H12	1.0373	0.7063	0.6212	0.074*
C13	0.8998 (4)	0.61541 (15)	0.5606 (2)	0.0494 (7)
H13	0.9236	0.5867	0.6270	0.059*
C14	0.6210 (5)	0.63421 (19)	0.1741 (3)	0.0685 (9)
H141	0.5616	0.6010	0.1171	0.103*
H142	0.7178	0.6555	0.1465	0.103*
H143	0.5465	0.6742	0.1899	0.103*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0319 (2)	0.01876 (17)	0.03134 (19)	−0.00072 (14)	0.00039 (13)	0.00013 (13)
N1	0.0360 (11)	0.0208 (8)	0.0301 (9)	−0.0031 (7)	−0.0014 (7)	−0.0001 (7)
N2	0.0580 (14)	0.0230 (9)	0.0320 (10)	−0.0104 (9)	−0.0059 (9)	0.0001 (7)
N3	0.0596 (14)	0.0224 (9)	0.0374 (11)	−0.0087 (9)	−0.0005 (9)	0.0005 (8)
N4	0.0534 (15)	0.0390 (12)	0.0420 (12)	0.0053 (10)	−0.0039 (10)	−0.0036 (9)
O1	0.0787 (14)	0.0295 (9)	0.0347 (9)	−0.0137 (9)	−0.0128 (9)	0.0005 (7)
O2	0.144 (3)	0.0406 (12)	0.0522 (13)	−0.0262 (14)	−0.0281 (14)	0.0150 (9)
O3	0.0534 (12)	0.0781 (15)	0.0476 (11)	−0.0089 (11)	0.0027 (9)	−0.0230 (10)
O4	0.0555 (16)	0.101 (2)	0.0851 (17)	−0.0147 (14)	−0.0039 (12)	−0.0202 (15)
O5	0.0921 (18)	0.0979 (19)	0.0391 (11)	0.0547 (15)	−0.0002 (11)	−0.0087 (11)
O6	0.0329 (9)	0.0440 (10)	0.0510 (10)	0.0008 (7)	0.0014 (7)	−0.0118 (8)
O7	0.0533 (11)	0.0350 (8)	0.0354 (9)	0.0093 (8)	0.0043 (7)	0.0047 (7)
C1	0.0445 (14)	0.0263 (11)	0.0348 (12)	−0.0010 (10)	−0.0082 (10)	−0.0009 (9)
C2	0.0492 (15)	0.0234 (10)	0.0337 (11)	−0.0011 (10)	−0.0097 (10)	0.0027 (8)
C3	0.0403 (13)	0.0218 (10)	0.0288 (10)	−0.0016 (9)	0.0001 (9)	−0.0001 (8)
C4	0.0435 (14)	0.0279 (11)	0.0322 (11)	−0.0054 (10)	−0.0076 (9)	0.0012 (8)
C5	0.0440 (14)	0.0239 (10)	0.0330 (11)	−0.0018 (9)	−0.0032 (9)	0.0047 (8)
C6	0.0470 (14)	0.0227 (10)	0.0314 (11)	−0.0046 (9)	−0.0016 (9)	−0.0003 (8)
C7	0.0610 (17)	0.0271 (12)	0.0371 (13)	−0.0070 (11)	−0.0029 (11)	0.0009 (9)
C8	0.0494 (15)	0.0249 (11)	0.0409 (13)	−0.0031 (10)	0.0040 (10)	0.0021 (9)

C9	0.0620 (18)	0.0283 (12)	0.0448 (14)	−0.0049 (11)	0.0024 (12)	0.0029 (10)
C10	0.077 (2)	0.0312 (13)	0.0550 (17)	−0.0067 (13)	0.0116 (14)	0.0105 (11)
C11	0.074 (2)	0.0289 (13)	0.073 (2)	−0.0169 (13)	0.0128 (16)	0.0012 (13)
C12	0.075 (2)	0.0404 (16)	0.0641 (19)	−0.0207 (15)	−0.0071 (15)	−0.0045 (13)
C13	0.0639 (19)	0.0334 (13)	0.0474 (15)	−0.0093 (12)	−0.0025 (13)	0.0028 (10)
C14	0.098 (3)	0.0541 (19)	0.0482 (17)	−0.0007 (18)	−0.0056 (16)	0.0134 (14)

Geometric parameters (Å, °)

Zn1—O6^{i}	2.0816 (19)	C1—H1	0.9300
Zn1—O6	2.0816 (19)	C2—C3	1.384 (3)
Zn1—O7	2.1356 (18)	C2—H2	0.9300
Zn1—O7^{i}	2.1356 (18)	C3—C4	1.382 (3)
Zn1—N1^{i}	2.166 (2)	C3—C6	1.506 (3)
Zn1—N1	2.166 (2)	C4—C5	1.376 (3)
N1—C5	1.330 (3)	C4—H4	0.9300
N1—C1	1.343 (3)	C5—H5	0.9300
N2—C6	1.335 (3)	C7—C8	1.457 (3)
N2—N3	1.383 (3)	C7—H7	0.9300
N2—H21	0.8600	C8—C13	1.378 (4)
N3—C7	1.260 (3)	C8—C9	1.397 (3)
N4—O5	1.219 (3)	C9—C10	1.386 (4)
N4—O4	1.240 (3)	C10—C11	1.372 (4)
N4—O3	1.250 (3)	C10—H10	0.9300
O1—C6	1.225 (3)	C11—C12	1.368 (4)
O2—C9	1.365 (3)	C11—H11	0.9300
O2—C14	1.399 (3)	C12—C13	1.376 (4)
O6—H61	0.8884	C12—H12	0.9300
O6—H62	0.8270	C13—H13	0.9300
O7—H71	0.8673	C14—H141	0.9600
O7—H72	0.8106	C14—H142	0.9600
C1—C2	1.383 (3)	C14—H143	0.9600
O6^{i}—Zn1—O6	180.0	C4—C3—C6	117.45 (19)
O6^{i}—Zn1—O7	92.82 (7)	C2—C3—C6	124.96 (19)
O6—Zn1—O7	87.18 (7)	C5—C4—C3	119.5 (2)
O6^{i}—Zn1—O7^{i}	87.18 (7)	C5—C4—H4	120.3
O6—Zn1—O7^{i}	92.82 (7)	C3—C4—H4	120.3
O7—Zn1—O7^{i}	180.0	N1—C5—C4	123.4 (2)
O6^{i}—Zn1—N1^{i}	89.33 (7)	N1—C5—H5	118.3
O6—Zn1—N1^{i}	90.67 (7)	C4—C5—H5	118.3
O7—Zn1—N1^{i}	88.97 (7)	O1—C6—N2	123.9 (2)
O7^{i}—Zn1—N1^{i}	91.03 (7)	O1—C6—C3	120.5 (2)
O6^{i}—Zn1—N1	90.67 (7)	N2—C6—C3	115.54 (19)
O6—Zn1—N1	89.33 (7)	N3—C7—C8	122.0 (2)
O7—Zn1—N1	91.03 (7)	N3—C7—H7	119.0
O7^{i}—Zn1—N1	88.97 (7)	C8—C7—H7	119.0

N1^{i}—Zn1—N1	180.00 (9)	C13—C8—C9	118.8 (2)
C5—N1—C1	117.29 (19)	C13—C8—C7	121.8 (2)
C5—N1—Zn1	119.97 (14)	C9—C8—C7	119.4 (2)
C1—N1—Zn1	122.44 (15)	O2—C9—C10	124.6 (2)
C6—N2—N3	119.29 (19)	O2—C9—C8	115.0 (2)
C6—N2—H21	120.4	C10—C9—C8	120.3 (3)
N3—N2—H21	120.4	C11—C10—C9	119.2 (3)
C7—N3—N2	113.8 (2)	C11—C10—H10	120.4
O5—N4—O4	120.5 (2)	C9—C10—H10	120.4
O5—N4—O3	120.9 (3)	C12—C11—C10	121.0 (3)
O4—N4—O3	118.6 (2)	C12—C11—H11	119.5
C9—O2—C14	119.5 (2)	C10—C11—H11	119.5
Zn1—O6—H61	116.6	C11—C12—C13	119.9 (3)
Zn1—O6—H62	126.6	C11—C12—H12	120.1
H61—O6—H62	108.1	C13—C12—H12	120.1
Zn1—O7—H71	117.2	C12—C13—C8	120.7 (3)
Zn1—O7—H72	129.4	C12—C13—H13	119.6
H71—O7—H72	113.3	C8—C13—H13	119.6
N1—C1—C2	122.7 (2)	O2—C14—H141	109.5
N1—C1—H1	118.6	O2—C14—H142	109.5
C2—C1—H1	118.6	H141—C14—H142	109.5
C1—C2—C3	119.4 (2)	O2—C14—H143	109.5
C1—C2—H2	120.3	H141—C14—H143	109.5
C3—C2—H2	120.3	H142—C14—H143	109.5
C4—C3—C2	117.6 (2)		
O6^{i}—Zn1—N1—C5	−46.33 (18)	C4—C3—C6—O1	−19.0 (4)
O6—Zn1—N1—C5	133.67 (18)	C2—C3—C6—O1	162.2 (3)
O7—Zn1—N1—C5	−139.16 (18)	C4—C3—C6—N2	158.8 (2)
O7^{i}—Zn1—N1—C5	40.84 (18)	C2—C3—C6—N2	−20.0 (4)
O6^{i}—Zn1—N1—C1	127.22 (19)	N2—N3—C7—C8	−176.6 (2)
O6—Zn1—N1—C1	−52.78 (19)	N3—C7—C8—C13	0.3 (4)
O7—Zn1—N1—C1	34.38 (19)	N3—C7—C8—C9	178.2 (3)
O7^{i}—Zn1—N1—C1	−145.62 (19)	C14—O2—C9—C10	−9.4 (5)
C6—N2—N3—C7	179.2 (3)	C14—O2—C9—C8	172.3 (3)
C5—N1—C1—C2	2.4 (4)	C13—C8—C9—O2	175.3 (3)
Zn1—N1—C1—C2	−171.35 (19)	C7—C8—C9—O2	−2.6 (4)
N1—C1—C2—C3	−0.5 (4)	C13—C8—C9—C10	−3.1 (4)
C1—C2—C3—C4	−1.9 (4)	C7—C8—C9—C10	179.0 (3)
C1—C2—C3—C6	176.8 (2)	O2—C9—C10—C11	−176.8 (3)
C2—C3—C4—C5	2.4 (4)	C8—C9—C10—C11	1.4 (5)
C6—C3—C4—C5	−176.5 (2)	C9—C10—C11—C12	1.3 (5)
C1—N1—C5—C4	−1.9 (4)	C10—C11—C12—C13	−2.3 (5)
Zn1—N1—C5—C4	171.99 (19)	C11—C12—C13—C8	0.5 (5)
C3—C4—C5—N1	−0.5 (4)	C9—C8—C13—C12	2.1 (5)
N3—N2—C6—O1	4.3 (4)	C7—C8—C13—C12	179.9 (3)
N3—N2—C6—C3	−173.4 (2)		

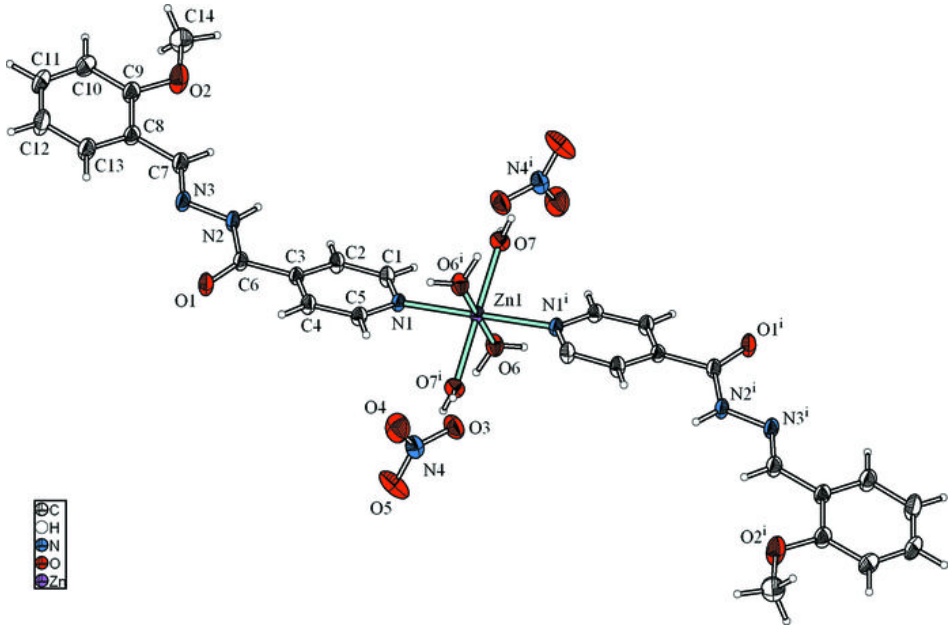
Symmetry codes: (i) −*x*+1, −*y*, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H61···O3	0.89	1.87	2.720 (3)	159
N2—H21···O5^{ii}	0.86	2.19	3.022 (3)	162
O6—H62···O3^{iii}	0.83	2.00	2.811 (3)	165
O7—H71···O4^{i}	0.87	2.24	3.014 (3)	148
O7—H72···O1^{iv}	0.81	2.01	2.788 (3)	159

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

Fig. 1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C9
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C8
C12
C13
C7
N3
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C6
O1
C3
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C5
C4
N1
O6i
Zn1
N1i
O7
N4i
O6
O7i
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C
H
N
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Zn

Fig. 2

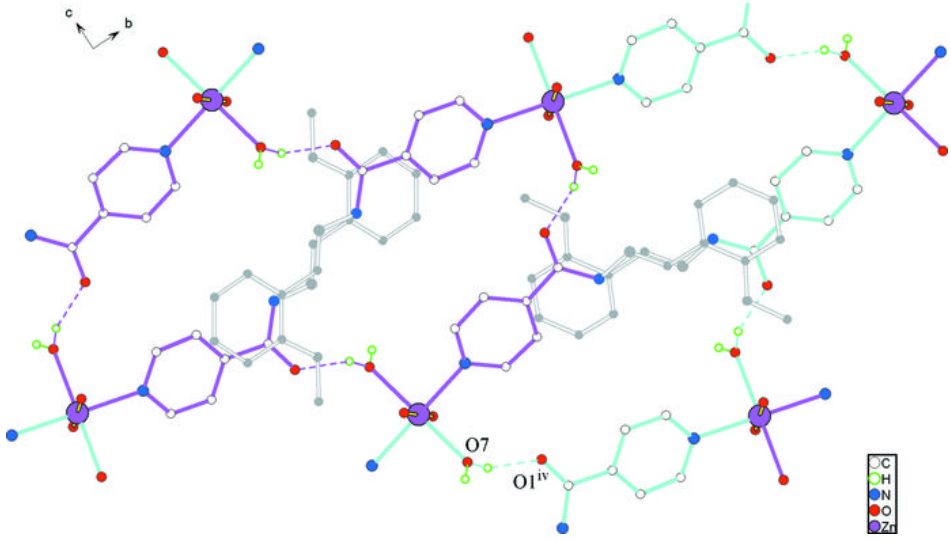

Fig. 3