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Poly[tetrabromidohexakis(μ_2-isonicotinato)bis(μ_2-pyridinium-4-carboxylato)-pentazinc(II)]

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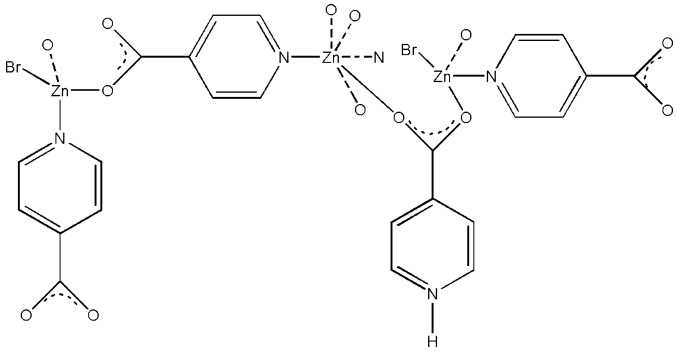
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.037; wR factor = 0.093; data-to-parameter ratio = 16.0.

In the title compound, $[Zn_5(IN)_6Br_4(1H\text{-}IN)_2]$, (where IN is isonicotinate, $C_6H_4NO_2$, and 1H-IN is pyridinium-4-carboxylate, $C_6H_5NO_2$), one Zn atom is located on an inversion center and has a six-coordinated ZnO_4N_2 geometry, while two other Zn atoms adopt a four-coordinated ZnO_2NBr pyramidal geometry. In the crystal structure, the metal centers are connected by intermolecular N—H···O hydrogen bonds, and IN and 1H-IN units, forming a two-dimensional bilayer structure.

Related literature

For a related structure, see: Lu & Babb (2001). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Zn_5(C_6H_4NO_2)_6Br_4(C_6H_5NO_2)_2]$
M_r = 1625.32
Monoclinic, $P2_1/c$
a = 14.096 (3) Å
b = 13.614 (3) Å
c = 14.781 (3) Å
β = 114.53 (3)°
V = 2580.5 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 5.47 mm^{-1}
T = 298 (2) K
0.47 × 0.42 × 0.29 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.123, T_{max} = 0.205
24795 measured reflections
5899 independent reflections
4756 reflections with $I > 2\sigma(I)$
R_{int} = 0.059

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.093
S = 1.06
5899 reflections
368 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.01 e Å^{-3}
$\Delta\rho_{min}$ = −1.05 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N2^{i}	2.118 (3)	Zn2—Br1	2.3798 (10)
Zn1—O2^{ii}	2.158 (3)	Zn3—O1^{ii}	1.948 (2)
Zn1—O7^{i}	2.191 (3)	Zn3—O8	1.955 (3)
Zn2—O4	1.933 (3)	Zn3—N3	2.037 (3)
Zn2—O5^{iii}	1.938 (3)	Zn3—Br2	2.3369 (9)
Zn2—N1	2.075 (3)		
N2—Zn1—O2^{ii}	84.93 (11)	O4—Zn2—Br1	110.08 (10)
N2^{i}—Zn1—O2^{ii}	95.07 (11)	O5^{iii}—Zn2—Br1	114.30 (9)
N2—Zn1—O7	86.31 (10)	N1—Zn2—Br1	107.59 (9)
N2^{i}—Zn1—O7	93.69 (10)	O1^{ii}—Zn3—O8	129.35 (12)
O2^{ii}—Zn1—O7	95.36 (11)	O1^{ii}—Zn3—N3	95.37 (11)
O2^{iv}—Zn1—O7	84.64 (11)	O8—Zn3—N3	96.52 (11)
O4—Zn2—O5^{iii}	127.98 (14)	O1^{ii}—Zn3—Br2	108.65 (9)
O4—Zn2—N1	96.22 (11)	O8—Zn3—Br2	107.89 (9)
O5^{iii}—Zn2—N1	95.07 (11)	N3—Zn3—Br2	118.85 (10)

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $x, y+1, z$; (iii) $x-1, y-1, z$; (iv) $-x, -y, -z+1$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···O6^{v}	0.86	2.23	2.758 (4)	119
N4—H4A···O3^{vi}	0.86	2.39	2.957 (4)	124

Symmetry codes: (v) $x, y-1, z$; (vi) $x+1, y, z$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2280).

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supplementary materials

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Poly[tetrabromidohexakis(μ_2-isonicotinato)bis(μ_2-pyridinium-4-carboxylato)pentazinc(II)]

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Comment

In recent years, isonicotinic acid (HIN) have been extensively studied, because of its ability of acting either as monodentate, bidentate, tridentate bridging or as chelating ligand. Novel complexes such as $[Cu_2(IN)_4(H_2O)_3][Cu_2(IN)_4(H_2O)_2].3H_2O$ (Lu & Babb, 2001) have been reported. The title compound, (I), was synthesized by hydrothermal synthesis at about 443 K. It was air stable and insoluble in most solvents. We report herein its crystal structure.

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles are generally within normal ranges (Allen *et al.*, 1987). Zn1 is located on an inversion centre and has ZnO_4N_2 octahedral geometry, which is completed by IN and 1*H*-IN oxygen atoms (where IN is isonicotinate), as well as IN nitrogen atoms, while Zn2 and Zn3 adopt the four-coordinated ZnO_2NBr pyramidal geometry, which is completed by IN oxygen and nitrogen atoms, as well as bromine ions.

The Zn—O/N bonds for Zn2 and Zn3 are in the range of 1.933 (3)–2.075 (3) Å, which are shorter than that observed for Zn1 within 2.118 (3)–2.191 (3) Å. The Zn—Br bonds are 2.3369 (9) Å for Zn3, and 2.3798 (10) Å for Zn2 (Table 1).

Furthermore, these metal centers are in turn connected by intermolecular N—H···O hydrogen bonds (Table 2), IN and 1*H*-IN to construct the two-dimensional bilayer structure (Fig. 2), where the 1*H*-IN ligands contribute to bidentate coordinated mode, while IN ligands to bidentate and tridentate coordinated modes. In addition, the closest Zn—Zn distance is *ca* 4.031 Å, and the edges of the present two-dimensional bilayer stucture is *ca* 8.8 *x* 8.5 Å.

Experimental

For the preparation of the title compound, (I), $ZnBr_2$ (1 mmol) and HIN (1.5 mmol) were dissolved in water (10 ml). The solution was heated in a 25 ml Teflon lined reaction vessel at 433 K for *ca* 3 d, and then cooled to room temperature. Colorless crystals of (I) were obtained (yield; 72%).

Refinement

H4A (for NH) was located in a difference syntheses, and only its thermal parameter was refined [N—H = 0.8622 Å and U_{iso}(H) = 0.10 (2) Å^2]. The remaining H atoms were positioned geometrically, with C—H = 0.93 Å, for aromatic H atoms, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

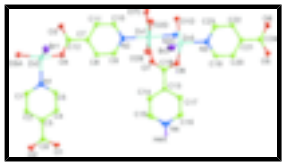


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level [symmetry codes: (A) $x-1, y-1, z$; (B) $-x, -y, -z+1$; (C) $-x, -y+1, -z+1$; (D) $x, y+1, z$.].

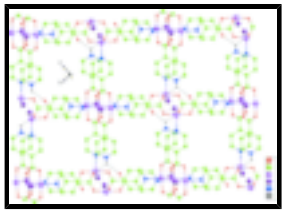


Fig. 2. Packing diagram for (I). Hydrogen bonds are shown as dashed lines.

catena-poly[tetrabromido-hexakis(isonicotinato)-bis(1*H*-\ isonicotinato)pentazinc(II)]

Crystal data

$[Zn_5Br_4(C_6H_4NO_2)_6(C_6H_5NO_2)_2]$	$F_{000} = 1592$
$M_r = 1625.32$	$D_x = 2.092$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 19365 reflections
$a = 14.096$ (3) Å	$\theta = 3.0$–27.5º
$b = 13.614$ (3) Å	$\mu = 5.47$ mm^{-1}
$c = 14.781$ (3) Å	$T = 298$ (2) K
$\beta = 114.53$ (3)º	Block, colorless
$V = 2580.5$ (11) Å^3	0.47 × 0.42 × 0.29 mm
$Z = 2$	

Data collection

Bruker SMART CCD area-detector diffractometer	5899 independent reflections
Radiation source: fine-focus sealed tube	4756 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.059$
$T = 298$(2) K	$\theta_{max} = 27.5$º
φ and ω scans	$\theta_{min} = 3.0$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -18 \rightarrow 18$
$T_{min} = 0.123$, $T_{max} = 0.205$	$k = -17 \rightarrow 16$
24795 measured reflections	$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.037$	H-atom parameters constrained
$wR(F^2) = 0.093$	$w = 1/[\sigma^2(F_o^2) + (0.0355P)^2 + 3.1559P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.001$
5899 reflections	$\Delta\rho_{max} = 1.01$ e Å^{-3}
368 parameters	$\Delta\rho_{min} = -1.05$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	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}
Zn1	0.0000	0.5000	0.5000	0.02606 (14)
Zn2	−0.42512 (3)	−0.01650 (3)	0.32550 (4)	0.02699 (11)
Zn3	0.05811 (3)	0.60169 (3)	0.27190 (3)	0.02547 (11)
Br1	−0.50694 (3)	0.03530 (3)	0.15671 (4)	0.04128 (12)
Br2	−0.02848 (3)	0.54039 (3)	0.11049 (3)	0.04207 (12)
O1	−0.03829 (18)	−0.31624 (18)	0.3020 (2)	0.0328 (6)
O2	−0.10618 (19)	−0.43045 (18)	0.3646 (2)	0.0340 (6)
O3	−0.4360 (2)	0.1908 (2)	0.3990 (3)	0.0490 (9)
O4	−0.32061 (18)	0.07798 (18)	0.4031 (2)	0.0383 (7)
O5	0.48779 (19)	0.90252 (19)	0.3679 (2)	0.0380 (7)
O6	0.3734 (2)	1.0190 (2)	0.3589 (3)	0.0557 (10)
O7	0.07644 (19)	0.40797 (18)	0.4283 (2)	0.0351 (6)
O8	0.15352 (19)	0.49998 (18)	0.3529 (2)	0.0343 (6)
N1	−0.3216 (2)	−0.1282 (2)	0.3338 (2)	0.0248 (6)
N2	−0.1145 (2)	0.3882 (2)	0.4622 (2)	0.0265 (6)
N3	0.1677 (2)	0.7084 (2)	0.2982 (2)	0.0266 (6)
N4	0.3694 (2)	0.2063 (2)	0.4284 (3)	0.0362 (8)
H4A	0.4172	0.1632	0.4369	0.10 (2)*
C1	−0.3497 (3)	−0.2229 (2)	0.3181 (3)	0.0278 (8)
H1	−0.4179	−0.2398	0.3060	0.033*
C2	−0.2817 (3)	−0.2966 (2)	0.3190 (3)	0.0268 (8)
H2	−0.3031	−0.3619	0.3099	0.032*
C3	−0.1811 (2)	−0.2712 (2)	0.3338 (3)	0.0217 (7)
C4	−0.1525 (3)	−0.1733 (3)	0.3487 (3)	0.0274 (8)

H4	−0.0858	−0.1542	0.3580	0.033*
C5	−0.2234 (3)	−0.1045 (2)	0.3498 (3)	0.0283 (8)
H5	−0.2026	−0.0392	0.3620	0.034*
C6	−0.1033 (2)	−0.3465 (2)	0.3341 (3)	0.0235 (7)
C7	−0.2650 (2)	0.2425 (2)	0.4292 (3)	0.0241 (7)
C8	−0.1620 (3)	0.2180 (2)	0.4520 (3)	0.0266 (8)
H8	−0.1416	0.1525	0.4569	0.032*
C9	−0.0904 (3)	0.2923 (2)	0.4674 (3)	0.0270 (8)
H9	−0.0217	0.2751	0.4821	0.032*
C10	−0.2148 (3)	0.4110 (2)	0.4362 (3)	0.0279 (8)
H10	−0.2339	0.4769	0.4283	0.033*
C11	−0.2909 (3)	0.3415 (3)	0.4205 (3)	0.0282 (8)
H11	−0.3593	0.3608	0.4041	0.034*
C12	−0.3486 (3)	0.1654 (3)	0.4097 (3)	0.0297 (8)
C13	0.2260 (2)	0.3467 (2)	0.4124 (3)	0.0204 (7)
C14	0.2064 (3)	0.2487 (2)	0.4237 (3)	0.0275 (8)
H14	0.1442	0.2303	0.4267	0.033*
C15	0.2793 (3)	0.1791 (3)	0.4305 (3)	0.0358 (9)
H15	0.2660	0.1131	0.4366	0.043*
C16	0.3927 (3)	0.3009 (3)	0.4220 (3)	0.0361 (9)
H16	0.4573	0.3177	0.4236	0.043*
C17	0.3216 (3)	0.3721 (3)	0.4132 (3)	0.0297 (8)
H17	0.3372	0.4376	0.4078	0.036*
C18	0.1439 (2)	0.4238 (2)	0.3974 (3)	0.0244 (7)
C19	0.2674 (3)	0.6857 (3)	0.3206 (3)	0.0320 (9)
H19	0.2856	0.6199	0.3220	0.038*
C20	0.3436 (3)	0.7555 (3)	0.3415 (3)	0.0335 (9)
H20	0.4121	0.7370	0.3568	0.040*
C21	0.3179 (3)	0.8534 (2)	0.3394 (3)	0.0263 (8)
C22	0.2149 (3)	0.8774 (3)	0.3152 (3)	0.0364 (10)
H22	0.1946	0.9428	0.3125	0.044*
C23	0.1431 (3)	0.8032 (3)	0.2953 (3)	0.0366 (10)
H23	0.0739	0.8199	0.2790	0.044*
C24	0.3993 (3)	0.9333 (3)	0.3577 (3)	0.0320 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0207 (3)	0.0190 (3)	0.0406 (4)	−0.0014 (2)	0.0148 (2)	0.0005 (2)
Zn2	0.01712 (19)	0.01695 (19)	0.0482 (3)	−0.00093 (15)	0.01486 (18)	−0.00226 (18)
Zn3	0.01996 (19)	0.01928 (19)	0.0404 (3)	0.00171 (15)	0.01574 (17)	−0.00049 (17)
Br1	0.0345 (2)	0.0343 (2)	0.0505 (3)	−0.00131 (17)	0.01318 (19)	0.00503 (18)
Br2	0.0394 (2)	0.0388 (2)	0.0445 (3)	0.00509 (18)	0.01385 (19)	−0.00973 (19)
O1	0.0283 (12)	0.0258 (13)	0.0546 (18)	0.0055 (11)	0.0274 (13)	0.0006 (12)
O2	0.0282 (13)	0.0210 (12)	0.0506 (18)	0.0057 (11)	0.0142 (12)	0.0068 (12)
O3	0.0237 (13)	0.0311 (15)	0.097 (3)	−0.0053 (12)	0.0304 (15)	−0.0130 (16)
O4	0.0205 (12)	0.0209 (12)	0.068 (2)	−0.0041 (10)	0.0136 (13)	−0.0096 (13)
O5	0.0247 (13)	0.0273 (13)	0.068 (2)	0.0002 (11)	0.0255 (13)	0.0047 (13)

O6	0.0386 (16)	0.0200 (14)	0.118 (3)	−0.0047 (12)	0.0417 (19)	−0.0116 (16)
O7	0.0267 (13)	0.0267 (13)	0.062 (2)	−0.0002 (11)	0.0280 (13)	−0.0013 (13)
O8	0.0281 (13)	0.0245 (12)	0.0543 (18)	0.0080 (11)	0.0210 (13)	0.0118 (13)
N1	0.0190 (13)	0.0192 (13)	0.0377 (18)	0.0021 (11)	0.0133 (12)	−0.0018 (13)
N2	0.0210 (13)	0.0222 (14)	0.0391 (18)	−0.0010 (12)	0.0151 (13)	0.0020 (13)
N3	0.0206 (13)	0.0221 (14)	0.0396 (18)	−0.0010 (12)	0.0151 (13)	0.0000 (13)
N4	0.0336 (17)	0.0340 (17)	0.039 (2)	0.0187 (15)	0.0134 (15)	0.0022 (15)
C1	0.0176 (15)	0.0231 (17)	0.043 (2)	−0.0011 (13)	0.0127 (15)	−0.0023 (16)
C2	0.0247 (16)	0.0180 (16)	0.039 (2)	0.0000 (13)	0.0142 (15)	−0.0009 (15)
C3	0.0187 (14)	0.0217 (16)	0.0258 (18)	0.0036 (13)	0.0105 (13)	0.0016 (14)
C4	0.0192 (15)	0.0222 (16)	0.043 (2)	−0.0006 (14)	0.0148 (15)	0.0008 (16)
C5	0.0252 (17)	0.0184 (16)	0.046 (2)	−0.0024 (14)	0.0193 (16)	−0.0020 (16)
C6	0.0194 (15)	0.0221 (16)	0.0283 (19)	−0.0011 (13)	0.0093 (14)	−0.0037 (14)
C7	0.0184 (15)	0.0213 (16)	0.033 (2)	−0.0042 (13)	0.0116 (14)	−0.0048 (14)
C8	0.0221 (16)	0.0196 (16)	0.039 (2)	0.0022 (13)	0.0134 (15)	−0.0014 (15)
C9	0.0189 (15)	0.0240 (17)	0.039 (2)	−0.0007 (13)	0.0132 (15)	−0.0013 (16)
C10	0.0239 (16)	0.0184 (16)	0.044 (2)	0.0002 (14)	0.0169 (16)	0.0001 (15)
C11	0.0175 (15)	0.0258 (17)	0.042 (2)	0.0006 (14)	0.0129 (15)	−0.0036 (16)
C12	0.0224 (17)	0.0250 (17)	0.043 (2)	−0.0026 (14)	0.0146 (16)	−0.0048 (16)
C13	0.0192 (15)	0.0185 (15)	0.0235 (17)	0.0023 (13)	0.0089 (13)	−0.0006 (13)
C14	0.0288 (17)	0.0223 (17)	0.035 (2)	−0.0006 (14)	0.0167 (16)	−0.0015 (15)
C15	0.047 (2)	0.0225 (18)	0.041 (2)	0.0056 (17)	0.0215 (19)	0.0015 (17)
C16	0.0232 (17)	0.038 (2)	0.049 (3)	0.0034 (16)	0.0174 (17)	−0.0029 (19)
C17	0.0244 (17)	0.0262 (18)	0.040 (2)	0.0016 (14)	0.0148 (16)	0.0001 (16)
C18	0.0201 (15)	0.0224 (16)	0.0304 (19)	0.0000 (14)	0.0101 (14)	−0.0037 (15)
C19	0.0267 (17)	0.0185 (16)	0.056 (3)	0.0038 (14)	0.0218 (17)	0.0021 (17)
C20	0.0243 (17)	0.0233 (17)	0.059 (3)	0.0026 (15)	0.0238 (18)	0.0021 (18)
C21	0.0218 (16)	0.0212 (16)	0.041 (2)	−0.0017 (14)	0.0179 (15)	0.0003 (15)
C22	0.0267 (18)	0.0181 (17)	0.069 (3)	0.0051 (14)	0.0242 (19)	0.0054 (18)
C23	0.0218 (17)	0.0271 (19)	0.063 (3)	0.0036 (15)	0.0203 (18)	0.0042 (19)
C24	0.0282 (18)	0.0242 (17)	0.051 (3)	−0.0011 (15)	0.0239 (17)	−0.0011 (17)

Geometric parameters (Å, °)

Zn1—N2^{i}	2.118 (3)	C2—C1	1.384 (5)
Zn1—O2^{ii}	2.158 (3)	C2—H2	0.9300
Zn1—O2^{iii}	2.158 (3)	C3—C4	1.383 (5)
Zn1—O7^{i}	2.191 (3)	C3—C2	1.386 (4)
Zn2—O4	1.933 (3)	C4—H4	0.9300
Zn2—O5^{iv}	1.938 (3)	C5—C4	1.374 (5)
Zn2—N1	2.075 (3)	C5—H5	0.9300
Zn2—Br1	2.3798 (10)	C6—C3	1.500 (4)
Zn3—O1^{ii}	1.948 (2)	C7—C11	1.389 (5)
Zn3—O8	1.955 (3)	C7—C12	1.513 (5)
Zn3—N3	2.037 (3)	C8—C9	1.380 (5)
Zn3—Br2	2.3369 (9)	C8—C7	1.388 (4)
O1—C6	1.263 (4)	C8—H8	0.9300
O1—Zn3^{v}	1.948 (2)	C9—H9	0.9300

O2—C6	1.236 (4)	C10—C11	1.376 (5)
O2—Zn1^{v}	2.158 (3)	C10—H10	0.9300
O3—C12	1.225 (4)	C11—H11	0.9300
O4—C12	1.270 (4)	C13—C17	1.387 (4)
O5—C24	1.265 (4)	C13—C14	1.387 (5)
O5—Zn2^{vi}	1.938 (3)	C13—C18	1.508 (4)
O6—C24	1.224 (4)	C14—C15	1.371 (5)
O7—C18	1.233 (4)	C14—H14	0.9300
O7—Zn1	2.191 (3)	C15—H15	0.9300
O8—C18	1.266 (4)	C16—H16	0.9300
N1—C1	1.341 (4)	C17—C16	1.360 (5)
N1—C5	1.344 (4)	C17—H17	0.9300
N2—C10	1.338 (4)	C19—H19	0.9300
N2—C9	1.343 (4)	C20—C19	1.371 (5)
N2—Zn1	2.118 (3)	C20—H20	0.9300
N3—C23	1.334 (5)	C21—C20	1.378 (5)
N3—C19	1.338 (4)	C21—C22	1.383 (5)
N4—C15	1.336 (5)	C21—C24	1.521 (5)
N4—C16	1.342 (5)	C22—C23	1.373 (5)
N4—H4A	0.8622	C22—H22	0.9300
C1—H1	0.9300	C23—H23	0.9300
N2—Zn1—N2^{i}	180.0	C4—C5—H5	118.8
N2—Zn1—O2^{ii}	84.93 (11)	O2—C6—O1	125.3 (3)
N2^{i}—Zn1—O2^{ii}	95.07 (11)	O2—C6—C3	119.9 (3)
N2—Zn1—O2^{iii}	95.07 (11)	O1—C6—C3	114.8 (3)
N2^{i}—Zn1—O2^{iii}	84.93 (11)	C8—C7—C11	117.6 (3)
O2^{ii}—Zn1—O2^{iii}	180.000 (1)	C8—C7—C12	122.2 (3)
N2—Zn1—O7	86.31 (10)	C11—C7—C12	120.1 (3)
N2^{i}—Zn1—O7	93.69 (10)	C9—C8—C7	118.9 (3)
O2^{ii}—Zn1—O7	95.36 (11)	C9—C8—H8	120.5
O2^{iii}—Zn1—O7	84.64 (11)	C7—C8—H8	120.5
N2—Zn1—O7^{i}	93.69 (10)	N2—C9—C8	123.6 (3)
N2^{i}—Zn1—O7^{i}	86.31 (10)	N2—C9—H9	118.2
O2^{ii}—Zn1—O7^{i}	84.64 (11)	C8—C9—H9	118.2
O2^{iii}—Zn1—O7^{i}	95.36 (11)	N2—C10—C11	123.1 (3)
O7—Zn1—O7^{i}	180.00 (13)	N2—C10—H10	118.5
O4—Zn2—O5^{iv}	127.98 (14)	C11—C10—H10	118.5
O4—Zn2—N1	96.22 (11)	C10—C11—C7	119.7 (3)
O5^{iv}—Zn2—N1	95.07 (11)	C10—C11—H11	120.1
O4—Zn2—Br1	110.08 (10)	C7—C11—H11	120.1
O5^{iv}—Zn2—Br1	114.30 (9)	O3—C12—O4	125.6 (3)
N1—Zn2—Br1	107.59 (9)	O3—C12—C7	119.4 (3)
O1^{ii}—Zn3—O8	129.35 (12)	O4—C12—C7	115.0 (3)
O1^{ii}—Zn3—N3	95.37 (11)	C17—C13—C14	118.7 (3)

O8—Zn3—N3	96.52 (11)	C17—C13—C18	120.8 (3)
O1^{ii}—Zn3—Br2	108.65 (9)	C14—C13—C18	120.5 (3)
O8—Zn3—Br2	107.89 (9)	C15—C14—C13	119.6 (3)
N3—Zn3—Br2	118.85 (10)	C15—C14—H14	120.2
C6—O1—Zn3^{v}	125.6 (2)	C13—C14—H14	120.2
C6—O2—Zn1^{v}	129.0 (2)	N4—C15—C14	119.9 (3)
C12—O4—Zn2	119.0 (2)	N4—C15—H15	120.1
C24—O5—Zn2^{vi}	120.0 (2)	C14—C15—H15	120.1
C18—O7—Zn1	133.6 (2)	N4—C16—C17	119.9 (3)
C18—O8—Zn3	134.8 (2)	N4—C16—H16	120.0
C1—N1—C5	118.0 (3)	C17—C16—H16	120.0
C1—N1—Zn2	123.0 (2)	C16—C17—C13	119.9 (3)
C5—N1—Zn2	118.9 (2)	C16—C17—H17	120.1
C10—N2—C9	117.0 (3)	C13—C17—H17	120.1
C10—N2—Zn1	120.5 (2)	O7—C18—O8	126.9 (3)
C9—N2—Zn1	122.4 (2)	O7—C18—C13	119.1 (3)
C23—N3—C19	117.7 (3)	O8—C18—C13	113.9 (3)
C23—N3—Zn3	121.1 (2)	N3—C19—C20	122.7 (3)
C19—N3—Zn3	121.2 (2)	N3—C19—H19	118.7
C15—N4—C16	122.0 (3)	C20—C19—H19	118.7
C15—N4—H4A	120.1	C19—C20—C21	119.4 (3)
C16—N4—H4A	117.7	C19—C20—H20	120.3
N1—C1—C2	122.8 (3)	C21—C20—H20	120.3
N1—C1—H1	118.6	C20—C21—C22	118.2 (3)
C2—C1—H1	118.6	C20—C21—C24	121.0 (3)
C1—C2—C3	118.7 (3)	C22—C21—C24	120.7 (3)
C1—C2—H2	120.7	C23—C22—C21	118.9 (3)
C3—C2—H2	120.7	C23—C22—H22	120.6
C4—C3—C2	118.5 (3)	C21—C22—H22	120.6
C4—C3—C6	119.6 (3)	N3—C23—C22	123.1 (3)
C2—C3—C6	122.0 (3)	N3—C23—H23	118.4
C5—C4—C3	119.6 (3)	C22—C23—H23	118.4
C5—C4—H4	120.2	O6—C24—O5	126.8 (3)
C3—C4—H4	120.2	O6—C24—C21	118.5 (3)
N1—C5—C4	122.4 (3)	O5—C24—C21	114.7 (3)
N1—C5—H5	118.8		
O4—Zn2—N1—C1	159.6 (3)	C9—N2—C10—C11	3.7 (6)
O5^{iv}—Zn2—N1—C1	30.5 (3)	Zn1—N2—C10—C11	−173.4 (3)
Br1—Zn2—N1—C1	−87.0 (3)	C23—N3—C19—C20	0.8 (6)
O4—Zn2—N1—C5	−24.6 (3)	Zn3—N3—C19—C20	−178.1 (3)
O5^{iv}—Zn2—N1—C5	−153.7 (3)	C19—N3—C23—C22	−0.8 (7)
Br1—Zn2—N1—C5	88.8 (3)	Zn3—N3—C23—C22	178.1 (4)
O5^{iv}—Zn2—O4—C12	−86.0 (3)	C16—N4—C15—C14	1.6 (6)
N1—Zn2—O4—C12	172.6 (3)	C15—N4—C16—C17	−2.8 (6)
Br1—Zn2—O4—C12	61.3 (3)	C3—C2—C1—N1	−2.1 (6)
O1^{ii}—Zn3—O8—C18	53.0 (4)	C4—C3—C2—C1	1.1 (6)
N3—Zn3—O8—C18	155.5 (4)	C6—C3—C2—C1	−179.0 (3)

Br2—Zn3—O8—C18	−81.4 (4)	C2—C3—C4—C5	0.8 (6)
O1^{ii}—Zn3—N3—C23	−21.3 (3)	C6—C3—C4—C5	−179.1 (4)
O8—Zn3—N3—C23	−152.0 (3)	N1—C5—C4—C3	−2.0 (6)
Br2—Zn3—N3—C23	93.5 (3)	O2—C6—C3—C4	147.9 (4)
O1^{ii}—Zn3—N3—C19	157.5 (3)	O1—C6—C3—C4	−32.0 (5)
O8—Zn3—N3—C19	26.9 (3)	O2—C6—C3—C2	−32.0 (5)
Br2—Zn3—N3—C19	−87.7 (3)	O1—C6—C3—C2	148.2 (4)
Zn3^{v}—O1—C6—O2	10.7 (5)	C8—C7—C11—C10	−1.1 (6)
Zn3^{v}—O1—C6—C3	−169.4 (2)	C12—C7—C11—C10	−178.5 (4)
Zn1^{v}—O2—C6—O1	71.3 (5)	C8—C7—C12—O3	173.2 (4)
Zn1^{v}—O2—C6—C3	−108.6 (3)	C11—C7—C12—O3	−9.5 (6)
Zn2—O4—C12—O3	24.3 (6)	C8—C7—C12—O4	−8.6 (6)
Zn2—O4—C12—C7	−153.7 (3)	C11—C7—C12—O4	168.7 (4)
Zn2^{vi}—O5—C24—O6	−29.5 (6)	C9—C8—C7—C11	1.6 (6)
Zn2^{vi}—O5—C24—C21	148.7 (3)	C9—C8—C7—C12	179.0 (4)
C18—O7—Zn1—N2	163.4 (4)	C7—C8—C9—N2	0.5 (6)
C18—O7—Zn1—N2^{i}	−16.6 (4)	N2—C10—C11—C7	−1.7 (6)
C18—O7—Zn1—O2^{ii}	78.8 (4)	C17—C13—C14—C15	−3.2 (6)
C18—O7—Zn1—O2^{iii}	−101.2 (4)	C18—C13—C14—C15	175.6 (4)
Zn1—O7—C18—O8	−38.8 (6)	C14—C13—C17—C16	2.0 (6)
Zn1—O7—C18—C13	141.1 (3)	C18—C13—C17—C16	−176.8 (4)
Zn3—O8—C18—O7	−25.3 (6)	C17—C13—C18—O7	−156.4 (4)
Zn3—O8—C18—C13	154.9 (3)	C14—C13—C18—O7	24.9 (5)
C5—N1—C1—C2	1.0 (6)	C17—C13—C18—O8	23.5 (5)
Zn2—N1—C1—C2	176.8 (3)	C14—C13—C18—O8	−155.3 (3)
C1—N1—C5—C4	1.1 (6)	C13—C14—C15—N4	1.5 (6)
Zn2—N1—C5—C4	−174.9 (3)	C13—C17—C16—N4	1.0 (6)
C10—N2—Zn1—O2^{ii}	−48.6 (3)	C21—C20—C19—N3	−0.1 (7)
C9—N2—Zn1—O2^{ii}	134.4 (3)	C20—C21—C24—O6	−177.2 (4)
C10—N2—Zn1—O2^{iii}	131.4 (3)	C22—C21—C24—O6	6.1 (6)
C9—N2—Zn1—O2^{iii}	−45.6 (3)	C20—C21—C24—O5	4.4 (6)
C10—N2—Zn1—O7	−144.4 (3)	C22—C21—C24—O5	−172.2 (4)
C9—N2—Zn1—O7	38.7 (3)	C22—C21—C20—C19	−0.6 (6)
C10—N2—Zn1—O7^{i}	35.6 (3)	C24—C21—C20—C19	−177.3 (4)
C9—N2—Zn1—O7^{i}	−141.3 (3)	C20—C21—C22—C23	0.6 (7)
C10—N2—C9—C8	−3.2 (6)	C24—C21—C22—C23	177.3 (4)
Zn1—N2—C9—C8	173.9 (3)	C21—C22—C23—N3	0.1 (7)

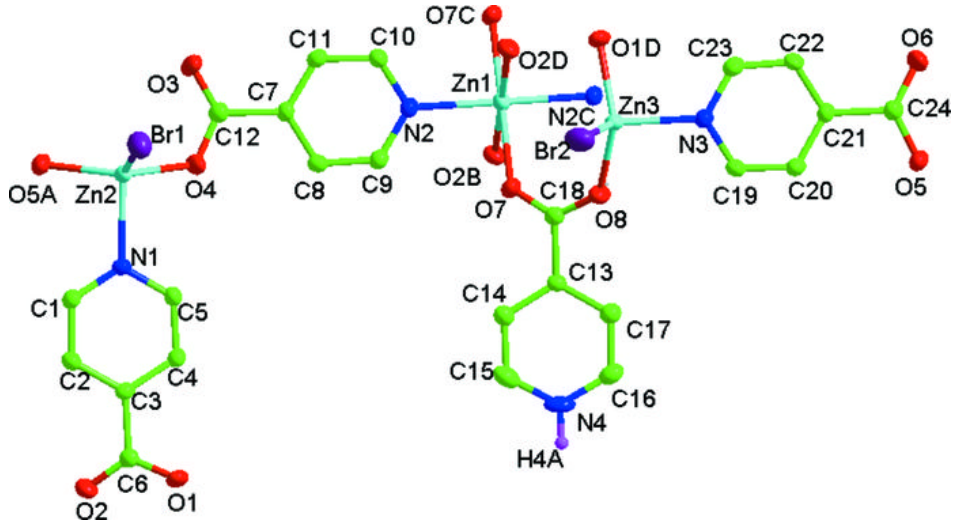
Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) *x*, *y*+1, *z*; (iii) −*x*, −*y*, −*z*+1; (iv) *x*−1, *y*−1, *z*; (v) *x*, *y*−1, *z*; (vi) *x*+1, *y*+1, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4A···O6^{v}	0.86	2.23	2.758 (4)	119
N4—H4A···O3^{vii}	0.86	2.39	2.957 (4)	124

Symmetry codes: (v) *x*, *y*−1, *z*; (vii) *x*+1, *y*, *z*.

Fig. 1


O7C
C11
C10
O2D
O1D
C23
C22
O6
O3
C7
Zn1
Zn3
C24
Br1
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N2
N2C
N3
C21
Br2
O5A
Zn2
O4
C8
C9
O2B
C18
C19
C20
O5
O7
O8
N1
C13
C1
C5
C14
C17
C2
C4
C15
C16
C3
N4
H4A
C6
O2
O1

Fig. 2