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Poly[(nitrato-κO)tris(μ_3-1*H*-1,2,4-triazolato)dizinc(II)]: a three-dimensional coordination polymer

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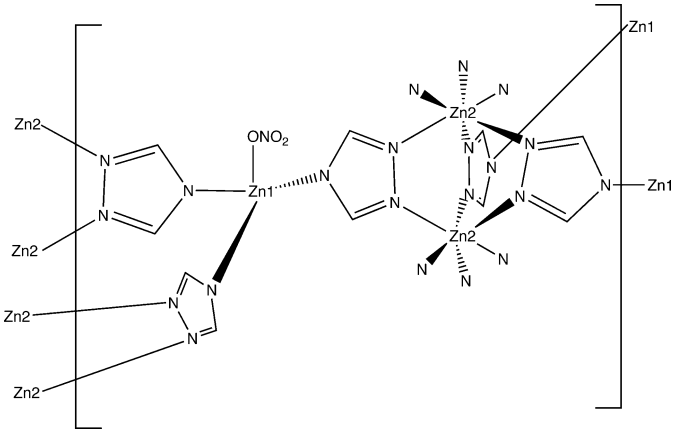
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(N–C) = 0.003 Å; disorder in main residue; R factor = 0.024; wR factor = 0.062; data-to-parameter ratio = 13.5.

In the title compound, $[Zn_2(C_2H_2N_3)_3(NO_3)]$, there are two unique Zn atoms, both with site symmetry *m*. One forms a ZnN_3O tetrahedron and the other a ZnN_6 octahedron. One and a half 1*H*-1,2,4-triazolate ligands, with the half-ligand located on a mirror plane, and a disordered nitrate anion complete the asymmetric unit of the structure. The polymeric connectivity is three-dimensional.

Related literature

For the isostructural Co phase, see: Ouellette *et al.* (2006). For related literature, see: Goforth *et al.* (2005); Su *et al.* (2004).



Experimental

Crystal data

$[Zn_2(C_2H_2N_3)_3(NO_3)]$
M_r = 396.95
Orthorhombic, *Pnma*
a = 7.6001 (4) Å
b = 9.9758 (5) Å
c = 17.5108 (8) Å
V = 1327.62 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.64 mm^{-1}
T = 150 (1) K
0.36 × 0.28 × 0.22 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.808, T_{max} = 1.000
(expected range = 0.363–0.449)
12217 measured reflections
1752 independent reflections
1627 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.062
S = 1.08
1752 reflections
130 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.84 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—N1	1.968 (2)	Zn2—N3^{ii}	2.109 (2)
Zn1—N4^{i}	1.9814 (16)	Zn2—N6^{iii}	2.1415 (15)
Zn1—N4	1.9815 (15)	Zn2—N6^{iv}	2.1415 (15)
Zn1—O1*A*^{i}	2.021 (4)	Zn2—N5^{v}	2.1634 (15)
Zn1—O1*A*	2.021 (4)	Zn2—N5^{vi}	2.1635 (15)
Zn1—O1*B*	2.033 (12)	Zn2—N2	2.221 (2)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: various; software used to prepare material for publication: *SHELXTL* (Bruker, 2000).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2547).

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supplementary materials

Acta Cryst. (2007). E**63**, m2744 [**doi:10.1107/S1600536807049574**]

Poly[(nitrato-κO)tris(μ_3-1H-1,2,4-triazolato)dizinc(II)]: a three-dimensional coordination polymer

J. M. Ellsworth, M. D. Smith and H.-C. zur Loye

Comment

The title compound, (I), was solvothermally synthesized from $Zn(NO_3)_2$ and 1,2,4–1H-triazole (Htrz) in a 1:1 molar ratio in an ethanol/water solvent mixture. Single crystal X-ray analysis determined that the transparent crystals contain a complicated three-dimensional atomic network whose asymmetric unit is shown in **Figure 1**. There are two crystallographically distinct Zn centers (**Figure 2**). Zn1 atoms are in a tetrahedral coordination sphere, coordinated to three trz ligands and one disordered NO_3. Zn2 atoms are in an octahedral coordination sphere, coordinated to six trz ligands (**Figure 2 b**). The nitrate anion coordinated to Zn1 is disordered over two independent positions in the asymmetric unit, and three positions when the mirror symmetry of the crystal is taken into account, in the proportion 40/40/20 (**Figure 2a**). Each Zn center forms its own one-dimensional chain/column along the *a* axis through the anionic bridging mode of the trz ligands, whose connectives generate a three-dimensional structure (**Figure 3**). Zn2 and its ligands form infinite one-dimensional chains down the *a* axis. These one-dimensional chains propagate by the N1,N2 bridging mode (see **Figure 4**) of the trz ligands. Each Zn2 one-dimensional chain is bridged *via* a N4 mode to columns of tetrahedrally coordinated Zn1 atoms. The Zn—O and Zn—N bond distances (Table 1) are comparable to those in an isostructural complex synthesized with Co (Ouellette *et al.*, 2006). Additionally, the bridging characteristics of trz in $[Zn_2(trz)_3(NO_3)]$ are similar to our previous work involving trz and ZnF, in that all trz ring nitrogen atoms coordinate to the Zn centers through an N1,N2,N4 bridging mode (Goforth *et al.*, 2005; Su *et al.*, 2004).

Experimental

In a typical procedure trz (0.5 mmol) and $Zn(NO_3)_2$ (0.5 mmol) were weighed and placed in a 23 ml Teflon lined autoclave together with 5 ml water and 5 ml e thanol, which functioned as the reaction solvent. The autoclave was subsequently sealed and heated at a rate of 1 K/min to 433 K. The temperature was held at 433 K for three days before it was decreased, at a rate of 0.1 K/min, to 353 K where it was then held for 6 h. Finally, the temperature was decreased at a rate of 0.1 K/min to room temperature. Colorless blocks of (I) were hand picked from the reaction and used for single-crystal analyses.

Refinement

The atoms of the minor nitrate disorder component were refined with U_{iso} values. The hydrogen atoms were placed in geometrically idealized positions and included as riding atoms. The final difference map extrema are +0.84 e-/Å3 (0.98 Å from Zn1) and −0.52 e-/Å3 (0.51 Å from O1B).

Figures

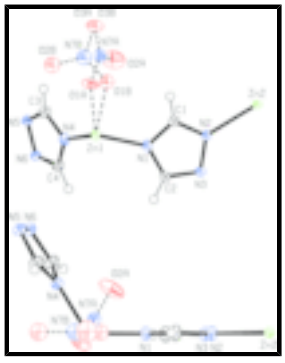


Fig. 1. Two views of the asymmetric unit of (I). Displacement ellipsoids are drawn at the 50% probability level. The asymmetric unit is on a mirror plane containing Zn1, Zn2 trz ligand {N1}, and component N7B of the disordered nitrate anion.

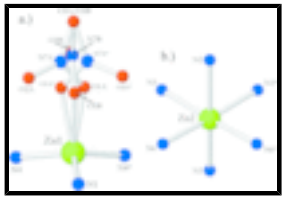


Fig. 2. (*a*) Tetrahedral coordination around Zn2. Disordered nitrate mirror plane is vertical and nearly perpendicular to figure. Occupancies: N7A = N7A* = 40%, N7B = 20%. (*b*) Octahedral coordination around Zn2. Mirror plane is vertical and nearly perpendicular to figure.

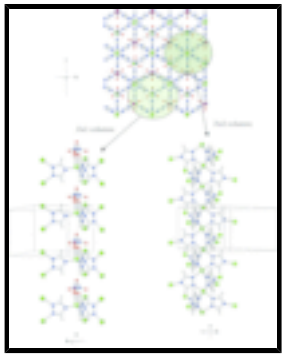


Fig. 3. View down *a* axis of the three-dimensional structure (top). Columns of tetrahedrally coordinated Zn1 atoms (bottom left). one-dimensional chains of Zn1 atoms (bottom right). Zn1 lighter green; Zn2 darker green.

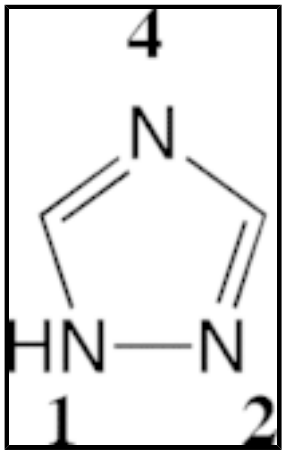


Fig. 4. Labeling scheme of coordination modes in 1,2,4-triazoles

Poly[(nitrato-κ*O*)tris(μ$_3$-1*H*-1,2,4-triazolato)dizinc(II)]

Crystal data

$[Zn_2(C_2H_2N_3)_3(NO_3)]$ $F_{000} = 784$

M_r = 396.95	D_x = 1.986 Mg m^{-3}
Orthorhombic, *Pnma*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2n	Cell parameters from 5133 reflections
a = 7.6001 (4) Å	θ = 2.4–28.3º
b = 9.9758 (5) Å	μ = 3.64 mm^{-1}
c = 17.5108 (8) Å	*T* = 150 (1) K
V = 1327.62 (11) Å^3	Block, colorless
Z = 4	0.36 × 0.28 × 0.22 mm

Data collection

Bruker SMART APEX CCD diffractometer	1752 independent reflections
Radiation source: fine-focus sealed tube	1627 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.037
T = 150(1) K	θ_{max} = 28.3º
ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Bruker, 2001)	*h* = −10→10
T_{min} = 0.808, T_{max} = 1.000	*k* = −13→13
12217 measured reflections	*l* = −22→23

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.025	H-atom parameters constrained
$wR(F^2)$ = 0.062	$w = 1/[\sigma^2(F_o^2) + (0.0321P)^2 + 0.8204P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.08	$(\Delta/\sigma)_{max}$ = 0.001
1752 reflections	$\Delta\rho_{max}$ = 0.84 e Å^{-3}
130 parameters	$\Delta\rho_{min}$ = −0.52 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}	Occ. (<1)
Zn1	0.65025 (4)	0.7500	0.580742 (16)	0.01318 (10)	
Zn2	0.51023 (3)	0.7500	0.237037 (17)	0.01112 (9)	
C1	0.5883 (3)	0.7500	0.41412 (15)	0.0190 (6)	
H1	0.4647	0.7500	0.4223	0.023*	
C2	0.8619 (3)	0.7500	0.43286 (16)	0.0187 (5)	
H2	0.9738	0.7500	0.4571	0.022*	
C3	0.5824 (2)	0.51411 (19)	0.67750 (11)	0.0180 (4)	
H3	0.4628	0.5408	0.6816	0.022*	
C4	0.8505 (2)	0.5094 (2)	0.64855 (11)	0.0180 (4)	
H4	0.9621	0.5317	0.6277	0.022*	
N1	0.7073 (3)	0.7500	0.47113 (13)	0.0161 (4)	
N2	0.6611 (3)	0.7500	0.34565 (13)	0.0157 (4)	
N3	0.8397 (3)	0.7500	0.35800 (13)	0.0156 (4)	
N4	0.7043 (2)	0.58402 (15)	0.63830 (9)	0.0158 (3)	
N5	0.64612 (18)	0.40513 (15)	0.70959 (9)	0.0149 (3)	
N6	0.82168 (19)	0.40187 (15)	0.69069 (9)	0.0147 (3)	
N7A	0.2668 (6)	0.7091 (4)	0.5694 (2)	0.0247 (11)	0.40
O1A	0.3900 (4)	0.7852 (3)	0.5936 (2)	0.0270 (10)	0.40
O2A	0.3091 (7)	0.6066 (5)	0.5355 (3)	0.0520 (13)	0.40
O3A	0.1108 (3)	0.7500	0.58235 (14)	0.0383 (6)	0.80
N7B	0.2657 (13)	0.7500	0.6055 (6)	0.029 (3)*	0.20
O1B	0.3885 (15)	0.7500	0.5567 (7)	0.026 (3)*	0.20
O2B	0.3006 (15)	0.7500	0.6737 (6)	0.033 (3)*	0.20
O3B	0.1108 (3)	0.7500	0.58235 (14)	0.0383 (6)	0.20

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.01843 (17)	0.01104 (16)	0.01007 (16)	0.000	0.00027 (10)	0.000
Zn2	0.00955 (15)	0.01216 (16)	0.01165 (17)	0.000	0.00029 (9)	0.000
C1	0.0141 (12)	0.0284 (15)	0.0145 (13)	0.000	0.0019 (9)	0.000
C2	0.0138 (11)	0.0277 (15)	0.0146 (13)	0.000	−0.0020 (9)	0.000
C3	0.0145 (8)	0.0166 (9)	0.0229 (10)	0.0028 (7)	0.0014 (7)	0.0048 (8)
C4	0.0160 (8)	0.0179 (9)	0.0201 (10)	−0.0005 (7)	0.0029 (7)	0.0052 (8)
N1	0.0179 (10)	0.0191 (11)	0.0114 (10)	0.000	−0.0003 (8)	0.000
N2	0.0121 (10)	0.0237 (12)	0.0114 (10)	0.000	0.0001 (8)	0.000
N3	0.0123 (10)	0.0201 (11)	0.0143 (11)	0.000	0.0002 (8)	0.000
N4	0.0181 (7)	0.0137 (8)	0.0155 (8)	0.0009 (6)	−0.0004 (6)	0.0013 (6)
N5	0.0117 (7)	0.0152 (8)	0.0179 (8)	0.0008 (5)	0.0008 (6)	0.0032 (6)
N6	0.0121 (7)	0.0157 (8)	0.0164 (8)	−0.0002 (5)	0.0004 (5)	0.0022 (6)
N7A	0.030 (2)	0.027 (3)	0.018 (2)	−0.0082 (16)	−0.0016 (17)	0.0046 (17)
O1A	0.0148 (16)	0.026 (3)	0.040 (2)	−0.0033 (12)	−0.0037 (15)	−0.0135 (16)

O2A	0.047 (3)	0.039 (3)	0.070 (4)	−0.009 (2)	−0.002 (3)	−0.029 (3)
O3A	0.0173 (10)	0.0551 (17)	0.0425 (15)	0.000	−0.0022 (10)	0.000
O3B	0.0173 (10)	0.0551 (17)	0.0425 (15)	0.000	−0.0022 (10)	0.000

Geometric parameters (Å, °)

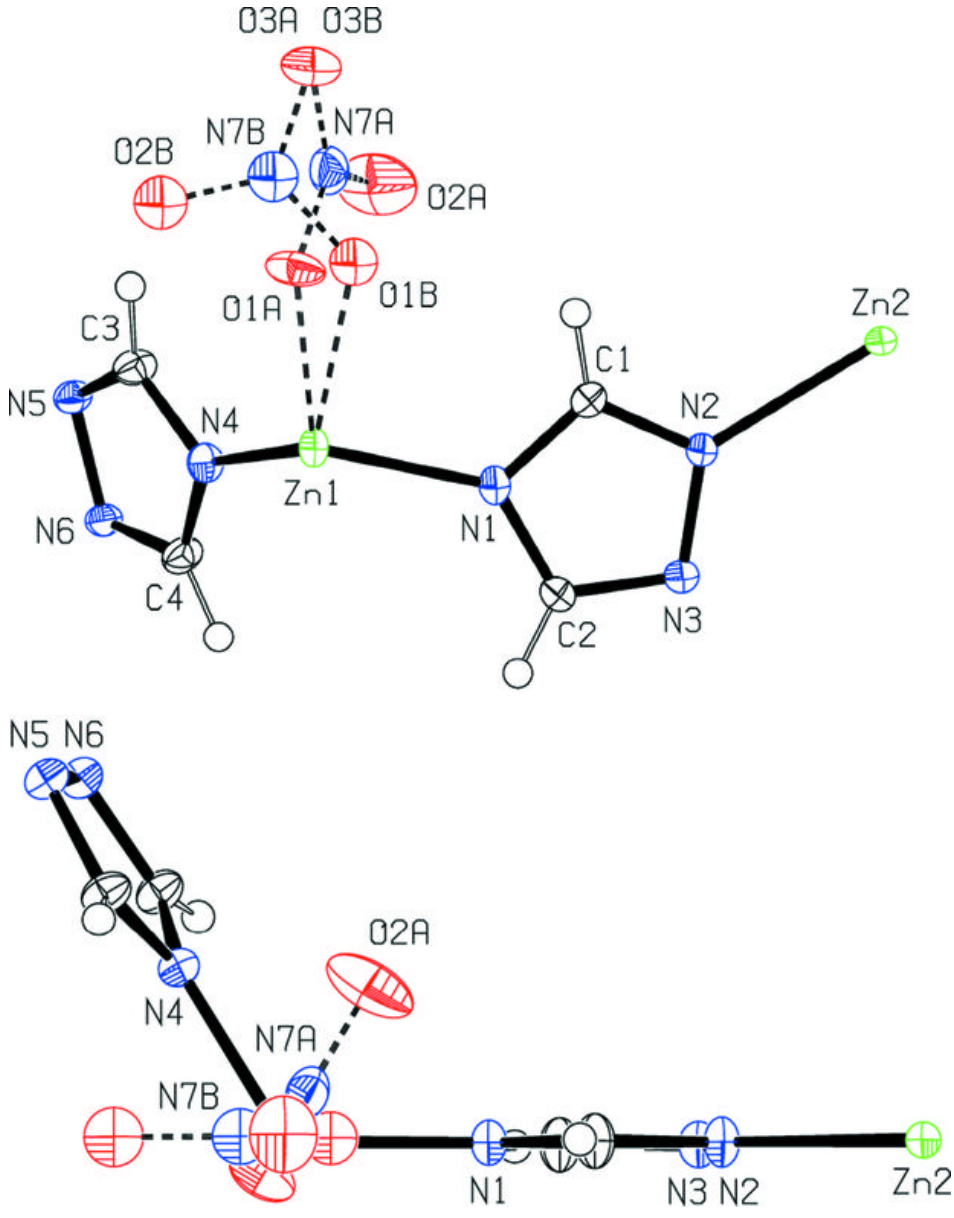
Zn1—N1	1.968 (2)	C3—N5	1.316 (2)
Zn1—N4^{i}	1.9814 (16)	C3—N4	1.348 (2)
Zn1—N4	1.9815 (15)	C3—H3	0.9500
Zn1—O1A^{i}	2.021 (4)	C4—N6	1.320 (2)
Zn1—O1A	2.021 (4)	C4—N4	1.349 (2)
Zn1—O1B	2.033 (12)	C4—H4	0.9500
Zn2—N3^{ii}	2.109 (2)	N2—N3	1.375 (3)
Zn2—N6^{iii}	2.1415 (15)	N3—Zn2^{vii}	2.109 (2)
Zn2—N6^{iv}	2.1415 (15)	N5—N6	1.375 (2)
Zn2—N5^{v}	2.1634 (15)	N5—Zn2^{vi}	2.1635 (15)
Zn2—N5^{vi}	2.1635 (15)	N6—Zn2^{viii}	2.1415 (15)
Zn2—N2	2.221 (2)	N7A—O2A	1.225 (6)
C1—N2	1.321 (3)	N7A—O3A	1.274 (5)
C1—N1	1.347 (3)	N7A—O1A	1.277 (5)
C1—H1	0.9500	O3A—N7A^{i}	1.274 (5)
C2—N3	1.322 (3)	N7B—O2B	1.222 (11)
C2—N1	1.353 (3)	N7B—O1B	1.266 (11)
C2—H2	0.9500		
N1—Zn1—N4^{i}	116.77 (5)	C1—N1—C2	102.5 (2)
N1—Zn1—N4	116.77 (5)	C1—N1—Zn1	125.11 (18)
N4^{i}—Zn1—N4	113.36 (9)	C2—N1—Zn1	132.41 (19)
N1—Zn1—O1A^{i}	108.90 (13)	C1—N2—N3	105.7 (2)
N4^{i}—Zn1—O1A^{i}	106.94 (11)	C1—N2—Zn2	124.16 (17)
N4—Zn1—O1A^{i}	90.08 (11)	N3—N2—Zn2	130.14 (17)
N1—Zn1—O1A	108.90 (13)	C2—N3—N2	106.4 (2)
N4^{i}—Zn1—O1A	90.08 (11)	C2—N3—Zn2^{vii}	134.77 (17)
N4—Zn1—O1A	106.94 (12)	N2—N3—Zn2^{vii}	118.86 (17)
N1—Zn1—O1B	90.8 (3)	C3—N4—C4	102.28 (15)
N4^{i}—Zn1—O1B	107.94 (17)	C3—N4—Zn1	123.29 (12)
N4—Zn1—O1B	107.94 (17)	C4—N4—Zn1	134.40 (13)
N3^{ii}—Zn2—N6^{iii}	93.87 (6)	C3—N5—N6	105.90 (15)
N3^{ii}—Zn2—N6^{iv}	93.87 (6)	C3—N5—Zn2^{vi}	124.97 (12)
N6^{iii}—Zn2—N6^{iv}	90.06 (8)	N6—N5—Zn2^{vi}	128.32 (11)
N3^{ii}—Zn2—N5^{v}	90.20 (6)	C4—N6—N5	106.04 (14)
N6^{iii}—Zn2—N5^{v}	89.16 (6)	C4—N6—Zn2^{viii}	133.44 (12)
N6^{iv}—Zn2—N5^{v}	175.90 (6)	N5—N6—Zn2^{viii}	120.29 (11)
N3^{ii}—Zn2—N5^{vi}	90.20 (6)	N7A^{i}—N7A—O1A^{i}	86.8 (3)
N6^{iii}—Zn2—N5^{vi}	175.90 (6)	N7A^{i}—N7A—O2A	146.6 (3)

N6^{iv}—Zn2—N5^{vi}	89.16 (6)	O1A^{i}—N7A—O2A	90.4 (4)
N5^{v}—Zn2—N5^{vi}	91.34 (8)	N7A^{i}—N7A—O3A	71.34 (19)
N3^{ii}—Zn2—N2	173.18 (8)	O1A^{i}—N7A—O3A	139.1 (5)
N6^{iii}—Zn2—N2	90.95 (6)	O2A—N7A—O3A	126.7 (4)
N6^{iv}—Zn2—N2	90.95 (6)	N7A^{i}—N7A—O1A	53.6 (3)
N5^{v}—Zn2—N2	85.04 (6)	O2A—N7A—O1A	117.6 (4)
N5^{vi}—Zn2—N2	85.04 (6)	O3A—N7A—O1A	115.7 (4)
N2—C1—N1	113.1 (2)	O1A^{i}—O1A—N7A^{i}	93.2 (3)
N2—C1—H1	123.5	O1A^{i}—O1A—N7A	53.6 (3)
N1—C1—H1	123.5	O1A^{i}—O1A—O2A^{i}	132.2 (3)
N3—C2—N1	112.4 (2)	N7A^{i}—O1A—O2A^{i}	49.7 (3)
N3—C2—H2	123.8	N7A—O1A—O2A^{i}	84.7 (3)
N1—C2—H2	123.8	O1A^{i}—O1A—Zn1	80.01 (10)
N5—C3—N4	113.07 (16)	N7A^{i}—O1A—Zn1	148.6 (4)
N5—C3—H3	123.5	N7A—O1A—Zn1	125.3 (3)
N4—C3—H3	123.5	O2A^{i}—O1A—Zn1	114.9 (3)
N6—C4—N4	112.71 (16)	O2B—N7B—O1B	119.9 (12)
N6—C4—H4	123.6	N7B—O1B—Zn1	125.6 (10)
N4—C4—H4	123.6		
N2—C1—N1—C2	0.0	Zn2^{vi}—N5—N6—C4	169.93 (14)
N2—C1—N1—Zn1	180.0	C3—N5—N6—Zn2^{viii}	175.21 (12)
N3—C2—N1—C1	0.0	Zn2^{vi}—N5—N6—Zn2^{viii}	−14.9 (2)
N3—C2—N1—Zn1	180.0	N7A^{i}—N7A—O1A—O1A^{i}	−179.988 (2)
N4^{i}—Zn1—N1—C1	−110.62 (6)	O2A—N7A—O1A—O1A^{i}	−38.3 (4)
N4—Zn1—N1—C1	110.62 (6)	O3A—N7A—O1A—O1A^{i}	142.7 (5)
O1A^{i}—Zn1—N1—C1	10.57 (10)	O1A^{i}—N7A—O1A—N7A^{i}	180.0
O1A—Zn1—N1—C1	−10.57 (10)	O2A—N7A—O1A—N7A^{i}	141.7 (4)
O1B—Zn1—N1—C1	0.0	O3A—N7A—O1A—N7A^{i}	−37.3 (5)
N4^{i}—Zn1—N1—C2	69.38 (6)	N7A^{i}—N7A—O1A—O2A^{i}	−24.9 (3)
N4—Zn1—N1—C2	−69.38 (6)	O1A^{i}—N7A—O1A—O2A^{i}	155.1 (3)
O1A^{i}—Zn1—N1—C2	−169.43 (10)	O2A—N7A—O1A—O2A^{i}	116.8 (6)
O1A—Zn1—N1—C2	169.43 (10)	O3A—N7A—O1A—O2A^{i}	−62.2 (4)
O1B—Zn1—N1—C2	180.0	N7A^{i}—N7A—O1A—Zn1	−141.8 (5)
N1—C1—N2—N3	0.000 (1)	O1A^{i}—N7A—O1A—Zn1	38.2 (5)
N1—C1—N2—Zn2	180.0	O2A—N7A—O1A—Zn1	−0.2 (7)
N6^{iii}—Zn2—N2—C1	134.96 (4)	O3A—N7A—O1A—Zn1	−179.1 (3)
N6^{iv}—Zn2—N2—C1	−134.96 (4)	N1—Zn1—O1A—O1A^{i}	93.45 (4)
N5^{v}—Zn2—N2—C1	45.89 (4)	N4^{i}—Zn1—O1A—O1A^{i}	−148.08 (5)
N5^{vi}—Zn2—N2—C1	−45.89 (4)	N4—Zn1—O1A—O1A^{i}	−33.57 (5)
N6^{iii}—Zn2—N2—N3	−45.04 (4)	O1B—Zn1—O1A—O1A^{i}	62.5 (6)
N6^{iv}—Zn2—N2—N3	45.04 (4)	N1—Zn1—O1A—N7A^{i}	13.9 (7)

N5^{v}—Zn2—N2—N3	−134.11 (4)	N4^{i}—Zn1—O1A—N7A^{i}	132.4 (7)
N5^{vi}—Zn2—N2—N3	134.11 (4)	N4—Zn1—O1A—N7A^{i}	−113.1 (7)
N1—C2—N3—N2	0.0	O1A^{i}—Zn1—O1A—N7A^{i}	−79.6 (7)
N1—C2—N3—Zn2^{vii}	180.0	O1B—Zn1—O1A—N7A^{i}	−17.1 (6)
C1—N2—N3—C2	0.000 (1)	N1—Zn1—O1A—N7A	63.1 (4)
Zn2—N2—N3—C2	180.0	N4^{i}—Zn1—O1A—N7A	−178.4 (4)
C1—N2—N3—Zn2^{vii}	180.0	N4—Zn1—O1A—N7A	−63.9 (4)
Zn2—N2—N3—Zn2^{vii}	0.0	O1A^{i}—Zn1—O1A—N7A	−30.3 (4)
N5—C3—N4—C4	0.0 (2)	O1B—Zn1—O1A—N7A	32.1 (6)
N5—C3—N4—Zn1	178.11 (13)	N1—Zn1—O1A—O2A^{i}	−38.7 (3)
N6—C4—N4—C3	0.0 (2)	N4^{i}—Zn1—O1A—O2A^{i}	79.8 (3)
N6—C4—N4—Zn1	−177.80 (14)	N4—Zn1—O1A—O2A^{i}	−165.7 (3)
N1—Zn1—N4—C3	−122.50 (16)	O1A^{i}—Zn1—O1A—O2A^{i}	−132.1 (3)
N4^{i}—Zn1—N4—C3	97.36 (16)	O1B—Zn1—O1A—O2A^{i}	−69.6 (6)
O1A^{i}—Zn1—N4—C3	−11.19 (19)	N7A^{i}—N7A—O2A—O1A^{i}	84.9 (6)
O1A—Zn1—N4—C3	−0.29 (19)	O3A—N7A—O2A—O1A^{i}	−161.3 (7)
O1B—Zn1—N4—C3	−22.2 (3)	O1A—N7A—O2A—O1A^{i}	19.9 (3)
N1—Zn1—N4—C4	54.9 (2)	O1A^{i}—N7A—O3A—N7A^{i}	61.4 (7)
N4^{i}—Zn1—N4—C4	−85.2 (2)	O2A—N7A—O3A—N7A^{i}	−147.9 (5)
O1A^{i}—Zn1—N4—C4	166.2 (2)	O1A—N7A—O3A—N7A^{i}	31.0 (4)
O1A—Zn1—N4—C4	177.1 (2)	O2B—N7B—O1B—Zn1	0.000 (4)
O1B—Zn1—N4—C4	155.3 (4)	N1—Zn1—O1B—N7B	180.000 (3)
N4—C3—N5—N6	0.0 (2)	N4^{i}—Zn1—O1B—N7B	−61.44 (11)
N4—C3—N5—Zn2^{vi}	−170.37 (13)	N4—Zn1—O1B—N7B	61.44 (11)
N4—C4—N6—N5	0.0 (2)	O1A^{i}—Zn1—O1B—N7B	29.2 (5)
N4—C4—N6—Zn2^{viii}	−174.30 (13)	O1A—Zn1—O1B—N7B	−29.2 (5)
C3—N5—N6—C4	0.0 (2)		

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

Fig. 1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N7B
N7A
O2B
O2A
O1A
O1B
C3
N5
N4
Zn1
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C4
C1
N2
Zn2
N1
C2
N3
N5
N6
O2A
N4
N7A
N7B
N1
N3
N2
Zn2

Fig. 2

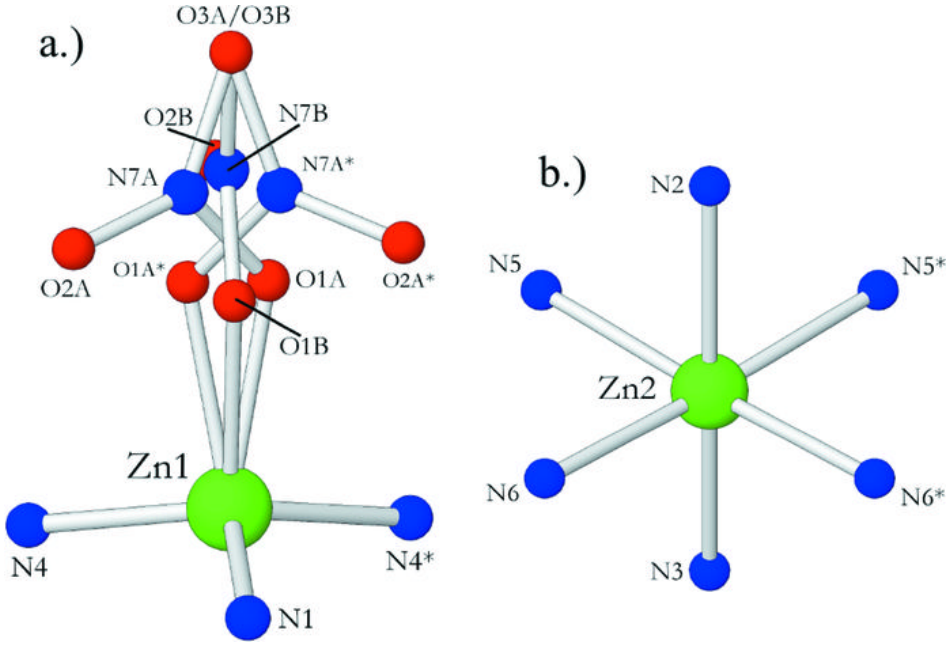
a.)
O3A/O3B
O2B
N7B
N7A
N7A*
O2A
O1A*
O1A
O2A*
O1B
Zn1
N4
N4*
N1
b.)
N2
N5
N5*
Zn2
N6
N6*
N3

Fig. 3

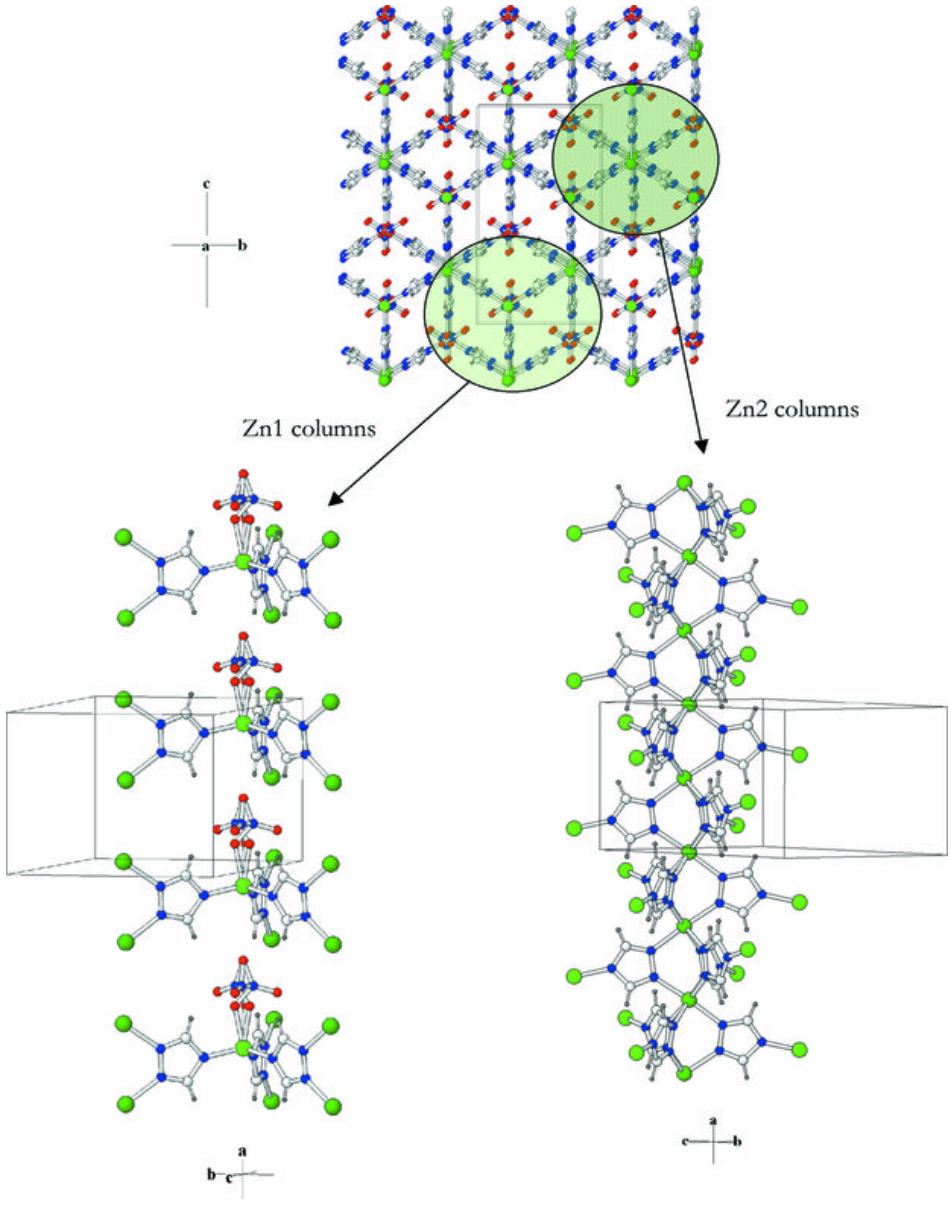

Fig. 4