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Poly[tris{μ-2-[(dimethylamino)methyl]imidazolato-$\kappa^3N^1,N^2:N^3$}(nitrato-κO)dizinc(II)]

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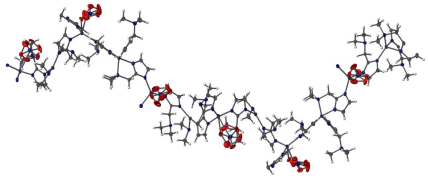
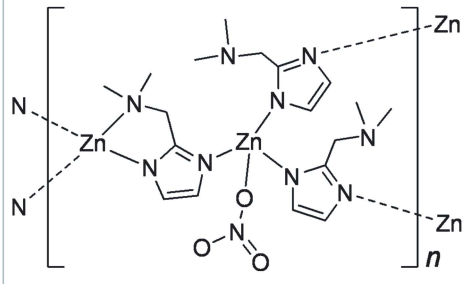
In the title coordination polymer, $[Zn_2(C_6H_{10}N_3)_3(NO_3)]_n$, two independent Zn^{II} ions are tetrahedrally coordinated by the anionic ligands, *viz*. 2-[(dimethylamino)methyl]imidazolate or nitrate ions. One Zn^{II} ion is coordinated by the imidazolate N atoms of three anions and an O atom of the nitrate ion. The second Zn^{II} ion is coordinated by imidazolate N atoms of three anions and one amino N atom of one such ligand. The 2-[(dimethylamino)methyl]imidazolate anions are bridging the Zn^{II} ions to form a helical chain structure along [001]. The chains are further linked by the bridging ligands into a three-dimensional framework structure. The nitrate anion is disordered over two sets of sites and was refined with two pairs of three O atoms using half-occupancy for each O atom.

3D view



Chemical scheme



Structure description

Metal–organic compounds with framework structures and in particular coordination polymers containing imidazolate linkers have been widely studied to create various zeolite-like compounds (Park *et al.*, 2006) because the bridging angle of the imidazolate ligands (145°) is close to that of Si—O—Si in zeolites. In the present study, the structure of a new imidazolate-bridged coordination polymer, $[Zn_2(C_6H_{10}N_3)_3(NO_3)]_n$, is reported.

In the crystal structure, three unique 2-[(dimethylamino)methyl]imidazolate ligands bridge two unique Zn^{II} ions. Since the 2-[(dimethylamino)methyl]imidazolate ligand also has an amino group as an additional coordination site, Zn2 is tetrahedrally coordinated by three imidazolate N atoms and one amino N atom, and thus Zn2 is bridged to three adjacent Zn1 ions. Zn1, on the other hand, is tetrahedrally coordinated by three imidazolate N atoms and one nitrate O atom, whereby the nitrate anion is positionally disordered over two sites (Fig. 1). The Zn1 and Zn2 ions construct helical chains along

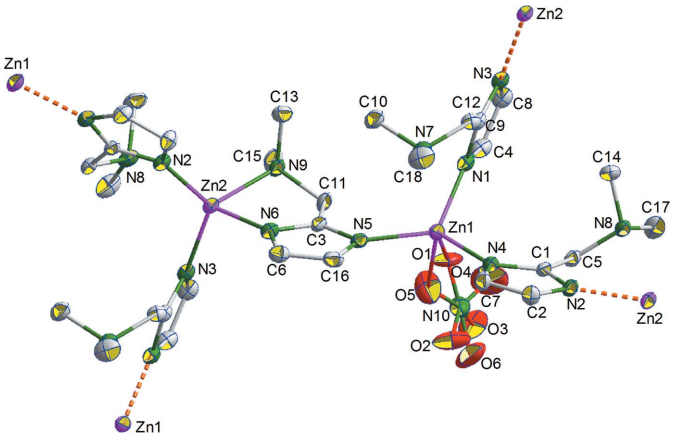


Figure 1
The molecular structure of the main structural motif in $[Zn_2(C_6N_3H_{10})_3(NO_3)]_n$, with displacement ellipsoids drawn at the 50% probability level. H atoms have been omitted for clarity.

[001] (Fig. 2). These chains are further connected to neighboring chains through the imidazolato ligands to build up a three-dimensional framework structure (Fig. 3).

Synthesis and crystallization

For the preparation of 2-[(dimethylamino)methyl]imidazole, see: Quan *et al.* (2005).

A mixture of imidazole-2-carbaldehyde (9.609 g, 100 mmol) in methanol (100 ml) was put in a 500 ml two-neck round-bottomed flask equipped with a reflux condenser. To this suspension, a solution of dimethylamine (40% aqueous solution, 100 ml) was slowly added at room temperature. After that, sodium borohydride (11.349 g, 300 mmol) was cautiously added portionwise over 45 min. The reaction mixture was then refluxed for two days. The reaction contents were concentrated by evaporation and added to a 500 ml separatory funnel containing brine (200 ml). The contents were extracted with ethyl acetate (2 × 200 ml) and the ethyl acetate extract was discarded. The aqueous layer was extracted with $CHCl_3$ (4 × 150 ml) and the organic layer dried over Na_2SO_4, filtered, and concentrated under vacuum to give 2-[(dimethylamino)-methyl]imidazole as a yellow solid. ^{1}H NMR(D_2O): δ = 7.07(*s*, 2H), 3.60(*s*, 2H), and 2.21(*s*, 6H) p.p.m.

Crystals of $[Zn_2(C_6H_{10}N_3)_3(NO_3)]_n$ were grown by pouring a solution of 2-[(dimethylamino)methyl]imidazole (0.520 g, 4.14 mmol) with methanol (5.0 ml) slowly onto a solution of $Zn(NO_3)_2{\cdot}6H_2O$ (0.496 g, 1.67 mmol) in methanol (5.0 ml) in a test tube. After keeping the solution at 323 K for two days, colorless hexagonal-shaped single crystals were obtained.

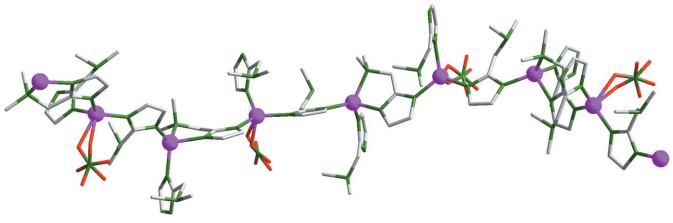


Figure 2
The one-dimensional helical chain consisting of the ligands and Zn^{II} ions.

Table 1
Experimental details.

Crystal data	
Chemical formula	$[Zn_2(C_6H_{10}N_3)_3(NO_3)]$
M_r	565.26
Crystal system, space group	Hexagonal, $P6_1$
Temperature (K)	100
a, c (Å)	9.2437 (8), 47.683 (4)
V (Å^3)	3528.5 (5)
Z	6
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.08
Crystal size (mm)	0.10 × 0.10 × 0.10
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2007)
T_{min}, T_{max}	0.819, 0.819
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	21198, 5835, 5595
R_{int}	0.023
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.682
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.025, 0.061, 1.03
No. of reflections	5835
No. of parameters	331
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.86, −0.26
Absolute structure	Flack (1983), 2004 Friedel pairs
Absolute structure parameter	0.010 (8)

Computer programs: *APEX2* and *SAINT* (Bruker, 2007), *SIR2002* (Burla *et al.*, 2003), *SHELXL97* (Sheldrick, 2008), *DIAMOND* (Brandenburg, 1999) and *Yadokari-XG* (Kabuto *et al.*, 2009).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The Flack parameter refined to 0.010 (8), indicating that the determination of the absolute

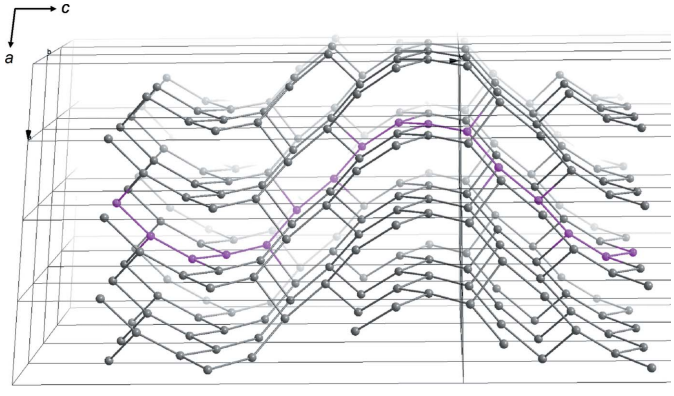


Figure 3
Three-dimensional arrangements of Zn^{II} ions (displayed as spheres) and connections between the helical chains. Gray and pink colours show zinc atoms and an example of a helical chain along [001], respectively.

structure is correct. The nitrate anion is disordered over two sets of sites and was refined with two pairs of three O atoms using half-occupancy for each O atom.

Acknowledgements

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References

Brandenburg, K. (1999). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.

Bruker (2007). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Burla, M. C., Camalli, M., Carrozzini, B., Cascarano, G. L., Giacovazzo, C., Polidori, G. & Spagna, R. (2003). *SIR2002*. University of Bari, Italy.

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.

Kabuto, C., Akine, S., Nemoto, T. & Kwon, E. (2009). *J. Crystallogr. Soc. Japan*, **51**, 218–224.

Park, K. S., Ni, Z., Côté, A. P., Choi, J. Y., Huang, R., Uribe-Romo, F. J., Chae, H. K., O'Keeffe, M. & Yaghi, O. M. (2006). *PNAS*, **103**, 10186–10191.

Quan, M. L., Lam, P. Y. S., Han, Q., Pinto, D. J. P., He, M. Y., Li, R., Ellis, C. D., Clark, C. G., Teleha, C. A., Sun, J.-H., Alexander, R. S., Bai, S., Luettgen, J. M., Knabb, R. M., Wong, P. C. & Wexler, R. R. (2005). *J. Med. Chem.* **48**, 1729–1744.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

full crystallographic data

IUCrData (2016). **1**, x161626 [https://doi.org/10.1107/S2414314616016266]

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Poly[tris{μ-2-[(dimethylamino)methyl]imidazolato-$\kappa^3N^1,N^2:N^3$}(nitrato-κO)dizinc(II)]

Crystal data

$[Zn_2(C_6H_{10}N_3)_3(NO_3)]$
M_r = 565.26
Hexagonal, $P6_1$
Hall symbol: P 61
a = 9.2437 (8) Å
c = 47.683 (4) Å
V = 3528.5 (5) Å^3
Z = 6
$F(000)$ = 1752
D_x = 1.596 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71069 Å
Cell parameters from 9942 reflections
θ = 2.5–28.8°
μ = 2.08 mm^{-1}
T = 100 K
Block, colorless
0.10 × 0.10 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.819, T_{max} = 0.819
21198 measured reflections
5835 independent reflections
5595 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 29.0°, θ_{min} = 2.5°
h = −9→12
k = −11→12
l = −64→64

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.061
S = 1.03
5835 reflections
331 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0286P)^2 + 1.2071P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.86 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Absolute structure: Flack (1983), 2004 Friedel pairs
Absolute structure parameter: 0.010 (8)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Zn1	0.96338 (4)	0.51358 (3)	0.423976 (5)	0.02299 (7)	
Zn2	0.91659 (3)	0.90826 (3)	0.517388 (5)	0.01875 (6)	
N1	1.0431 (2)	0.7009 (2)	0.39668 (4)	0.0187 (4)	
N2	0.8514 (2)	0.7160 (2)	0.49260 (4)	0.0189 (4)	
N3	1.1380 (2)	1.0233 (2)	0.53585 (4)	0.0191 (4)	
N4	0.8770 (2)	0.5671 (2)	0.45813 (4)	0.0188 (4)	
N5	0.8621 (3)	0.2810 (2)	0.41073 (4)	0.0227 (4)	
N6	0.7489 (2)	0.8132 (2)	0.55003 (4)	0.0204 (4)	
N7	0.6872 (2)	0.4885 (2)	0.39504 (4)	0.0213 (4)	
C1	0.9489 (3)	0.7127 (3)	0.47207 (5)	0.0172 (4)	
N8	1.1186 (2)	1.0145 (2)	0.46746 (4)	0.0215 (4)	
N9	0.8060 (2)	1.0574 (2)	0.51150 (4)	0.0214 (4)	
C2	0.7078 (3)	0.5625 (3)	0.49164 (5)	0.0220 (4)	
H1	0.6137	0.5261	0.5036	0.026*	
N10	1.2858 (3)	0.5830 (3)	0.44997 (5)	0.0295 (5)	
C3	0.9140 (3)	0.2259 (3)	0.38929 (5)	0.0201 (4)	
C4	1.2009 (3)	0.8129 (3)	0.38672 (5)	0.0233 (5)	
H2	1.3008	0.8116	0.3908	0.028*	
C5	1.1198 (3)	0.8562 (3)	0.46715 (5)	0.0192 (4)	
H3	1.1962	0.8583	0.4819	0.023*	
H4	1.1617	0.8426	0.4488	0.023*	
C6	0.6743 (3)	0.6850 (3)	0.56929 (5)	0.0238 (5)	
H5	0.6916	0.5922	0.5708	0.029*	
C7	0.7236 (3)	0.4722 (3)	0.47082 (5)	0.0234 (5)	
H6	0.6422	0.3615	0.4657	0.028*	
C8	1.2627 (3)	1.1880 (3)	0.53668 (5)	0.0237 (5)	
H7	1.2616	1.2777	0.5272	0.028*	
C9	0.9425 (3)	0.7511 (3)	0.38563 (5)	0.0170 (4)	
C10	0.6820 (3)	0.4142 (3)	0.36753 (5)	0.0280 (5)	
H8	0.6079	0.4310	0.3550	0.042*	
H9	0.6400	0.2943	0.3698	0.042*	
H10	0.7948	0.4677	0.3595	0.042*	
C11	0.7485 (3)	1.0731 (3)	0.53982 (5)	0.0235 (5)	
H11	0.6570	1.0987	0.5380	0.028*	
H12	0.8417	1.1662	0.5501	0.028*	

C12	0.7593 (3)	0.6679 (3)	0.39220 (5)	0.0198 (4)	
H13	0.7430	0.7142	0.4099	0.024*	
H14	0.7011	0.6917	0.3770	0.024*	
C13	0.6598 (3)	0.9608 (3)	0.49275 (5)	0.0292 (5)	
H15	0.5967	1.0196	0.4910	0.044*	
H16	0.5877	0.8496	0.5007	0.044*	
H17	0.6989	0.9496	0.4742	0.044*	
C14	1.0359 (3)	1.0285 (3)	0.44220 (5)	0.0285 (5)	
H18	1.0997	1.0314	0.4256	0.043*	
H19	1.0301	1.1314	0.4431	0.043*	
H20	0.9227	0.9321	0.4410	0.043*	
C15	0.9136 (4)	1.2257 (3)	0.49959 (6)	0.0308 (5)	
H21	0.9518	1.2155	0.4809	0.046*	
H22	1.0105	1.2891	0.5118	0.046*	
H23	0.8499	1.2841	0.4981	0.046*	
C16	0.7148 (3)	0.1427 (3)	0.41900 (5)	0.0260 (5)	
H24	0.6451	0.1404	0.4338	0.031*	
C17	1.2918 (3)	1.1527 (3)	0.46788 (6)	0.0322 (6)	
H25	1.3490	1.1496	0.4508	0.048*	
H26	1.3493	1.1417	0.4843	0.048*	
H27	1.2927	1.2591	0.4688	0.048*	
C18	0.5178 (3)	0.4166 (4)	0.40630 (6)	0.0340 (6)	
H28	0.5221	0.4640	0.4249	0.051*	
H29	0.4678	0.2952	0.4079	0.051*	
H30	0.4500	0.4424	0.3937	0.051*	
O1	1.2289 (5)	0.5962 (6)	0.42732 (8)	0.0351 (9)	0.50
O2	1.1877 (7)	0.4844 (8)	0.46768 (10)	0.0545 (13)	0.50
O3	1.4340 (5)	0.6432 (7)	0.45486 (11)	0.0483 (11)	0.50
O4	1.3830 (9)	0.7235 (7)	0.44125 (15)	0.092 (2)	0.50
O5	1.1560 (6)	0.4869 (6)	0.43798 (13)	0.0569 (14)	0.50
O6	1.3130 (11)	0.5543 (7)	0.47393 (11)	0.086 (2)	0.50

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.03698 (15)	0.02441 (13)	0.01474 (11)	0.02071 (12)	0.00109 (11)	−0.00093 (10)
Zn2	0.02086 (12)	0.02111 (12)	0.01535 (11)	0.01129 (10)	−0.00115 (10)	−0.00447 (10)
N1	0.0165 (8)	0.0235 (9)	0.0162 (9)	0.0102 (7)	−0.0002 (7)	−0.0016 (7)
N2	0.0209 (9)	0.0191 (9)	0.0143 (8)	0.0081 (7)	0.0009 (7)	−0.0018 (7)
N3	0.0217 (9)	0.0173 (8)	0.0167 (9)	0.0085 (7)	0.0011 (7)	−0.0010 (7)
N4	0.0225 (9)	0.0179 (8)	0.0151 (9)	0.0095 (7)	−0.0004 (7)	−0.0016 (7)
N5	0.0373 (11)	0.0253 (10)	0.0122 (9)	0.0206 (9)	0.0016 (8)	0.0011 (7)
N6	0.0213 (9)	0.0212 (9)	0.0170 (9)	0.0093 (8)	0.0006 (7)	−0.0003 (7)
N7	0.0167 (9)	0.0220 (9)	0.0206 (9)	0.0063 (7)	−0.0016 (7)	0.0009 (8)
C1	0.0226 (10)	0.0197 (9)	0.0114 (9)	0.0122 (8)	−0.0005 (8)	−0.0003 (7)
N8	0.0263 (10)	0.0178 (8)	0.0156 (9)	0.0074 (7)	−0.0008 (7)	−0.0011 (7)
N9	0.0264 (9)	0.0254 (9)	0.0150 (9)	0.0149 (8)	0.0030 (7)	−0.0003 (7)
C2	0.0203 (10)	0.0197 (10)	0.0215 (11)	0.0067 (9)	0.0060 (9)	0.0007 (9)

N10	0.0276 (11)	0.0275 (10)	0.0348 (13)	0.0148 (9)	−0.0076 (9)	−0.0033 (9)
C3	0.0261 (11)	0.0236 (11)	0.0142 (10)	0.0151 (9)	−0.0047 (8)	−0.0041 (8)
C4	0.0164 (10)	0.0322 (12)	0.0213 (11)	0.0121 (9)	−0.0007 (9)	−0.0020 (9)
C5	0.0224 (10)	0.0230 (10)	0.0135 (10)	0.0124 (9)	0.0014 (8)	−0.0020 (8)
C6	0.0207 (10)	0.0254 (11)	0.0220 (11)	0.0091 (9)	−0.0002 (9)	0.0035 (9)
C7	0.0247 (11)	0.0180 (10)	0.0232 (12)	0.0074 (9)	−0.0009 (9)	−0.0034 (9)
C8	0.0289 (12)	0.0174 (10)	0.0224 (12)	0.0097 (9)	0.0035 (9)	0.0027 (9)
C9	0.0164 (9)	0.0191 (9)	0.0151 (10)	0.0087 (8)	−0.0019 (8)	−0.0042 (8)
C10	0.0284 (12)	0.0265 (12)	0.0217 (12)	0.0082 (10)	−0.0052 (10)	−0.0029 (9)
C11	0.0301 (12)	0.0281 (11)	0.0164 (11)	0.0177 (10)	0.0054 (9)	−0.0011 (9)
C12	0.0169 (10)	0.0237 (11)	0.0198 (11)	0.0109 (8)	−0.0003 (8)	0.0010 (9)
C13	0.0307 (12)	0.0433 (14)	0.0183 (11)	0.0221 (11)	−0.0015 (10)	0.0029 (10)
C14	0.0416 (14)	0.0278 (12)	0.0172 (11)	0.0181 (11)	−0.0037 (10)	0.0023 (9)
C15	0.0392 (14)	0.0317 (13)	0.0265 (13)	0.0216 (11)	0.0098 (11)	0.0072 (10)
C16	0.0379 (13)	0.0328 (12)	0.0171 (11)	0.0252 (11)	0.0046 (9)	0.0050 (9)
C17	0.0306 (13)	0.0243 (12)	0.0254 (13)	0.0014 (10)	0.0080 (10)	0.0022 (10)
C18	0.0194 (11)	0.0378 (14)	0.0333 (15)	0.0055 (10)	0.0016 (10)	0.0053 (11)
O1	0.034 (2)	0.055 (3)	0.0236 (19)	0.027 (2)	−0.0030 (15)	0.0123 (18)
O2	0.049 (3)	0.084 (4)	0.028 (2)	0.033 (3)	0.010 (2)	0.026 (2)
O3	0.0231 (19)	0.068 (3)	0.056 (3)	0.025 (2)	−0.0217 (19)	−0.017 (2)
O4	0.091 (5)	0.045 (3)	0.072 (4)	−0.017 (3)	−0.008 (4)	0.028 (3)
O5	0.032 (2)	0.045 (3)	0.090 (4)	0.017 (2)	−0.024 (3)	−0.015 (3)
O6	0.128 (6)	0.051 (3)	0.031 (3)	0.008 (4)	−0.028 (4)	−0.004 (2)

Geometric parameters (Å, º)

Zn1—N5	1.971 (2)	C4—H2	0.9500
Zn1—N4	1.9827 (19)	C5—H3	0.9900
Zn1—N1	1.9898 (19)	C5—H4	0.9900
Zn1—O5	2.029 (4)	C6—C16^{ii}	1.357 (3)
Zn1—O1	2.182 (4)	C6—H5	0.9500
Zn2—N2	1.9611 (19)	C7—H6	0.9500
Zn2—N3	1.979 (2)	C8—C4^{i}	1.361 (4)
Zn2—N6	2.058 (2)	C8—H7	0.9500
Zn2—N9	2.1054 (19)	C9—N3^{iv}	1.336 (3)
N1—C9	1.338 (3)	C9—C12	1.502 (3)
N1—C4	1.383 (3)	C10—H8	0.9800
N2—C1	1.341 (3)	C10—H9	0.9800
N2—C2	1.376 (3)	C10—H10	0.9800
N3—C9^{i}	1.336 (3)	C11—C3^{ii}	1.499 (3)
N3—C8	1.376 (3)	C11—H11	0.9900
N4—C1	1.342 (3)	C11—H12	0.9900
N4—C7	1.379 (3)	C12—H13	0.9900
N5—C3	1.333 (3)	C12—H14	0.9900
N5—C16	1.379 (3)	C13—H15	0.9800
N6—C3^{ii}	1.337 (3)	C13—H16	0.9800
N6—C6	1.381 (3)	C13—H17	0.9800
N7—C12	1.451 (3)	C14—H18	0.9800

N7—C18	1.463 (3)	C14—H19	0.9800
N7—C10	1.470 (3)	C14—H20	0.9800
C1—C5	1.489 (3)	C15—H21	0.9800
N8—C17	1.466 (3)	C15—H22	0.9800
N8—C14	1.466 (3)	C15—H23	0.9800
N8—C5	1.468 (3)	C16—C6^{iii}	1.357 (3)
N9—C15	1.479 (3)	C16—H24	0.9500
N9—C11	1.484 (3)	C17—H25	0.9800
N9—C13	1.489 (3)	C17—H26	0.9800
C2—C7	1.351 (3)	C17—H27	0.9800
C2—H1	0.9500	C18—H28	0.9800
N10—O3	1.216 (4)	C18—H29	0.9800
N10—O5	1.220 (5)	C18—H30	0.9800
N10—O4	1.225 (5)	O1—O5	1.026 (6)
N10—O6	1.227 (6)	O1—O4	1.476 (8)
N10—O1	1.234 (4)	O2—O6	1.049 (9)
N10—O2	1.240 (5)	O2—O5	1.448 (8)
C3—N6^{iii}	1.337 (3)	O3—O4	1.243 (9)
C3—C11^{iii}	1.499 (3)	O3—O6	1.354 (9)
C4—C8^{iv}	1.361 (4)		

N5—Zn1—N4	120.32 (8)	C2—C7—H6	125.6
N5—Zn1—N1	120.45 (8)	N4—C7—H6	125.6
N4—Zn1—N1	109.89 (8)	C4^{i}—C8—N3	108.6 (2)
N5—Zn1—O5	86.57 (15)	C4^{i}—C8—H7	125.7
N4—Zn1—O5	104.32 (19)	N3—C8—H7	125.7
N1—Zn1—O5	110.81 (19)	N3^{iv}—C9—N1	112.97 (19)
N5—Zn1—O1	104.05 (14)	N3^{iv}—C9—C12	124.2 (2)
N4—Zn1—O1	112.07 (12)	N1—C9—C12	122.8 (2)
N1—Zn1—O1	83.14 (12)	N7—C10—H8	109.5
O5—Zn1—O1	27.90 (18)	N7—C10—H9	109.5
N2—Zn2—N3	121.43 (8)	H8—C10—H9	109.5
N2—Zn2—N6	104.15 (8)	N7—C10—H10	109.5
N3—Zn2—N6	104.40 (8)	H8—C10—H10	109.5
N2—Zn2—N9	118.88 (8)	H9—C10—H10	109.5
N3—Zn2—N9	114.69 (8)	N9—C11—C3^{ii}	110.31 (18)
N6—Zn2—N9	82.62 (8)	N9—C11—H11	109.6
C9—N1—C4	105.11 (19)	C3^{ii}—C11—H11	109.6
C9—N1—Zn1	122.68 (15)	N9—C11—H12	109.6
C4—N1—Zn1	132.00 (16)	C3^{ii}—C11—H12	109.6
C1—N2—C2	105.33 (19)	H11—C11—H12	108.1
C1—N2—Zn2	123.71 (15)	N7—C12—C9	111.15 (18)
C2—N2—Zn2	130.96 (15)	N7—C12—H13	109.4
C9^{i}—N3—C8	105.18 (19)	C9—C12—H13	109.4
C9^{i}—N3—Zn2	122.17 (15)	N7—C12—H14	109.4
C8—N3—Zn2	132.59 (16)	C9—C12—H14	109.4
C1—N4—C7	104.87 (18)	H13—C12—H14	108.0
C1—N4—Zn1	126.74 (15)	N9—C13—H15	109.5

C7—N4—Zn1	128.02 (15)	N9—C13—H16	109.5
C3—N5—C16	104.0 (2)	H15—C13—H16	109.5
C3—N5—Zn1	126.65 (17)	N9—C13—H17	109.5
C16—N5—Zn1	128.99 (16)	H15—C13—H17	109.5
C3^{ii}—N6—C6	104.74 (19)	H16—C13—H17	109.5
C3^{ii}—N6—Zn2	110.60 (15)	N8—C14—H18	109.5
C6—N6—Zn2	144.64 (17)	N8—C14—H19	109.5
C12—N7—C18	109.21 (19)	H18—C14—H19	109.5
C12—N7—C10	109.88 (19)	N8—C14—H20	109.5
C18—N7—C10	109.74 (19)	H18—C14—H20	109.5
N2—C1—N4	112.5 (2)	H19—C14—H20	109.5
N2—C1—C5	121.4 (2)	N9—C15—H21	109.5
N4—C1—C5	126.0 (2)	N9—C15—H22	109.5
C17—N8—C14	108.9 (2)	H21—C15—H22	109.5
C17—N8—C5	108.6 (2)	N9—C15—H23	109.5
C14—N8—C5	110.11 (18)	H21—C15—H23	109.5
C15—N9—C11	109.38 (19)	H22—C15—H23	109.5
C15—N9—C13	109.37 (19)	C6^{iii}—C16—N5	109.3 (2)
C11—N9—C13	110.07 (19)	C6^{iii}—C16—H24	125.3
C15—N9—Zn2	116.67 (15)	N5—C16—H24	125.3
C11—N9—Zn2	104.92 (14)	N8—C17—H25	109.5
C13—N9—Zn2	106.24 (15)	N8—C17—H26	109.5
C7—C2—N2	108.4 (2)	H25—C17—H26	109.5
C7—C2—H1	125.8	N8—C17—H27	109.5
N2—C2—H1	125.8	H25—C17—H27	109.5
O3—N10—O5	153.6 (4)	H26—C17—H27	109.5
O3—N10—O4	61.2 (5)	N7—C18—H28	109.5
O5—N10—O4	123.1 (5)	N7—C18—H29	109.5
O3—N10—O6	67.3 (5)	H28—C18—H29	109.5
O5—N10—O6	120.8 (5)	N7—C18—H30	109.5
O4—N10—O6	115.1 (5)	H28—C18—H30	109.5
O3—N10—O1	124.1 (4)	H29—C18—H30	109.5
O5—N10—O1	49.4 (3)	O5—O1—N10	64.6 (3)
O4—N10—O1	73.8 (4)	O5—O1—O4	117.3 (5)
O6—N10—O1	168.6 (5)	N10—O1—O4	52.8 (3)
O3—N10—O2	116.7 (4)	O5—O1—Zn1	67.8 (3)
O5—N10—O2	72.1 (4)	N10—O1—Zn1	119.3 (3)
O4—N10—O2	152.8 (5)	O4—O1—Zn1	141.3 (5)
O6—N10—O2	50.3 (4)	O6—O2—N10	64.2 (4)
O1—N10—O2	118.5 (4)	O6—O2—O5	116.0 (5)
N5—C3—N6^{iii}	113.9 (2)	N10—O2—O5	53.3 (3)
N5—C3—C11^{iii}	126.3 (2)	N10—O3—O4	59.7 (3)
N6^{iii}—C3—C11^{iii}	119.7 (2)	N10—O3—O6	56.7 (4)
C8^{iv}—C4—N1	108.1 (2)	O4—O3—O6	105.5 (6)
C8^{iv}—C4—H2	125.9	N10—O4—O3	59.1 (4)
N1—C4—H2	125.9	N10—O4—O1	53.4 (3)
N8—C5—C1	110.65 (18)	O3—O4—O1	105.2 (5)
N8—C5—H3	109.5	O1—O5—N10	66.0 (3)

C1—C5—H3	109.5	O1—O5—O2	117.5 (5)
N8—C5—H4	109.5	N10—O5—O2	54.6 (3)
C1—C5—H4	109.5	O1—O5—Zn1	84.3 (4)
H3—C5—H4	108.1	N10—O5—Zn1	132.0 (4)
C16^{ii}—C6—N6	107.9 (2)	O2—O5—Zn1	121.4 (4)
C16^{ii}—C6—H5	126.0	O2—O6—N10	65.5 (4)
N6—C6—H5	126.0	O2—O6—O3	120.4 (6)
C2—C7—N4	108.9 (2)	N10—O6—O3	56.0 (3)
N5—Zn1—N1—C9	85.68 (19)	O3—N10—O1—Zn1	−170.8 (3)
N4—Zn1—N1—C9	−60.98 (19)	O5—N10—O1—Zn1	41.6 (4)
O5—Zn1—N1—C9	−175.8 (2)	O4—N10—O1—Zn1	−134.2 (5)
O1—Zn1—N1—C9	−172.0 (2)	O6—N10—O1—Zn1	8 (2)
N5—Zn1—N1—C4	−100.4 (2)	O2—N10—O1—Zn1	19.4 (6)
N4—Zn1—N1—C4	113.0 (2)	N5—Zn1—O1—O5	−52.8 (4)
O5—Zn1—N1—C4	−1.8 (3)	N4—Zn1—O1—O5	78.7 (4)
O1—Zn1—N1—C4	1.9 (2)	N1—Zn1—O1—O5	−172.5 (4)
N3—Zn2—N2—C1	−47.6 (2)	N5—Zn1—O1—N10	−93.2 (3)
N6—Zn2—N2—C1	−164.67 (18)	N4—Zn1—O1—N10	38.4 (4)
N9—Zn2—N2—C1	106.03 (18)	N1—Zn1—O1—N10	147.1 (4)
N3—Zn2—N2—C2	132.1 (2)	O5—Zn1—O1—N10	−40.4 (4)
N6—Zn2—N2—C2	15.0 (2)	N5—Zn1—O1—O4	−159.2 (5)
N9—Zn2—N2—C2	−74.3 (2)	N4—Zn1—O1—O4	−27.6 (6)
N2—Zn2—N3—C9^{i}	−56.5 (2)	N1—Zn1—O1—O4	81.1 (5)
N6—Zn2—N3—C9^{i}	60.37 (18)	O5—Zn1—O1—O4	−106.4 (7)
N9—Zn2—N3—C9^{i}	148.78 (16)	O3—N10—O2—O6	12.4 (7)
N2—Zn2—N3—C8	126.6 (2)	O5—N10—O2—O6	165.4 (7)
N6—Zn2—N3—C8	−116.5 (2)	O4—N10—O2—O6	−65.9 (12)
N9—Zn2—N3—C8	−28.1 (2)	O1—N10—O2—O6	−177.1 (6)
N5—Zn1—N4—C1	168.46 (17)	O3—N10—O2—O5	−153.0 (4)
N1—Zn1—N4—C1	−44.8 (2)	O4—N10—O2—O5	128.7 (11)
O5—Zn1—N4—C1	74.0 (2)	O6—N10—O2—O5	−165.4 (7)
O1—Zn1—N4—C1	45.7 (2)	O1—N10—O2—O5	17.6 (4)
N5—Zn1—N4—C7	−19.6 (2)	O5—N10—O3—O4	107.0 (11)
N1—Zn1—N4—C7	127.07 (19)	O6—N10—O3—O4	−138.9 (6)
O5—Zn1—N4—C7	−114.1 (2)	O1—N10—O3—O4	40.8 (6)
O1—Zn1—N4—C7	−142.4 (2)	O2—N10—O3—O4	−149.2 (6)
N4—Zn1—N5—C3	−175.44 (18)	O5—N10—O3—O6	−114.0 (11)
N1—Zn1—N5—C3	41.3 (2)	O4—N10—O3—O6	138.9 (6)
O5—Zn1—N5—C3	−70.8 (3)	O1—N10—O3—O6	179.7 (5)
O1—Zn1—N5—C3	−48.9 (2)	O2—N10—O3—O6	−10.3 (6)
N4—Zn1—N5—C16	12.3 (2)	O5—N10—O4—O3	−149.5 (5)
N1—Zn1—N5—C16	−130.93 (19)	O6—N10—O4—O3	42.0 (7)
O5—Zn1—N5—C16	116.9 (3)	O1—N10—O4—O3	−145.7 (5)
O1—Zn1—N5—C16	138.8 (2)	O2—N10—O4—O3	92.9 (11)
N2—Zn2—N6—C3^{ii}	−133.67 (16)	O3—N10—O4—O1	145.7 (5)
N3—Zn2—N6—C3^{ii}	98.02 (16)	O5—N10—O4—O1	−3.8 (6)
N9—Zn2—N6—C3^{ii}	−15.66 (15)	O6—N10—O4—O1	−172.3 (6)

N2—Zn2—N6—C6	48.5 (3)	O2—N10—O4—O1	−121.4 (10)
N3—Zn2—N6—C6	−79.8 (3)	O6—O3—O4—N10	−34.8 (4)
N9—Zn2—N6—C6	166.5 (3)	N10—O3—O4—O1	−28.0 (4)
C2—N2—C1—N4	−0.1 (3)	O6—O3—O4—O1	−62.7 (7)
Zn2—N2—C1—N4	179.66 (15)	O5—O1—O4—N10	4.2 (6)
C2—N2—C1—C5	−177.7 (2)	Zn1—O1—O4—N10	92.1 (6)
Zn2—N2—C1—C5	2.1 (3)	O5—O1—O4—O3	34.3 (9)
C7—N4—C1—N2	0.0 (3)	N10—O1—O4—O3	30.1 (4)
Zn1—N4—C1—N2	173.36 (15)	Zn1—O1—O4—O3	122.2 (6)
C7—N4—C1—C5	177.4 (2)	O4—O1—O5—N10	−3.7 (6)
Zn1—N4—C1—C5	−9.2 (3)	Zn1—O1—O5—N10	−141.3 (3)
N2—Zn2—N9—C15	−108.29 (17)	N10—O1—O5—O2	18.7 (4)
N3—Zn2—N9—C15	47.08 (19)	O4—O1—O5—O2	15.0 (8)
N6—Zn2—N9—C15	149.58 (18)	Zn1—O1—O5—O2	−122.6 (5)
N2—Zn2—N9—C11	130.50 (14)	N10—O1—O5—Zn1	141.3 (3)
N3—Zn2—N9—C11	−74.13 (16)	O4—O1—O5—Zn1	137.5 (5)
N6—Zn2—N9—C11	28.38 (14)	O3—N10—O5—O1	−86.3 (10)
N2—Zn2—N9—C13	13.91 (17)	O4—N10—O5—O1	4.8 (7)
N3—Zn2—N9—C13	169.28 (14)	O6—N10—O5—O1	172.7 (6)
N6—Zn2—N9—C13	−88.21 (15)	O2—N10—O5—O1	159.6 (5)
C1—N2—C2—C7	0.2 (3)	O3—N10—O5—O2	114.2 (10)
Zn2—N2—C2—C7	−179.52 (17)	O4—N10—O5—O2	−154.8 (7)
C16—N5—C3—N6^{iii}	−0.6 (3)	O6—N10—O5—O2	13.1 (6)
Zn1—N5—C3—N6^{iii}	−174.38 (15)	O1—N10—O5—O2	−159.6 (5)
C16—N5—C3—C11^{iii}	−177.3 (2)	O3—N10—O5—Zn1	−143.2 (8)
Zn1—N5—C3—C11^{iii}	8.8 (3)	O4—N10—O5—Zn1	−52.1 (9)
C9—N1—C4—C8^{iv}	−0.3 (3)	O6—N10—O5—Zn1	115.8 (7)
Zn1—N1—C4—C8^{iv}	−175.00 (17)	O1—N10—O5—Zn1	−56.9 (5)
C17—N8—C5—C1	169.44 (19)	O2—N10—O5—Zn1	102.7 (6)
C14—N8—C5—C1	−71.4 (2)	O6—O2—O5—O1	−35.7 (10)
N2—C1—C5—N8	−46.1 (3)	N10—O2—O5—O1	−21.1 (5)
N4—C1—C5—N8	136.6 (2)	O6—O2—O5—N10	−14.7 (7)
C3^{ii}—N6—C6—C16^{ii}	0.3 (3)	O6—O2—O5—Zn1	−136.5 (7)
Zn2—N6—C6—C16^{ii}	178.2 (2)	N10—O2—O5—Zn1	−121.9 (4)
N2—C2—C7—N4	−0.3 (3)	N5—Zn1—O5—O1	129.3 (4)
C1—N4—C7—C2	0.2 (3)	N4—Zn1—O5—O1	−110.3 (4)
Zn1—N4—C7—C2	−173.11 (16)	N1—Zn1—O5—O1	7.9 (5)
C9^{i}—N3—C8—C4^{i}	0.6 (3)	N5—Zn1—O5—N10	179.5 (6)
Zn2—N3—C8—C4^{i}	177.79 (17)	N4—Zn1—O5—N10	−60.0 (6)
C4—N1—C9—N3^{iv}	0.7 (3)	N1—Zn1—O5—N10	58.2 (7)
Zn1—N1—C9—N3^{iv}	176.01 (14)	O1—Zn1—O5—N10	50.3 (5)
C4—N1—C9—C12	−177.1 (2)	N5—Zn1—O5—O2	−111.8 (5)
Zn1—N1—C9—C12	−1.7 (3)	N4—Zn1—O5—O2	8.7 (5)
C15—N9—C11—C3^{ii}	−161.6 (2)	N1—Zn1—O5—O2	126.9 (4)
C13—N9—C11—C3^{ii}	78.2 (2)	O1—Zn1—O5—O2	118.9 (6)
Zn2—N9—C11—C3^{ii}	−35.8 (2)	O5—O2—O6—N10	13.0 (6)
C18—N7—C12—C9	169.90 (19)	N10—O2—O6—O3	−11.5 (6)
C10—N7—C12—C9	−69.7 (2)	O5—O2—O6—O3	1.5 (12)

N3^{iv}—C9—C12—N7	145.6 (2)	O3—N10—O6—O2	−168.0 (7)
N1—C9—C12—N7	−36.9 (3)	O5—N10—O6—O2	−16.3 (8)
C3—N5—C16—C6^{iii}	0.7 (3)	O4—N10—O6—O2	152.5 (7)
Zn1—N5—C16—C6^{iii}	174.34 (17)	O1—N10—O6—O2	13 (2)
O3—N10—O1—O5	147.6 (5)	O5—N10—O6—O3	151.7 (5)
O4—N10—O1—O5	−175.8 (6)	O4—N10—O6—O3	−39.5 (6)
O6—N10—O1—O5	−34 (2)	O1—N10—O6—O3	−179 (73)
O2—N10—O1—O5	−22.2 (6)	O2—N10—O6—O3	168.0 (7)
O3—N10—O1—O4	−36.6 (6)	N10—O3—O6—O2	12.7 (7)
O5—N10—O1—O4	175.8 (6)	O4—O3—O6—O2	48.8 (10)
O6—N10—O1—O4	142 (2)	O4—O3—O6—N10	36.1 (5)
O2—N10—O1—O4	153.6 (6)		

Symmetry codes: (i) $x-y+1, x, z+1/6$; (ii) $x-y, x, z+1/6$; (iii) $y, -x+y, z-1/6$; (iv) $y, -x+y+1, z-1/6$.