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Bis[6-(3,5-dimethyl-1*H*-pyrazol-1-yl-κN^2)picolinato-$\kappa^2 N,O$]zinc(II) trihydrate

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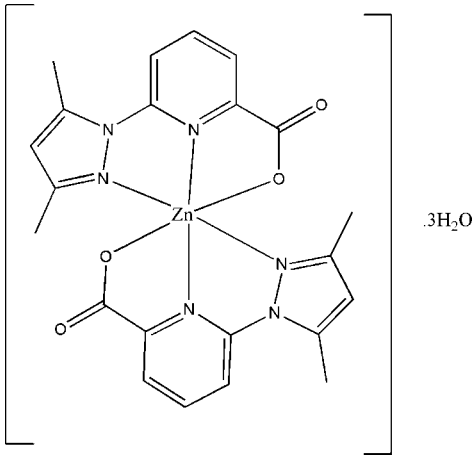
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; disorder in solvent or counterion; R factor = 0.042; wR factor = 0.125; data-to-parameter ratio = 12.7.

In the title compound, $[Zn(C_{11}H_{10}N_3O_2)_2]\cdot 3H_2O$, the Zn^{II} atom is coordinated by four N and two O atoms in a distorted octahedral geometry. One water molecule is disordered equally over two positions.

Related literature

For related literature, see: Bhatia *et al.* (1981); Costamagna *et al.* (1992).



Experimental

Crystal data

$[Zn(C_{11}H_{10}N_3O_2)_2]\cdot 3H_2O$
M_r = 551.86
Triclinic, $P\overline{1}$
a = 9.8071 (9) Å
b = 10.8388 (12) Å
c = 12.6766 (16) Å
α = 71.334 (2)°
β = 74.505 (2)°
γ = 84.772 (3)°
V = 1230.2 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.05 mm^{-1}
T = 298 (2) K
0.50 × 0.48 × 0.34 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.621, T_{max} = 0.716
6315 measured reflections
4251 independent reflections
3192 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.125
S = 1.04
4251 reflections
334 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—N1	2.077 (3)	Zn1—O1	2.122 (3)
Zn1—N4	2.084 (3)	Zn1—N6	2.200 (3)
Zn1—O3	2.109 (3)	Zn1—N3	2.219 (3)

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SG2196).

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supplementary materials

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Bis[6-(3,5-dimethyl-1*H*-pyrazol-1-yl-κN^2)picolinato-$\kappa^2 N,O$]zinc(II) trihydrate

X.-H. Yin, K. Zhao, Y. Feng and J. Zhu

Comment

In recent years, there has been an increasing interest in the coordination chemistry due to the increased recognition of it's role in catalysis enzymatic reactions, magnetism and molecular architectures (Costamagna *et al.*, 1992; Bhatia *et al.*, 1981). We report here the crystal structure of a new zinc(II) complex with the ligand 6- (3,5-dimethyl-1*H*-pyrazol-1-yl) picolinic acid(DPPA)·(I) (Fig.1).

The title compound, (I), consists of a zinc(II) complex cation and three uncoordinated water molecules. In the cation(Fig. 1), the Co atom is six-coordinated by four N atoms and two O atoms from two DPPA ligands. The Zn(II) atom is a slightly distorted octahedral environment. The Zn—O bond length is 2.109 (3) and 2.122 (3) Å,The Zn—N distances range from 2.077 (3) to 2.219 (3) Å, *i.e.* normal values. The C1—C2 bond length is 1.528 (5) Å, being in the normal C—C ranges in cobaltcarboxylate complexes·The angles around Zn(II) atom are from 73.01 (10) to 177.31 (10)°. The DPPA molecule acts as a bidentate ligand.

Experimental

6-(3,5-dimethyl-1*H*-pyrazol-1-yl)picolinic acid, and $ZnCl_2$. $6H_2O$ were available commercially and were used without further purification. Equimolar 6-(3,5-dimethyl-1*H*-pyrazol-1-yl)picolinic acid (1 mmol, 217 mg) was dissolved in anhydrous alcohol (15 ml). The mixture was stirred to give a clear solution, To this solution was added $ZnCl_2{\cdot}6H_2O$ (0.5 mmol, 119 mg) in anhydrous alcohol (10 ml). After keeping the resulting solution in air to evaporate about half of the solvents, dark red prisms of the title compound were formed. The crystals were isolated, washed with alcohol three times and dried in a vacuum desiccator using silica gel (Yield 75%). Elemental analysis: found: C, 47.78; H, 4.85; N, 15.13; O, 20.39; calc. for $C_{22}H_{26}Zn_N6_O7$: C, 47.88; H, 4.75; N, 15.23; O, 20.29

Refinement

All the H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with N—H and C—H distances of 0.90 Å and 0.96 Å, respectively. They were treated as riding atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$, $U_{iso}(H) = 1.2U_{eq}(N)$ and $U_{iso}(H) = 1.5U_{eq}(O)$.

Figures

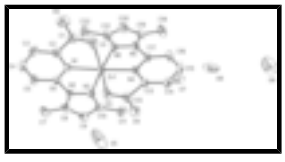


Fig. 1. The structure of the title compound (I) showing 50% probability displacement ellipsoids and the atom-numbering scheme.

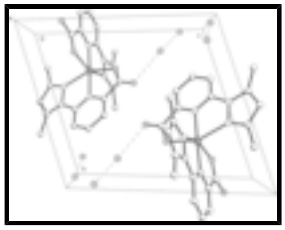


Fig. 2. Crystal packing of (I) showing the hydrogen bonded interactions as dashed lines.

Bis[6-(3,5-dimethyl-1*H*-pyrazol-1-yl-κN^2)picolinato-κ^2*N*,*O*]zinc(II) trihydrate

Crystal data

$[Zn(C_{11}H_{10}N_3O_2)_2]\cdot 3H_2O_1$	$Z = 2$
$M_r = 551.86$	$F_{000} = 572$
Triclinic, $P\bar{1}$	$D_x = 1.490$ Mg m^{-3}
$a = 9.8071$ (9) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 10.8388$ (12) Å	Cell parameters from 3006 reflections
$c = 12.6766$ (16) Å	$\theta = 2.2$–25.9º
$\alpha = 71.334$ (2)º	$\mu = 1.05$ mm^{-1}
$\beta = 74.505$ (2)º	$T = 298$ (2) K
$\gamma = 84.772$ (3)º	Block, colorless
$V = 1230.2$ (2) Å^3	0.50 × 0.48 × 0.34 mm

Data collection

Bruker SMART CCD area-detector diffractometer	4251 independent reflections
Radiation source: fine-focus sealed tube	3192 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.021$
$T = 298$(2) K	$\theta_{max} = 25.0$º
phi and ω scans	$\theta_{min} = 1.8$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -11 \rightarrow 11$
$T_{min} = 0.621$, $T_{max} = 0.716$	$k = -12 \rightarrow 12$
6315 measured reflections	$l = -15 \rightarrow 12$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.042$	H-atom parameters constrained
$wR(F^2) = 0.125$	$w = 1/[\sigma^2(F_o^2) + (0.0638P)^2 + 0.5328P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.001$
4251 reflections	$\Delta\rho_{max} = 0.50$ e Å^{-3}

334 parameters	$\Delta\rho_{min} = -0.38$ 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}	Occ. (<1)
Zn1	0.78562 (4)	0.71982 (4)	0.72699 (4)	0.04776 (17)	
N1	0.8809 (3)	0.8979 (2)	0.6879 (2)	0.0383 (6)	
N2	1.0937 (3)	0.8039 (3)	0.6297 (2)	0.0415 (6)	
N3	1.0155 (3)	0.6935 (3)	0.6573 (2)	0.0432 (7)	
N4	0.6810 (3)	0.5449 (2)	0.7692 (2)	0.0382 (6)	
N5	0.7234 (3)	0.4926 (3)	0.9470 (2)	0.0445 (7)	
N6	0.7831 (3)	0.6137 (3)	0.9073 (3)	0.0500 (7)	
O1	0.6140 (3)	0.8407 (3)	0.7764 (3)	0.0775 (9)	
O2	0.5565 (3)	1.0410 (3)	0.7860 (3)	0.0882 (10)	
O3	0.7335 (3)	0.7301 (3)	0.5734 (2)	0.0631 (7)	
O4	0.6151 (3)	0.6316 (3)	0.4964 (2)	0.0604 (7)	
O5	0.6801 (4)	0.8398 (4)	0.2929 (3)	0.1290 (17)	
H5A	0.6557	0.7771	0.3548	0.155*	
H5B	0.6060	0.8730	0.2720	0.155*	
O6	0.0977 (5)	0.0193 (5)	0.8593 (4)	0.1492 (18)	
H6A	0.1701	0.0622	0.8137	0.179*	
H6B	0.1187	−0.0245	0.9216	0.179*	
O7	0.8467 (7)	0.1337 (7)	0.9299 (5)	0.095 (2)	0.50
H7D	0.7748	0.0855	0.9498	0.113*	0.50
H7E	0.9202	0.0906	0.9094	0.113*	0.50
O8	0.6242 (9)	0.0134 (8)	0.9945 (6)	0.131 (3)	0.50
H8A	0.5892	0.0190	0.9386	0.157*	0.50
H8B	0.5582	−0.0035	1.0561	0.157*	0.50
C1	0.6401 (4)	0.9559 (4)	0.7605 (4)	0.0607 (10)	
C2	0.7947 (4)	0.9962 (3)	0.7060 (3)	0.0471 (8)	
C3	0.8450 (5)	1.1204 (4)	0.6748 (4)	0.0624 (11)	
H3	0.7846	1.1883	0.6876	0.075*	
C4	0.9862 (5)	1.1418 (4)	0.6245 (4)	0.0698 (12)	
H4	1.0222	1.2254	0.6014	0.084*	
C5	1.0746 (4)	1.0412 (3)	0.6078 (3)	0.0586 (10)	

H5	1.1709	1.0549	0.5745	0.070*
C6	1.0172 (3)	0.9183 (3)	0.6419 (3)	0.0401 (7)
C7	1.3505 (4)	0.8774 (4)	0.5519 (4)	0.0664 (11)
H7A	1.4403	0.8362	0.5319	0.100*
H7B	1.3475	0.9097	0.6147	0.100*
H7C	1.3378	0.9484	0.4867	0.100*
C8	1.2346 (4)	0.7804 (4)	0.5869 (3)	0.0479 (8)
C9	1.2439 (4)	0.6538 (4)	0.5886 (3)	0.0542 (9)
H9	1.3260	0.6091	0.5650	0.065*
C10	1.1074 (4)	0.6037 (3)	0.6322 (3)	0.0466 (8)
C11	1.0586 (5)	0.4695 (4)	0.6528 (4)	0.0672 (11)
H11A	1.0213	0.4290	0.7338	0.101*
H11B	1.1370	0.4190	0.6243	0.101*
H11C	0.9862	0.4742	0.6135	0.101*
C12	0.6603 (3)	0.6400 (4)	0.5754 (3)	0.0475 (8)
C13	0.6244 (3)	0.5298 (3)	0.6900 (3)	0.0409 (8)
C14	0.5401 (4)	0.4242 (3)	0.7133 (3)	0.0506 (9)
H14	0.5027	0.4128	0.6570	0.061*
C15	0.5132 (4)	0.3362 (3)	0.8224 (4)	0.0581 (10)
H15	0.4557	0.2649	0.8403	0.070*
C16	0.5703 (4)	0.3526 (3)	0.9051 (4)	0.0562 (10)
H16	0.5516	0.2943	0.9792	0.067*
C17	0.6566 (3)	0.4596 (3)	0.8736 (3)	0.0410 (8)
C18	0.6907 (5)	0.2913 (5)	1.1241 (4)	0.0839 (15)
H18A	0.5892	0.2888	1.1455	0.126*
H18B	0.7252	0.2645	1.1922	0.126*
H18C	0.7268	0.2334	1.0793	0.126*
C19	0.7389 (4)	0.4274 (4)	1.0543 (3)	0.0550 (9)
C20	0.8090 (5)	0.5092 (4)	1.0815 (4)	0.0683 (11)
H20	0.8359	0.4921	1.1499	0.082*
C21	0.8344 (4)	0.6234 (4)	0.9900 (3)	0.0586 (10)
C22	0.9040 (6)	0.7455 (5)	0.9796 (4)	0.0874 (15)
H22A	0.9557	0.7839	0.9012	0.131*
H22B	0.9678	0.7251	1.0286	0.131*
H22C	0.8331	0.8057	1.0022	0.131*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0398 (3)	0.0390 (2)	0.0616 (3)	−0.01119 (17)	−0.00741 (19)	−0.01302 (19)
N1	0.0382 (15)	0.0338 (14)	0.0419 (15)	−0.0030 (11)	−0.0058 (12)	−0.0131 (12)
N2	0.0337 (15)	0.0418 (15)	0.0484 (17)	−0.0082 (12)	−0.0060 (12)	−0.0147 (13)
N3	0.0382 (15)	0.0382 (15)	0.0549 (17)	−0.0030 (12)	−0.0093 (13)	−0.0181 (13)
N4	0.0299 (14)	0.0380 (14)	0.0459 (16)	−0.0034 (11)	−0.0060 (12)	−0.0139 (13)
N5	0.0404 (16)	0.0452 (16)	0.0454 (17)	−0.0098 (13)	−0.0081 (13)	−0.0104 (13)
N6	0.0505 (18)	0.0460 (17)	0.0533 (18)	−0.0136 (14)	−0.0101 (14)	−0.0139 (14)
O1	0.0384 (15)	0.0589 (18)	0.116 (3)	−0.0053 (13)	0.0062 (15)	−0.0210 (17)
O2	0.072 (2)	0.077 (2)	0.099 (2)	0.0321 (17)	−0.0020 (18)	−0.0289 (18)

O3	0.0582 (16)	0.0646 (17)	0.0608 (17)	−0.0278 (13)	−0.0192 (13)	−0.0005 (13)
O4	0.0574 (16)	0.0719 (18)	0.0553 (16)	−0.0067 (13)	−0.0205 (13)	−0.0173 (14)
O5	0.080 (2)	0.153 (4)	0.115 (3)	−0.041 (2)	−0.044 (2)	0.038 (3)
O6	0.129 (4)	0.166 (5)	0.126 (4)	−0.039 (3)	−0.019 (3)	−0.010 (3)
O7	0.091 (5)	0.140 (6)	0.073 (4)	0.026 (4)	−0.025 (4)	−0.064 (4)
O8	0.148 (7)	0.145 (7)	0.065 (5)	0.030 (6)	0.015 (5)	−0.028 (5)
C1	0.053 (2)	0.054 (2)	0.063 (3)	0.0125 (19)	−0.0038 (19)	−0.014 (2)
C2	0.054 (2)	0.0384 (19)	0.047 (2)	0.0061 (16)	−0.0117 (17)	−0.0136 (16)
C3	0.083 (3)	0.038 (2)	0.070 (3)	0.006 (2)	−0.020 (2)	−0.0228 (19)
C4	0.086 (3)	0.041 (2)	0.083 (3)	−0.020 (2)	−0.014 (3)	−0.021 (2)
C5	0.053 (2)	0.050 (2)	0.073 (3)	−0.0167 (18)	−0.006 (2)	−0.022 (2)
C6	0.0387 (18)	0.0407 (18)	0.0419 (19)	−0.0071 (14)	−0.0069 (15)	−0.0147 (15)
C7	0.036 (2)	0.080 (3)	0.070 (3)	−0.0162 (19)	−0.0033 (18)	−0.010 (2)
C8	0.0353 (19)	0.065 (2)	0.040 (2)	−0.0056 (16)	−0.0071 (15)	−0.0127 (17)
C9	0.041 (2)	0.066 (3)	0.054 (2)	0.0098 (18)	−0.0102 (17)	−0.0214 (19)
C10	0.046 (2)	0.047 (2)	0.051 (2)	0.0061 (16)	−0.0133 (16)	−0.0218 (17)
C11	0.067 (3)	0.050 (2)	0.091 (3)	0.0059 (19)	−0.021 (2)	−0.032 (2)
C12	0.0327 (18)	0.057 (2)	0.053 (2)	−0.0024 (16)	−0.0107 (16)	−0.0168 (17)
C13	0.0324 (17)	0.0436 (18)	0.051 (2)	0.0008 (14)	−0.0089 (15)	−0.0212 (16)
C14	0.048 (2)	0.045 (2)	0.069 (3)	−0.0004 (16)	−0.0194 (18)	−0.0272 (19)
C15	0.059 (2)	0.0376 (19)	0.080 (3)	−0.0138 (17)	−0.023 (2)	−0.0139 (19)
C16	0.058 (2)	0.0375 (19)	0.067 (3)	−0.0127 (17)	−0.0168 (19)	−0.0049 (18)
C17	0.0358 (18)	0.0367 (17)	0.048 (2)	−0.0010 (14)	−0.0079 (15)	−0.0117 (15)
C18	0.096 (4)	0.083 (3)	0.060 (3)	−0.036 (3)	−0.026 (3)	0.011 (2)
C19	0.051 (2)	0.061 (2)	0.047 (2)	−0.0128 (18)	−0.0057 (17)	−0.0093 (18)
C20	0.072 (3)	0.086 (3)	0.049 (2)	−0.018 (2)	−0.019 (2)	−0.015 (2)
C21	0.055 (2)	0.068 (3)	0.058 (2)	−0.0155 (19)	−0.0137 (19)	−0.023 (2)
C22	0.105 (4)	0.082 (3)	0.088 (3)	−0.035 (3)	−0.036 (3)	−0.025 (3)

Geometric parameters (Å, °)

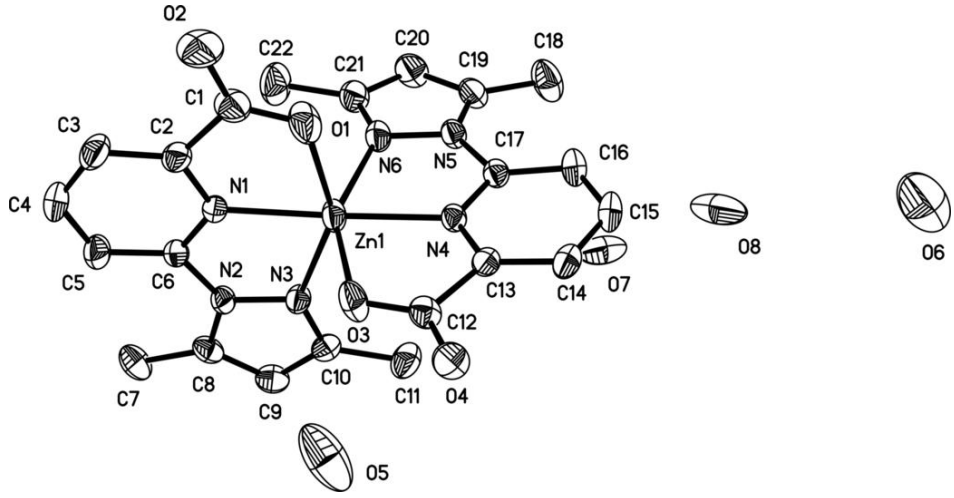
Zn1—N1	2.077 (3)	C4—C5	1.364 (6)
Zn1—N4	2.084 (3)	C4—H4	0.9300
Zn1—O3	2.109 (3)	C5—C6	1.385 (4)
Zn1—O1	2.122 (3)	C5—H5	0.9300
Zn1—N6	2.200 (3)	C7—C8	1.498 (5)
Zn1—N3	2.219 (3)	C7—H7A	0.9600
N1—C6	1.315 (4)	C7—H7B	0.9600
N1—C2	1.339 (4)	C7—H7C	0.9600
N2—C8	1.376 (4)	C8—C9	1.361 (5)
N2—N3	1.377 (3)	C9—C10	1.392 (5)
N2—C6	1.420 (4)	C9—H9	0.9300
N3—C10	1.322 (4)	C10—C11	1.493 (5)
N4—C17	1.323 (4)	C11—H11A	0.9600
N4—C13	1.328 (4)	C11—H11B	0.9600
N5—C19	1.359 (5)	C11—H11C	0.9600
N5—N6	1.371 (4)	C12—C13	1.534 (5)
N5—C17	1.416 (4)	C13—C14	1.380 (5)
N6—C21	1.313 (5)	C14—C15	1.378 (5)

O1—C1	1.239 (5)	C14—H14	0.9300
O2—C1	1.240 (5)	C15—C16	1.377 (5)
O3—C12	1.253 (4)	C15—H15	0.9300
O4—C12	1.230 (4)	C16—C17	1.387 (5)
O5—H5A	0.8500	C16—H16	0.9300
O5—H5B	0.8500	C18—C19	1.500 (5)
O6—H6A	0.8500	C18—H18A	0.9600
O6—H6B	0.8499	C18—H18B	0.9600
O7—H7D	0.8499	C18—H18C	0.9600
O7—H7E	0.8499	C19—C20	1.346 (6)
O8—H8A	0.8500	C20—C21	1.387 (6)
O8—H8B	0.8500	C20—H20	0.9300
C1—C2	1.528 (5)	C21—C22	1.496 (5)
C2—C3	1.374 (5)	C22—H22A	0.9600
C3—C4	1.367 (6)	C22—H22B	0.9600
C3—H3	0.9300	C22—H22C	0.9600
N1—Zn1—N4	177.31 (10)	H7A—C7—H7B	109.5
N1—Zn1—O3	103.44 (10)	C8—C7—H7C	109.5
N4—Zn1—O3	76.71 (10)	H7A—C7—H7C	109.5
N1—Zn1—O1	76.63 (10)	H7B—C7—H7C	109.5
N4—Zn1—O1	100.68 (11)	C9—C8—N2	106.2 (3)
O3—Zn1—O1	93.81 (12)	C9—C8—C7	129.0 (4)
N1—Zn1—N6	106.66 (10)	N2—C8—C7	124.7 (3)
N4—Zn1—N6	73.18 (10)	C8—C9—C10	107.1 (3)
O3—Zn1—N6	149.89 (10)	C8—C9—H9	126.5
O1—Zn1—N6	92.03 (12)	C10—C9—H9	126.5
N1—Zn1—N3	73.01 (10)	N3—C10—C9	110.7 (3)
N4—Zn1—N3	109.68 (10)	N3—C10—C11	120.3 (3)
O3—Zn1—N3	94.08 (10)	C9—C10—C11	129.0 (3)
O1—Zn1—N3	149.62 (11)	C10—C11—H11A	109.5
N6—Zn1—N3	95.67 (11)	C10—C11—H11B	109.5
C6—N1—C2	120.2 (3)	H11A—C11—H11B	109.5
C6—N1—Zn1	123.3 (2)	C10—C11—H11C	109.5
C2—N1—Zn1	116.4 (2)	H11A—C11—H11C	109.5
C8—N2—N3	110.3 (3)	H11B—C11—H11C	109.5
C8—N2—C6	132.7 (3)	O4—C12—O3	127.0 (3)
N3—N2—C6	116.8 (2)	O4—C12—C13	117.7 (3)
C10—N3—N2	105.8 (3)	O3—C12—C13	115.3 (3)
C10—N3—Zn1	140.6 (2)	N4—C13—C14	121.2 (3)
N2—N3—Zn1	113.60 (18)	N4—C13—C12	113.6 (3)
C17—N4—C13	120.8 (3)	C14—C13—C12	125.2 (3)
C17—N4—Zn1	122.4 (2)	C15—C14—C13	118.1 (3)
C13—N4—Zn1	116.4 (2)	C15—C14—H14	120.9
C19—N5—N6	110.9 (3)	C13—C14—H14	120.9
C19—N5—C17	132.4 (3)	C16—C15—C14	120.8 (3)
N6—N5—C17	116.7 (3)	C16—C15—H15	119.6
C21—N6—N5	105.8 (3)	C14—C15—H15	119.6
C21—N6—Zn1	139.6 (3)	C15—C16—C17	117.4 (3)
N5—N6—Zn1	114.1 (2)	C15—C16—H16	121.3

C1—O1—Zn1	117.6 (2)	C17—C16—H16	121.3
C12—O3—Zn1	117.6 (2)	N4—C17—C16	121.8 (3)
H5A—O5—H5B	108.5	N4—C17—N5	112.9 (3)
H6A—O6—H6B	108.5	C16—C17—N5	125.3 (3)
H7D—O7—H7E	108.6	C19—C18—H18A	109.5
H8A—O8—H8B	108.7	C19—C18—H18B	109.5
O1—C1—O2	127.8 (4)	H18A—C18—H18B	109.5
O1—C1—C2	115.7 (3)	C19—C18—H18C	109.5
O2—C1—C2	116.5 (4)	H18A—C18—H18C	109.5
N1—C2—C3	121.2 (3)	H18B—C18—H18C	109.5
N1—C2—C1	113.5 (3)	C20—C19—N5	105.4 (3)
C3—C2—C1	125.3 (3)	C20—C19—C18	128.3 (4)
C4—C3—C2	118.4 (4)	N5—C19—C18	126.3 (4)
C4—C3—H3	120.8	C19—C20—C21	108.2 (4)
C2—C3—H3	120.8	C19—C20—H20	125.9
C5—C4—C3	120.4 (4)	C21—C20—H20	125.9
C5—C4—H4	119.8	N6—C21—C20	109.7 (3)
C3—C4—H4	119.8	N6—C21—C22	121.4 (4)
C4—C5—C6	118.2 (4)	C20—C21—C22	128.9 (4)
C4—C5—H5	120.9	C21—C22—H22A	109.5
C6—C5—H5	120.9	C21—C22—H22B	109.5
N1—C6—C5	121.5 (3)	H22A—C22—H22B	109.5
N1—C6—N2	113.0 (3)	C21—C22—H22C	109.5
C5—C6—N2	125.4 (3)	H22A—C22—H22C	109.5
C8—C7—H7A	109.5	H22B—C22—H22C	109.5
C8—C7—H7B	109.5		
N4—Zn1—N1—C6	179 (100)	O2—C1—C2—N1	175.7 (3)
O3—Zn1—N1—C6	−88.5 (3)	O1—C1—C2—C3	175.9 (4)
O1—Zn1—N1—C6	−179.2 (3)	O2—C1—C2—C3	−5.6 (6)
N6—Zn1—N1—C6	92.7 (3)	N1—C2—C3—C4	0.0 (6)
N3—Zn1—N1—C6	1.7 (2)	C1—C2—C3—C4	−178.6 (4)
N4—Zn1—N1—C2	−5(2)	C2—C3—C4—C5	−1.2 (6)
O3—Zn1—N1—C2	87.9 (2)	C3—C4—C5—C6	0.8 (6)
O1—Zn1—N1—C2	−2.8 (2)	C2—N1—C6—C5	−2.0 (5)
N6—Zn1—N1—C2	−90.9 (2)	Zn1—N1—C6—C5	174.2 (3)
N3—Zn1—N1—C2	178.1 (3)	C2—N1—C6—N2	179.4 (3)
C8—N2—N3—C10	0.2 (3)	Zn1—N1—C6—N2	−4.4 (4)
C6—N2—N3—C10	176.0 (3)	C4—C5—C6—N1	0.8 (6)
C8—N2—N3—Zn1	−179.8 (2)	C4—C5—C6—N2	179.2 (3)
C6—N2—N3—Zn1	−4.1 (3)	C8—N2—C6—N1	180.0 (3)
N1—Zn1—N3—C10	−178.7 (4)	N3—N2—C6—N1	5.4 (4)
N4—Zn1—N3—C10	1.5 (4)	C8—N2—C6—C5	1.5 (6)
O3—Zn1—N3—C10	−75.9 (4)	N3—N2—C6—C5	−173.1 (3)
O1—Zn1—N3—C10	179.5 (3)	N3—N2—C8—C9	−0.3 (4)
N6—Zn1—N3—C10	75.6 (4)	C6—N2—C8—C9	−175.1 (3)
N1—Zn1—N3—N2	1.4 (2)	N3—N2—C8—C7	−177.8 (3)
N4—Zn1—N3—N2	−178.5 (2)	C6—N2—C8—C7	7.3 (6)
O3—Zn1—N3—N2	104.2 (2)	N2—C8—C9—C10	0.2 (4)
O1—Zn1—N3—N2	−0.5 (4)	C7—C8—C9—C10	177.6 (4)

N6—Zn1—N3—N2	−104.3 (2)	N2—N3—C10—C9	−0.1 (4)
N1—Zn1—N4—C17	−84 (2)	Zn1—N3—C10—C9	−180.0 (3)
O3—Zn1—N4—C17	−177.9 (3)	N2—N3—C10—C11	179.4 (3)
O1—Zn1—N4—C17	−86.4 (3)	Zn1—N3—C10—C11	−0.6 (6)
N6—Zn1—N4—C17	2.4 (2)	C8—C9—C10—N3	−0.1 (4)
N3—Zn1—N4—C17	92.5 (3)	C8—C9—C10—C11	−179.5 (4)
N1—Zn1—N4—C13	88 (2)	Zn1—O3—C12—O4	177.0 (3)
O3—Zn1—N4—C13	−5.7 (2)	Zn1—O3—C12—C13	−2.9 (4)
O1—Zn1—N4—C13	85.7 (2)	C17—N4—C13—C14	−0.8 (5)
N6—Zn1—N4—C13	174.6 (2)	Zn1—N4—C13—C14	−173.1 (2)
N3—Zn1—N4—C13	−95.3 (2)	C17—N4—C13—C12	178.3 (3)
C19—N5—N6—C21	−0.4 (4)	Zn1—N4—C13—C12	6.0 (3)
C17—N5—N6—C21	178.3 (3)	O4—C12—C13—N4	178.1 (3)
C19—N5—N6—Zn1	173.5 (2)	O3—C12—C13—N4	−2.1 (4)
C17—N5—N6—Zn1	−7.7 (3)	O4—C12—C13—C14	−2.9 (5)
N1—Zn1—N6—C21	−8.9 (4)	O3—C12—C13—C14	177.0 (3)
N4—Zn1—N6—C21	173.9 (4)	N4—C13—C14—C15	1.6 (5)
O3—Zn1—N6—C21	173.4 (4)	C12—C13—C14—C15	−177.3 (3)
O1—Zn1—N6—C21	−85.5 (4)	C13—C14—C15—C16	−0.8 (6)
N3—Zn1—N6—C21	65.1 (4)	C14—C15—C16—C17	−0.8 (6)
N1—Zn1—N6—N5	−179.8 (2)	C13—N4—C17—C16	−0.9 (5)
N4—Zn1—N6—N5	3.0 (2)	Zn1—N4—C17—C16	170.9 (3)
O3—Zn1—N6—N5	2.4 (4)	C13—N4—C17—N5	−179.0 (3)
O1—Zn1—N6—N5	103.5 (2)	Zn1—N4—C17—N5	−7.2 (4)
N3—Zn1—N6—N5	−105.9 (2)	C15—C16—C17—N4	1.7 (5)
N1—Zn1—O1—C1	1.3 (3)	C15—C16—C17—N5	179.5 (3)
N4—Zn1—O1—C1	−178.8 (3)	C19—N5—C17—N4	−172.0 (3)
O3—Zn1—O1—C1	−101.6 (3)	N6—N5—C17—N4	9.6 (4)
N6—Zn1—O1—C1	107.9 (3)	C19—N5—C17—C16	10.0 (6)
N3—Zn1—O1—C1	3.1 (5)	N6—N5—C17—C16	−168.4 (3)
N1—Zn1—O3—C12	−172.6 (3)	N6—N5—C19—C20	0.1 (4)
N4—Zn1—O3—C12	4.6 (3)	C17—N5—C19—C20	−178.4 (4)
O1—Zn1—O3—C12	−95.5 (3)	N6—N5—C19—C18	−178.3 (4)
N6—Zn1—O3—C12	5.2 (4)	C17—N5—C19—C18	3.2 (7)
N3—Zn1—O3—C12	113.9 (3)	N5—C19—C20—C21	0.3 (5)
Zn1—O1—C1—O2	−177.9 (4)	C18—C19—C20—C21	178.6 (4)
Zn1—O1—C1—C2	0.3 (5)	N5—N6—C21—C20	0.6 (4)
C6—N1—C2—C3	1.6 (5)	Zn1—N6—C21—C20	−170.8 (3)
Zn1—N1—C2—C3	−174.9 (3)	N5—N6—C21—C22	−177.8 (4)
C6—N1—C2—C1	−179.7 (3)	Zn1—N6—C21—C22	10.8 (7)
Zn1—N1—C2—C1	3.8 (4)	C19—C20—C21—N6	−0.6 (5)
O1—C1—C2—N1	−2.7 (5)	C19—C20—C21—C22	177.7 (4)

Fig. 1


O2
C22
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Zn1
C15
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C6
N2
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C13
C14
O7
C12
O3
C7
C8
C10
C11
O4
C9
O5

Fig. 2