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Poly[bis[μ_2-5-(pyrimidin-2-yl)tetrazolato]zinc(II)]

Xiu-Ling Zhang,* Cun-Lan Zhang, Yu-E Qiu and Ning An

Department of Chemistry, Dezhou University, Dezhou 253011, People's Republic of China
Correspondence e-mail: xlzhang99@126.com

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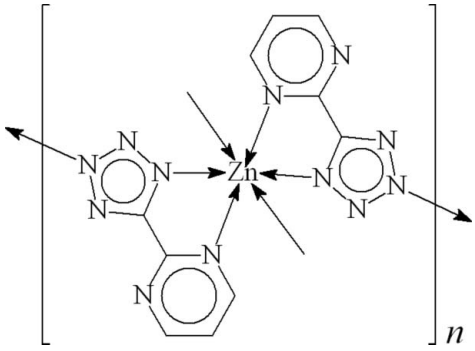
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.059; wR factor = 0.081; data-to-parameter ratio = 15.3.

The title compound, $[Zn(C_5H_3N_6)_2]_n$, has a neutral two-dimensional square grid-like network structure, in which the central Zn^{II} atom is located on an inversion centre and coordinated by six N atoms from four 5-(pyrimidin-2-yl)tetrazolate ligands in a distorted octahedral geometry [Zn—N = 2.114 (3)–2.193 (3) Å and N—Zn—N = 77.78 (9)–102.22 (9)°]. The tetrazolate ligand adopts an $N,N':N''$-tridentate chelating–bridging coordination mode. This complex is isostructural with the iron(II), cobalt(II) and nickel(II) analogues.

Related literature

For ligand preparation, see: Demko & Sharpless (2001). For related literature, see: Rodríguez & Colacio (2006); Rodríguez *et al.* (2005, 2007); Liu & Fan (2007).



Experimental

Crystal data

$[Zn(C_5H_3N_6)_2]$
M_r = 359.64
Orthorhombic, *Pbca*
a = 8.3490 (17) Å
b = 9.4760 (19) Å
c = 17.828 (4) Å
V = 1410.5 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.76 mm^{-1}
T = 293 (2) K
0.20 × 0.20 × 0.18 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.720, T_{max} = 0.742
13281 measured reflections
1619 independent reflections
1162 reflections with $I > 2\sigma(I)$
R_{int} = 0.085

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.081
S = 1.19
1619 reflections
106 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	2.114 (3)	Zn1—N5	2.169 (3)
N1^{i}—Zn1—N5	102.22 (9)	N5—Zn1—N3^{ii}	88.44 (10)
N1—Zn1—N5	77.78 (9)	N1—Zn1—N3^{iii}	91.63 (11)
N1—Zn1—N3^{ii}	88.37 (11)	N5—Zn1—N3^{iii}	91.56 (10)

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

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

The authors thank Dezhou University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2105).

References

Bruker (1998). *SMART* (Version 5.051), *SAINT* (Version 5.01), *SADABS* (Version 2.03) and *SHELXTL* (Version 6.1). Bruker AXS Inc., Madison, Wisconsin, USA.
Demko, Z. P. & Sharpless, K. B. (2001). *J. Org. Chem.* **66**, 7945–7950.
Liu, J.-T. & Fan, S.-D. (2007). *Acta Cryst.* E**63**, m1632.
Rodríguez, A., Kivekäsb, R. & Colacio, E. (2005). *Chem. Commun.* pp. 5228–5230.
Rodríguez, A., Salinas-Castillo, A., Galli, A. S., Masciocchi, N., Gutíerrez-Zorrilla, J. M., Vitoriad, P. & Colacio, E. (2007). *Dalton Trans.* pp. 1821–1828.
Rodríguez, A. & Colacio, E. (2006). *Chem. Commun.* pp. 4140–4142.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.

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supplementary materials

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Poly[bis[μ_2-5-(pyrimidin-2-yl)tetrazolato]zinc(II)]

X.-L. Zhang, C.-L. Zhang, Y.-E. Qiu and N. An

Comment

Recently, several complexes of 5-(pyrimidin-2-yl)tetrazolato ligand have been reported containing iron(II), cobalt(II), nickel(II), zinc(II) and cadmium(II) metal ion [Rodríguez & Colacio (2006); Rodríguez *et al.*, 2005, 2007; Liu & Fan, 2007]. The title compound poly[5-(pyrimidin-2-yl)tetrazolato]zinc(II)] (I, Fig. 1 and 2) is isostructural with the iron(II), cobalt(II) and nickel(II) analogs. The structure features a two-dimensional square-grid-like network with the grid side length of 6.315 (3) Å, in which Zn^{II} atom is located on an inversion centre and exhibits a distorted octahedral coordination geometry around by six N atoms. Each Zn^{II} atom coordinates to four ligands and each ligand bonds to two Zn^{II} atoms through one of the pyrimidyl N atoms and the 1-positon tetrazole N for one, and one 3-position tetrazole N atom for the other. Selected bond distances and angles are listed in Table 1. In addition, in crystal structure such two-dimensional layers stack in an ABAB sequence.

Experimental

The ligand, 2-(1*H*-tetrazol-5-yl)pyrimidine was synthesized by the literature method (Demko & Sharpless, 2001). A mixture of $ZnCl_2$ (27 mg, 0.2 mmol) and the ligand (60 mg, 0.4 mmol) in *N*,*N*-dimethylformamide/ethanol (*v*/*v* = 3:1, 8 ml) in presence of a drop of triethylamine was placed in a Teflon-lined stainless-steel Parr bomb that was heated at 413 K for 36 h. Colorless crystals were collected after the bomb allowed to cool to room temperature during a period of 24 h. Yield, 30%.

Refinement

H atoms were included in calculated positions and treated in the subsequent refinement as riding atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C,*N*).

Figures

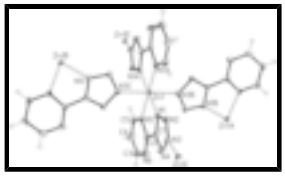


Fig. 1. Displacement ellipsoid plot (30% probability) of a fragment of the layer structure of (I) showing the coordination environment of the metal and ligands. [symmetry codes: (A) 2 − *x*, 1 − *y*, 1 − *z*; (B) 1/2 + *x*, 1/2 − *y*, 1 − *z*; (C) 3/2 − *x*, 1/2 + *y*, *z*.]

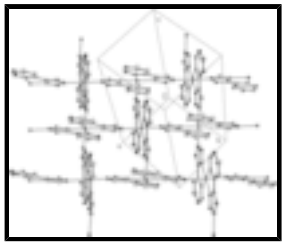


Fig. 2. Two-dimensional layer of (I). For clarity, all H atoms have been omitted.

Poly[bis[μ$_2$-5-(pyrimidin-2-yl)tetrazolato]zinc(II)]

Crystal data

$[Zn(C_5H_3N_6)_2]$	F_{000} = 720
M_r = 359.64	D_x = 1.694 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 10696 reflections
a = 8.3490 (17) Å	θ = 3.1–27.5º
b = 9.4760 (19) Å	μ = 1.76 mm^{-1}
c = 17.828 (4) Å	*T* = 293 (2) K
V = 1410.5 (5) Å^3	Block, colourless
Z = 4	0.20 × 0.20 × 0.18 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	1619 independent reflections
Radiation source: fine-focus sealed tube	1162 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.085
T = 293(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 3.3º
Absorption correction: multi-scan (SADABS; Bruker, 1998)	*h* = −10→10
T_{min} = 0.720, T_{max} = 0.742	*k* = −12→12
13281 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
$R[F^2 > 2\sigma(F^2)]$ = 0.059	H-atom parameters constrained
$wR(F^2)$ = 0.081	$w = 1/[\sigma^2(F_o^2) + (0.0173P)^2 + 1.2986P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.19	$(\Delta/\sigma)_{max} < 0.001$
1619 reflections	$\Delta\rho_{max}$ = 0.28 e Å^{-3}
106 parameters	$\Delta\rho_{min}$ = −0.25 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	1.0000	0.5000	0.5000	0.02321 (15)
N1	0.8536 (3)	0.3208 (3)	0.48306 (14)	0.0251 (6)
N2	0.7488 (3)	0.2405 (3)	0.51939 (13)	0.0293 (6)
N3	0.6979 (3)	0.1430 (3)	0.47237 (15)	0.0277 (7)
N4	0.7676 (3)	0.1574 (3)	0.40459 (15)	0.0286 (7)
N5	1.0407 (3)	0.4532 (3)	0.38246 (14)	0.0229 (6)
N6	0.9801 (4)	0.2806 (3)	0.28978 (16)	0.0442 (8)
C1	0.8634 (4)	0.2684 (3)	0.41356 (17)	0.0241 (7)
C2	0.9676 (4)	0.3365 (3)	0.35780 (18)	0.0264 (8)
C3	1.0735 (5)	0.3528 (4)	0.2425 (2)	0.0491 (11)
H3A	1.0860	0.3182	0.1940	0.059*
C4	1.1517 (5)	0.4744 (4)	0.2612 (2)	0.0435 (10)
H4A	1.2141	0.5230	0.2265	0.052*
C5	1.1340 (4)	0.5217 (4)	0.3333 (2)	0.0355 (9)
H5A	1.1878	0.6028	0.3484	0.043*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0251 (2)	0.0189 (2)	0.0256 (3)	−0.0015 (3)	−0.0001 (3)	−0.0023 (3)
N1	0.0259 (14)	0.0229 (14)	0.0264 (16)	−0.0039 (13)	0.0022 (12)	−0.0011 (12)
N2	0.0332 (14)	0.0247 (14)	0.0299 (15)	−0.0076 (13)	0.0055 (16)	−0.0035 (15)
N3	0.0261 (15)	0.0267 (15)	0.0303 (15)	−0.0067 (13)	0.0073 (13)	−0.0046 (13)
N4	0.0312 (16)	0.0278 (15)	0.0269 (15)	−0.0085 (13)	0.0058 (13)	−0.0063 (13)
N5	0.0237 (16)	0.0194 (13)	0.0256 (14)	−0.0004 (10)	0.0035 (12)	0.0043 (11)
N6	0.054 (2)	0.0475 (19)	0.0310 (17)	−0.0108 (18)	0.0148 (16)	−0.0130 (15)
C1	0.0259 (17)	0.0225 (17)	0.0239 (17)	−0.0016 (15)	0.0015 (15)	−0.0036 (15)
C2	0.026 (2)	0.0256 (18)	0.0276 (18)	−0.0002 (15)	0.0024 (14)	−0.0004 (14)
C3	0.064 (3)	0.056 (3)	0.027 (2)	−0.003 (2)	0.017 (2)	−0.010 (2)
C4	0.054 (3)	0.040 (2)	0.037 (2)	0.000 (2)	0.0209 (19)	0.0069 (18)
C5	0.038 (2)	0.026 (2)	0.043 (2)	−0.0001 (17)	0.0066 (17)	0.0049 (17)

Geometric parameters (Å, °)

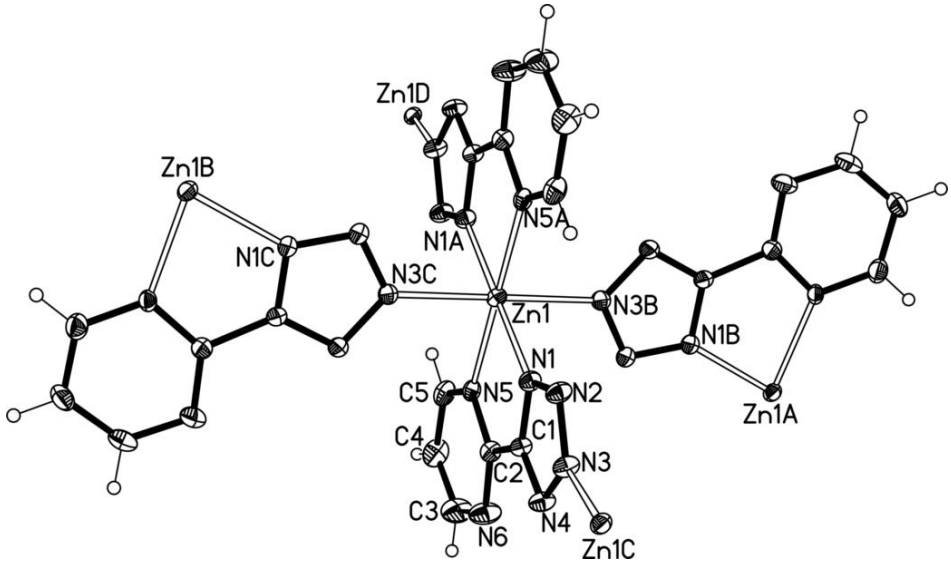
Zn1—N1^{i}	2.114 (3)	N4—C1	1.331 (4)
Zn1—N1	2.114 (3)	N5—C2	1.338 (4)
Zn1—N5	2.169 (3)	N5—C5	1.340 (4)

Zn1—N5^{i}	2.169 (3)	N6—C2	1.327 (4)
Zn1—N3^{ii}	2.193 (3)	N6—C3	1.337 (5)
Zn1—N3^{iii}	2.193 (3)	C1—C2	1.470 (4)
N1—N2	1.329 (3)	C3—C4	1.366 (5)
N1—C1	1.337 (4)	C3—H3A	0.9300
N2—N3	1.318 (4)	C4—C5	1.370 (5)
N3—N4	1.348 (3)	C4—H4A	0.9300
N3—Zn1^{iv}	2.193 (3)	C5—H5A	0.9300
N1^{i}—Zn1—N1	180.0	N4—N3—Zn1^{iv}	126.1 (2)
N1^{i}—Zn1—N5	102.22 (9)	C1—N4—N3	103.4 (2)
N1—Zn1—N5	77.78 (9)	C2—N5—C5	116.8 (3)
N1^{i}—Zn1—N5^{i}	77.78 (9)	C2—N5—Zn1	114.5 (2)
N1—Zn1—N5^{i}	102.22 (9)	C5—N5—Zn1	128.6 (2)
N5—Zn1—N5^{i}	180.00 (3)	C2—N6—C3	114.7 (3)
N1^{i}—Zn1—N3^{ii}	91.63 (11)	N4—C1—N1	111.6 (3)
N1—Zn1—N3^{ii}	88.37 (11)	N4—C1—C2	128.4 (3)
N5—Zn1—N3^{ii}	88.44 (10)	N1—C1—C2	120.0 (3)
N5^{i}—Zn1—N3^{ii}	91.56 (10)	N6—C2—N5	126.5 (3)
N1^{i}—Zn1—N3^{iii}	88.37 (11)	N6—C2—C1	119.3 (3)
N1—Zn1—N3^{iii}	91.63 (11)	N5—C2—C1	114.2 (3)
N5—Zn1—N3^{iii}	91.56 (10)	N6—C3—C4	123.8 (4)
N5^{i}—Zn1—N3^{iii}	88.44 (10)	N6—C3—H3A	118.1
N3^{ii}—Zn1—N3^{iii}	180.00 (14)	C4—C3—H3A	118.1
N2—N1—C1	106.2 (3)	C3—C4—C5	117.0 (3)
N2—N1—Zn1	140.5 (2)	C3—C4—H4A	121.5
C1—N1—Zn1	113.3 (2)	C5—C4—H4A	121.5
N3—N2—N1	107.7 (2)	N5—C5—C4	121.2 (3)
N2—N3—N4	111.1 (2)	N5—C5—H5A	119.4
N2—N3—Zn1^{iv}	122.2 (2)	C4—C5—H5A	119.4
N5—Zn1—N1—N2	−176.3 (4)	N3—N4—C1—N1	−0.2 (4)
N5^{i}—Zn1—N1—N2	3.7 (4)	N3—N4—C1—C2	−178.3 (3)
N3^{ii}—Zn1—N1—N2	95.0 (3)	N2—N1—C1—N4	0.2 (4)
N3^{iii}—Zn1—N1—N2	−85.0 (3)	Zn1—N1—C1—N4	−178.9 (2)
N5—Zn1—N1—C1	2.3 (2)	N2—N1—C1—C2	178.4 (3)
N5^{i}—Zn1—N1—C1	−177.7 (2)	Zn1—N1—C1—C2	−0.6 (4)
N3^{ii}—Zn1—N1—C1	−86.5 (2)	C3—N6—C2—N5	−1.4 (5)
N3^{iii}—Zn1—N1—C1	93.5 (2)	C3—N6—C2—C1	177.9 (3)
C1—N1—N2—N3	0.0 (3)	C5—N5—C2—N6	1.0 (5)
Zn1—N1—N2—N3	178.6 (3)	Zn1—N5—C2—N6	−176.1 (3)
N1—N2—N3—N4	−0.2 (4)	C5—N5—C2—C1	−178.3 (3)
N1—N2—N3—Zn1^{iv}	−171.9 (2)	Zn1—N5—C2—C1	4.6 (3)
N2—N3—N4—C1	0.2 (4)	N4—C1—C2—N6	−4.2 (5)
Zn1^{iv}—N3—N4—C1	171.6 (2)	N1—C1—C2—N6	177.8 (3)

N1^{i}—Zn1—N5—C2	176.1 (2)	N4—C1—C2—N5	175.2 (3)
N1—Zn1—N5—C2	−3.9 (2)	N1—C1—C2—N5	−2.8 (4)
N3^{ii}—Zn1—N5—C2	84.8 (2)	C2—N6—C3—C4	0.2 (6)
N3^{iii}—Zn1—N5—C2	−95.2 (2)	N6—C3—C4—C5	1.3 (6)
N1^{i}—Zn1—N5—C5	−0.5 (3)	C2—N5—C5—C4	0.7 (5)
N1—Zn1—N5—C5	179.5 (3)	Zn1—N5—C5—C4	177.2 (3)
N3^{ii}—Zn1—N5—C5	−91.8 (3)	C3—C4—C5—N5	−1.7 (6)
N3^{iii}—Zn1—N5—C5	88.2 (3)		

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

Fig. 1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C1
C2
N3
C3
N6
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Zn1C

Fig. 2