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

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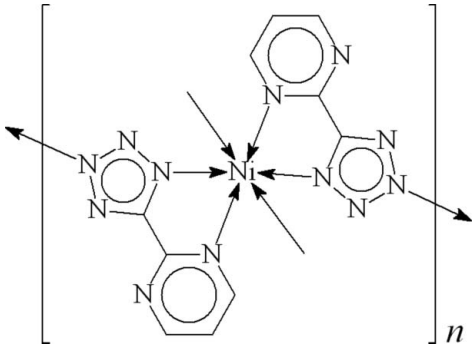
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.053; wR factor = 0.105; data-to-parameter ratio = 15.1.

In the title compound, $[Ni(C_5H_3N_6)_2]_n$, the Ni^{II} atom is located on an inversion centre and exhibits a distorted octahedral geometry. The crystal structure features a two-dimensional square-grid-like network. The compound is isostructural with the iron(II) and cobalt(II) analogues, whose structures and magnetic properties have been reported [Rodríguez, Kivekäsb & Colacio (2005). *Chem. Commun.* pp. 5228–5230].

Related literature

For compound preparation, see: Demko & Sharpless (2001). For related literature, see: Rodríguez *et al.* (2005).



Experimental

Crystal data

$[Ni(C_5H_3N_6)_2]$
M_r = 352.98
Orthorhombic, *Pbca*
a = 8.2054 (16) Å
b = 9.1736 (18) Å
c = 17.846 (4) Å
V = 1343.3 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.47 mm^{-1}
T = 293 (2) K
0.18 × 0.16 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.974, T_{max} = 1.000
(expected range = 0.771–0.791)
9528 measured reflections
1598 independent reflections
1396 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.105
S = 1.20
1598 reflections
106 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—N1	2.054 (3)	Ni1—N6	2.098 (3)
Ni1—N3^{i}	2.089 (2)		
N1—Ni1—N3^{ii}	91.02 (10)	N1—Ni1—N6	79.12 (10)
N1—Ni1—N3^{i}	88.98 (10)	N3^{ii}—Ni1—N6	91.13 (10)
N1—Ni1—N6^{iii}	100.88 (10)	N3^{i}—Ni1—N6	88.87 (10)

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

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2385).

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.
Rodríguez, A., Kivekäsb, R. & Colacio, E. (2005). *Chem. Commun.* pp. 5228–5230.
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supplementary materials

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

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Comment

Poly[5-(pyrimidin-2-yl)tetrazolato]nickel(II)], (I) (Fig. 1), is isostructural with the iron(II) and cobalt(II) analogs (Rodríguez *et al.*, 2005). The three structures feature a two-dimensional square-grid-like network, in which each metal atom is located on an inversion centre and exhibits a distorted octahedral geometry. Each metal atom bonds to four ligands, and each ligand is coordinated to two metal atoms through one of the pyrimidyl nitrogen atoms and the 1-positon tetrazole nitrogen atom in *cis* position for one, and one 3-position tetrazole nitrogen atom for the other.

Experimental

The ligand, 2-(1*H*-tetrazol-5-yl)pyrimidine (*L*), was synthesized according to the literature method (Demko & Sharpless, 2001). A mixture of $NiCl_2{\cdot}6H_2O$ (48 mg, 0.2 mmol) and ligand *L* (60 mg, 0.4 mmol) in water (10 ml) was placed in a Teflon-lined stainless-steel Parr bomb that was heated at 413 K for 72 h. The bomb was then cooled to room temperature. Pink crystals were isolated in about 20% yield.

Refinement

H atoms bound to C atoms were placed in calculated positions (C—H = 0.93 Å) and refined in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

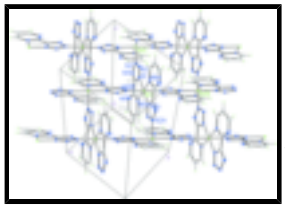

Fig. 1. Part of the two-dimensional network structure of (I). Displacement ellipsoids are drawn at the 40% probability level. [symmetry codes: (A) −*x*, 1 − *y*, 1 − *z*; (B) 1/2 + *x*, 1/2 − *y*, 1 − *z*.]

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

Crystal data

$[Ni(C_5H_3N_6)_2]$	F_{000} = 712
M_r = 352.98	D_x = 1.745 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 3035 reflections
a = 8.2054 (16) Å	θ = 2.5–26.4°

b = 9.1736 (18) Å	μ = 1.47 mm^{-1}
c = 17.846 (4) Å	T = 293 (2) K
V = 1343.3 (5) Å^3	Block, pink
Z = 4	0.18 × 0.16 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer	1598 independent reflections
Radiation source: fine-focus sealed tube	1396 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.058
T = 293(2) K	θ_{max} = 27.9º
φ and ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Bruker, 1998)	$h = -10 \rightarrow 9$
T_{min} = 0.974, T_{max} = 1.000	$k = -12 \rightarrow 10$
9528 measured reflections	$l = -23 \rightarrow 22$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.053	H-atom parameters constrained
$wR(F^2)$ = 0.105	$w = 1/[\sigma^2(F_o^2) + (0.032P)^2 + 2.6446P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.20	$(\Delta/\sigma)_{max}$ = 0.001
1598 reflections	$\Delta\rho_{max}$ = 0.56 e Å^{-3}
106 parameters	$\Delta\rho_{min}$ = −0.40 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}
Ni1	0.0000	0.5000	0.5000	0.00927 (16)

N1	−0.1491 (3)	0.3232 (3)	0.48286 (15)	0.0130 (6)
C2	−0.0291 (4)	0.3372 (3)	0.35937 (19)	0.0142 (6)
N6	0.0456 (3)	0.4562 (3)	0.38656 (15)	0.0116 (5)
N5	−0.0129 (3)	0.2818 (3)	0.29133 (16)	0.0196 (6)
C5	0.1446 (4)	0.5280 (3)	0.3397 (2)	0.0175 (7)
H5	0.1993	0.6105	0.3565	0.021*
C1	−0.1385 (4)	0.2677 (3)	0.41376 (17)	0.0121 (6)
C4	0.1666 (4)	0.4812 (4)	0.2669 (2)	0.0213 (7)
H4	0.2334	0.5320	0.2338	0.026*
N2	−0.2581 (3)	0.2430 (3)	0.51904 (14)	0.0128 (5)
N4	−0.2388 (3)	0.1549 (3)	0.40478 (15)	0.0148 (6)
C3	0.0857 (4)	0.3563 (4)	0.2450 (2)	0.0236 (8)
H3	0.1000	0.3225	0.1963	0.028*
N3	−0.3114 (3)	0.1428 (3)	0.47178 (16)	0.0126 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0094 (3)	0.0073 (3)	0.0111 (3)	0.0006 (2)	−0.0003 (2)	−0.0005 (2)
N1	0.0116 (12)	0.0106 (11)	0.0169 (15)	0.0001 (10)	0.0008 (10)	−0.0004 (10)
C2	0.0143 (14)	0.0136 (14)	0.0148 (16)	−0.0025 (12)	0.0006 (12)	0.0005 (12)
N6	0.0129 (12)	0.0080 (11)	0.0139 (14)	0.0016 (9)	−0.0010 (10)	0.0007 (9)
N5	0.0216 (15)	0.0220 (14)	0.0153 (15)	−0.0032 (12)	0.0039 (12)	−0.0051 (11)
C5	0.0191 (16)	0.0108 (14)	0.0227 (18)	0.0004 (12)	0.0033 (13)	0.0008 (12)
C1	0.0129 (14)	0.0127 (14)	0.0106 (16)	−0.0006 (12)	0.0002 (12)	−0.0003 (11)
C4	0.0224 (17)	0.0219 (16)	0.0195 (18)	0.0017 (14)	0.0079 (14)	0.0040 (14)
N2	0.0118 (12)	0.0114 (12)	0.0152 (14)	−0.0031 (10)	0.0012 (11)	−0.0004 (10)
N4	0.0157 (13)	0.0153 (12)	0.0134 (14)	−0.0015 (11)	0.0024 (11)	−0.0015 (10)
C3	0.0272 (18)	0.0290 (18)	0.0146 (18)	−0.0029 (16)	0.0060 (14)	−0.0019 (15)
N3	0.0138 (12)	0.0095 (11)	0.0144 (14)	−0.0033 (10)	0.0018 (10)	−0.0013 (10)

Geometric parameters (Å, °)

Ni1—N1^{i}	2.054 (3)	N6—C5	1.338 (4)
Ni1—N1	2.054 (3)	N5—C3	1.344 (4)
Ni1—N3^{ii}	2.089 (2)	C5—C4	1.382 (5)
Ni1—N3^{iii}	2.089 (2)	C5—H5	0.93
Ni1—N6^{i}	2.098 (3)	C1—N4	1.332 (4)
Ni1—N6	2.098 (3)	C4—C3	1.381 (5)
N1—N2	1.326 (3)	C4—H4	0.93
N1—C1	1.337 (4)	N2—N3	1.322 (4)
C2—N5	1.323 (4)	N4—N3	1.340 (4)
C2—N6	1.343 (4)	C3—H3	0.93
C2—C1	1.468 (4)	N3—Ni1^{iv}	2.089 (2)
N1^{i}—Ni1—N1	180	C5—N6—C2	116.8 (3)
N1^{i}—Ni1—N3^{ii}	88.98 (10)	C5—N6—Ni1	128.1 (2)
N1—Ni1—N3^{ii}	91.02 (10)	C2—N6—Ni1	115.0 (2)

N1^{i}—Ni1—N3^{iii}	91.02 (10)	C2—N5—C3	115.5 (3)
N1—Ni1—N3^{iii}	88.98 (10)	N6—C5—C4	121.0 (3)
N3^{ii}—Ni1—N3^{iii}	180	N6—C5—H5	119.5
N1^{i}—Ni1—N6^{i}	79.12 (10)	C4—C5—H5	119.5
N1—Ni1—N6^{i}	100.88 (10)	N4—C1—N1	111.5 (3)
N3^{ii}—Ni1—N6^{i}	88.87 (10)	N4—C1—C2	129.5 (3)
N3^{iii}—Ni1—N6^{i}	91.13 (10)	N1—C1—C2	119.0 (3)
N1^{i}—Ni1—N6	100.88 (10)	C3—C4—C5	117.4 (3)
N1—Ni1—N6	79.12 (10)	C3—C4—H4	121.3
N3^{ii}—Ni1—N6	91.13 (10)	C5—C4—H4	121.3
N3^{iii}—Ni1—N6	88.87 (10)	N3—N2—N1	107.4 (2)
N6^{i}—Ni1—N6	180	C1—N4—N3	103.4 (2)
N2—N1—C1	106.4 (2)	N5—C3—C4	122.5 (3)
N2—N1—Ni1	140.1 (2)	N5—C3—H3	118.7
C1—N1—Ni1	113.5 (2)	C4—C3—H3	118.7
N5—C2—N6	126.7 (3)	N2—N3—N4	111.4 (2)
N5—C2—C1	120.1 (3)	N2—N3—Ni1^{iv}	121.8 (2)
N6—C2—C1	113.2 (3)	N4—N3—Ni1^{iv}	126.6 (2)
N3^{ii}—Ni1—N1—N2	−85.7 (3)	C2—N6—C5—C4	0.5 (5)
N3^{iii}—Ni1—N1—N2	94.3 (3)	Ni1—N6—C5—C4	177.2 (2)
N6^{i}—Ni1—N1—N2	3.4 (3)	N2—N1—C1—N4	0.5 (3)
N6—Ni1—N1—N2	−176.6 (3)	Ni1—N1—C1—N4	−179.06 (19)
N3^{ii}—Ni1—N1—C1	93.6 (2)	N2—N1—C1—C2	178.4 (3)
N3^{iii}—Ni1—N1—C1	−86.4 (2)	Ni1—N1—C1—C2	−1.2 (3)
N6^{i}—Ni1—N1—C1	−177.3 (2)	N5—C2—C1—N4	−4.5 (5)
N6—Ni1—N1—C1	2.7 (2)	N6—C2—C1—N4	175.3 (3)
N5—C2—N6—C5	1.3 (5)	N5—C2—C1—N1	178.0 (3)
C1—C2—N6—C5	−178.4 (3)	N6—C2—C1—N1	−2.2 (4)
N5—C2—N6—Ni1	−175.8 (3)	N6—C5—C4—C3	−1.4 (5)
C1—C2—N6—Ni1	4.4 (3)	C1—N1—N2—N3	−0.4 (3)
N1^{i}—Ni1—N6—C5	−0.8 (3)	Ni1—N1—N2—N3	178.9 (2)
N1—Ni1—N6—C5	179.2 (3)	N1—C1—N4—N3	−0.3 (3)
N3^{ii}—Ni1—N6—C5	88.4 (3)	C2—C1—N4—N3	−177.9 (3)
N3^{iii}—Ni1—N6—C5	−91.6 (3)	C2—N5—C3—C4	0.8 (5)
N1^{i}—Ni1—N6—C2	176.0 (2)	C5—C4—C3—N5	0.7 (5)
N1—Ni1—N6—C2	−4.0 (2)	N1—N2—N3—N4	0.2 (3)
N3^{ii}—Ni1—N6—C2	−94.8 (2)	N1—N2—N3—Ni1^{iv}	−174.80 (18)
N3^{iii}—Ni1—N6—C2	85.2 (2)	C1—N4—N3—N2	0.0 (3)
N6—C2—N5—C3	−2.0 (5)	C1—N4—N3—Ni1^{iv}	174.8 (2)
C1—C2—N5—C3	177.8 (3)		

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

Fig. 1