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Poly[bis[μ-1,4-bis(1,2,4-triazol-1-ylmethyl)benzene]dicyanatonickel(II)]

Wen-Bao Wang,[a,b] Li-Yan Wang,[a] Bao-Long Li[a]* and Yong Zhang[a]

[a]Key Laboratory of Organic Synthesis of Jiangsu Province, College of Chemistry and Chemical Engineering, Suzhou University, Suzhou 215123, People's Republic of China, and [b]Center of Analysis and Measurement, Suzhou University, Suzhou 215123, People's Republic of China
Correspondence e-mail: libaolong@suda.edu.cn

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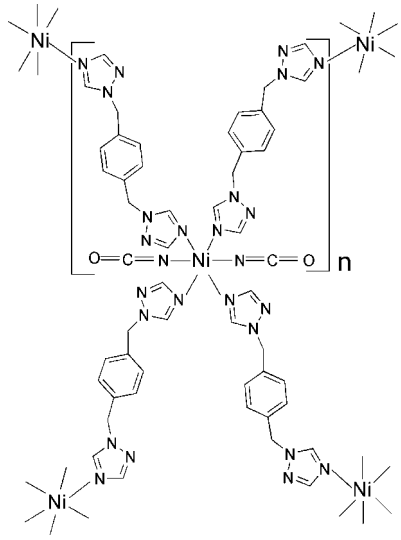
Key indicators: single-crystal X-ray study; T = 193 K; mean σ(C–C) = 0.003 Å; R factor = 0.035; wR factor = 0.092; data-to-parameter ratio = 16.1.

The coordination geometry of the Ni^{II} atom in the title complex, $[Ni(NCO)_2(C_{12}H_{12}N_6)_2]_n$ or $[Ni(NCO)_2(bbtz)_2]_n$, where bbtz is 1,4-bis(1,2,4-triazol-1-ylmethyl)benzene, is distorted octahedral, in which the Ni^{II} atom lies on an inversion center and is bonded to four N atoms from the triazole rings of four symmetry-related bbtz ligands and two N atoms from two symmetry-related monodentate NCO^- ligands. The Ni^{II} atoms are bridged by four bbtz ligands to form a two-dimensional (4,4) network.

Related literature

The synthesis of the ligand 1,4-bis(1,2,4-triazol-1-ylmethyl)-benzene (bbtz) was described by Peng *et al.* (2004). Several bbtz complexes have been synthesized and structurally characterized (Li *et al.*, 2004, 2005; Wang *et al.*, 2007). The complex $[Ni(bbtz)_2(N_3)_2]_n$ has a similar two-dimensional (4,4) network (Wang *et al.*, 2007). For flexible bis(triazole) ligands, see: Haasnoot (2000); Albada *et al.* (2000); Zhao *et al.* (2002); Meng *et al.* (2004).



Experimental

Crystal data

$[Ni(CNO)_2(C_{12}H_{12}N_6)_2]$
M_r = 623.30
Monoclinic, $P2_1/c$
a = 8.3857 (7) Å
b = 20.1913 (14) Å
c = 8.4229 (7) Å
β = 103.836 (2)°
V = 1384.77 (19) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.75 mm^{-1}
T = 193 (2) K
0.50 × 0.20 × 0.20 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.704, T_{max} = 0.864
15292 measured reflections
3168 independent reflections
2828 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.092
S = 1.06
3168 reflections
197 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: BT2480).

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supplementary materials

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Poly[bis[μ-1,4-bis(1,2,4-triazol-1-ylmethyl)benzene]dicyanatonickel(II)]

W.-B. Wang, L.-Y. Wang, B.-L. Li and Y. Zhang

Comment

The design and assembly of coordination polymers have been intensely studied for their interesting topologies and potential application as functional materials. The structural motifs of coordination polymers rest on several factors, such as the central atom, the performance of the ligands, the coordinated and/or non-coordinated counter ions and the reaction conditions. The ligand is no doubt the key factor of manipulating the topologies of the coordination polymers. Some novel coordination polymers with the flexible bis(triazole) ligands have been synthesized (Haasnoot, 2000; Albada *et al.*, 2000; Zhao *et al.*, 2002; Meng *et al.*, 2004; Li *et al.*, 2005).

In our previous studies, we synthesized several coordination polymers with the flexible ligands 1,4-bis(1,2,4-triazol-1-ylmethyl)benzene (bbtz) (Li *et al.*, 2004; Li *et al.*, 2005; Wang *et al.*, 2007). In the present paper, we report the preparation and crystal structure of a two-dimensional (4,4) network coordination polymer $[Ni(bbtz)_2(NCO)_2]_n$ (I).

The structure of (I) is similar to that of $[Ni(bbtz)_2(N_3)_2]_n$ (Wang *et al.*, 2007). Fig. 1 shows the local coordination of the Ni^{II} atom in (I). The complex has a center of symmetry and the Ni^{II} atom occupies an inversion center. The coordination geometry of the Ni^{II} atom is distorted octahedral; it is coordinated equatorially by four nitrogen atoms from the triazole rings of four symmetry-related bbtz ligands [Ni1—N3, 2.1156 (3) Å; Ni1—N6 ($-x+1$, $y-1/2$, $-z-1/2$), 2.1195 (14) Å], and axially by two nitrogen atoms from two symmetry-related cyanate anions [Ni1—N7, 2.0672 (16) Å]. The Ni—N(triazole) bond lengths [2.1156 (3) and 2.1195 (14) Å] at equatorial plane in (I) are corresponding to the values [2.1012 (16) and 2.1162 (16) Å] reported in $[Ni(bbtz)_2(N_3)_2]_n$ (Wang *et al.*, 2007). The cyanato ligand in (I) is quasi-linear as expected [the N—C—O bond angle is 178.3 (2)°]. The Ni—N—C (NCO) bond angle is 169.80 (15)°.

Because the methyl carbon atoms of bbtz can freely rotate to adjust itself to the coordination environment, bbtz can exhibit the *trans-gauche* and *gauche-gauche* conformations. The bbtz ligands exhibit the *trans-gauche* conformation in (I), similar to the situation in the free bbtz molecule (Peng *et al.*, 2004), $[Ni(bbtz)_2(N_3)_2]_n$ (Wang *et al.*, 2007) and $[Co(bbtz)_2(N_3)_2]_n$ (Li *et al.*, 2004). The three rings (two triazole rings and one benzene ring) of one bbtz ligand are not coplanar in (I), $[Ni(bbtz)_2(N_3)_2]_n$, $[Co(bbtz)_2(N_3)_2]_n$ and the free bbtz molecule. The dihedral angle between the two triazole planes in (I) is 58.8 (1)°, compared with the values 63.70 (9)° in $[Ni(bbtz)_2(N_3)_2]_n$, 61.94 (19)° in $[Co(bbtz)_2(N_3)_2]_n$, but 0° in free bbtz molecule by imposed crystallographic symmetry. The dihedral angles between the benzene plane and triazole planes in (I) are 67.6 (1) and 65.8 (1)°, compared with the values 66.46 (9) and 66.10 (7)° in $[Ni(bbtz)_2(N_3)_2]_n$, 67.26 (9) and 66.96 (7)° in $[Co(bbtz)_2(N_3)_2]_n$, and 77.81 (9)° in the free bbtz molecule.

As illustrated in Fig. 2, each bbtz ligand in (I) coordinates to the Ni^{II} atoms through its two triazole nitrogen atoms, thus acting as a bridging bidentate ligand to form a two-dimensional neutral (4,4) network. The networks contain square grids (52-membered ring), with a Ni^{II} atom at each corner and a bbtz ligand at each edge connecting two Ni^{II} atoms. As a consequence of the symmetry of the crystal structure, the edge lengths are equal, with a value of 14.383 (1) Å, similar to the

M···*M* separations [14.3646 (15) Å] in $[Ni(bbtz)_2(N_3)_2]_n$ (Wang *et al.*, 2007), and [14.4156 (18) Å] in $[Co(bbtz)_2(N_3)_2]_n$ (Li *et al.*, 2004).

The diagonal lengths of the square grid are 20.191 (1) and 20.489 (1) Å; the square angles are 90.8 (1) and 89.2 (1)°. The square-grid sheets are stacked in an off-set fashion parallel to the c direction. The off-set half-cell superposition of each pair of adjacent networks divides the voids into smaller rectangle. The cyanate anions of one sheet project into the holes of the next sheet. In the superposition structure, the sheets are arranged in the sequence ··· A—B—A—B ···(Fig.3).

Experimental

A 25 ml H_2O/EtOH solution (*v*/*v*, 1:1) of 1,4-bis(1,2,4-triazol-1- ylmethyl)benzene (bbtz) (0.240 g, 1.0 mmol) was added to one leg of a H-shape tube, and 25 ml H_2O/EtOH (*v*/*v*, 1:1) solution of $Ni(NO_3)_2{\cdot}6H_2O$ (0.145 g, 0.5 mmol) and NaOCN (0.088 g, 1.4 mmol) was added to the other leg of the tube. The tube was allowed to stand in air at the room temperature for about one month. The light-blue crystals $[Ni(bbtz)_2(NCO)_2]_n$ (I) suitable for X-ray diffraction were obtained. Yield 73%. Elemental analysis confirmed the organic content (Found: C, 49.96; H, 3.82; N, 31.38%. Calcd. for $C_{26}H_{24}N_{14}NiO_2$: C, 50.10; H, 3.88; N, 31.47%).

Refinement

H atom were placed in idealized positions and refined as riding, with C—H distances of 0.95 (triazole and benzene) and 0.99Å (methyl), and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

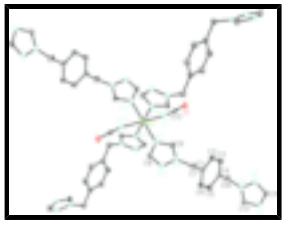

Fig. 1. The coordination environment of the Ni^{II} atom of (I) at the 30% probability level. [Symmetry codes: # −*x*, −*y* + 1, −*z* + 1 $ −*x* + 1, *y* − 1/2, −*z* + 1/2 & *x* − 1, −*y* + 3/2, *z* + 1/2]. The hydrogen atoms have been omitted for clarity.

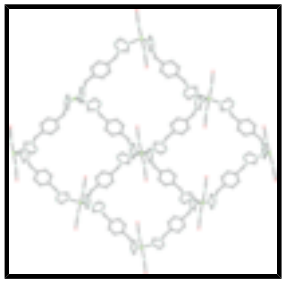

Fig. 2. Viewing the two-dimensional (4,4) network of the title compound along the c direction.

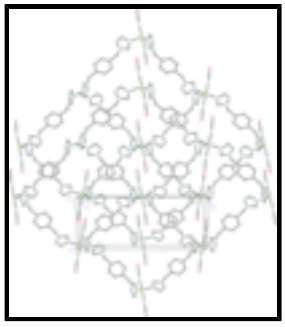

Fig. 3. The cell packing of the title compound

Poly[bis[μ-1,4-bis(1,2,4-triazol-1-ylmethyl)benzene]dicyanatonickel(II)]

Crystal data

$[Ni(CNO)_2(C_{12}H_{12}N_6)_2]$	F_{000} = 644
M_r = 623.30	D_x = 1.495 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 5408 reflections
a = 8.3857 (7) Å	θ = 3.0–27.5º
b = 20.1913 (14) Å	μ = 0.75 mm^{-1}
c = 8.4229 (7) Å	T = 193 (2) K
β = 103.836 (2)º	Prism, light-blue
V = 1384.77 (19) Å^3	0.50 × 0.20 × 0.20 mm
Z = 2	

Data collection

Rigaku Mercury CCD diffractometer	3168 independent reflections
Radiation source: fine-focus sealed tube	2828 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.027
Detector resolution: 7.31 pixels mm^{-1}	θ_{max} = 27.5º
T = 193(2) K	θ_{min} = 3.2º
ω scans	h = −10→10
Absorption correction: multi-scan (Jacobson, 1998)	k = −23→26
T_{min} = 0.704, T_{max} = 0.864	l = −8→10
15292 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.035	H-atom parameters constrained
$wR(F^2)$ = 0.092	$w = 1/[\sigma^2(F_o^2) + (0.047P)^2 + 0.5612P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} < 0.001$
3168 reflections	$\Delta\rho_{max} = 0.28$ e Å^{-3}
197 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}
Ni1	0.0000	0.5000	0.5000	0.02367 (11)
O1	0.51308 (17)	0.53499 (8)	0.77007 (19)	0.0498 (4)
N1	0.14183 (18)	0.58347 (7)	0.09373 (17)	0.0285 (3)
N2	−0.0216 (2)	0.58482 (9)	0.0260 (2)	0.0395 (4)
N3	0.02897 (17)	0.54577 (7)	0.28271 (17)	0.0270 (3)
N4	0.80765 (18)	0.83698 (7)	0.20798 (18)	0.0302 (3)
N5	0.9361 (2)	0.80325 (8)	0.1727 (2)	0.0388 (4)
N6	0.92675 (17)	0.90787 (7)	0.08018 (17)	0.0275 (3)
N7	0.24273 (19)	0.52223 (8)	0.60611 (19)	0.0337 (3)
C1	0.3763 (2)	0.65567 (9)	0.0773 (2)	0.0295 (4)
C2	0.5224 (2)	0.64025 (9)	0.1849 (3)	0.0390 (4)
H2A	0.5502	0.5952	0.2091	0.047*
C3	0.6300 (2)	0.68970 (10)	0.2586 (2)	0.0388 (4)
H3A	0.7306	0.6781	0.3324	0.047*
C4	0.5919 (2)	0.75545 (9)	0.2256 (2)	0.0312 (4)
C5	0.4459 (3)	0.77098 (10)	0.1158 (3)	0.0435 (5)
H5A	0.4185	0.8161	0.0911	0.052*
C6	0.3389 (3)	0.72163 (10)	0.0412 (3)	0.0435 (5)
H6A	0.2396	0.7331	−0.0348	0.052*
C7	0.2624 (2)	0.60073 (10)	−0.0015 (2)	0.0370 (4)
H7A	0.2033	0.6147	−0.1127	0.044*
H7B	0.3282	0.5610	−0.0123	0.044*
C8	−0.0831 (2)	0.56153 (10)	0.1443 (2)	0.0347 (4)
H8A	−0.1978	0.5562	0.1333	0.042*
C9	0.1696 (2)	0.56019 (9)	0.2452 (2)	0.0311 (4)
H9A	0.2752	0.5547	0.3164	0.037*

C10	0.7068 (3)	0.80889 (10)	0.3107 (2)	0.0382 (4)
H10A	0.6415	0.8447	0.3445	0.046*
H10B	0.7797	0.7902	0.4107	0.046*
C11	1.0026 (2)	0.84856 (9)	0.0954 (2)	0.0349 (4)
H11A	1.0964	0.8400	0.0539	0.042*
C12	0.8044 (2)	0.89849 (9)	0.1525 (2)	0.0288 (4)
H12A	0.7260	0.9311	0.1630	0.035*
C13	0.3752 (2)	0.52878 (8)	0.6844 (2)	0.0275 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.02108 (17)	0.02854 (18)	0.02304 (17)	0.00161 (11)	0.00850 (12)	0.00138 (11)
O1	0.0248 (7)	0.0645 (10)	0.0567 (9)	−0.0067 (7)	0.0029 (6)	0.0001 (8)
N1	0.0284 (7)	0.0334 (8)	0.0251 (7)	−0.0067 (6)	0.0090 (6)	0.0005 (6)
N2	0.0329 (9)	0.0497 (10)	0.0341 (8)	−0.0023 (7)	0.0045 (7)	0.0115 (7)
N3	0.0267 (7)	0.0296 (7)	0.0265 (7)	0.0014 (6)	0.0099 (6)	0.0027 (6)
N4	0.0312 (8)	0.0307 (8)	0.0299 (7)	−0.0074 (6)	0.0097 (6)	−0.0030 (6)
N5	0.0357 (9)	0.0328 (8)	0.0495 (10)	−0.0002 (7)	0.0133 (8)	−0.0016 (7)
N6	0.0253 (7)	0.0305 (7)	0.0283 (7)	−0.0027 (6)	0.0094 (6)	−0.0013 (6)
N7	0.0260 (8)	0.0438 (9)	0.0318 (8)	−0.0009 (7)	0.0080 (6)	0.0012 (7)
C1	0.0314 (9)	0.0327 (9)	0.0272 (8)	−0.0065 (7)	0.0127 (7)	0.0027 (7)
C2	0.0404 (11)	0.0285 (9)	0.0472 (11)	−0.0008 (8)	0.0089 (9)	0.0058 (8)
C3	0.0333 (10)	0.0380 (10)	0.0411 (10)	−0.0027 (8)	0.0007 (8)	0.0089 (8)
C4	0.0343 (9)	0.0333 (9)	0.0288 (8)	−0.0070 (7)	0.0132 (7)	0.0011 (7)
C5	0.0406 (11)	0.0298 (10)	0.0576 (13)	0.0006 (8)	0.0071 (10)	0.0090 (9)
C6	0.0329 (10)	0.0426 (11)	0.0503 (12)	−0.0016 (8)	0.0010 (9)	0.0096 (9)
C7	0.0396 (10)	0.0469 (11)	0.0289 (9)	−0.0135 (9)	0.0168 (8)	−0.0041 (8)
C8	0.0263 (9)	0.0429 (10)	0.0352 (9)	0.0020 (8)	0.0080 (7)	0.0089 (8)
C9	0.0254 (8)	0.0418 (10)	0.0268 (8)	−0.0027 (7)	0.0079 (7)	0.0029 (7)
C10	0.0481 (11)	0.0390 (10)	0.0310 (9)	−0.0141 (9)	0.0164 (8)	−0.0021 (8)
C11	0.0294 (9)	0.0347 (10)	0.0427 (10)	−0.0022 (7)	0.0128 (8)	−0.0038 (8)
C12	0.0269 (8)	0.0305 (9)	0.0301 (9)	−0.0031 (7)	0.0092 (7)	−0.0028 (7)
C13	0.0277 (9)	0.0258 (9)	0.0322 (9)	−0.0004 (7)	0.0134 (7)	0.0025 (7)

Geometric parameters (Å, °)

Ni1—N7^{i}	2.0672 (15)	C1—C2	1.374 (3)
Ni1—N7	2.0672 (16)	C1—C6	1.385 (3)
Ni1—N3^{i}	2.1156 (13)	C1—C7	1.510 (3)
Ni1—N3	2.1156 (13)	C2—C3	1.388 (3)
Ni1—N6^{ii}	2.1195 (14)	C2—H2A	0.9500
Ni1—N6^{iii}	2.1195 (14)	C3—C4	1.378 (3)
O1—C13	1.214 (2)	C3—H3A	0.9500
N1—C9	1.327 (2)	C4—C5	1.382 (3)
N1—N2	1.353 (2)	C4—C10	1.509 (3)
N1—C7	1.475 (2)	C5—C6	1.387 (3)
N2—C8	1.314 (2)	C5—H5A	0.9500

N3—C9	1.325 (2)	C6—H6A	0.9500
N3—C8	1.349 (2)	C7—H7A	0.9900
N4—C12	1.325 (2)	C7—H7B	0.9900
N4—N5	1.366 (2)	C8—H8A	0.9500
N4—C10	1.461 (2)	C9—H9A	0.9500
N5—C11	1.321 (2)	C10—H10A	0.9900
N6—C12	1.326 (2)	C10—H10B	0.9900
N6—C11	1.347 (2)	C11—H11A	0.9500
N6—Ni1^{iv}	2.1195 (14)	C12—H12A	0.9500
N7—C13	1.156 (2)		
N7^{i}—Ni1—N7	180.0	C4—C3—H3A	119.7
N7^{i}—Ni1—N3^{i}	88.53 (6)	C2—C3—H3A	119.7
N7—Ni1—N3^{i}	91.47 (6)	C3—C4—C5	118.61 (17)
N7^{i}—Ni1—N3	91.47 (6)	C3—C4—C10	120.15 (18)
N7—Ni1—N3	88.53 (6)	C5—C4—C10	121.23 (18)
N3^{i}—Ni1—N3	180.0	C4—C5—C6	120.90 (18)
N7^{i}—Ni1—N6^{ii}	90.12 (6)	C4—C5—H5A	119.5
N7—Ni1—N6^{ii}	89.88 (6)	C6—C5—H5A	119.5
N3^{i}—Ni1—N6^{ii}	89.67 (5)	C1—C6—C5	120.22 (19)
N3—Ni1—N6^{ii}	90.33 (5)	C1—C6—H6A	119.9
N7^{i}—Ni1—N6^{iii}	89.88 (6)	C5—C6—H6A	119.9
N7—Ni1—N6^{iii}	90.12 (6)	N1—C7—C1	112.26 (14)
N3^{i}—Ni1—N6^{iii}	90.33 (5)	N1—C7—H7A	109.2
N3—Ni1—N6^{iii}	89.67 (5)	C1—C7—H7A	109.2
N6^{ii}—Ni1—N6^{iii}	180.0	N1—C7—H7B	109.2
C9—N1—N2	109.87 (14)	C1—C7—H7B	109.2
C9—N1—C7	128.37 (16)	H7A—C7—H7B	107.9
N2—N1—C7	121.56 (15)	N2—C8—N3	114.90 (16)
C8—N2—N1	102.41 (14)	N2—C8—H8A	122.6
C9—N3—C8	102.61 (14)	N3—C8—H8A	122.6
C9—N3—Ni1	126.55 (12)	N3—C9—N1	110.21 (16)
C8—N3—Ni1	130.56 (12)	N3—C9—H9A	124.9
C12—N4—N5	109.95 (14)	N1—C9—H9A	124.9
C12—N4—C10	127.36 (16)	N4—C10—C4	113.01 (15)
N5—N4—C10	122.24 (16)	N4—C10—H10A	109.0
C11—N5—N4	102.10 (15)	C4—C10—H10A	109.0
C12—N6—C11	103.21 (15)	N4—C10—H10B	109.0
C12—N6—Ni1^{iv}	125.93 (12)	C4—C10—H10B	109.0
C11—N6—Ni1^{iv}	130.10 (12)	H10A—C10—H10B	107.8
C13—N7—Ni1	169.80 (15)	N5—C11—N6	114.67 (16)
C2—C1—C6	118.82 (17)	N5—C11—H11A	122.7
C2—C1—C7	119.59 (17)	N6—C11—H11A	122.7
C6—C1—C7	121.57 (18)	N6—C12—N4	110.07 (16)
C1—C2—C3	120.89 (18)	N6—C12—H12A	125.0
C1—C2—H2A	119.6	N4—C12—H12A	125.0

C3—C2—H2A	119.6	N7—C13—O1	178.3 (2)
C4—C3—C2	120.54 (18)		
C9—N1—N2—C8	−0.1 (2)	C7—C1—C6—C5	179.90 (19)
C7—N1—N2—C8	175.07 (17)	C4—C5—C6—C1	0.7 (3)
N7^{i}—Ni1—N3—C9	−163.56 (15)	C9—N1—C7—C1	−61.6 (3)
N7—Ni1—N3—C9	16.44 (15)	N2—N1—C7—C1	124.14 (19)
N6^{ii}—Ni1—N3—C9	−73.44 (15)	C2—C1—C7—N1	91.4 (2)
N6^{iii}—Ni1—N3—C9	106.56 (15)	C6—C1—C7—N1	−89.9 (2)
N7^{i}—Ni1—N3—C8	9.20 (17)	N1—N2—C8—N3	0.3 (2)
N7—Ni1—N3—C8	−170.80 (17)	C9—N3—C8—N2	−0.4 (2)
N6^{ii}—Ni1—N3—C8	99.33 (17)	Ni1—N3—C8—N2	−174.48 (13)
N6^{iii}—Ni1—N3—C8	−80.67 (17)	C8—N3—C9—N1	0.3 (2)
C12—N4—N5—C11	−0.2 (2)	Ni1—N3—C9—N1	174.71 (11)
C10—N4—N5—C11	−173.03 (16)	N2—N1—C9—N3	−0.2 (2)
N3^{i}—Ni1—N7—C13	8.8 (9)	C7—N1—C9—N3	−174.92 (16)
N3—Ni1—N7—C13	−171.2 (9)	C12—N4—C10—C4	115.0 (2)
N6^{ii}—Ni1—N7—C13	−80.8 (9)	N5—N4—C10—C4	−73.5 (2)
N6^{iii}—Ni1—N7—C13	99.2 (9)	C3—C4—C10—N4	101.5 (2)
C6—C1—C2—C3	1.0 (3)	C5—C4—C10—N4	−79.7 (2)
C7—C1—C2—C3	179.69 (18)	N4—N5—C11—N6	0.3 (2)
C1—C2—C3—C4	0.2 (3)	C12—N6—C11—N5	−0.2 (2)
C2—C3—C4—C5	−1.0 (3)	Ni1^{iv}—N6—C11—N5	170.08 (13)
C2—C3—C4—C10	177.90 (18)	C11—N6—C12—N4	0.11 (19)
C3—C4—C5—C6	0.6 (3)	Ni1^{iv}—N6—C12—N4	−170.75 (11)
C10—C4—C5—C6	−178.32 (19)	N5—N4—C12—N6	0.0 (2)
C2—C1—C6—C5	−1.5 (3)	C10—N4—C12—N6	172.43 (16)

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

Fig. 1

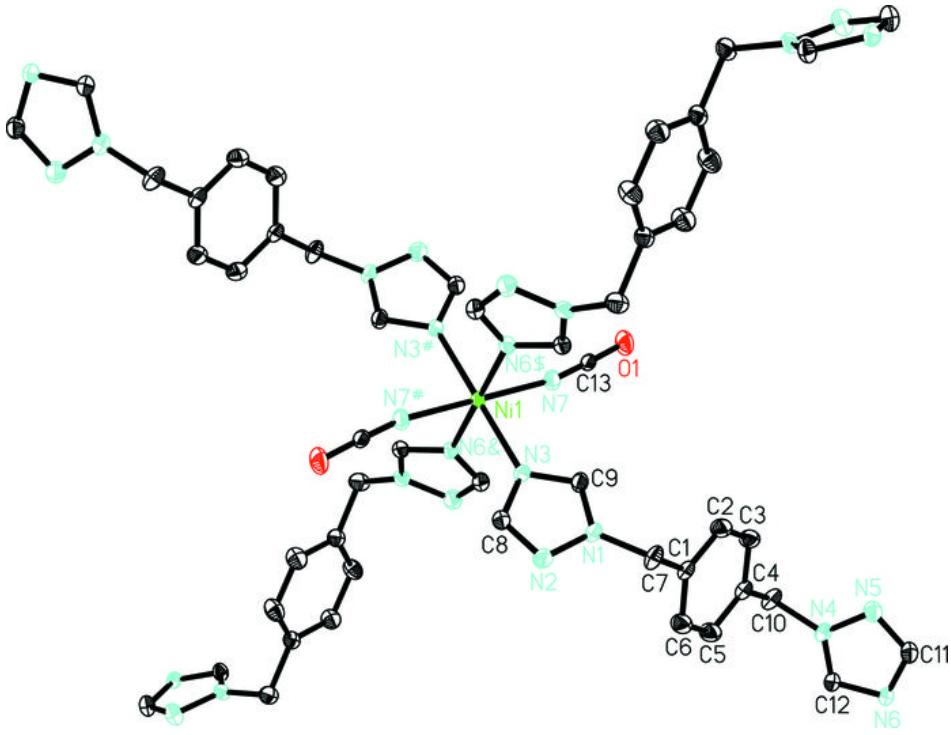
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Fig. 2

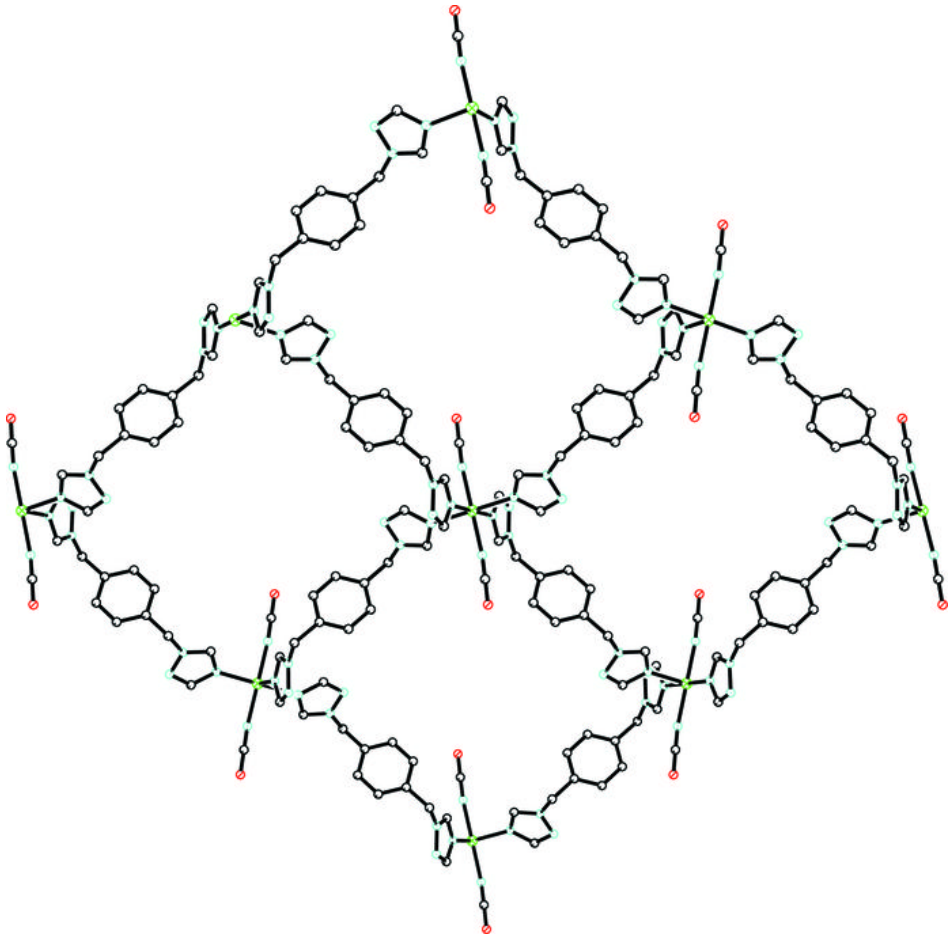

Fig. 3