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An Ni-based coordination polymer with a bamboo-like crystal structure

Yi Li,[a] Wang Xie[b] and Chen Lin[b]*

[a]Nanjing Petmedicine Technology Co., Ltd, Nanjing, People's Republic of China, and [b]School of Chemistry and Chemical Engineering, Nanjing University, Nanjing, 210023, People's Republic of China. *Correspondence e-mail: linchen@nju.edu.cn

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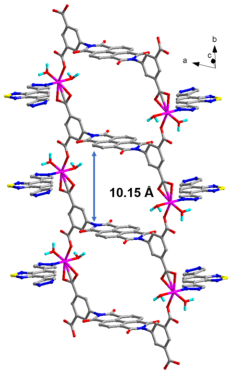
An Ni-based coordination polymer, namely, poly[tetraaquabis[4,7-bis(1*H*-pyrazol-4-yl)benzo[*c*][1,2,5]thiadiazole][μ_4-5,5′-(1,3,6,8-tetraoxo-1,3,6,8-tetrahydrobenzo[*lmn*][3,8]phenanthroline-2,7-diyl)diisophthalato]dinickel(II)], $\{[Ni_2(C_{30}H_{10}N_2O_{12})(C_{12}H_8N_6S)_2(H_2O)_4]\cdot 2C_3H_7NO\cdot H_2O\}_n$ or **Ni-BIBT-BINDI**, with a crystal structure reminiscent of bamboo has been synthesized, the Ni^{2+} ions exhibiting a slightly distorted octahedral coordination geometry with N atoms and O atoms. The bond lengths of the Ni—O bonds range from 2.032 to 2.121 Å, and those of the Ni—N bonds are approximately 2.080 Å. The BINDI ligands are connected to each other by the Ni—O bonds, which form the backbone of the bamboo, while the BIBT ligands are connected to the backbone of the bamboo through Ni—N bonds and grows on both sides of the bamboo, constituting the bamboo leaves.

1. Chemical context

Coordination polymers are defined as polymers formed by the association of inorganic metal ions and organic ligands with coordination bonds (Xia *et al.*, 2022). Currently, coordination polymers are being widely used in the fields of catalysis (Li *et al.*, 2024), sensing (Tian *et al.*, 2023) and gas storage (Dong *et al.*, 2023). In particular, Ni-based coordination polymers have received much attention from researchers in recent years because of their excellent catalytic properties (Shah *et al.*, 2019) and electrical conductivity (Khokhar *et al.*, 2022).



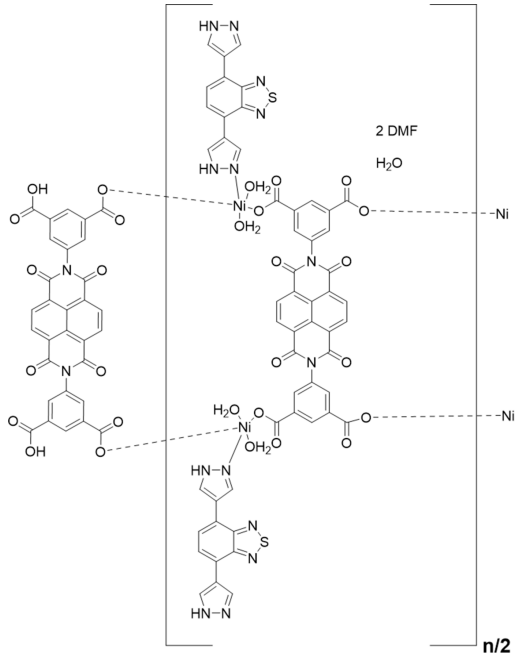


Table 1
Selected geometric parameters (Å, °).

Ni1—O1	2.042 (3)	Ni1—O5^{i}	2.115 (3)
Ni1—O3	2.101 (3)	Ni1—O6^{i}	2.122 (3)
Ni1—O4	2.032 (3)	Ni1—N1	2.079 (4)
O1—Ni1—O3	89.17 (14)	O4—Ni1—O5^{i}	103.05 (13)
O1—Ni1—O5^{i}	160.93 (13)	O4—Ni1—O6^{i}	164.09 (13)
O1—Ni1—O6^{i}	98.70 (12)	O4—Ni1—N1	96.72 (15)
O1—Ni1—N1	89.40 (15)	O5^{i}—Ni1—O6^{i}	62.43 (12)
O3—Ni1—O5^{i}	87.54 (13)	N1—Ni1—O3	178.02 (14)
O3—Ni1—O6^{i}	87.96 (13)	N1—Ni1—O5^{i}	93.37 (15)
O4—Ni1—O1	95.34 (13)	N1—Ni1—O6^{i}	90.90 (15)
O4—Ni1—O3	84.78 (14)		

Symmetry code: (i) $x, y-1, z$.

In this context, a novel one-dimensional Ni-based coordination polymer with the formula {[Ni (BINDI)$_{0.5}$(BIBT)(H$_2$O)$_2$]·DMF·0.5H$_2$O]}$_n$ [DMF = *N*,*N*-dimethylformamide, BIBT = 4,7-di(1*H*-pyrazol-4-yl)benzo[*c*][1,2,5]-thiadiazole and H$_4$BINDI = 5,5′-(1,3,6,8-tetraoxo-1,3,6,8-tetrahydrobenzo[lmn][3,8]phenanthroline-2,7-diyl)diisophthalic acid], namely **Ni-BIBT-BINDI**, was synthesized. The crystal structure of **Ni-BIBT-BINDI** exhibits a bamboo-like morphology, with BINDI^{4-} ions and Ni^{2+} ions connected to form the bamboo trunk, and BIBT ligands and Ni^{2+} ions coordinated to form the bamboo leaves.

2. Structural commentary

Ni-BIBT-BINDI crystallizes in the triclinic crystal system, space group $P\overline{1}$. The asymmetric unit contains one Ni^{II} ion, one BIBT ligand and half a BINDI^{4-} ion, one DMF molecule, as well as two coordinated H$_2$O molecules and half of a free H$_2$O molecule (Fig. 1). The Ni^{II} ion is surrounded by one nitrogen atom (N1) from one BIBT molecule, two oxygen atoms (O3, O4) from two different H$_2$O molecules, and three oxygen (O1, O5, O6) atoms from two different BINDI^{4-} ions (Fig. 1), resulting in a distorted octahedral coordination

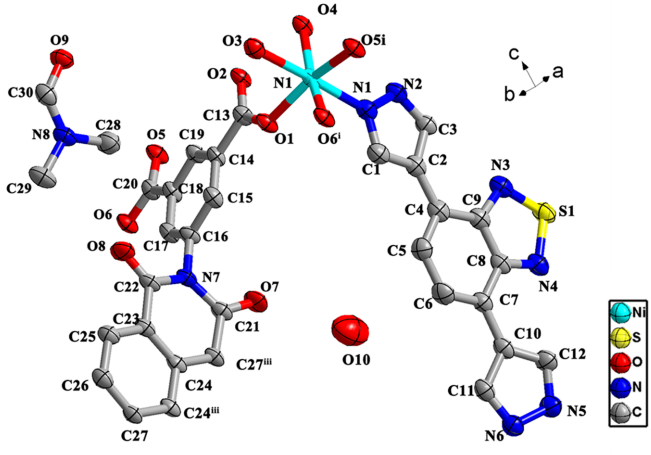


Figure 1
[The coordination environment of **Ni-BIBT-BINDI**, Symmetry codes: (i) $x, y-1, z$?(ii) $x, y+1, z$; (iii) $-x, -y+2, -z$]

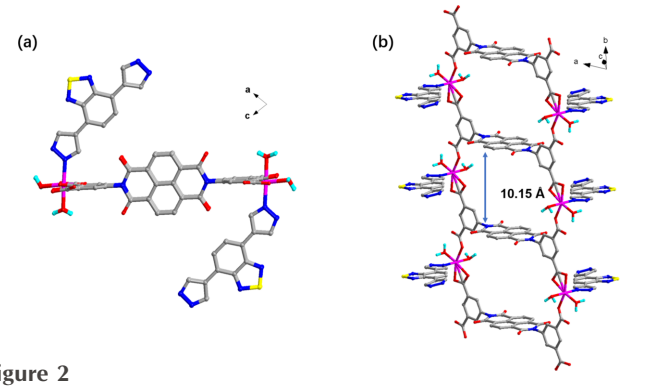


Figure 2
[(*a*)The Ni—BT-BINDI chain was observed from the *b* axis direction. (*b*) The Ni—BT-BINDI chain exhibits a structural similarity to bamboo, with nodes positioned at intervals of 10.15 Å]

geometry (Fig. 1). The Ni—O bond lengths range from 2.032 (3) to 2.122 (3) Å, while the Ni—N bond length is 2.079 (4) Å (Table 1), which is consistent with previously reported Ni-based coordination complexes (Wang *et al.*, 2020). The BINDI^{4-} ions are linked by the Ni^{2+} ions, extending along the *b*-axis direction (Fig. 2*a*), forming a structure comparable to that of bamboo, while the naphthalene diimide functional group is almost perpendicular to the *b*-axis, resembling a bamboo joint (Fig. 2*b*). The distance between adjacent naphthalene diimide functional groups is 10.15 Å (Fig. 2*b*). The N atom at the terminal end of the BIBT ligand on the bamboo coordinates with the Ni^{2+} ion and grows in a manner analogous to a bamboo leaf (Fig. 2*b*). It has been established that only one end of the N atom of the BIBT ligand is coordinated to the Ni^{2+} ion, thus resulting in the formation of a mono-periodic chain.

3. Supramolecular features

In the crystal structure of **Ni-BIBT-BINDI**, the coordination polymer chains are oriented along the *b*-axis direction. The chains are linked by face-to-face π–π stacking interactions [centroid–centroid distance = 3.515 (3) Å] between the BIBT ligand and BINDI ion, as shown in Fig. 3*a*. Within an Ni-BIBT-BINDI chain, the pore between two neighbouring ligand

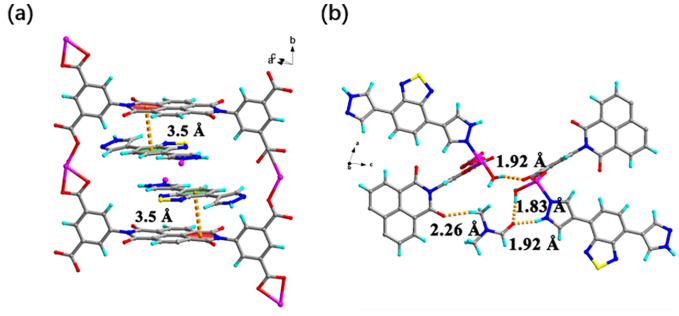


Figure 3
[(*a*) The π-π stacking interactions between the ligand BIBT and BINDI, (*b*) The H-bond interactions between a DMF molecule and two distinct Ni—BT-BINDI chains.]

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O2^{ii}	0.87	1.92	2.758 (5)	162
O3—H3B···N6^{iii}	0.87	2.18	2.986 (5)	154
O4—H4A···O2	0.87	1.86	2.640 (4)	148
O4—H4B···O9^{ii}	0.87	1.83	2.695 (5)	173
N2—H2···O9^{ii}	0.88	1.92	2.779 (5)	166
N5—H5···N6^{iv}	0.88	2.20	2.956 (6)	144
C1—H1···O10^{iii}	0.95	2.57	3.46 (3)	155
C11—H11···O1^{iii}	0.95	2.54	3.210 (6)	127
C11—H11···O6^{v}	0.95	2.49	3.279 (6)	141
C12—H12···O2^{vi}	0.95	2.46	3.168 (6)	131
C28—H28A···N5^{iii}	0.98	2.65	3.426 (8)	136
C28—H28B···O4^{ii}	0.98	2.72	3.414 (6)	128
C28—H28C···O8	0.98	2.26	3.157 (7)	151
O10—H10A···O7	0.87	2.08	2.95 (3)	180
O10—H10B···O6^{v}	0.87	2.20	3.01 (3)	155

Symmetry codes: (ii) $-x+1, -y+1, -z+2$; (iii) $-x+1, -y+1, -z+1$; (iv) $-x+2, -y+1, -z$; (v) $-x+1, -y+2, -z+1$; (vi) $-x+2, -y+1, -z+1$.

BINDIs contains two ligand BIBTs, which are from different Ni-BIBT-BINDI chains. The distance between the BIBT ligand and the neighbouring BINDI ligand is 3.5 Å, as shown in Fig. 3*b*. In addition to these π–π stacking interactions, there is also evidence of hydrogen-bonding interactions between a DMF molecule and two distinct Ni-BIBT-BINDI chains (C28—H28C···O8, 2.26 Å; O4—H4B···O9^{ii}, 1.83 Å; N2—H2···O9^{ii}, 1.92 Å; Table 2). Hydrogen bonding is also present between two different Ni-BIBT-BINDI chains (O3—H3A···O2^{ii}; Fig. 3*b*, Table 2). These weak interactions connect Ni-BIBT-BINDI chains and build the 3D framework structure of **Ni-BIBT-BINDI**.

4. Database survey

A search in CSD (version 5.46, last update November 2024; Groom *et al.*, 2016) using CONQUEST (Bruno *et al.*, 2002) for compounds based on BIBT and BINDI ligands revealed that no identical compounds have been reported. However, there are two metal–organic frameworks assembled from ligand BT [4,7-di(1*H*-benzoimidazol-1-yl)benzo[*c*][1,2,5]thiadiazole, structurally analogous to BIBT] in combination with BINDI ligands. The structural unit of the first compound includes Ni^{2+} ions, BINDI and BT ligands (BODCOQ; Xiong *et al.*, 2024), while that of the second compound includes Cu^{2+} ions, BINDI and BT ligands (TILTHU; Huang *et al.*, 2023).

5. Synthesis and crystallization

The crystal of **Ni-BIBT-BINDI** was synthesized by the solvothermal method. 2.7 mg of BIBT, 6 mg of BINDI, 58 mg of $Ni(NO_3)_2{\cdot}6H_2O$, 3.5 mL of DMF and 2.5 mL of deionized water were added in a 10 mL glass tube. After sonication for about 10 min, the glass tube was sealed and heated at 368 K for 24 h. After cooling to room temperature, green crystals were collected.

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Ni_2(C_{30}H_{10}N_2O_{12})(C_{12}H_8N_6S)_2(H_2O)_4]{\cdot}2(C_3H_7NO){\cdot}H_2O$
M_r	1480.70
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	193
a, b, c (Å)	9.5384 (4), 10.1543 (4), 16.2521 (8)
α, β, γ (°)	81.511 (3), 75.790 (3), 75.920 (3)
V (Å^3)	1473.62 (12)
Z	1
Radiation type	Cu $K\alpha$
μ (mm^{-1})	2.27
Crystal size (mm)	0.16 × 0.12 × 0.11
Data collection	
Diffractometer	Bruker PHOTON-II area detector
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.544, 0.753
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	24224, 5414, 4005
R_{int}	0.068
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.604
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.076, 0.247, 1.06
No. of reflections	5414
No. of parameters	455
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.46, −1.04

Computer programs: *APEX2* and *SAINT* (Bruker, 2016), *OLEX2.solve* (Bourhis *et al.*, 2015), *SHELXL2018/3* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. H atoms were positioned geometrically and refined using a riding model.

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Computing details

Poly[tetraaquabis[4,7-bis(1*H*-pyrazol-4-yl)benzo[*c*][1,2,5]thiadiazole][μ_4-5,5′-(1,3,6,8-tetraoxo-1,3,6,8-tetrahydrobenzo[*lmn*][3,8]phenanthroline-2,7-diyl)diisophthalato]dinickel(II)]

Crystal data

$[Ni_2(C_{30}H_{10}N_2O_{12})(C_{12}H_8N_6S)_2(H_2O)_4]\cdot 2(C_3H_7NO)\cdot H_2O$
M_r = 1480.70
Triclinic, $P\overline{1}$
a = 9.5384 (4) Å
b = 10.1543 (4) Å
c = 16.2521 (8) Å
α = 81.511 (3)°
β = 75.790 (3)°
γ = 75.920 (3)°
V = 1473.62 (12) Å^3
Z = 1
$F(000)$ = 762
D_x = 1.669 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 7699 reflections
θ = 4.5–68.1°
μ = 2.27 mm^{-1}
T = 193 K
Block, dull greenish green
0.16 × 0.12 × 0.11 mm

Data collection

Bruker PHOTON-II area detector diffractometer
Detector resolution: 7.4 pixels mm^{-1}
phi and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.544, T_{max} = 0.753
24224 measured reflections
5414 independent reflections
4005 reflections with $I > 2\sigma(I)$
R_{int} = 0.068
θ_{max} = 68.6°, θ_{min} = 2.8°
h = −11→11
k = −12→12
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.076
$wR(F^2)$ = 0.247
S = 1.06
5414 reflections
455 parameters
0 restraints
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1781P)^2 + 0.7895P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.46 e Å^{-3}
$\Delta\rho_{min}$ = −1.04 e Å^{-3}

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ni1	0.57153 (8)	0.31000 (7)	0.84217 (5)	0.0304 (3)	
S1	1.29018 (14)	0.30007 (14)	0.39030 (9)	0.0450 (4)	
O1	0.4971 (4)	0.5137 (3)	0.8127 (2)	0.0341 (7)	
O2	0.5865 (3)	0.6001 (3)	0.9027 (2)	0.0335 (7)	
O3	0.3923 (4)	0.3157 (3)	0.9478 (2)	0.0378 (8)	
H3A	0.418410	0.332432	0.992361	0.057*	
H3B	0.321320	0.385253	0.939452	0.057*	
O4	0.6859 (4)	0.3342 (3)	0.9272 (2)	0.0359 (7)	
H4A	0.680119	0.420791	0.928462	0.054*	
H4B	0.779938	0.300760	0.908602	0.054*	
O5	0.5926 (4)	1.0963 (3)	0.8525 (2)	0.0349 (7)	
O6	0.4480 (4)	1.2335 (3)	0.7751 (2)	0.0337 (7)	
O7	0.4323 (4)	0.8766 (4)	0.5411 (2)	0.0492 (9)	
O8	0.0255 (4)	0.9415 (4)	0.7567 (2)	0.0496 (10)	
N1	0.7439 (4)	0.3085 (4)	0.7351 (3)	0.0359 (9)	
N2	0.8912 (5)	0.2834 (4)	0.7296 (3)	0.0393 (9)	
H2	0.933374	0.260189	0.773567	0.047*	
N3	1.1602 (5)	0.3014 (4)	0.4758 (3)	0.0423 (10)	
N4	1.1933 (5)	0.3483 (4)	0.3182 (3)	0.0408 (10)	
N5	1.0322 (5)	0.4553 (5)	0.0894 (3)	0.0454 (10)	
H5	1.094565	0.446406	0.039685	0.055*	
N6	0.8855 (5)	0.5163 (5)	0.0989 (3)	0.0416 (10)	
N7	0.2282 (4)	0.9214 (4)	0.6484 (2)	0.0311 (8)	
C1	0.7268 (6)	0.3386 (5)	0.6562 (3)	0.0396 (11)	
H1	0.633402	0.359982	0.640809	0.048*	
C2	0.8620 (5)	0.3357 (5)	0.5972 (3)	0.0358 (10)	
C3	0.9646 (6)	0.2981 (5)	0.6490 (3)	0.0372 (10)	
H3	1.069080	0.285286	0.630045	0.045*	
C4	0.8869 (5)	0.3612 (5)	0.5052 (3)	0.0363 (10)	
C5	0.7710 (6)	0.4059 (5)	0.4641 (3)	0.0410 (11)	
H5A	0.672881	0.419811	0.497727	0.049*	
C6	0.7905 (6)	0.4322 (6)	0.3745 (3)	0.0434 (12)	
H6	0.704894	0.463219	0.351132	0.052*	
C7	0.9277 (5)	0.4149 (5)	0.3194 (3)	0.0346 (10)	
C8	1.0512 (6)	0.3685 (5)	0.3594 (3)	0.0356 (10)	
C9	1.0309 (6)	0.3426 (5)	0.4498 (3)	0.0361 (10)	
C10	0.9456 (5)	0.4426 (5)	0.2269 (3)	0.0368 (10)	
C11	0.8347 (6)	0.5097 (5)	0.1819 (3)	0.0393 (11)	
H11	0.734986	0.545945	0.208585	0.047*	

C12	1.0702 (6)	0.4106 (6)	0.1641 (3)	0.0434 (12)	
H12	1.166018	0.364911	0.172088	0.052*	
C13	0.5182 (5)	0.6112 (4)	0.8442 (3)	0.0292 (9)	
C14	0.4599 (5)	0.7526 (4)	0.8049 (3)	0.0293 (9)	
C15	0.3696 (5)	0.7719 (4)	0.7469 (3)	0.0313 (9)	
H15	0.340778	0.696185	0.732957	0.038*	
C16	0.3218 (5)	0.9009 (5)	0.7094 (3)	0.0320 (10)	
C17	0.3612 (5)	1.0118 (4)	0.7286 (3)	0.0323 (10)	
H17	0.326368	1.100122	0.702890	0.039*	
C18	0.4529 (5)	0.9944 (4)	0.7863 (3)	0.0295 (9)	
C19	0.5010 (5)	0.8645 (4)	0.8249 (3)	0.0306 (9)	
H19	0.561972	0.852347	0.864919	0.037*	
C20	0.5006 (5)	1.1154 (4)	0.8060 (3)	0.0309 (9)	
C21	0.2983 (5)	0.9141 (5)	0.5622 (3)	0.0344 (10)	
C22	0.0752 (5)	0.9435 (5)	0.6811 (3)	0.0323 (10)	
C23	−0.0198 (5)	0.9732 (4)	0.6173 (3)	0.0314 (10)	
C24	0.0452 (5)	0.9811 (4)	0.5302 (3)	0.0298 (9)	
C25	−0.1718 (5)	0.9988 (5)	0.6451 (3)	0.0358 (10)	
H25	−0.214907	0.991401	0.704439	0.043*	
C26	−0.2624 (6)	1.0358 (5)	0.5860 (3)	0.0381 (11)	
H26	−0.367033	1.053781	0.605420	0.046*	
C27	−0.2012 (5)	1.0462 (4)	0.5001 (3)	0.0309 (9)	
O9	0.0216 (4)	0.7746 (4)	1.1156 (2)	0.0448 (9)	
N8	−0.0606 (5)	0.8531 (5)	0.9943 (3)	0.0427 (10)	
C28	0.0864 (7)	0.8243 (7)	0.9386 (4)	0.0523 (14)	
H28A	0.112379	0.728549	0.926460	0.078*	
H28B	0.159091	0.841639	0.966780	0.078*	
H28C	0.086624	0.883241	0.885104	0.078*	
C29	−0.1853 (7)	0.9179 (6)	0.9545 (4)	0.0526 (14)	
H29A	−0.168246	1.004746	0.923080	0.079*	
H29B	−0.276681	0.934675	0.998658	0.079*	
H29C	−0.194565	0.857833	0.915068	0.079*	
C30	−0.0785 (6)	0.8241 (5)	1.0773 (3)	0.0415 (11)	
H30	−0.176878	0.842806	1.110522	0.050*	
O10	0.584 (3)	0.692 (2)	0.4066 (17)	0.217 (12)	0.5
H10A	0.539592	0.746254	0.446417	0.326*	0.5
H10B	0.557502	0.736204	0.360787	0.326*	0.5

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0285 (5)	0.0232 (4)	0.0429 (5)	−0.0058 (3)	−0.0149 (3)	−0.0012 (3)
S1	0.0326 (7)	0.0497 (8)	0.0521 (8)	−0.0048 (5)	−0.0156 (5)	0.0007 (6)
O1	0.0359 (18)	0.0220 (15)	0.0500 (19)	−0.0064 (13)	−0.0215 (14)	−0.0001 (13)
O2	0.0311 (17)	0.0249 (15)	0.0477 (18)	−0.0025 (13)	−0.0198 (14)	−0.0004 (13)
O3	0.0331 (17)	0.0382 (18)	0.0457 (19)	−0.0060 (14)	−0.0160 (14)	−0.0057 (14)
O4	0.0321 (17)	0.0288 (16)	0.0497 (19)	−0.0045 (13)	−0.0172 (14)	−0.0027 (13)
O5	0.0336 (17)	0.0254 (16)	0.0515 (19)	−0.0069 (13)	−0.0217 (14)	−0.0001 (13)

O6	0.0335 (17)	0.0216 (15)	0.0504 (19)	−0.0044 (12)	−0.0202 (14)	−0.0015 (13)
O7	0.0244 (18)	0.069 (3)	0.054 (2)	−0.0009 (17)	−0.0190 (15)	−0.0023 (18)
O8	0.0354 (19)	0.071 (3)	0.042 (2)	−0.0040 (18)	−0.0182 (15)	0.0006 (17)
N1	0.032 (2)	0.033 (2)	0.045 (2)	−0.0080 (16)	−0.0119 (17)	−0.0034 (16)
N2	0.037 (2)	0.036 (2)	0.047 (2)	−0.0058 (18)	−0.0170 (18)	−0.0021 (17)
N3	0.042 (2)	0.036 (2)	0.052 (2)	−0.0081 (18)	−0.0181 (19)	0.0003 (18)
N4	0.032 (2)	0.038 (2)	0.054 (3)	−0.0078 (17)	−0.0136 (18)	−0.0016 (18)
N5	0.036 (2)	0.057 (3)	0.042 (2)	−0.010 (2)	−0.0089 (18)	−0.0025 (19)
N6	0.035 (2)	0.046 (2)	0.045 (2)	−0.0084 (19)	−0.0124 (18)	−0.0032 (18)
N7	0.0269 (19)	0.0271 (18)	0.043 (2)	−0.0060 (15)	−0.0174 (15)	0.0019 (15)
C1	0.040 (3)	0.034 (2)	0.048 (3)	−0.007 (2)	−0.017 (2)	−0.003 (2)
C2	0.035 (3)	0.028 (2)	0.047 (3)	−0.0097 (19)	−0.014 (2)	−0.0032 (19)
C3	0.035 (3)	0.034 (2)	0.045 (3)	−0.009 (2)	−0.014 (2)	−0.0008 (19)
C4	0.035 (3)	0.030 (2)	0.049 (3)	−0.0120 (19)	−0.013 (2)	−0.0020 (19)
C5	0.031 (3)	0.047 (3)	0.047 (3)	−0.011 (2)	−0.008 (2)	−0.004 (2)
C6	0.033 (3)	0.049 (3)	0.053 (3)	−0.008 (2)	−0.018 (2)	−0.006 (2)
C7	0.030 (2)	0.031 (2)	0.045 (3)	−0.0070 (19)	−0.0131 (19)	−0.0036 (19)
C8	0.034 (2)	0.028 (2)	0.046 (3)	−0.0090 (19)	−0.012 (2)	−0.0013 (19)
C9	0.037 (3)	0.028 (2)	0.048 (3)	−0.0105 (19)	−0.015 (2)	−0.0026 (19)
C10	0.030 (2)	0.033 (2)	0.049 (3)	−0.0072 (19)	−0.014 (2)	−0.002 (2)
C11	0.032 (2)	0.037 (3)	0.051 (3)	−0.005 (2)	−0.014 (2)	−0.005 (2)
C12	0.033 (3)	0.052 (3)	0.047 (3)	−0.008 (2)	−0.014 (2)	−0.003 (2)
C13	0.026 (2)	0.024 (2)	0.041 (2)	−0.0089 (17)	−0.0120 (17)	0.0002 (17)
C14	0.023 (2)	0.024 (2)	0.041 (2)	−0.0011 (17)	−0.0110 (17)	−0.0022 (17)
C15	0.026 (2)	0.025 (2)	0.046 (3)	−0.0068 (17)	−0.0114 (18)	−0.0031 (18)
C16	0.029 (2)	0.031 (2)	0.040 (2)	−0.0063 (18)	−0.0171 (18)	−0.0003 (18)
C17	0.028 (2)	0.023 (2)	0.044 (3)	−0.0019 (17)	−0.0125 (18)	0.0003 (17)
C18	0.022 (2)	0.023 (2)	0.046 (2)	−0.0056 (16)	−0.0113 (17)	−0.0028 (17)
C19	0.026 (2)	0.029 (2)	0.039 (2)	−0.0058 (17)	−0.0133 (18)	−0.0024 (18)
C20	0.026 (2)	0.026 (2)	0.041 (2)	−0.0044 (17)	−0.0091 (18)	−0.0024 (17)
C21	0.032 (2)	0.030 (2)	0.046 (3)	−0.0068 (19)	−0.0196 (19)	−0.0001 (18)
C22	0.029 (2)	0.029 (2)	0.043 (3)	−0.0054 (18)	−0.0180 (19)	0.0018 (18)
C23	0.028 (2)	0.025 (2)	0.044 (2)	−0.0060 (18)	−0.0168 (19)	−0.0001 (17)
C24	0.028 (2)	0.021 (2)	0.044 (2)	−0.0057 (17)	−0.0159 (19)	0.0002 (17)
C25	0.031 (2)	0.034 (2)	0.043 (3)	−0.0076 (19)	−0.0123 (19)	0.0021 (19)
C26	0.029 (2)	0.038 (3)	0.047 (3)	−0.005 (2)	−0.012 (2)	−0.001 (2)
C27	0.025 (2)	0.028 (2)	0.043 (2)	−0.0047 (17)	−0.0150 (18)	−0.0008 (17)
O9	0.0387 (19)	0.050 (2)	0.047 (2)	−0.0044 (16)	−0.0193 (16)	0.0019 (15)
N8	0.038 (2)	0.044 (2)	0.048 (2)	−0.0057 (19)	−0.0194 (19)	0.0007 (18)
C28	0.043 (3)	0.062 (4)	0.049 (3)	−0.007 (3)	−0.014 (2)	0.001 (3)
C29	0.046 (3)	0.050 (3)	0.065 (4)	−0.005 (3)	−0.029 (3)	0.006 (3)
C30	0.032 (3)	0.038 (3)	0.056 (3)	−0.008 (2)	−0.013 (2)	−0.001 (2)
O10	0.29 (3)	0.16 (2)	0.22 (2)	−0.02 (2)	−0.11 (2)	−0.028 (17)

Geometric parameters (Å, º)

Ni1—O1	2.042 (3)	C6—C7	1.380 (7)
Ni1—O3	2.101 (3)	C7—C8	1.432 (7)

Ni1—O4	2.032 (3)	C7—C10	1.462 (7)
Ni1—O5^{i}	2.115 (3)	C8—C9	1.428 (7)
Ni1—O6^{i}	2.122 (3)	C10—C11	1.415 (7)
Ni1—N1	2.079 (4)	C10—C12	1.370 (7)
Ni1—C20^{i}	2.428 (5)	C11—H11	0.9500
S1—N3	1.618 (5)	C12—H12	0.9500
S1—N4	1.615 (4)	C13—C14	1.515 (6)
O1—C13	1.257 (5)	C14—C15	1.390 (6)
O2—C13	1.257 (5)	C14—C19	1.393 (6)
O3—H3A	0.8717	C15—H15	0.9500
O3—H3B	0.8720	C15—C16	1.380 (6)
O4—H4A	0.8703	C16—C17	1.368 (7)
O4—H4B	0.8715	C17—H17	0.9500
O5—C20	1.256 (6)	C17—C18	1.398 (6)
O6—C20	1.263 (5)	C18—C19	1.395 (6)
O7—C21	1.217 (6)	C18—C20	1.510 (6)
O8—C22	1.202 (6)	C19—H19	0.9500
N1—N2	1.348 (6)	C21—C27^{ii}	1.484 (6)
N1—C1	1.314 (6)	C22—C23	1.491 (6)
N2—H2	0.8800	C23—C24	1.398 (7)
N2—C3	1.330 (7)	C23—C25	1.380 (7)
N3—C9	1.351 (6)	C24—C24^{ii}	1.413 (8)
N4—C8	1.336 (6)	C24—C27^{ii}	1.419 (6)
N5—H5	0.8800	C25—H25	0.9500
N5—N6	1.366 (6)	C25—C26	1.397 (7)
N5—C12	1.335 (7)	C26—H26	0.9500
N6—C11	1.314 (7)	C26—C27	1.375 (7)
N7—C16	1.452 (5)	O9—C30	1.232 (6)
N7—C21	1.401 (6)	N8—C28	1.459 (7)
N7—C22	1.399 (6)	N8—C29	1.462 (6)
C1—H1	0.9500	N8—C30	1.315 (7)
C1—C2	1.401 (7)	C28—H28A	0.9800
C2—C3	1.393 (7)	C28—H28B	0.9800
C2—C4	1.450 (7)	C28—H28C	0.9800
C3—H3	0.9500	C29—H29A	0.9800
C4—C5	1.380 (7)	C29—H29B	0.9800
C4—C9	1.431 (7)	C29—H29C	0.9800
C5—H5A	0.9500	C30—H30	0.9500
C5—C6	1.415 (7)	O10—H10A	0.8701
C6—H6	0.9500	O10—H10B	0.8699

O1—Ni1—O3	89.17 (14)	C12—C10—C11	103.9 (4)
O1—Ni1—O5^{i}	160.93 (13)	N6—C11—C10	112.2 (5)
O1—Ni1—O6^{i}	98.70 (12)	N6—C11—H11	123.9
O1—Ni1—N1	89.40 (15)	C10—C11—H11	123.9
O1—Ni1—C20^{i}	129.91 (14)	N5—C12—C10	107.5 (5)
O3—Ni1—O5^{i}	87.54 (13)	N5—C12—H12	126.3
O3—Ni1—O6^{i}	87.96 (13)	C10—C12—H12	126.3

O3—Ni1—C20^{i}	86.63 (14)	O1—C13—O2	125.5 (4)
O4—Ni1—O1	95.34 (13)	O1—C13—C14	116.0 (4)
O4—Ni1—O3	84.78 (14)	O2—C13—C14	118.5 (4)
O4—Ni1—O5^{i}	103.05 (13)	C15—C14—C13	120.9 (4)
O4—Ni1—O6^{i}	164.09 (13)	C15—C14—C19	119.4 (4)
O4—Ni1—N1	96.72 (15)	C19—C14—C13	119.7 (4)
O4—Ni1—C20^{i}	133.75 (14)	C14—C15—H15	120.0
O5^{i}—Ni1—O6^{i}	62.43 (12)	C16—C15—C14	120.1 (4)
O5^{i}—Ni1—C20^{i}	31.13 (13)	C16—C15—H15	120.0
O6^{i}—Ni1—C20^{i}	31.31 (14)	C15—C16—N7	120.3 (4)
N1—Ni1—O3	178.02 (14)	C17—C16—N7	118.6 (4)
N1—Ni1—O5^{i}	93.37 (15)	C17—C16—C15	121.1 (4)
N1—Ni1—O6^{i}	90.90 (15)	C16—C17—H17	120.2
N1—Ni1—C20^{i}	93.24 (16)	C16—C17—C18	119.7 (4)
N4—S1—N3	100.7 (2)	C18—C17—H17	120.2
C13—O1—Ni1	127.5 (3)	C17—C18—C20	120.1 (4)
Ni1—O3—H3A	109.5	C19—C18—C17	119.6 (4)
Ni1—O3—H3B	109.5	C19—C18—C20	120.3 (4)
H3A—O3—H3B	104.4	C14—C19—C18	120.1 (4)
Ni1—O4—H4A	109.2	C14—C19—H19	119.9
Ni1—O4—H4B	109.3	C18—C19—H19	119.9
H4A—O4—H4B	104.5	O5—C20—Ni1^{iii}	60.6 (2)
C20—O5—Ni1^{iii}	88.3 (3)	O5—C20—O6	121.4 (4)
C20—O6—Ni1^{iii}	87.8 (3)	O5—C20—C18	119.1 (4)
N2—N1—Ni1	129.7 (3)	O6—C20—Ni1^{iii}	60.9 (2)
C1—N1—Ni1	124.8 (4)	O6—C20—C18	119.5 (4)
C1—N1—N2	105.4 (4)	C18—C20—Ni1^{iii}	178.1 (3)
N1—N2—H2	124.3	O7—C21—N7	120.4 (4)
C3—N2—N1	111.3 (4)	O7—C21—C27^{ii}	123.0 (5)
C3—N2—H2	124.3	N7—C21—C27^{ii}	116.6 (4)
C9—N3—S1	106.3 (4)	O8—C22—N7	120.7 (4)
C8—N4—S1	106.5 (4)	O8—C22—C23	123.0 (4)
N6—N5—H5	123.8	N7—C22—C23	116.3 (4)
C12—N5—H5	123.8	C24—C23—C22	119.9 (4)
C12—N5—N6	112.4 (4)	C25—C23—C22	119.3 (4)
C11—N6—N5	104.0 (4)	C25—C23—C24	120.7 (4)
C21—N7—C16	117.5 (4)	C23—C24—C24^{ii}	119.9 (5)
C22—N7—C16	117.0 (4)	C23—C24—C27^{ii}	121.8 (4)
C22—N7—C21	125.5 (4)	C24^{ii}—C24—C27^{ii}	118.3 (5)
N1—C1—H1	123.8	C23—C25—H25	120.0
N1—C1—C2	112.4 (5)	C23—C25—C26	120.0 (5)
C2—C1—H1	123.8	C26—C25—H25	120.0
C1—C2—C4	128.0 (4)	C25—C26—H26	119.8
C3—C2—C1	102.7 (4)	C27—C26—C25	120.5 (5)
C3—C2—C4	129.3 (5)	C27—C26—H26	119.8
N2—C3—C2	108.2 (5)	C24^{ii}—C27—C21^{ii}	119.3 (4)
N2—C3—H3	125.9	C26—C27—C21^{ii}	120.1 (4)
C2—C3—H3	125.9	C26—C27—C24^{ii}	120.6 (4)

C5—C4—C2	121.7 (5)	C28—N8—C29	117.5 (5)
C5—C4—C9	114.7 (5)	C30—N8—C28	120.7 (4)
C9—C4—C2	123.6 (4)	C30—N8—C29	121.8 (5)
C4—C5—H5A	118.2	N8—C28—H28A	109.5
C4—C5—C6	123.5 (5)	N8—C28—H28B	109.5
C6—C5—H5A	118.2	N8—C28—H28C	109.5
C5—C6—H6	118.3	H28A—C28—H28B	109.5
C7—C6—C5	123.3 (5)	H28A—C28—H28C	109.5
C7—C6—H6	118.3	H28B—C28—H28C	109.5
C6—C7—C8	115.0 (4)	N8—C29—H29A	109.5
C6—C7—C10	122.5 (4)	N8—C29—H29B	109.5
C8—C7—C10	122.4 (4)	N8—C29—H29C	109.5
N4—C8—C7	124.9 (5)	H29A—C29—H29B	109.5
N4—C8—C9	113.7 (4)	H29A—C29—H29C	109.5
C9—C8—C7	121.4 (4)	H29B—C29—H29C	109.5
N3—C9—C4	125.1 (5)	O9—C30—N8	125.4 (5)
N3—C9—C8	112.8 (4)	O9—C30—H30	117.3
C8—C9—C4	122.1 (4)	N8—C30—H30	117.3
C11—C10—C7	127.0 (5)	H10A—O10—H10B	104.5
C12—C10—C7	129.1 (4)		

Ni1—O1—C13—O2	−2.5 (7)	C7—C8—C9—N3	−179.1 (4)
Ni1—O1—C13—C14	175.2 (3)	C7—C8—C9—C4	0.1 (7)
Ni1^{iii}—O5—C20—O6	2.5 (4)	C7—C10—C11—N6	−178.7 (5)
Ni1^{iii}—O5—C20—C18	−177.8 (4)	C7—C10—C12—N5	179.4 (5)
Ni1^{iii}—O6—C20—O5	−2.5 (4)	C8—C7—C10—C11	−168.5 (5)
Ni1^{iii}—O6—C20—C18	177.8 (4)	C8—C7—C10—C12	11.8 (8)
Ni1—N1—N2—C3	−177.3 (3)	C9—C4—C5—C6	−0.1 (7)
Ni1—N1—C1—C2	177.0 (3)	C10—C7—C8—N4	1.4 (8)
S1—N3—C9—C4	−178.5 (4)	C10—C7—C8—C9	179.8 (4)
S1—N3—C9—C8	0.7 (5)	C11—C10—C12—N5	−0.4 (6)
S1—N4—C8—C7	178.6 (4)	C12—N5—N6—C11	1.0 (6)
S1—N4—C8—C9	0.1 (5)	C12—C10—C11—N6	1.1 (6)
O1—C13—C14—C15	9.4 (6)	C13—C14—C15—C16	−177.7 (4)
O1—C13—C14—C19	−168.5 (4)	C13—C14—C19—C18	177.3 (4)
O2—C13—C14—C15	−172.8 (4)	C14—C15—C16—N7	179.7 (4)
O2—C13—C14—C19	9.4 (7)	C14—C15—C16—C17	−0.3 (7)
O8—C22—C23—C24	176.5 (5)	C15—C14—C19—C18	−0.6 (7)
O8—C22—C23—C25	−0.5 (7)	C15—C16—C17—C18	0.8 (7)
N1—N2—C3—C2	0.2 (5)	C16—N7—C21—O7	8.2 (7)
N1—C1—C2—C3	0.9 (6)	C16—N7—C21—C27^{ii}	−171.9 (4)
N1—C1—C2—C4	179.0 (4)	C16—N7—C22—O8	−1.9 (6)
N2—N1—C1—C2	−0.8 (5)	C16—N7—C22—C23	176.2 (4)
N3—S1—N4—C8	0.2 (4)	C16—C17—C18—C19	−1.2 (7)
N4—S1—N3—C9	−0.5 (4)	C16—C17—C18—C20	178.2 (4)
N4—C8—C9—N3	−0.6 (6)	C17—C18—C19—C14	1.1 (7)
N4—C8—C9—C4	178.7 (4)	C17—C18—C20—O5	−174.2 (4)
N5—N6—C11—C10	−1.2 (6)	C17—C18—C20—O6	5.5 (7)

N6—N5—C12—C10	−0.3 (6)	C19—C14—C15—C16	0.2 (7)
N7—C16—C17—C18	−179.2 (4)	C19—C18—C20—O5	5.2 (7)
N7—C22—C23—C24	−1.6 (6)	C19—C18—C20—O6	−175.1 (4)
N7—C22—C23—C25	−178.6 (4)	C20—C18—C19—C14	−178.3 (4)
C1—N1—N2—C3	0.3 (5)	C21—N7—C16—C15	−90.6 (5)
C1—C2—C3—N2	−0.6 (5)	C21—N7—C16—C17	89.4 (5)
C1—C2—C4—C5	6.4 (8)	C21—N7—C22—O8	176.4 (4)
C1—C2—C4—C9	−173.6 (5)	C21—N7—C22—C23	−5.5 (6)
C2—C4—C5—C6	179.9 (5)	C22—N7—C16—C15	87.8 (5)
C2—C4—C9—N3	−1.0 (8)	C22—N7—C16—C17	−92.2 (5)
C2—C4—C9—C8	179.9 (4)	C22—N7—C21—O7	−170.1 (5)
C3—C2—C4—C5	−176.0 (5)	C22—N7—C21—C27^{ii}	9.8 (6)
C3—C2—C4—C9	4.0 (8)	C22—C23—C24—C24^{ii}	−175.5 (5)
C4—C2—C3—N2	−178.7 (5)	C22—C23—C24—C27^{ii}	3.7 (6)
C4—C5—C6—C7	0.3 (9)	C22—C23—C25—C26	175.8 (4)
C5—C4—C9—N3	179.1 (5)	C23—C25—C26—C27	0.3 (7)
C5—C4—C9—C8	−0.1 (7)	C24—C23—C25—C26	−1.3 (7)
C5—C6—C7—C8	−0.3 (8)	C25—C23—C24—C24^{ii}	1.5 (8)
C5—C6—C7—C10	180.0 (5)	C25—C23—C24—C27^{ii}	−179.3 (4)
C6—C7—C8—N4	−178.3 (5)	C25—C26—C27—C21^{ii}	−179.8 (5)
C6—C7—C8—C9	0.1 (7)	C25—C26—C27—C24^{ii}	0.4 (7)
C6—C7—C10—C11	11.2 (8)	C28—N8—C30—O9	1.6 (9)
C6—C7—C10—C12	−168.5 (5)	C29—N8—C30—O9	−177.0 (5)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*A*···O2^{iv}	0.87	1.92	2.758 (5)	162
O3—H3*B*···N6^{v}	0.87	2.18	2.986 (5)	154
O4—H4*A*···O2	0.87	1.86	2.640 (4)	148
O4—H4*B*···O9^{iv}	0.87	1.83	2.695 (5)	173
N2—H2···O9^{iv}	0.88	1.92	2.779 (5)	166
N5—H5···N6^{vi}	0.88	2.20	2.956 (6)	144
C1—H1···O10^{v}	0.95	2.57	3.46 (3)	155
C11—H11···O1^{v}	0.95	2.54	3.210 (6)	127
C11—H11···O6^{vii}	0.95	2.49	3.279 (6)	141
C12—H12···O2^{viii}	0.95	2.46	3.168 (6)	131
C28—H28*A*···N5^{v}	0.98	2.65	3.426 (8)	136
C28—H28*B*···O4^{iv}	0.98	2.72	3.414 (6)	128
C28—H28*C*···O8	0.98	2.26	3.157 (7)	151
O10—H10*A*···O7	0.87	2.08	2.95 (3)	180
O10—H10*B*···O6^{vii}	0.87	2.20	3.01 (3)	155

Symmetry codes: (iv) −*x*+1, −*y*+1, −*z*+2; (v) −*x*+1, −*y*+1, −*z*+1; (vi) −*x*+2, −*y*+1, −*z*; (vii) −*x*+1, −*y*+2, −*z*+1; (viii) −*x*+2, −*y*+1, −*z*+1.