Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS
ISSN 2056-9890

A new one-dimensional Ni^{II} coordination polymer with a two-dimensional supramolecular architecture

Kai-Long Zhong*

Department of Applied Chemistry, Nanjing Polytechnic Institute, Nanjing 210048, People's Republic of China. *Correspondence e-mail: zklong76@163.com

Received 18 December 2016
Accepted 10 January 2017

Edited by M. Zeller, Purdue University, USA

Keywords: crystal structure; coordination polymer; nickel complex; one-dimensional coordination polymer.

CCDC reference: 1470095

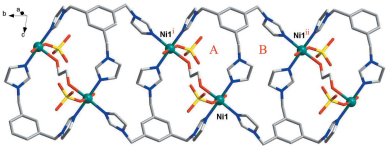
Supporting information: this article has supporting information at journals.iucr.org/e

A new one-dimensional Ni^{II} coordination polymer of 1,3,5-tris(imidazol-1-ylmethyl)benzene, namely *catena*-poly[[aqua(sulfato-κO)hemi(μ-ethane-1,2-diol-$\kappa^2 O:O'$)[μ_3-1,3,5-tris(1*H*-imidazol-1-ylmethyl)benzene-$\kappa^3 N^3,N^{3'},N^{3''}$]nickel(II)] ethane-1,2-diol monosolvate monohydrate], $\{[Ni(SO_4)(C_{18}H_{18}N_6)(C_2H_6O_2)_{0.5}(H_2O)]\cdot C_2H_6O_2\cdot H_2O\}_n$, was synthesized and characterized by elemental analysis, IR spectroscopy and single-crystal X-ray diffraction. The Ni^{II} cation is coordinated by three N atoms of three different 1,3,5-tris(imidazol-1-ylmethyl)benzene ligands, one O atom of an ethane-1,2-diol molecule, by a sulfate anion and a water molecule, forming a distorted octahedral NiN_3O_3 coordination geometry. The tripodal 1,3,5-tris(imidazol-1-ylmethyl)benzene ligands link the Ni^{II} cations, generating metal–organic chains running along the [100] direction. Adjacent chains are further connected by O—H···O hydrogen bonds, resulting in a two-dimensional supermolecular architecture running parallel to the (001) plane. Another water molecule and a second ethane-1,2-diol molecule are non-coordinating and are linked to the coordinating sulfate ions *via* O—H···O hydrogen bonds.

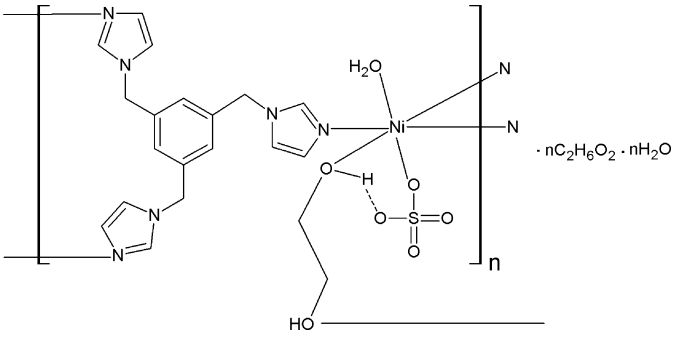
1. Chemical context

In recent years, the self-assembly of coordination polymers and crystal engineering of metal-organic coordination frameworks have attracted great interest, owing to their intriguing molecular topologies and the potential applications of these polymers as functional materials (Pan *et al.*, 2004; Jiang *et al.*, 2011; Du *et al.*, 2014). Previously reported studies a major strategy to be the use of multidentate organic ligands and metal ions to construct inorganic–organic hybrid materials through metal–ligand coordination and hydrogen-bonding interactions. Imidazole-containing multidentate ligands that contain an aromatic core have received much attention, such as 1,3-bis(1-imidazolyl)-5-(imidazol-1-ylmethyl)benzene (Fan *et al.*, 2003), 2,4,6-tris[4-(imidazol-1-ylmethyl)phenyl-1,3,5-triazine (Wan *et al.*, 2004), 1,3,5-tris(imidazol-1-ylmethyl)-2,4,6-trimethylbenzene (Zhao *et al.*, 2004), 4,4′-bis(imidazol-1-ylmethyl)biphenyl (Carlucci *et al.*, 2008), 1,3,5-tri(1-imidazolyl)benzene (Su *et al.*, 2010), 1,2,4,5-tetrakis(imidazol-1-ylmethyl)benzene (Hua *et al.*, 2010) and 1,3,5-tris(imidazol-1-ylmethyl)benzene (Xu *et al.*, 2009; Zhong, 2014).

Hydrothermal (solvothermal) synthesis is an effective method for the construction of new metal–organic coordination polymers because it can provide ideal conditions for crystal growth due to the enhanced transport ability of solvents in superheated systems. In the present work, we carried out the solvothermal reaction between $NiSO_4\cdot 6H_2O$



and imidazole-containing multidentate ligands, 1,3,5-tris-(imidazol-1-ylmethyl)benzene (timb) and successfully obtained a new Ni^{II} one-dimensional coordination polymer, $\{[Ni(SO_4)(C_{18}H_{18}N_6)(C_2H_6O_2)_{0.5}(H_2O)]\cdot C_2H_6O_2\cdot H_2O\}_n$, (I). Herein we report its crystal structure and its elemental and IR spectroscopic analysis data.



2. Structural commentary

The title complex (I) crystallizes in the triclinic space group $P\overline{1}$ and the asymmetric unit of the structure consists of one Ni^{II} ion, one sulfate anion, one timb ligand, half a coordinating ethane-1,2-diol molecule, one coordinating water molecules, one additional lattice water molecule and one non-coordinating ethane-1,2-diol solvent molecule. As shown in Fig. 1, each Ni^{II} cation exhibits an irregular octahedral NiN_3O_3 coordination geometry and is coordinated by three N atoms (N1, $N5^i$ and $N3^{ii}$) from three different tripodal timb ligands and three O atoms (O1*W*, O1 and O5) from a coordinating water molecule, a sulfate anion and a coordinating ethane-1,2-diol molecule, respectively (see Fig. 1 and Table 1 for symmetry codes). The Ni—O [2.0904 (12)–2.1458 (12) Å; Table 1] and Ni—N bond lengths [2.0597 (15)–2.0777 (15) Å] are in accord with corresponding bond lengths found in previously reported Ni^{II} coordination polymers $\{[Ni(tib)(H_2O)_2(SO_4)]\cdot EtOH\cdot H_2O\}_n$ [tib = 1,3,5-tris(imidazol-1-ylmethyl) benzene; Ni—O = 2.0911 (14)–2.1368 (12) Å and Ni—N = 2.0709 (15)–2.0728 (14) Å; Xu *et al.*, 2009] and $[Ni(timpt)_2](ClO_4)_2$ [timpt = 2,4,6-tri[4-(imidazol-1-ylmethyl)phenyl]-1,3,5-triazine; Ni—N = 2.097 (5)–2.151 (4) Å; Wan *et al.*, 2004].

Table 1
Selected geometric parameters (Å, °).

Ni1—N5^i	2.0597 (15)	Ni1—O5	2.0904 (12)
Ni1—N3^{ii}	2.0735 (15)	Ni1—O1*W*	2.1048 (12)
Ni1—N1	2.0777 (15)	Ni1—O1	2.1458 (12)
N5^i—Ni1—N3^{ii}	89.38 (6)	N1—Ni1—O1*W*	87.11 (5)
N5^i—Ni1—N1	175.70 (6)	O5—Ni1—O1*W*	89.54 (5)
N3^{ii}—Ni1—N1	92.36 (6)	N5^i—Ni1—O1	93.10 (6)
N5^i—Ni1—O5	88.70 (6)	N3^{ii}—Ni1—O1	90.67 (5)
N3^{ii}—Ni1—O5	176.18 (5)	N1—Ni1—O1	90.82 (5)
N1—Ni1—O5	89.79 (5)	O5—Ni1—O1	86.13 (5)
N5^i—Ni1—O1*W*	88.85 (6)	O1*W*—Ni1—O1	175.21 (5)
N3^{ii}—Ni1—O1*W*	93.73 (6)		

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $-x, -y, -z+1$.

Each Ni^{II} atom is coordinated to three individual timb ligands and each timb ligand in turn connects three nickel(II) atoms to generate an infinite laddered chain along the [010] direction (Fig. 2). Each timb ligand adopts *cis*, *cis*, *cis* substituent conformations and coordinates to three Ni^{II} atoms (Ni1, $Ni1^i$ and $Ni1^{ii}$), as observed in the Ni compound reported by Xu *et al.* (2009). The metal–metal distances (Ni···Ni) in the above-mentioned chain are 7.1003 (4) Å (Ni1···$Ni1^i$), 8.7577 (4) Å (Ni1···$Ni1^{ii}$) and 11.7296 (6) Å ($Ni1^i$···$Ni1^{ii}$) (see Fig. 2 for symmetry codes). The three imidazole groups within each timb ligand are inclined to the central benzene ring plane at dihedral angles of 67.60 (6)° (N2/C12/N1/C11/C10), 77.54 (6)° (N4/C15/N3/C14/C13) and 71.75 (6)° (N6/C18/N5/C17/C16), which are different from the values found in a

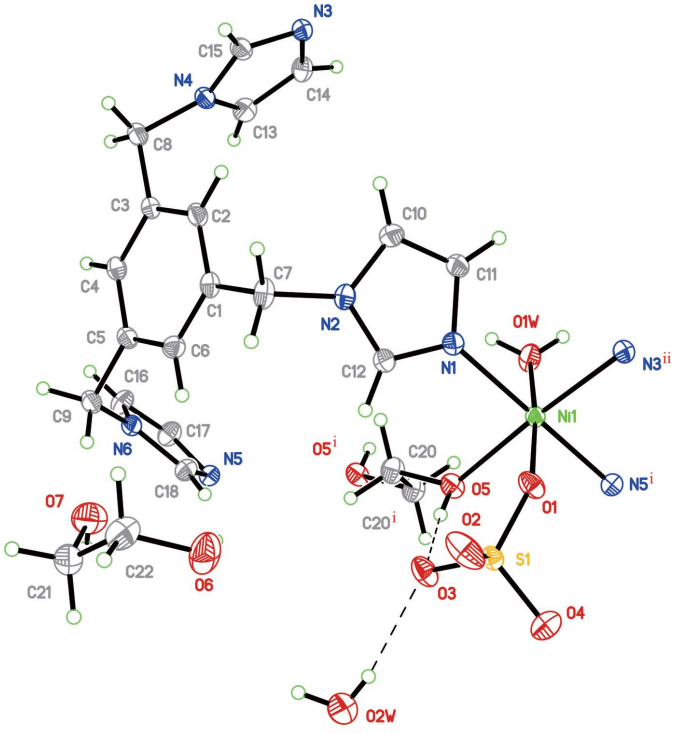


Figure 1
The asymmetric unit of (I), showing the atom-numbering scheme and with displacement ellipsoids drawn at the 25% probability level. All H atoms have been omitted for clarity. [Symmetry codes: (i) $-x, 1-y, 1-z$; (ii) $-x, -y, 1-z$.]

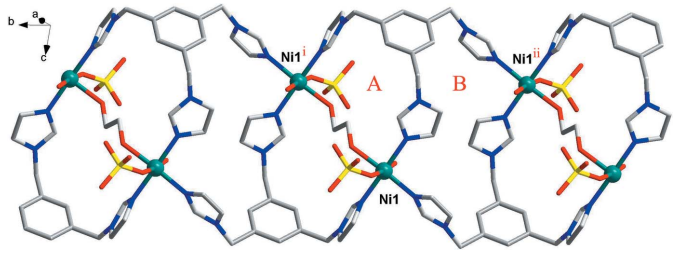


Figure 2
The one-dimensional polymeric chain along the [010] direction. The 17-membered (*A*) and 24-membered (*B*) macrocyclic rings are indicated. [Symmetry codes: (i) $-x, 1-y, 1-z$; (ii) $-x, -y, 1-z$.]

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O6^{iii}	0.82	1.93	2.743 (2)	172
O1W—H1WB···O2^{iii}	0.82	1.88	2.6995 (19)	178
O2W—H2WA···O3^{iv}	0.83	2.00	2.827 (2)	176
O2W—H2WB···O3	0.83	2.13	2.928 (2)	163
O5—H1A···O3	0.81	1.81	2.6168 (18)	169
O7—H7C···O4^{iv}	0.82	2.07	2.884 (3)	174

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

previously reported tib–cadmium compound with the same *cis*, *cis*, *cis* ligand conformations (66.15, 75.58 and 86.33°; Xu *et al.*, 2009). The three least-square planes of the terminal imidazole rings of the timb ligand are oriented with respect to each other at 56.46 (6)° (N2/C12/N1/C11/C10 and N4/C15/N3/C14/C13), 74.95 (7)° (N2/C12/N1/C11/C10 and N6/C18/N5/C17/C16) and 75.78 (7)° (N4/C15/N3/C14/C13 and N6/C18/N5/C17/C16), respectively.

It can be seen clearly that one 17-membered macrocyclic ring (*A*) and one 24-membered macrocyclic ring (*B*) exist in the above-mentioned chain (see Fig. 2), which are evidently different from that observed in the previously noted nickel compound $\{[Ni(tib)(H_2O)_2(SO_4)]\cdot EtOH\cdot(H_2O)\}_n$ in which *A* and *B* are 24-membered macrocyclic rings (Xu *et al.*, 2009).

3. Supramolecular features

In the crystal structure of the title compound, the above-mentioned neighbouring chains are further connected to each other by O_{water}—H···$O_{sulfate}$ hydrogen bonds (O1W—H1WB···O2^{iii}), giving rise to a two-dimensional supermolecular structure running parallel to (001) plane (Fig. 3). Other O—H···O hydrogen-bonding interactions involve the coordinating water and ethane-1,2-diol molecules, the lattice water molecule, the solvent ethane-1,2-diol molecule and the sulfate anion, *viz.* O1W—H1WA···O6^{iii}, O2W—H2WA···O3^{iv}, O2W—H2WB···O3, O5—H1A···O3, and O7—H7C···O4^{iv} (see Table 2 for symmetry codes).

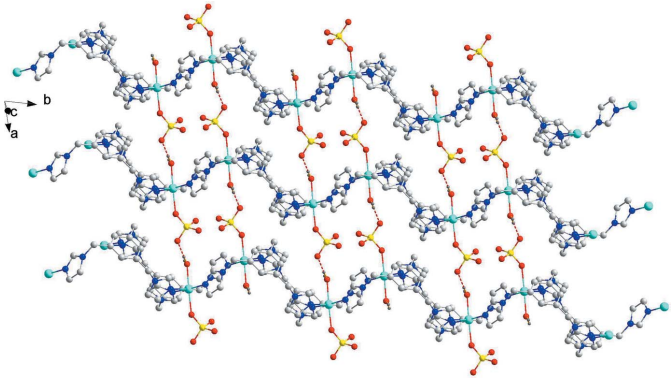


Figure 3
Two-dimensional structure of (I), running parallel to (001) plane. Hydrogen bonds are represented by dashed lines. All lattice water and solvent ethane-1,2-diol molecules have been omitted for clarity.

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Ni(SO_4)(C_{18}H_{18}N_6)(C_2H_6O_2)_{0.5}(H_2O)]\cdot C_2H_6O_2\cdot H_2O$
M_r	602.29
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	223
a, b, c (Å)	8.6910 (4), 11.7296 (5), 13.1200 (6)
α, β, γ (°)	83.922 (1), 77.829 (1), 74.064 (1)
V (Å^3)	1255.53 (10)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.92
Crystal size (mm)	0.30 × 0.25 × 0.20
Data collection	
Diffractometer	Rigaku Mercury CCD
Absorption correction	Multi-scan (*REQAB*; Jacobson, 1998)
T_{min}, T_{max}	0.770, 0.837
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10288, 5701, 5102
R_{int}	0.015
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.031, 0.077, 1.05
No. of reflections	5701
No. of parameters	346
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.64, −0.35

Computer programs: *CrystalClear* (Rigaku, 2007), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*) and *XP* in *SHELXTL* (Sheldrick, 2008).

4. Synthesis and crystallization

$NiSO_4\cdot 6H_2O$ (0.1 mmol), 1,3,5-tris(imidazol-1-ylmethyl)-benzene (0.1 mmol), water (6 ml) and ethane-1,2-diol (2 ml) were mixed and placed in a thick Pyrex tube, which was sealed and heated to 413 K for 72 h. After cooling to room temperature, blue block-shaped crystals (45% yield, based on Ni) suitable for X-ray analysis were obtained. Elemental analysis calculated for $C_{21}H_{31}N_6NiO_9S$: C 41.86, H 5.15, N 13.95%; found: C 41.90, H 5.12, N 13.86%. IR (KBr disc, ν, cm^{-1}): 3378 (*s*), 1612 (*m*), 1521 (*s*), 1445 (*m*), 1400 (*w*), 1283 (*w*), 1234 (*m*), 1119 (*s*), 1055 (*s*), 963 (*w*), 830 (*m*), 750 (*s*), 661 (*s*), 637 (*m*).

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. C-bound H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 or 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C). O-bound H atoms of the water and ethane-1,2-diol molecules were either located in difference Fourier maps or placed in calculated positions so as to form a reasonable hydrogen-bonding network, as far as possible. Initially, their positions were refined with tight restraints on the O—H and H···H distances [0.82 (1) and 1.35 (1) Å, respectively] in order to ensure a reasonable geometry. They were then constrained to ride on their parent O atoms, with U_{iso}(H) = 1.5U_{eq}(O).

Funding information

Funding for this research was provided by: Scientific Research Foundation of Nanjing Polytechnic Institute (award No. NHKY-2016–11).

References

Carlucci, L., Ciani, G., Maggini, S. & Proserpio, D. M. (2008). *CrystEngComm*, **10**, 1191–1203.
Du, M., Li, C.-P., Chen, M., Ge, Z.-W., Wang, X., Wang, L. & Liu, C.-S. (2014). *J. Am. Chem. Soc.* **136**, 10906–10909.
Fan, J., Sun, W.-Y., Okamura, T., Tang, W.-X. & Ueyama, N. (2003). *Inorg. Chem.* **42**, 3168–3175.
Hua, Q., Su, Z., Zhao, Y., Okamura, T., Xu, G.-C., Sun, W.-Y. & Ueyama, N. (2010). *Inorg. Chim. Acta*, **363**, 3550–3557.
Jacobson, R. (1998). *REQAB*. Molecular Structure Corporation, The Woodlands, Texas, USA.
Jiang, H.-L., Liu, B., Lan, Y.-Q., Kuratani, K., Akita, T., Shioyama, H., Zong, F. & Xu, Q. (2011). *J. Am. Chem. Soc.* **133**, 11854–11857.
Pan, L., Sander, M.-B., Huang, X.-Y., Li, J., Smith, M., Bittner, E., Bockrath, B. & Johnson, J.-K. (2004). *J. Am. Chem. Soc.* **126**, 1308–1309.
Rigaku (2007). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Su, Z., Wang, Z.-B. & Sun, W.-Y. (2010). *Inorg. Chem. Commun.* **13**, 1278–1280.
Wan, S.-Y., Huang, Y.-T., Li, Y.-Z. & Sun, W.-Y. (2004). *Microporous Mesoporous Mater.* **73**, 101–108.
Xu, G.-C., Ding, Y.-J., Okamura, T., Huang, Y.-Q., Bai, Z.-S., Hua, Q., Liu, G.-X., Sun, W.-Y. & Ueyama, N. (2009). *Cryst. Growth Des.* **9**, 395–403.
Zhao, W., Fan, J., Okamura, T., Sun, W.-Y. & Ueyama, N. (2004). *J. Solid State Chem.* **177**, 2358–2365.
Zhong, K.-L. (2014). *Acta Cryst.* C**70**, 189–193.

supporting information

Acta Cryst. (2017). E**73**, 192-195 [https://doi.org/10.1107/S2056989017000470]

A new one-dimensional Ni^{II} coordination polymer with a two-dimensional supramolecular architecture

Kai-Long Zhong

Computing details

Data collection: *CrystalClear* (Rigaku, 2007); cell refinement: *CrystalClear* (Rigaku, 2007); data reduction: *CrystalClear* (Rigaku, 2007); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015b); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015b).

***catena*-Poly[[aqua(sulfato-κO)hemi(μ-ethane-1,2-diol-κ^2O:O')[μ_3-1,3,5-tris(1*H*-imidazol-1-ylmethyl)benzene-$\kappa^3N^3,N^{3'},N^{3''}$]nickel(II)] ethane-1,2-diol monosolvate monohydrate]**

Crystal data

$[Ni(SO_4)(C_{18}H_{18}N_6)(C_2H_6O_2)_{0.5}(H_2O)]\cdot C_2H_6O_2\cdot H_2O$
M_r = 602.29
Triclinic, $P\overline{1}$
a = 8.6910 (4) Å
b = 11.7296 (5) Å
c = 13.1200 (6) Å
α = 83.922 (1)°
β = 77.829 (1)°
γ = 74.064 (1)°
V = 1255.53 (10) Å^3
Z = 2
$F(000)$ = 630
D_x = 1.593 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5689 reflections
θ = 3.6–27.5°
μ = 0.92 mm^{-1}
T = 223 K
Block, blue
0.30 × 0.25 × 0.20 mm

Data collection

Rigaku Mercury CCD diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 28.5714 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*REQAB*; Jacobson, 1998)
T_{min} = 0.770, T_{max} = 0.837
10288 measured reflections
5701 independent reflections
5102 reflections with $I > 2\sigma(I)$
R_{int} = 0.015
θ_{max} = 27.5°, θ_{min} = 2.5°
h = −11→3
k = −15→14
l = −17→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.077
S = 1.05
5701 reflections
346 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0339P)^2 + 0.5937P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.64$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ 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}
Ni1	0.04969 (2)	0.26468 (2)	0.69398 (2)	0.02264 (7)
S1	0.39700 (5)	0.31684 (4)	0.73486 (3)	0.02532 (10)
N1	0.17497 (17)	0.15324 (13)	0.57365 (11)	0.0264 (3)
N2	0.35427 (17)	0.07352 (13)	0.43798 (11)	0.0272 (3)
N3	−0.00592 (17)	−0.12373 (13)	0.20513 (11)	0.0275 (3)
N4	0.12631 (18)	−0.00981 (14)	0.09797 (11)	0.0288 (3)
N5	0.08774 (18)	0.61960 (13)	0.19341 (11)	0.0280 (3)
N6	0.28790 (17)	0.48786 (13)	0.10352 (11)	0.0271 (3)
O1	0.27204 (14)	0.25000 (12)	0.74691 (10)	0.0332 (3)
O1W	−0.16019 (15)	0.28607 (13)	0.63045 (10)	0.0375 (3)
H1WA	−0.1485	0.2805	0.5674	0.045*
H1WB	−0.2450	0.2694	0.6602	0.045*
O2	0.55747 (16)	0.23427 (14)	0.72399 (15)	0.0551 (5)
O2W	0.4836 (2)	0.61941 (19)	0.57640 (16)	0.0644 (5)
H2WA	0.5186	0.6125	0.5127	0.091 (12)*
H2WB	0.4695	0.5551	0.6032	0.19 (2)*
O4	0.3645 (2)	0.39103 (17)	0.82364 (12)	0.0585 (5)
O3	0.38778 (17)	0.39792 (13)	0.63970 (11)	0.0405 (3)
O5	0.10109 (15)	0.40988 (11)	0.59967 (10)	0.0309 (3)
H1A	0.1896	0.4142	0.6075	0.066 (8)*
O7	0.7848 (2)	0.36115 (16)	0.21737 (13)	0.0581 (4)
H7C	0.7487	0.4328	0.2068	0.087*
O6	0.8462 (2)	0.27266 (19)	0.42207 (12)	0.0641 (5)
H6B	0.7551	0.3036	0.4092	0.096*
C1	0.44203 (19)	0.11243 (16)	0.24838 (13)	0.0270 (4)
C2	0.3776 (2)	0.05094 (16)	0.19147 (13)	0.0281 (4)
H2A	0.3650	−0.0240	0.2159	0.034*
C3	0.3312 (2)	0.10036 (16)	0.09739 (13)	0.0267 (3)
C4	0.3538 (2)	0.21075 (16)	0.06059 (13)	0.0272 (3)
H4A	0.3251	0.2435	−0.0026	0.033*
C5	0.4194 (2)	0.27334 (15)	0.11748 (14)	0.0264 (3)
C6	0.4632 (2)	0.22389 (16)	0.21129 (14)	0.0290 (4)
H6A	0.5068	0.2653	0.2496	0.035*
C7	0.4926 (2)	0.05685 (18)	0.34988 (13)	0.0321 (4)
H7A	0.5418	−0.0274	0.3423	0.039*
H7B	0.5740	0.0920	0.3645	0.039*

C8	0.2624 (2)	0.03201 (19)	0.03467 (14)	0.0349 (4)
H8A	0.2253	0.0826	−0.0235	0.042*
H8B	0.3478	−0.0356	0.0064	0.042*
C9	0.4402 (2)	0.39447 (16)	0.07772 (15)	0.0306 (4)
H9A	0.5237	0.4113	0.1080	0.037*
H9B	0.4765	0.3949	0.0025	0.037*
C10	0.2496 (2)	0.00224 (17)	0.46746 (14)	0.0323 (4)
H10A	0.2531	−0.0665	0.4367	0.039*
C11	0.1396 (2)	0.05254 (17)	0.55086 (14)	0.0307 (4)
H11A	0.0532	0.0232	0.5872	0.037*
C12	0.3053 (2)	0.16280 (16)	0.50339 (13)	0.0270 (3)
H12A	0.3563	0.2236	0.4998	0.032*
C13	−0.0332 (2)	0.05429 (17)	0.12110 (15)	0.0337 (4)
H13A	−0.0776	0.1313	0.0968	0.040*
C14	−0.1129 (2)	−0.01670 (17)	0.18614 (14)	0.0329 (4)
H14A	−0.2239	0.0037	0.2141	0.040*
C15	0.1375 (2)	−0.11575 (16)	0.15006 (14)	0.0299 (4)
H15A	0.2336	−0.1758	0.1478	0.036*
C16	0.1711 (2)	0.52835 (18)	0.04308 (15)	0.0362 (4)
H16A	0.1747	0.5047	−0.0230	0.043*
C17	0.0496 (2)	0.60986 (18)	0.09903 (15)	0.0356 (4)
H17A	−0.0456	0.6528	0.0767	0.043*
C18	0.2324 (2)	0.54442 (16)	0.19310 (14)	0.0298 (4)
H18A	0.2886	0.5322	0.2480	0.036*
C20	0.0760 (2)	0.45061 (18)	0.49659 (15)	0.0349 (4)
H20A	0.0660	0.3861	0.4600	0.042*
H20B	0.1682	0.4783	0.4581	0.042*
C21	0.9401 (3)	0.3387 (2)	0.24521 (18)	0.0498 (5)
H21A	0.9519	0.4103	0.2700	0.060*
H21B	1.0250	0.3158	0.1844	0.060*
C22	0.9574 (3)	0.2421 (2)	0.32855 (19)	0.0533 (6)
H22A	0.9415	0.1718	0.3039	0.064*
H22B	1.0673	0.2225	0.3422	0.064*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.02106 (11)	0.02523 (12)	0.02195 (11)	−0.00719 (8)	−0.00350 (8)	−0.00055 (8)
S1	0.02180 (18)	0.0309 (2)	0.0249 (2)	−0.00984 (16)	−0.00678 (15)	0.00368 (16)
N1	0.0254 (7)	0.0282 (8)	0.0252 (7)	−0.0072 (6)	−0.0043 (6)	−0.0008 (6)
N2	0.0267 (7)	0.0305 (8)	0.0220 (7)	−0.0043 (6)	−0.0040 (5)	0.0001 (6)
N3	0.0269 (7)	0.0299 (8)	0.0263 (7)	−0.0102 (6)	−0.0022 (6)	−0.0016 (6)
N4	0.0317 (7)	0.0313 (8)	0.0263 (7)	−0.0151 (6)	−0.0040 (6)	0.0008 (6)
N5	0.0293 (7)	0.0287 (8)	0.0261 (7)	−0.0077 (6)	−0.0049 (6)	−0.0026 (6)
N6	0.0296 (7)	0.0239 (7)	0.0265 (7)	−0.0075 (6)	−0.0019 (6)	−0.0011 (6)
O1	0.0261 (6)	0.0392 (8)	0.0386 (7)	−0.0155 (5)	−0.0128 (5)	0.0111 (6)
O1W	0.0257 (6)	0.0619 (9)	0.0279 (7)	−0.0159 (6)	−0.0043 (5)	−0.0058 (6)
O2	0.0231 (6)	0.0416 (9)	0.0939 (13)	−0.0063 (6)	−0.0090 (7)	0.0162 (9)

O2W	0.0637 (11)	0.0762 (14)	0.0583 (12)	−0.0359 (10)	0.0060 (9)	−0.0144 (10)
O4	0.0787 (12)	0.0705 (12)	0.0375 (8)	−0.0353 (10)	−0.0087 (8)	−0.0141 (8)
O3	0.0393 (7)	0.0474 (9)	0.0394 (8)	−0.0212 (6)	−0.0143 (6)	0.0181 (6)
O5	0.0320 (6)	0.0338 (7)	0.0301 (6)	−0.0112 (5)	−0.0153 (5)	0.0098 (5)
O7	0.0763 (12)	0.0541 (10)	0.0512 (10)	−0.0234 (9)	−0.0231 (9)	0.0046 (8)
O6	0.0594 (10)	0.1007 (15)	0.0345 (8)	−0.0213 (10)	−0.0141 (7)	−0.0020 (9)
C1	0.0224 (7)	0.0313 (9)	0.0232 (8)	−0.0035 (7)	−0.0013 (6)	0.0014 (7)
C2	0.0307 (8)	0.0271 (9)	0.0251 (8)	−0.0096 (7)	−0.0017 (7)	0.0035 (7)
C3	0.0269 (8)	0.0295 (9)	0.0235 (8)	−0.0107 (7)	−0.0004 (6)	−0.0004 (7)
C4	0.0273 (8)	0.0291 (9)	0.0240 (8)	−0.0074 (7)	−0.0044 (6)	0.0036 (7)
C5	0.0238 (7)	0.0234 (8)	0.0297 (9)	−0.0061 (6)	−0.0010 (6)	0.0005 (7)
C6	0.0278 (8)	0.0313 (9)	0.0291 (9)	−0.0088 (7)	−0.0048 (7)	−0.0043 (7)
C7	0.0254 (8)	0.0403 (11)	0.0236 (8)	0.0001 (7)	−0.0024 (7)	0.0019 (7)
C8	0.0425 (10)	0.0416 (11)	0.0259 (9)	−0.0241 (9)	−0.0008 (8)	−0.0013 (8)
C9	0.0279 (8)	0.0256 (9)	0.0351 (10)	−0.0081 (7)	0.0020 (7)	−0.0005 (7)
C10	0.0376 (9)	0.0329 (10)	0.0296 (9)	−0.0125 (8)	−0.0077 (7)	−0.0037 (7)
C11	0.0309 (8)	0.0357 (10)	0.0290 (9)	−0.0155 (8)	−0.0047 (7)	−0.0012 (7)
C12	0.0273 (8)	0.0270 (9)	0.0264 (8)	−0.0075 (7)	−0.0049 (7)	0.0010 (7)
C13	0.0361 (9)	0.0311 (10)	0.0319 (9)	−0.0042 (8)	−0.0092 (8)	0.0007 (8)
C14	0.0273 (8)	0.0389 (11)	0.0297 (9)	−0.0056 (8)	−0.0030 (7)	−0.0019 (8)
C15	0.0279 (8)	0.0290 (9)	0.0330 (9)	−0.0106 (7)	−0.0028 (7)	−0.0006 (7)
C16	0.0407 (10)	0.0413 (11)	0.0262 (9)	−0.0067 (9)	−0.0087 (8)	−0.0063 (8)
C17	0.0344 (9)	0.0411 (11)	0.0307 (9)	−0.0032 (8)	−0.0120 (8)	−0.0047 (8)
C18	0.0325 (9)	0.0299 (9)	0.0273 (9)	−0.0069 (7)	−0.0071 (7)	−0.0030 (7)
C20	0.0366 (10)	0.0364 (10)	0.0298 (9)	−0.0055 (8)	−0.0102 (8)	0.0031 (8)
C21	0.0546 (13)	0.0468 (13)	0.0463 (13)	−0.0177 (11)	0.0023 (10)	−0.0065 (10)
C22	0.0651 (15)	0.0489 (14)	0.0455 (13)	−0.0091 (12)	−0.0142 (11)	−0.0077 (11)

Geometric parameters (Å, º)

Ni1—N5^{i}	2.0597 (15)	C1—C6	1.393 (3)
Ni1—N3^{ii}	2.0735 (15)	C1—C7	1.516 (2)
Ni1—N1	2.0777 (15)	C2—C3	1.397 (2)
Ni1—O5	2.0904 (12)	C2—H2A	0.9300
Ni1—O1W	2.1048 (12)	C3—C4	1.384 (2)
Ni1—O1	2.1458 (12)	C3—C8	1.513 (2)
S1—O2	1.4516 (14)	C4—C5	1.395 (2)
S1—O4	1.4611 (16)	C4—H4A	0.9300
S1—O1	1.4792 (12)	C5—C6	1.386 (2)
S1—O3	1.4895 (13)	C5—C9	1.506 (2)
N1—C12	1.324 (2)	C6—H6A	0.9300
N1—C11	1.375 (2)	C7—H7A	0.9700
N2—C12	1.344 (2)	C7—H7B	0.9700
N2—C10	1.370 (2)	C8—H8A	0.9700
N2—C7	1.467 (2)	C8—H8B	0.9700
N3—C15	1.325 (2)	C9—H9A	0.9700
N3—C14	1.376 (2)	C9—H9B	0.9700
N3—Ni1^{ii}	2.0736 (15)	C10—C11	1.358 (3)

N4—C15	1.343 (2)	C10—H10A	0.9300
N4—C13	1.371 (2)	C11—H11A	0.9300
N4—C8	1.465 (2)	C12—H12A	0.9300
N5—C18	1.322 (2)	C13—C14	1.348 (3)
N5—C17	1.371 (2)	C13—H13A	0.9300
N5—Ni1^{i}	2.0597 (15)	C14—H14A	0.9300
N6—C18	1.343 (2)	C15—H15A	0.9300
N6—C16	1.371 (2)	C16—C17	1.355 (3)
N6—C9	1.469 (2)	C16—H16A	0.9300
O1W—H1WA	0.8187	C17—H17A	0.9300
O1W—H1WB	0.8219	C18—H18A	0.9300
O2W—H2WA	0.8318	C20—C20^{i}	1.492 (4)
O2W—H2WB	0.8269	C20—H20A	0.9700
O5—C20	1.427 (2)	C20—H20B	0.9700
O5—H1A	0.8129	C21—C22	1.489 (3)
O7—C21	1.420 (3)	C21—H21A	0.9700
O7—H7C	0.8200	C21—H21B	0.9700
O6—C22	1.404 (3)	C22—H22A	0.9700
O6—H6B	0.8200	C22—H22B	0.9700
C1—C2	1.379 (3)		

N5^{i}—Ni1—N3^{ii}	89.38 (6)	C5—C6—H6A	119.9
N5^{i}—Ni1—N1	175.70 (6)	C1—C6—H6A	119.9
N3^{ii}—Ni1—N1	92.36 (6)	N2—C7—C1	112.19 (14)
N5^{i}—Ni1—O5	88.70 (6)	N2—C7—H7A	109.2
N3^{ii}—Ni1—O5	176.18 (5)	C1—C7—H7A	109.2
N1—Ni1—O5	89.79 (5)	N2—C7—H7B	109.2
N5^{i}—Ni1—O1W	88.85 (6)	C1—C7—H7B	109.2
N3^{ii}—Ni1—O1W	93.73 (6)	H7A—C7—H7B	107.9
N1—Ni1—O1W	87.11 (5)	N4—C8—C3	112.00 (15)
O5—Ni1—O1W	89.54 (5)	N4—C8—H8A	109.2
N5^{i}—Ni1—O1	93.10 (6)	C3—C8—H8A	109.2
N3^{ii}—Ni1—O1	90.67 (5)	N4—C8—H8B	109.2
N1—Ni1—O1	90.82 (5)	C3—C8—H8B	109.2
O5—Ni1—O1	86.13 (5)	H8A—C8—H8B	107.9
O1W—Ni1—O1	175.21 (5)	N6—C9—C5	111.96 (14)
O2—S1—O4	111.46 (11)	N6—C9—H9A	109.2
O2—S1—O1	109.44 (9)	C5—C9—H9A	109.2
O4—S1—O1	110.26 (9)	N6—C9—H9B	109.2
O2—S1—O3	109.46 (9)	C5—C9—H9B	109.2
O4—S1—O3	107.10 (10)	H9A—C9—H9B	107.9
O1—S1—O3	109.06 (7)	C11—C10—N2	105.93 (16)
C12—N1—C11	105.32 (15)	C11—C10—H10A	127.0
C12—N1—Ni1	127.89 (12)	N2—C10—H10A	127.0
C11—N1—Ni1	126.79 (12)	C10—C11—N1	109.93 (16)
C12—N2—C10	107.46 (14)	C10—C11—H11A	125.0
C12—N2—C7	126.22 (16)	N1—C11—H11A	125.0
C10—N2—C7	126.31 (16)	N1—C12—N2	111.36 (15)

C15—N3—C14	105.22 (15)	N1—C12—H12A	124.3
C15—N3—Ni1^{ii}	126.02 (12)	N2—C12—H12A	124.3
C14—N3—Ni1^{ii}	128.61 (12)	C14—C13—N4	106.18 (16)
C15—N4—C13	107.33 (15)	C14—C13—H13A	126.9
C15—N4—C8	125.92 (16)	N4—C13—H13A	126.9
C13—N4—C8	126.61 (16)	C13—C14—N3	110.02 (16)
C18—N5—C17	105.44 (15)	C13—C14—H14A	125.0
C18—N5—Ni1^{i}	128.44 (12)	N3—C14—H14A	125.0
C17—N5—Ni1^{i}	126.04 (12)	N3—C15—N4	111.25 (16)
C18—N6—C16	107.12 (15)	N3—C15—H15A	124.4
C18—N6—C9	126.52 (15)	N4—C15—H15A	124.4
C16—N6—C9	126.24 (15)	C17—C16—N6	106.14 (16)
S1—O1—Ni1	138.40 (8)	C17—C16—H16A	126.9
Ni1—O1W—H1WA	118.1	N6—C16—H16A	126.9
Ni1—O1W—H1WB	126.3	C16—C17—N5	109.86 (16)
H1WA—O1W—H1WB	109.6	C16—C17—H17A	125.1
H2WA—O2W—H2WB	108.8	N5—C17—H17A	125.1
C20—O5—Ni1	131.31 (12)	N5—C18—N6	111.43 (15)
C20—O5—H1A	110.7	N5—C18—H18A	124.3
Ni1—O5—H1A	106.8	N6—C18—H18A	124.3
C21—O7—H7C	109.5	O5—C20—C20^{i}	108.89 (19)
C22—O6—H6B	109.5	O5—C20—H20A	109.9
C2—C1—C6	119.90 (16)	C20^{i}—C20—H20A	109.9
C2—C1—C7	119.62 (16)	O5—C20—H20B	109.9
C6—C1—C7	120.47 (16)	C20^{i}—C20—H20B	109.9
C1—C2—C3	120.49 (16)	H20A—C20—H20B	108.3
C1—C2—H2A	119.8	O7—C21—C22	109.84 (19)
C3—C2—H2A	119.8	O7—C21—H21A	109.7
C4—C3—C2	119.28 (16)	C22—C21—H21A	109.7
C4—C3—C8	120.40 (16)	O7—C21—H21B	109.7
C2—C3—C8	120.29 (16)	C22—C21—H21B	109.7
C3—C4—C5	120.59 (16)	H21A—C21—H21B	108.2
C3—C4—H4A	119.7	O6—C22—C21	113.0 (2)
C5—C4—H4A	119.7	O6—C22—H22A	109.0
C6—C5—C4	119.54 (16)	C21—C22—H22A	109.0
C6—C5—C9	120.37 (16)	O6—C22—H22B	109.0
C4—C5—C9	120.09 (16)	C21—C22—H22B	109.0
C5—C6—C1	120.19 (16)	H22A—C22—H22B	107.8

O2—S1—O1—Ni1	−139.62 (13)	C7—N2—C10—C11	−178.79 (16)
O4—S1—O1—Ni1	97.44 (15)	N2—C10—C11—N1	−0.3 (2)
O3—S1—O1—Ni1	−19.90 (16)	C12—N1—C11—C10	0.3 (2)
C6—C1—C2—C3	−0.9 (3)	Ni1—N1—C11—C10	−179.26 (12)
C7—C1—C2—C3	−179.63 (15)	C11—N1—C12—N2	−0.27 (19)
C1—C2—C3—C4	1.4 (3)	Ni1—N1—C12—N2	179.31 (11)
C1—C2—C3—C8	179.31 (16)	C10—N2—C12—N1	0.12 (19)
C2—C3—C4—C5	−1.2 (3)	C7—N2—C12—N1	179.00 (15)
C8—C3—C4—C5	−179.09 (16)	C15—N4—C13—C14	−0.6 (2)

C3—C4—C5—C6	0.5 (3)	C8—N4—C13—C14	−176.31 (17)
C3—C4—C5—C9	−178.73 (15)	N4—C13—C14—N3	0.7 (2)
C4—C5—C6—C1	0.1 (3)	C15—N3—C14—C13	−0.5 (2)
C9—C5—C6—C1	179.27 (15)	Ni1^{ii}—N3—C14—C13	175.22 (13)
C2—C1—C6—C5	0.2 (3)	C14—N3—C15—N4	0.1 (2)
C7—C1—C6—C5	178.86 (15)	Ni1^{ii}—N3—C15—N4	−175.73 (11)
C12—N2—C7—C1	−92.6 (2)	C13—N4—C15—N3	0.3 (2)
C10—N2—C7—C1	86.1 (2)	C8—N4—C15—N3	176.05 (16)
C2—C1—C7—N2	−82.8 (2)	C18—N6—C16—C17	0.8 (2)
C6—C1—C7—N2	98.5 (2)	C9—N6—C16—C17	177.19 (17)
C15—N4—C8—C3	−92.2 (2)	N6—C16—C17—N5	−0.7 (2)
C13—N4—C8—C3	82.8 (2)	C18—N5—C17—C16	0.4 (2)
C4—C3—C8—N4	−129.77 (17)	Ni1^{i}—N5—C17—C16	177.31 (13)
C2—C3—C8—N4	52.4 (2)	C17—N5—C18—N6	0.1 (2)
C18—N6—C9—C5	85.2 (2)	Ni1^{i}—N5—C18—N6	−176.68 (12)
C16—N6—C9—C5	−90.5 (2)	C16—N6—C18—N5	−0.6 (2)
C6—C5—C9—N6	−97.28 (19)	C9—N6—C18—N5	−176.97 (15)
C4—C5—C9—N6	81.9 (2)	Ni1—O5—C20—C20^{i}	99.0 (2)
C12—N2—C10—C11	0.09 (19)	O7—C21—C22—O6	−64.0 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O6^{iii}	0.82	1.93	2.743 (2)	172
O1*W*—H1*WB*···O2^{iii}	0.82	1.88	2.6995 (19)	178
O2*W*—H2*WA*···O3^{iv}	0.83	2.00	2.827 (2)	176
O2*W*—H2*WB*···O3	0.83	2.13	2.928 (2)	163
O5—H1*A*···O3	0.81	1.81	2.6168 (18)	169
O7—H7*C*···O4^{iv}	0.82	2.07	2.884 (3)	174

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