IUCrData

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(μ-2,2′,2″,2‴-{[Pyrazine-2,3,5,6-tetrayltetrakis(methylene)]tetrakis(sulfanediyl)}tetraacetato)-bis[aquanickel(II)] heptahydrate

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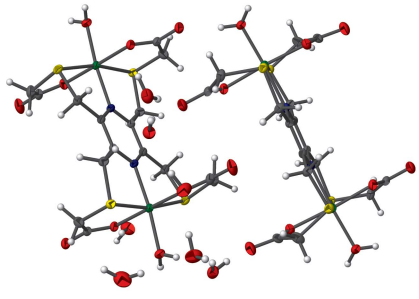
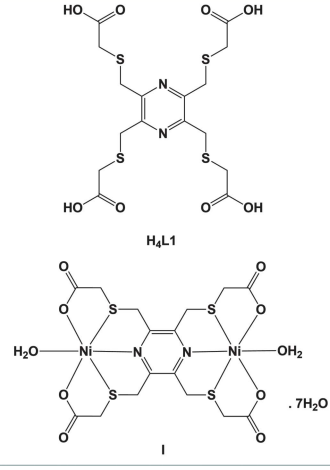
Reaction of the ligand 2,2′,2″,2‴-{[pyrazine-2,3,5,6-tetrayltetrakis(methylene)]-tetrakis(sulfanediyl)}tetraacetic acid (**H_4L1**), with $NiCl_2$ leads to the formation of a binuclear complex, (μ-2,2′,2″,2‴-{[pyrazine-2,3,5,6-tetrayltetrakis(methylene)]tetrakis(sulfanediyl)}tetraacetato-$\kappa^5O,S,N^1,S',O':\kappa^5O'',S'',N^4,S''',O'''$)bis-[aquanickel(II)] heptahydrate, $\{[Ni_2(C_{16}H_{16}N_2O_8S_4)(H_2O)_2]\cdot 7H_2O\}$ (**I**). It crystallizes with two half molecules in the asymmetric unit. The complete molecules are generated by inversion symmetry, with the center of the pyrazine rings being located at crystallographic centres of inversion. The ligand coordinates two Ni^{II} ions in a bis-pentadentate manner and the sixfold coordination sphere of each nickel(II) atom (NiS_2O_3N) is completed by a water molecule. The complex crystallized as a hepta-hydrate. The binuclear complexes are linked by O_{water}—H···$O_{carbonyl}$ hydrogen bonds, forming layers parallel to the (101) plane. This layered structure is additionally stabilized by weak C—H···O hydrogen bonds. Further O—H···O hydrogen bonds involving binuclear complexes and solvent water molecules, together with weak C—H···S hydrogen bonds, link the layers to form a supramolecular framework.

3D view



Chemical scheme



Structure description

The tetrakis-substituted pyrazine carboxylic acid ligand, 2,2′,2″,2‴-{[pyrazine-2,3,5,6-tetrayltetrakis(methylene)]tetrakis(sulfanediyl)}tetraacetic acid (**H_4L1**), is one of a series of tetrakis-substituted pyrazine ligands containing N_xS_4 and $N_2S_4O_8$ donor atoms synthesized to study their coordination behaviour with various first-row transition metals and the magnetic exchange properties of the complexes (Pacifico, 2003). Crystal struc-

Table 1
Selected geometric parameters (Å, °).

Ni1—O1*W*	2.0276 (19)	Ni2—O2*W*	2.033 (2)
Ni1—O2	2.0423 (18)	Ni2—O6	2.0440 (19)
Ni1—O4	2.0158 (19)	Ni2—O8	2.0287 (19)
Ni1—N1	2.081 (2)	Ni2—N2	2.057 (2)
Ni1—S1	2.3775 (7)	Ni2—S4	2.3674 (7)
Ni1—S2	2.3883 (8)	Ni2—S3	2.3685 (7)
N1—C1—C2—S1	−20.9 (3)	N2—C13—C14—S4	−1.3 (3)
N1—C5—C6—S2	−14.8 (3)	N2—C9—C10—S3	−7.0 (3)
S1—C3—C4—O2	−0.1 (3)	S4—C15—C16—O8	−21.9 (3)
S2—C7—C8—O4	−6.7 (4)	S3—C11—C12—O6	−27.6 (4)

tures of two polymorphs of the tetrapropionic acid analogue of the title ligand, 3,3′,3″,3‴-{[pyrazine-2,3,5,6-tetrayltetrakis(methylene)]tetrakis(sulfanediyl)}tetrapropionic acid (**H_4L2**), and of two potassium–organic frameworks have been reported (Pacifico & Stoeckli-Evans, 2021).

Reaction of **H_4L1** with $NiCl_2$ yielded the binuclear complex **I**, with the ligand coordinating two Ni^{II} ions in a bis-pentadentate manner. Complex **I** was shown to exhibit a weak antiferromagnetic coupling between the Ni centres *via* the pyrazine ring with a J value of -1.78 cm^{-1} (Pacifico, 2003).

A similar ligand, 2,2′,2″,2‴-{[pyrazine-2,3,5,6-tetrayltetrakis(methylene)] tetrakis(sulfanediyl)}tetrakis(ethan-1-amine) (**H_4L3**; CSD refcode PUXJUQ for the tetraperchlorate salt: Pacifico & Stoeckli-Evans, 2020), has also been shown to form binuclear nickel(II) complexes (TAGTUU and EHUBOB) with similar antiferromagnetic couplings (J = -1.78 cm^{-1}; Pacifico, 2003).

Reaction of **H_4L1** with nickel(II) chloride leads to the formation of the binuclear title compound **I**, which crystallizes with two half molecules in the asymmetric unit (Fig. 1 and Table 1). The complete molecules are generated by inversion symmetry, with the centres of the pyrazine rings being located at crystallographic centres of inversion.

The best fit for the molecular overlap of the two molecules is shown in Fig. 2. The r.m.s. deviation is 0.3168 Å, with a maximum deviation of 0.7435 Å (*Mercury*; Macrae *et al.*, 2020), The two molecules differ essentially in the conformations of the four chelate rings as shown by the torsion angles given in Table 1. The calculation of the mean planes of the chelate rings (*PLATON*; Spek, 2020) indicate that: ring Ni1/N1/C1/C2/S1 is twisted on the S1—C2 bond compared to ring Ni2/N2/C13//14/S4, which is flat; ring Ni1/N1/C5/C6/S2 has an envelope conformation with atom S2 as the flap, while ring Ni2/N2/C9/C10/S3 is flat; ring Ni1/S1/C3/C4/O2 is flat

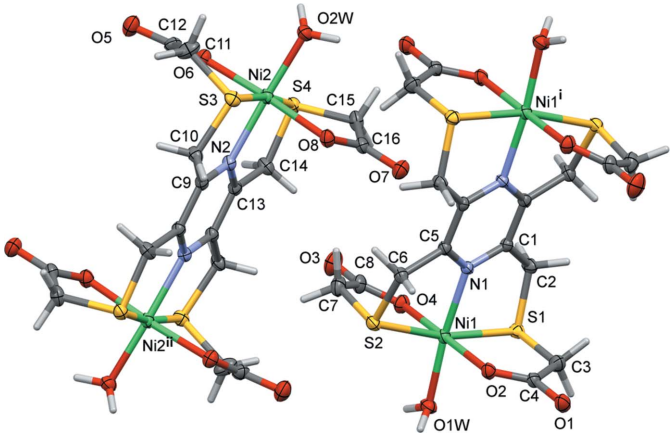


Figure 1
The molecular structure of the two independent molecules of complex **I**, with the atom labelling. Displacement ellipsoids are drawn at the 50% probability level [symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x, -y+1, -z$].

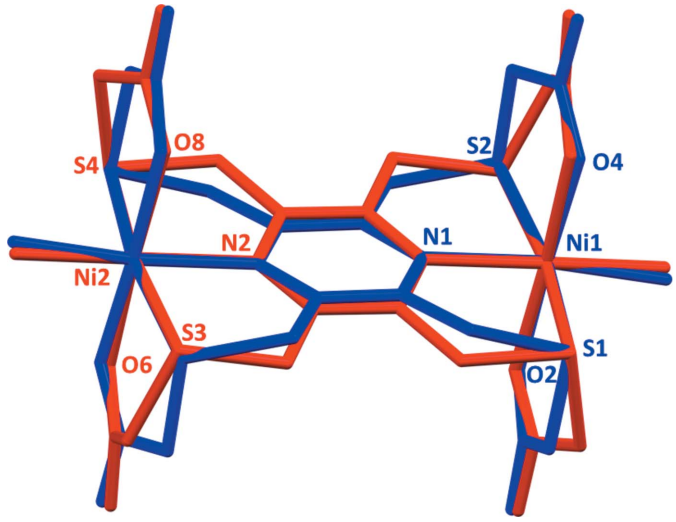


Figure 2
Molecular overlap of the two independent complex molecules of **I** (*Mercury*; Macrae *et al.*, 2020). (Molecule 1 involving atom Ni1 is in blue; Molecule 2 involving atom Ni2 is in red.)

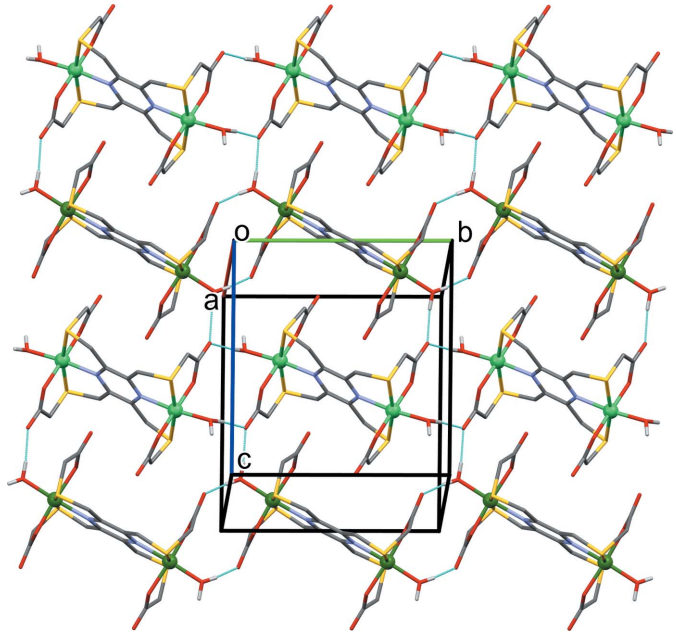


Figure 3
A view normal to the (101) plane of the crystal packing of the two independent molecules of complex **I** (atom Ni1 light-green ball; atom Ni2 dark-green ball). Hydrogen bonds (see Table 2) are shown as dashed lines. For clarity, solvent water molecules and C-bound H atoms have been omitted.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O1^{i}	0.90 (5)	1.78 (5)	2.672 (3)	174 (4)
O1W—H1WB···O5W	0.83 (5)	1.85 (5)	2.677 (3)	170 (5)
O2W—H2WA···O5^{ii}	0.88 (5)	1.80 (5)	2.673 (3)	168 (4)
O2W—H2WB···O1^{iii}	0.88 (6)	1.88 (6)	2.742 (3)	168 (6)
O3W—H3WA···O2	0.87 (4)	2.02 (4)	2.842 (3)	157 (4)
O3W—H3WB···O8W^{i}	0.98 (7)	1.87 (7)	2.785 (4)	154 (6)
O4W—H4WA···O8^{iv}	0.91 (5)	1.83 (5)	2.733 (3)	172 (4)
O4W—H4WB···O6W	0.86 (5)	1.88 (5)	2.724 (3)	166 (5)
O5W—H5WA···O7W	0.97 (7)	1.88 (7)	2.785 (3)	154 (6)
O5W—H5WB···O5^{v}	0.80 (5)	2.06 (5)	2.776 (3)	149 (5)
O6W—H6WA···O7	0.83 (5)	1.98 (5)	2.814 (3)	178 (4)
O6W—H6WB···O3W^{iii}	0.87 (6)	1.98 (6)	2.849 (4)	173 (5)
O7W—H7WA···O9W	0.86 (2)	1.85 (2)	2.698 (3)	169 (5)
O7W—H7WB···O6^{vi}	0.97 (6)	1.94 (6)	2.899 (3)	174 (5)
O8W—H8WA···O7W	0.85 (2)	2.32 (2)	3.159 (5)	173 (6)
O8W—H8WB···O3W^{iv}	0.86 (8)	2.19 (8)	3.019 (4)	164 (7)
O9W—H9WA···O4	0.82 (6)	1.93 (6)	2.752 (3)	174 (6)
O9W—H9WB···O4W	0.84 (5)	1.90 (5)	2.731 (3)	171 (5)
C2—H2A···O4W^{vii}	0.99	2.35	3.324 (3)	167
C2—H2B···O6W	0.99	2.55	3.308 (4)	133
C3—H3A···O8W^{viii}	0.99	2.55	3.488 (4)	159
C6—H6A···O4W^{ix}	0.99	2.43	3.413 (3)	173
C6—H6B···O3W	0.99	2.60	3.365 (4)	134
C6—H6B···O6W^{iii}	0.99	2.58	3.334 (3)	133
C10—H10B···O3^{v}	0.99	2.27	3.150 (4)	148
C11—H11B···O5W^{x}	0.99	2.52	3.303 (4)	136
C11—H11B···O7W^{x}	0.99	2.58	3.516 (4)	158
C14—H14A···O9W^{vi}	0.99	2.45	3.260 (4)	139
C14—H14B···O3	0.99	2.29	3.169 (4)	148
C15—H15A···S3^{iv}	0.99	2.84	3.609 (3)	135

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

compared to ring N12/S4/C15/C16 /O8, which has an envelope conformation with atom S4 as the flap, finally ring Ni1/S2/C7/C8/O4 is twisted on the Ni1—S2 bond, compared to ring Ni2/S3/C11/C12/O6, which is twisted on the S3—C11 bond.

The ligand coordinates two Ni^{II} ions in a bis-pentadentate manner and the sixfold coordination sphere of each nickel(II) atom (NiS_2O_3N) is completed by a water molecule. The

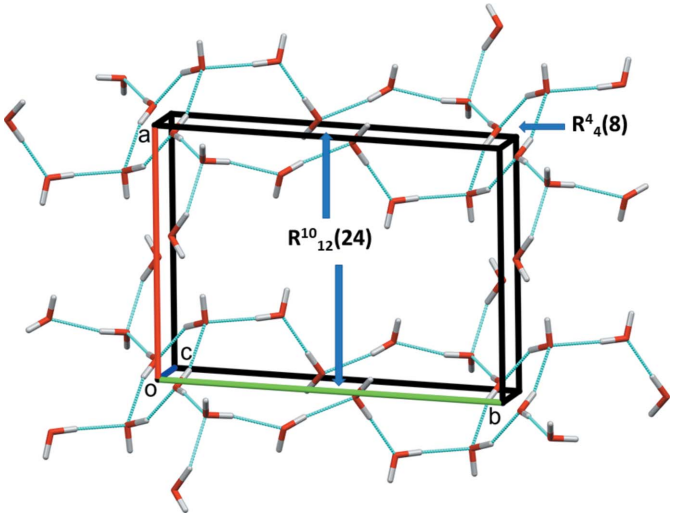


Figure 4
A view along the *c* axis of the hydrogen-bonded network of solvent water molecules (see Table 2).

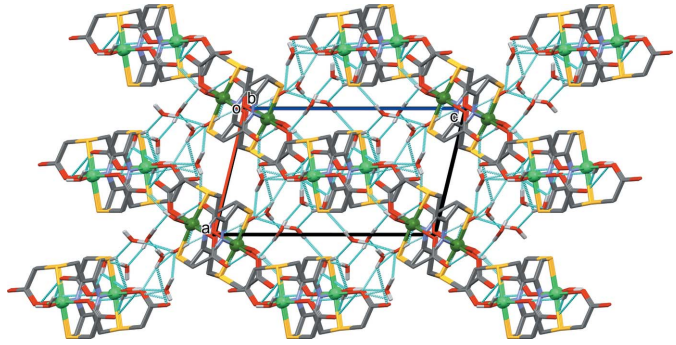


Figure 5
A view along the *b* axis of the crystal packing of complex **I**. Hydrogen bonds (see Table 2) are shown as dashed lines. For clarity, C-bound H atoms have been omitted. (atom Ni1 light-green ball; atom Ni2 dark-green ball).

complex crystallized as a hepta-hydrate. Selected bond lengths involving the nickel atoms of the two molecules are given in Table 1. There is a slight difference in the Ni—N bond lengths [Ni1—N1 = 2.081 (2) Å, Ni2—N2 = 2.057 (2) Å; Table 1], otherwise the bond lengths involving the nickel atoms are similar and close to those reported for the complex aqua(2,2′-{(pyridine-2,6-diyl)bis[methylene(sulfanediyl)]}dipropanoato)nickel(II) (CSD refcode DUYFOU; Rheingold, 2015).

In the crystal structure of **I**, binuclear nickel(II) complexes are linked by O_{water}—H···$O_{carbonyl}$ hydrogen bonds, forming layers parallel to the (101) plane (Fig. 3, Table 2). Within the layers, weak C—H···O hydrogen bonds are present (Table 2). Solvent water molecules are linked by O—H_{water}···O_{water} hydrogen bonds to form ribbons propagating along the *b*-axis direction that consist of eight and twenty-four membered rings of the $R^4_4(8)$ and $R^{10}_{12}(24)$ types (Fig. 4 and Table 2). Additional O—H_{water}···$O_{carbonyl}$ hydrogen bonds involving the binuclear complexes and solvent water molecules, together with weak C—H···S hydrogen bonds, link the layers to form a supramolecular framework (Fig. 5).

Synthesis and crystallization

The synthesis and crystal structure of the reagent tetra-2,3,5,6-bromomethyl-pyrazine (**TBr**) have been reported [Ferigo *et al.*, 1994; Assoumatine & Stoeckli-Evans, 2014 (CSD refcode: TOJXUN)].

Synthesis of ligand 2,2′,2″,2‴-{[pyrazine-2,3,5,6-tetrayltetrakis(methylene)]tetrakis(sulfanediyl)}tetraacetic acid (H_4L1): Thioglycolic acid (1.6313 g, 1.77 mol, 4 eq) was dissolved in 50 ml of THF, then NaOH (1.4166 g, 3.54 mol, 8 eq), dissolved in a minimum amount of water (a few ml) was added. The volume was increased to 100 ml adding THF and then the reaction was left to stir under reflux for 1 h. **TBr** (2 g, 4.42 mol, 1 eq) dissolved in 50 ml of THF, was then added dropwise using an addition funnel. The mixture was stirred under reflux for 6 h. After evaporation of the solvent, the mixture was dissolved in 50 ml of deionized water, and HCl (puriss.) was added dropwise until a clearly acidic pH was

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Ni_2(C_{16}H_{16}N_2O_8S_4)(H_2O)_2]\cdot 7H_2O$
M_r	772.11
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	153
a, b, c (Å)	8.6799 (8), 11.4092 (10), 14.7210 (13)
α, β, γ (°)	90.308 (7), 103.619 (7), 93.801 (7)
V (Å^3)	1413.4 (2)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.71
Crystal size (mm)	0.49 × 0.06 × 0.06
Data collection	
Diffractometer	Stoe IPDS 2
Absorption correction	Empirical (using intensity measurements) (*ShxAbs*; Spek, 2020)
T_{min}, T_{max}	0.261, 0.714
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19974, 7779, 6120
R_{int}	0.052
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.693
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.096, 1.02
No. of reflections	7779
No. of parameters	443
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.74, −0.64

Computer programs: *X-AREA* and *X-RED32* (Stoe & Cie, 2002), *SHELXS97* (Sheldrick, 2008), *SHELXL2018/3* (Sheldrick, 2015), *PLATON* (Spek, 2020), *Mercury* (Macrae *et al.*, 2020), *PLATON* (Spek, 2020) and *publCIF* (Westrip, 2010).

obtained. The mixture was then stirred at room temperature for at least 1–2 h. The yellow precipitate that slowly formed was filtered off and washed with a minimum amount of water and then with $CHCl_3$. The solid obtained (**H_4L1**) was dried *in vacuo* and was then recrystallized from methanol.

Spectroscopic data for H_4L1: ^{1}H-NMR(CD_3OD, 400 MHz, p.p.m.): 4.13 (s, 8H, H2); 3.37 (s, 8H, H3). ^{13}C-NMR(CD_3OD, 50 MHz, p.p.m.): 172.82 (4 C, C4); 150.01 (4 C, C1); 34.31 (4 C, C3); 33.26 (4 C, C2).

Analysis for $C_{16}H_{20}N_2O_8S_4$, M_W = 496.60 g/mol: Calculated (%) C 38.70, H 4.06, N5.64, Found (%) C 37.35, H 3.99, N 5.4.

ESI-MS: 534.97[M + K]$^+$; 519.00[M+Na]$^+$; 497.02[M + H]$^+$; 422.86, 407.04, 247.88.

IR (KBr disc, cm^{-1}) ν: 2984(s), 2922(s), 1690(s), 1431(s), 1395(s), 1321(s), 1289(s), 1202(s), 1181(s).

Synthesis of complex $[(H_2O)Ni(L1)Ni(H_2O)]\cdot 7H_2O$ (I): $NiCl_2\cdot 6\ H_2O$ (38.3 mg, 0.161 mmol, 2 eq) and **H_4L1** (40 mg, 0.080 mmol, 1 eq) were mixed together in 20 ml of degassed water. The mixture was left at 353 K under stirring and nitrogen conditions for 2.5 h. The mixture was then filtered and left to evaporate in air for two weeks, yielding purple needle-like crystals of complex **I** (m.p. 553 K decomposition).

Analysis for $(C_{16}H_{20}N_2Ni_2O_{10}S_4)\cdot 7\ (H_2O)$, M_w = 772.10 g mol^{-1}. Calculated (%) C 24.89, H 4.44, N 3.63. Found (%) C 28.17, H 3.90, N 4.18. Deviation due to the probable loss of water molecules of crystallization, for example, loss of five water molecules gives calculated (%) C 28.18, H 3.55, N 4.11.

ESI–MS: 703, 663, 615[$M - 2H_2O$], 601, 579, 565, 511, 499, 477, 461, 433, 165.

IR (KBr disc, cm^{-1}) ν: 3364(s), 2921(m), 1713(m), 1575(s), 1404(s), 1237(m), 1208(m), 1155(m), 1137(m), 928(m), 704(m).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. For complex **I**, the average *HKL* measurement multiplicity was low at 2.6, hence an empirical absorption correction was applied.

Acknowledgements

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full crystallographic data

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(*μ*-2,2′,2″,2‴-{[Pyrazine-2,3,5,6-tetrayltetrakis(methylene)]tetrakis-(sulfanediyl)}tetraacetato)bis[aquanickel(II)] heptahydrate

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(*μ*-2,2′,2″,2‴-{[Pyrazine-2,3,5,6-tetrayltetrakis(methylene)]tetrakis(sulfanediyl)}tetraacetato-*κ*^{5}*O*,*S*,*N*^{1},*S*′,*O*′:*κ*^{5}*O*″,*S*″,*N*^{4},*S*‴,*O*‴)bis[aquanickel(II)] heptahydrate

Crystal data

$[Ni_2(C_{16}H_{16}N_2O_8S_4)(H_2O)_2]\cdot 7H_2O$
M_r = 772.11
Triclinic, $P\overline{1}$
a = 8.6799 (8) Å
b = 11.4092 (10) Å
c = 14.7210 (13) Å
α = 90.308 (7)°
β = 103.619 (7)°
γ = 93.801 (7)°
V = 1413.4 (2) Å^3
Z = 2
$F(000)$ = 800
D_x = 1.814 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 19267 reflections
θ = 2.3–25.9°
μ = 1.71 mm^{-1}
T = 153 K
Needle, purple
0.49 × 0.06 × 0.06 mm

Data collection

STOE IPDS 2 diffractometer
Radiation source: fine-focus sealed tube
Plane graphite monochromator
$\varphi + \omega$ scans
Absorption correction: empirical (using intensity measurements) (*ShxAbs*; Spek, 2020)
T_{min} = 0.261, T_{max} = 0.714
19974 measured reflections
7779 independent reflections
6120 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 29.5°, θ_{min} = 1.8°
h = −12→11
k = −15→13
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.096
S = 1.02
7779 reflections
443 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0462P)^2 + 1.0506P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}
Extinction correction: (SHELXL-2018/3; Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0029 (6)

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.

Refinement. H atoms of coordinated and non-coordinated water molecules were all located from difference-Fourier maps and freely refined. The C-bound H atoms were included in calculated positions and treated as riding on their parent C atom: C—H = 0.97 - 0.99 Å with U_{iso}(H) = 1.2U_{eq}(C).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.53221 (4)	0.24084 (3)	0.38618 (2)	0.01578 (8)
S1	0.80929 (7)	0.27577 (5)	0.45193 (4)	0.01770 (12)
S2	0.25256 (8)	0.24883 (6)	0.32588 (5)	0.01966 (13)
O1	0.6527 (3)	0.09177 (18)	0.64400 (14)	0.0260 (4)
O2	0.5239 (2)	0.15751 (16)	0.50754 (13)	0.0189 (3)
O3	0.4421 (3)	0.4074 (2)	0.13485 (16)	0.0374 (5)
O4	0.5504 (2)	0.31920 (17)	0.26639 (13)	0.0218 (4)
O1W	0.5614 (2)	0.07971 (17)	0.33656 (14)	0.0214 (4)
H1WA	0.493 (5)	0.021 (4)	0.347 (3)	0.044 (12)*
H1WB	0.562 (5)	0.074 (4)	0.280 (4)	0.049 (13)*
N1	0.5120 (2)	0.39964 (18)	0.45117 (14)	0.0150 (4)
C1	0.6427 (3)	0.4640 (2)	0.49454 (16)	0.0150 (4)
C2	0.8013 (3)	0.4274 (2)	0.48542 (19)	0.0187 (5)
H2A	0.878607	0.443243	0.546080	0.022*
H2B	0.836746	0.477764	0.438614	0.022*
C3	0.8088 (3)	0.1985 (2)	0.5586 (2)	0.0243 (5)
H3A	0.881017	0.134074	0.562820	0.029*
H3B	0.854011	0.253460	0.611882	0.029*
C4	0.6478 (3)	0.1460 (2)	0.57012 (18)	0.0186 (5)
C5	0.3695 (3)	0.4333 (2)	0.45563 (17)	0.0157 (4)
C6	0.2232 (3)	0.3583 (2)	0.40844 (18)	0.0191 (5)
H6A	0.142444	0.410319	0.375290	0.023*
H6B	0.179663	0.317800	0.457218	0.023*
C7	0.2684 (3)	0.3386 (3)	0.22634 (19)	0.0267 (6)
H7A	0.195741	0.302037	0.169739	0.032*
H7B	0.230429	0.416684	0.235880	0.032*
C8	0.4334 (3)	0.3569 (3)	0.20767 (19)	0.0233 (5)
Ni2	0.08393 (4)	0.76880 (3)	0.11162 (2)	0.01682 (8)
S3	−0.17445 (8)	0.74194 (6)	0.13855 (4)	0.01891 (13)
S4	0.33203 (7)	0.76930 (6)	0.07086 (4)	0.01819 (12)
O5	−0.2463 (2)	0.9086 (2)	−0.09705 (16)	0.0298 (5)
O6	−0.0227 (2)	0.85094 (17)	−0.00750 (13)	0.0211 (4)
O7	0.4137 (2)	0.62254 (19)	0.31716 (15)	0.0272 (4)
O8	0.1895 (2)	0.67823 (17)	0.22496 (13)	0.0208 (4)
O2W	0.1272 (3)	0.92039 (18)	0.18933 (14)	0.0230 (4)
H2WA	0.159 (6)	0.984 (4)	0.162 (3)	0.052 (13)*

H2WB	0.187 (7)	0.910 (5)	0.245 (4)	0.078 (18)*
N2	0.0311 (2)	0.60923 (18)	0.04172 (14)	0.0161 (4)
C9	−0.1108 (3)	0.5517 (2)	0.03476 (17)	0.0161 (4)
C10	−0.2367 (3)	0.6057 (2)	0.07259 (18)	0.0191 (5)
H10A	−0.276242	0.548113	0.113293	0.023*
H10B	−0.326835	0.620196	0.019548	0.023*
C11	−0.2527 (4)	0.8505 (3)	0.0556 (2)	0.0288 (6)
H11A	−0.365699	0.826762	0.027239	0.035*
H11B	−0.249215	0.926009	0.089668	0.035*
C12	−0.1675 (3)	0.8705 (2)	−0.02232 (19)	0.0209 (5)
C13	0.1429 (3)	0.5602 (2)	0.00845 (17)	0.0162 (4)
C14	0.3030 (3)	0.6239 (2)	0.01658 (19)	0.0201 (5)
H14A	0.321931	0.630870	−0.046967	0.024*
H14B	0.384762	0.574769	0.052830	0.024*
C15	0.4378 (3)	0.7395 (3)	0.18853 (18)	0.0231 (5)
H15A	0.528662	0.692942	0.185131	0.028*
H15B	0.481816	0.815165	0.220452	0.028*
C16	0.3408 (3)	0.6741 (2)	0.24832 (18)	0.0189 (5)
O3W	0.2116 (3)	0.1139 (2)	0.53431 (19)	0.0364 (5)
H3WA	0.310 (5)	0.107 (3)	0.531 (3)	0.030 (9)*
H3WB	0.186 (8)	0.056 (6)	0.578 (5)	0.09 (2)*
O4W	0.9679 (3)	0.5567 (2)	0.29921 (16)	0.0274 (4)
H4WA	1.041 (6)	0.603 (4)	0.278 (3)	0.047 (12)*
H4WB	0.893 (6)	0.597 (4)	0.310 (4)	0.058 (14)*
O5W	0.5598 (3)	0.0350 (2)	0.15764 (15)	0.0283 (4)
H5WA	0.649 (8)	0.081 (6)	0.143 (4)	0.09 (2)*
H5WB	0.487 (6)	0.068 (4)	0.129 (4)	0.054 (14)*
O6W	0.7456 (3)	0.6695 (2)	0.36273 (17)	0.0315 (5)
H6WA	0.648 (6)	0.654 (4)	0.349 (3)	0.042 (12)*
H6WB	0.763 (6)	0.738 (5)	0.391 (4)	0.068 (16)*
O7W	0.8648 (3)	0.1299 (2)	0.16038 (19)	0.0370 (5)
H7WA	0.867 (6)	0.202 (2)	0.178 (3)	0.050 (13)*
H7WB	0.923 (7)	0.132 (5)	0.112 (4)	0.078 (17)*
O8W	0.9536 (3)	0.0333 (3)	0.3655 (3)	0.0467 (7)
H8WA	0.939 (8)	0.059 (6)	0.310 (2)	0.10 (2)*
H8WB	1.022 (9)	0.070 (7)	0.410 (5)	0.11 (3)*
O9W	0.8291 (3)	0.3532 (2)	0.20860 (18)	0.0339 (5)
H9WA	0.745 (7)	0.338 (5)	0.224 (4)	0.065 (16)*
H9WB	0.878 (6)	0.411 (4)	0.241 (3)	0.048 (13)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.01756 (15)	0.01571 (15)	0.01319 (15)	0.00010 (11)	0.00220 (11)	−0.00087 (11)
S1	0.0181 (3)	0.0171 (3)	0.0182 (3)	0.0016 (2)	0.0048 (2)	−0.0015 (2)
S2	0.0195 (3)	0.0176 (3)	0.0199 (3)	−0.0013 (2)	0.0015 (2)	−0.0045 (2)
O1	0.0324 (10)	0.0244 (10)	0.0177 (9)	−0.0046 (8)	0.0007 (8)	0.0025 (8)
O2	0.0206 (8)	0.0201 (9)	0.0149 (8)	−0.0013 (7)	0.0026 (7)	0.0003 (7)

O3	0.0421 (13)	0.0489 (14)	0.0205 (10)	0.0069 (11)	0.0048 (9)	0.0131 (10)
O4	0.0244 (9)	0.0253 (9)	0.0157 (8)	0.0010 (7)	0.0050 (7)	0.0047 (7)
O1W	0.0266 (9)	0.0174 (9)	0.0198 (9)	−0.0006 (7)	0.0052 (8)	−0.0035 (7)
N1	0.0163 (9)	0.0135 (9)	0.0143 (9)	−0.0011 (7)	0.0027 (7)	−0.0014 (7)
C1	0.0169 (10)	0.0150 (10)	0.0127 (10)	0.0012 (8)	0.0026 (8)	0.0007 (8)
C2	0.0157 (11)	0.0177 (11)	0.0223 (12)	0.0001 (9)	0.0040 (9)	−0.0017 (9)
C3	0.0232 (13)	0.0220 (12)	0.0256 (13)	0.0001 (10)	0.0021 (10)	0.0045 (10)
C4	0.0230 (12)	0.0168 (11)	0.0144 (11)	−0.0009 (9)	0.0021 (9)	−0.0011 (9)
C5	0.0173 (10)	0.0153 (10)	0.0136 (10)	−0.0011 (8)	0.0025 (8)	0.0000 (8)
C6	0.0190 (11)	0.0203 (12)	0.0167 (11)	−0.0003 (9)	0.0020 (9)	−0.0029 (9)
C7	0.0271 (13)	0.0351 (15)	0.0164 (12)	0.0059 (11)	0.0011 (10)	−0.0008 (11)
C8	0.0281 (13)	0.0262 (13)	0.0142 (11)	0.0017 (10)	0.0020 (10)	0.0005 (10)
Ni2	0.01780 (15)	0.01761 (16)	0.01431 (15)	0.00035 (11)	0.00256 (11)	−0.00098 (11)
S3	0.0210 (3)	0.0200 (3)	0.0168 (3)	0.0014 (2)	0.0069 (2)	−0.0016 (2)
S4	0.0185 (3)	0.0189 (3)	0.0162 (3)	−0.0023 (2)	0.0031 (2)	−0.0005 (2)
O5	0.0248 (10)	0.0340 (11)	0.0279 (11)	0.0016 (8)	0.0008 (8)	0.0106 (9)
O6	0.0209 (9)	0.0234 (9)	0.0189 (9)	0.0030 (7)	0.0040 (7)	0.0032 (7)
O7	0.0284 (10)	0.0290 (10)	0.0222 (10)	0.0049 (8)	0.0008 (8)	0.0059 (8)
O8	0.0205 (9)	0.0243 (9)	0.0164 (8)	−0.0017 (7)	0.0026 (7)	0.0015 (7)
O2W	0.0312 (10)	0.0183 (9)	0.0177 (9)	−0.0001 (8)	0.0025 (8)	−0.0027 (7)
N2	0.0165 (9)	0.0170 (9)	0.0140 (9)	0.0007 (7)	0.0019 (7)	−0.0008 (8)
C9	0.0165 (10)	0.0179 (11)	0.0128 (10)	−0.0002 (8)	0.0017 (8)	−0.0002 (9)
C10	0.0170 (11)	0.0212 (12)	0.0192 (11)	0.0003 (9)	0.0046 (9)	−0.0045 (9)
C11	0.0299 (14)	0.0270 (14)	0.0347 (16)	0.0108 (11)	0.0155 (12)	0.0101 (12)
C12	0.0229 (12)	0.0168 (11)	0.0228 (12)	0.0009 (9)	0.0047 (10)	0.0044 (10)
C13	0.0170 (10)	0.0175 (11)	0.0135 (10)	0.0007 (8)	0.0024 (8)	−0.0004 (9)
C14	0.0190 (11)	0.0215 (12)	0.0197 (12)	−0.0032 (9)	0.0056 (9)	−0.0053 (10)
C15	0.0184 (11)	0.0314 (14)	0.0170 (12)	−0.0032 (10)	0.0009 (9)	−0.0020 (10)
C16	0.0213 (11)	0.0191 (11)	0.0145 (11)	0.0004 (9)	0.0009 (9)	−0.0024 (9)
O3W	0.0268 (11)	0.0366 (13)	0.0473 (14)	0.0028 (9)	0.0113 (10)	0.0092 (11)
O4W	0.0258 (10)	0.0272 (10)	0.0281 (11)	−0.0019 (8)	0.0052 (8)	0.0017 (8)
O5W	0.0287 (11)	0.0321 (11)	0.0239 (10)	0.0034 (9)	0.0058 (8)	−0.0033 (9)
O6W	0.0272 (11)	0.0402 (13)	0.0276 (11)	0.0041 (9)	0.0066 (9)	0.0044 (10)
O7W	0.0386 (13)	0.0311 (12)	0.0462 (14)	−0.0009 (10)	0.0208 (11)	−0.0050 (11)
O8W	0.0367 (14)	0.0421 (15)	0.061 (2)	−0.0031 (11)	0.0130 (14)	0.0098 (14)
O9W	0.0352 (12)	0.0336 (12)	0.0345 (12)	−0.0043 (10)	0.0132 (10)	−0.0071 (10)

Geometric parameters (Å, º)

Ni1—O1W	2.0276 (19)	S3—C10	1.810 (3)
Ni1—O2	2.0423 (18)	S4—C15	1.805 (3)
Ni1—O4	2.0158 (19)	S4—C14	1.814 (3)
Ni1—N1	2.081 (2)	O5—C12	1.248 (3)
Ni1—S1	2.3775 (7)	O6—C12	1.260 (3)
Ni1—S2	2.3883 (8)	O7—C16	1.236 (3)
S1—C3	1.805 (3)	O8—C16	1.281 (3)
S1—C2	1.806 (3)	O2W—H2WA	0.88 (5)
S2—C6	1.809 (3)	O2W—H2WB	0.88 (6)

S2—C7	1.819 (3)	N2—C13	1.337 (3)
O1—C4	1.248 (3)	N2—C9	1.338 (3)
O2—C4	1.255 (3)	C9—C13^{ii}	1.405 (3)
O3—C8	1.235 (3)	C9—C10	1.502 (3)
O4—C8	1.270 (3)	C10—H10A	0.9900
O1W—H1WA	0.90 (5)	C10—H10B	0.9900
O1W—H1WB	0.83 (5)	C11—C12	1.515 (4)
N1—C1	1.333 (3)	C11—H11A	0.9900
N1—C5	1.335 (3)	C11—H11B	0.9900
C1—C5^{i}	1.403 (3)	C13—C14	1.503 (3)
C1—C2	1.500 (3)	C14—H14A	0.9900
C2—H2A	0.9900	C14—H14B	0.9900
C2—H2B	0.9900	C15—C16	1.521 (4)
C3—C4	1.531 (4)	C15—H15A	0.9900
C3—H3A	0.9900	C15—H15B	0.9900
C3—H3B	0.9900	O3W—H3WA	0.87 (4)
C5—C6	1.503 (3)	O3W—H3WB	0.98 (7)
C6—H6A	0.9900	O4W—H4WA	0.91 (5)
C6—H6B	0.9900	O4W—H4WB	0.86 (5)
C7—C8	1.523 (4)	O5W—H5WA	0.97 (7)
C7—H7A	0.9900	O5W—H5WB	0.80 (5)
C7—H7B	0.9900	O6W—H6WA	0.83 (5)
Ni2—O2W	2.033 (2)	O6W—H6WB	0.87 (6)
Ni2—O6	2.0440 (19)	O7W—H7WA	0.857 (19)
Ni2—O8	2.0287 (19)	O7W—H7WB	0.97 (6)
Ni2—N2	2.057 (2)	O8W—H8WA	0.85 (2)
Ni2—S4	2.3674 (7)	O8W—H8WB	0.86 (8)
Ni2—S3	2.3685 (7)	O9W—H9WA	0.82 (6)
S3—C11	1.795 (3)	O9W—H9WB	0.84 (5)

O4—Ni1—O1W	92.71 (8)	O2W—Ni2—N2	175.03 (9)
O4—Ni1—O2	177.15 (8)	O6—Ni2—N2	89.81 (8)
O1W—Ni1—O2	85.47 (8)	O8—Ni2—S4	85.30 (6)
O4—Ni1—N1	92.73 (8)	O2W—Ni2—S4	97.60 (6)
O1W—Ni1—N1	173.94 (8)	O6—Ni2—S4	93.64 (6)
O2—Ni1—N1	88.99 (8)	N2—Ni2—S4	86.11 (6)
O4—Ni1—S1	91.86 (6)	O8—Ni2—S3	94.92 (6)
O1W—Ni1—S1	92.11 (6)	O2W—Ni2—S3	91.04 (6)
O2—Ni1—S1	86.03 (6)	O6—Ni2—S3	85.63 (6)
N1—Ni1—S1	85.03 (6)	N2—Ni2—S3	85.28 (6)
O4—Ni1—S2	84.80 (6)	S4—Ni2—S3	171.37 (3)
O1W—Ni1—S2	99.55 (6)	C11—S3—C10	102.65 (14)
O2—Ni1—S2	97.65 (6)	C11—S3—Ni2	93.29 (10)
N1—Ni1—S2	83.62 (6)	C10—S3—Ni2	98.05 (8)
S1—Ni1—S2	167.99 (3)	C15—S4—C14	101.74 (13)
C3—S1—C2	103.12 (13)	C15—S4—Ni2	93.14 (9)
C3—S1—Ni1	95.52 (9)	C14—S4—Ni2	97.06 (8)
C2—S1—Ni1	96.06 (8)	C12—O6—Ni2	119.89 (17)

C6—S2—C7	101.48 (13)	C16—O8—Ni2	120.83 (17)
C6—S2—Ni1	96.67 (9)	Ni2—O2W—H2WA	117 (3)
C7—S2—Ni1	95.58 (10)	Ni2—O2W—H2WB	112 (4)
C4—O2—Ni1	121.22 (17)	H2WA—O2W—H2WB	113 (5)
C8—O4—Ni1	123.77 (18)	C13—N2—C9	120.3 (2)
Ni1—O1W—H1WA	116 (3)	C13—N2—Ni2	119.43 (17)
Ni1—O1W—H1WB	117 (3)	C9—N2—Ni2	120.15 (16)
H1WA—O1W—H1WB	106 (4)	N2—C9—C13^{ii}	119.9 (2)
C1—N1—C5	119.7 (2)	N2—C9—C10	120.7 (2)
C1—N1—Ni1	119.71 (16)	C13^{ii}—C9—C10	119.5 (2)
C5—N1—Ni1	120.41 (16)	C9—C10—S3	115.48 (18)
N1—C1—C5^{i}	120.2 (2)	C9—C10—H10A	108.4
N1—C1—C2	118.9 (2)	S3—C10—H10A	108.4
C5^{i}—C1—C2	120.9 (2)	C9—C10—H10B	108.4
C1—C2—S1	116.34 (18)	S3—C10—H10B	108.4
C1—C2—H2A	108.2	H10A—C10—H10B	107.5
S1—C2—H2A	108.2	C12—C11—S3	115.45 (19)
C1—C2—H2B	108.2	C12—C11—H11A	108.4
S1—C2—H2B	108.2	S3—C11—H11A	108.4
H2A—C2—H2B	107.4	C12—C11—H11B	108.4
C4—C3—S1	116.69 (19)	S3—C11—H11B	108.4
C4—C3—H3A	108.1	H11A—C11—H11B	107.5
S1—C3—H3A	108.1	O5—C12—O6	124.2 (3)
C4—C3—H3B	108.1	O5—C12—C11	116.9 (2)
S1—C3—H3B	108.1	O6—C12—C11	118.9 (2)
H3A—C3—H3B	107.3	N2—C13—C9^{ii}	119.8 (2)
O1—C4—O2	124.7 (2)	N2—C13—C14	120.6 (2)
O1—C4—C3	114.8 (2)	C9^{ii}—C13—C14	119.5 (2)
O2—C4—C3	120.5 (2)	C13—C14—S4	116.43 (18)
N1—C5—C1^{i}	120.1 (2)	C13—C14—H14A	108.2
N1—C5—C6	119.1 (2)	S4—C14—H14A	108.2
C1^{i}—C5—C6	120.7 (2)	C13—C14—H14B	108.2
C5—C6—S2	115.43 (17)	S4—C14—H14B	108.2
C5—C6—H6A	108.4	H14A—C14—H14B	107.3
S2—C6—H6A	108.4	C16—C15—S4	115.77 (18)
C5—C6—H6B	108.4	C16—C15—H15A	108.3
S2—C6—H6B	108.4	S4—C15—H15A	108.3
H6A—C6—H6B	107.5	C16—C15—H15B	108.3
C8—C7—S2	116.14 (19)	S4—C15—H15B	108.3
C8—C7—H7A	108.3	H15A—C15—H15B	107.4
S2—C7—H7A	108.3	O7—C16—O8	124.6 (3)
C8—C7—H7B	108.3	O7—C16—C15	117.7 (2)
S2—C7—H7B	108.3	O8—C16—C15	117.8 (2)
H7A—C7—H7B	107.4	H3WA—O3W—H3WB	108 (4)
O3—C8—O4	124.9 (3)	H4WA—O4W—H4WB	111 (4)
O3—C8—C7	116.4 (3)	H5WA—O5W—H5WB	101 (5)
O4—C8—C7	118.7 (2)	H6WA—O6W—H6WB	107 (4)
O8—Ni2—O2W	90.24 (8)	H7WA—O7W—H7WB	104 (5)

O8—Ni2—O6	176.47 (8)	H8WA—O8W—H8WB	120 (7)
O2W—Ni2—O6	93.24 (8)	H9WA—O9W—H9WB	109 (5)
O8—Ni2—N2	86.76 (8)		
N1—C1—C2—S1	−20.9 (3)	Ni1—S2—C7—C8	9.7 (2)
N1—C5—C6—S2	−14.8 (3)	Ni1—O4—C8—O3	178.4 (2)
S1—C3—C4—O2	−0.1 (3)	Ni1—O4—C8—C7	−2.2 (4)
S2—C7—C8—O4	−6.7 (4)	S2—C7—C8—O3	172.7 (2)
N2—C13—C14—S4	−1.3 (3)	C13—N2—C9—C13^{ii}	−0.6 (4)
N2—C9—C10—S3	−7.0 (3)	Ni2—N2—C9—C13^{ii}	−176.41 (18)
S4—C15—C16—O8	−21.9 (3)	C13—N2—C9—C10	179.5 (2)
S3—C11—C12—O6	−27.6 (4)	Ni2—N2—C9—C10	3.7 (3)
C5—N1—C1—C5^{i}	−0.2 (4)	C13^{ii}—C9—C10—S3	173.09 (19)
Ni1—N1—C1—C5^{i}	−175.32 (17)	C11—S3—C10—C9	101.2 (2)
C5—N1—C1—C2	−177.5 (2)	Ni2—S3—C10—C9	6.0 (2)
Ni1—N1—C1—C2	7.4 (3)	C10—S3—C11—C12	−72.7 (3)
C5^{i}—C1—C2—S1	161.87 (19)	Ni2—S3—C11—C12	26.3 (2)
C3—S1—C2—C1	−76.6 (2)	Ni2—O6—C12—O5	−172.1 (2)
Ni1—S1—C2—C1	20.51 (19)	Ni2—O6—C12—C11	9.8 (3)
C2—S1—C3—C4	96.0 (2)	S3—C11—C12—O5	154.2 (2)
Ni1—S1—C3—C4	−1.6 (2)	C9—N2—C13—C9^{ii}	0.6 (4)
Ni1—O2—C4—O1	−176.6 (2)	Ni2—N2—C13—C9^{ii}	176.44 (18)
Ni1—O2—C4—C3	2.3 (3)	C9—N2—C13—C14	−179.6 (2)
S1—C3—C4—O1	178.92 (19)	Ni2—N2—C13—C14	−3.7 (3)
C1—N1—C5—C1^{i}	0.2 (4)	C9^{ii}—C13—C14—S4	178.57 (19)
Ni1—N1—C5—C1^{i}	175.29 (17)	C15—S4—C14—C13	99.1 (2)
C1—N1—C5—C6	−178.5 (2)	Ni2—S4—C14—C13	4.4 (2)
Ni1—N1—C5—C6	−3.4 (3)	C14—S4—C15—C16	−71.2 (2)
C1^{i}—C5—C6—S2	166.52 (19)	Ni2—S4—C15—C16	26.7 (2)
C7—S2—C6—C5	−75.9 (2)	Ni2—O8—C16—O7	178.7 (2)
Ni1—S2—C6—C5	21.24 (19)	Ni2—O8—C16—C15	0.2 (3)
C6—S2—C7—C8	107.7 (2)	S4—C15—C16—O7	159.5 (2)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O1^{iii}	0.90 (5)	1.78 (5)	2.672 (3)	174 (4)
O1*W*—H1*WB*···O5*W*	0.83 (5)	1.85 (5)	2.677 (3)	170 (5)
O2*W*—H2*WA*···O5^{iv}	0.88 (5)	1.80 (5)	2.673 (3)	168 (4)
O2*W*—H2*WB*···O1^{i}	0.88 (6)	1.88 (6)	2.742 (3)	168 (6)
O3*W*—H3*WA*···O2	0.87 (4)	2.02 (4)	2.842 (3)	157 (4)
O3*W*—H3*WB*···O8*W*^{iii}	0.98 (7)	1.87 (7)	2.785 (4)	154 (6)
O4*W*—H4*WA*···O8^{v}	0.91 (5)	1.83 (5)	2.733 (3)	172 (4)
O4*W*—H4*WB*···O6*W*	0.86 (5)	1.88 (5)	2.724 (3)	166 (5)
O5*W*—H5*WA*···O7*W*	0.97 (7)	1.88 (7)	2.785 (3)	154 (6)
O5*W*—H5*WB*···O5^{ii}	0.80 (5)	2.06 (5)	2.776 (3)	149 (5)

O6*W*—H6*WA*···O7	0.83 (5)	1.98 (5)	2.814 (3)	178 (4)
O6*W*—H6*WB*···O3*W*^{i}	0.87 (6)	1.98 (6)	2.849 (4)	173 (5)
O7*W*—H7*WA*···O9*W*	0.86 (2)	1.85 (2)	2.698 (3)	169 (5)
O7*W*—H7*WB*···O6^{vi}	0.97 (6)	1.94 (6)	2.899 (3)	174 (5)
O8*W*—H8*WA*···O7*W*	0.85 (2)	2.32 (2)	3.159 (5)	173 (6)
O8*W*—H8*WB*···O3*W*^{v}	0.86 (8)	2.19 (8)	3.019 (4)	164 (7)
O9*W*—H9*WA*···O4	0.82 (6)	1.93 (6)	2.752 (3)	174 (6)
O9*W*—H9*WB*···O4*W*	0.84 (5)	1.90 (5)	2.731 (3)	171 (5)
C2—H2*A*···O4*W*^{vii}	0.99	2.35	3.324 (3)	167
C2—H2*B*···O6*W*	0.99	2.55	3.308 (4)	133
C3—H3*A*···O8*W*^{viii}	0.99	2.55	3.488 (4)	159
C6—H6*A*···O4*W*^{ix}	0.99	2.43	3.413 (3)	173
C6—H6*B*···O3*W*	0.99	2.60	3.365 (4)	134
C6—H6*B*···O6*W*^{i}	0.99	2.58	3.334 (3)	133
C10—H10*B*···O3^{ii}	0.99	2.27	3.150 (4)	148
C11—H11*B*···O5*W*^{x}	0.99	2.52	3.303 (4)	136
C11—H11*B*···O7*W*^{x}	0.99	2.58	3.516 (4)	158
C14—H14*A*···O9*W*^{vi}	0.99	2.45	3.260 (4)	139
C14—H14*B*···O3	0.99	2.29	3.169 (4)	148
C15—H15*A*···S3^{v}	0.99	2.84	3.609 (3)	135

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