

Tris(oxamide dioxime- κ^2N,N')nickel(II) sulfate pentahydrate

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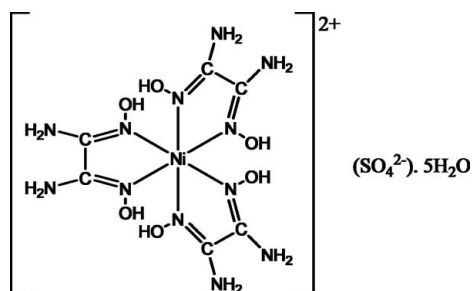
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(C-C) = 0.004$ Å; H-atom completeness 93%; disorder in solvent or counterion; R factor = 0.053; wR factor = 0.164; data-to-parameter ratio = 16.7.

The asymmetric unit of the title compound, $[Ni(C_2H_6N_4O_2)_3]SO_4 \cdot 5H_2O$, contains two complex cations, two sulfate anions and ten lattice water molecules. In both independent cations, the central Ni^{II} ion adopts a distorted octahedral coordination involving six imino N atoms of three bidentate oxamide dioxime ligands. The bulk structure is achieved by a three-dimensional network of $O-H \cdots O$ and $N-H \cdots O$ hydrogen bonds which interlink the ionic partners and some water molecules in such a manner that the lattice framework thus formed defines channels parallel to $[100]$. The other water molecules are lodged inside these channels. Two of the ten water molecules in the asymmetric unit are disordered over three sites, in 0.356 (3):0.324 (5):0.320 (5) and 0.247 (3):0.293 (6):0.460 (6) occupancy ratios, and one O atom of a sulfate ion is also disordered over two sites, with occupancies of 0.621 (5) and 0.379 (5).

Related literature

For general background, see: Akutsu-Sato *et al.* (2005); B elomb e *et al.* (2007); Ephraim (1889); Infantes & Motherwell (2002); Martin *et al.* (2007); Nenwa (2004); Rashid *et al.* (2001). For related structures, see: B elomb e *et al.* (2006); B elomb e *et al.* (2007); Endres & Jannack (1980).



Experimental

Crystal data

$[Ni(C_2H_6N_4O_2)_3]SO_4 \cdot 5H_2O$
 $M_r = 599.17$
 Triclinic, $P\bar{1}$
 $a = 12.3141$ (16) Å
 $b = 14.0458$ (17) Å
 $c = 14.7734$ (18) Å
 $\alpha = 86.077$ (3)°
 $\beta = 77.769$ (3)°

$\gamma = 72.868$ (3)°
 $V = 2386.4$ (5) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.99$ mm⁻¹
 $T = 293$ (2) K
 $0.25 \times 0.15 \times 0.10$ mm

Data collection

Bruker APEX CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2001)
 $T_{min} = 0.789$, $T_{max} = 0.907$

33235 measured reflections
 11834 independent reflections
 9771 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.029$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.164$
 $S = 1.12$
 11834 reflections
 707 parameters
 23 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{max} = 1.48$ e Å⁻³
 $\Delta\rho_{min} = -1.45$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H \cdots A$ | $D-H$ | $H \cdots A$ | $D \cdots A$ | $D-H \cdots A$ |
|---------------------------------|----------|--------------|--------------|----------------|
| O11—H11...O20 | 0.82 | 1.85 | 2.673 (4) | 177 |
| O12—H12...O2A | 0.82 | 1.85 | 2.663 (7) | 174 |
| O13—H13...O10 | 0.82 | 1.88 | 2.698 (3) | 174 |
| O15—H15...O30 | 0.82 | 1.90 | 2.716 (3) | 177 |
| O16—H16...O2B | 0.82 | 1.95 | 2.770 (5) | 178 |
| O16—H16...O4 | 0.82 | 2.37 | 2.857 (4) | 119 |
| O21—H21...O1 | 0.82 | 1.85 | 2.645 (4) | 163 |
| O23—H23...O3 | 0.82 | 1.94 | 2.744 (4) | 165 |
| O25—H25...O4 | 0.82 | 1.82 | 2.636 (5) | 177 |
| O22—H22...O4W ⁱ | 0.82 | 1.96 | 2.694 (4) | 148 |
| O24—H24...O5W ⁱ | 0.82 | 2.00 | 2.796 (5) | 164 |
| O26—H26...O4W ⁱ | 0.82 | 1.95 | 2.760 (4) | 167 |
| O1W—H1W1...O13 | 0.84 (2) | 1.98 (3) | 2.819 (3) | 174 (5) |
| O2W—H2W2...O21 | 0.84 (3) | 1.93 (3) | 2.764 (4) | 168 (4) |
| O4W—H2W4...O5W | 0.83 (3) | 1.98 (3) | 2.783 (5) | 160 (5) |
| O5W—H1W5...O7W | 0.88 (3) | 2.16 (6) | 2.827 (7) | 132 (6) |
| O7W—H7W1...O8W | 0.85 | 1.93 | 2.782 (8) | 175 |
| O8W—H2W8...O3 | 0.91 (3) | 1.92 (7) | 2.720 (7) | 147 (11) |
| O1W—H2W1...O10 ⁱⁱ | 0.82 (2) | 2.13 (3) | 2.944 (3) | 172 (5) |
| O2W—H1W2...O40 ⁱⁱⁱ | 0.86 (3) | 1.91 (3) | 2.764 (4) | 175 (5) |
| O3W—H2W3...O20 ⁱⁱ | 0.86 (3) | 2.29 (4) | 3.045 (4) | 146 (6) |
| O4W—H1W4...O2W ^{iv} | 0.85 (3) | 1.98 (3) | 2.825 (4) | 170 (5) |
| O6W—H2W6...O24 ^v | 0.82 (3) | 2.25 (4) | 3.038 (4) | 161 (7) |
| N17—H17B...O10 ⁱⁱ | 0.86 | 2.43 | 3.022 (4) | 126 |
| N18—H18A...O23 ^{vi} | 0.86 | 2.26 | 3.052 (3) | 154 |
| N19—H19A...O3 ^{vii} | 0.86 | 2.60 | 3.182 (4) | 125 |
| N19—H19B...O12 ^{vii} | 0.86 | 2.19 | 3.044 (4) | 175 |
| N50—H50A...O1W ^{vii} | 0.86 | 2.35 | 3.006 (4) | 134 |
| N50—H50B...O12 ^{vii} | 0.86 | 2.14 | 2.941 (3) | 155 |
| N51—H51B...O20 ^{viii} | 0.86 | 2.19 | 3.039 (4) | 172 |
| N112—H11A...O2W ^{ix} | 0.86 | 2.45 | 3.096 (4) | 132 |
| N112—H11B...O20 ^{viii} | 0.86 | 2.03 | 2.846 (4) | 158 |
| N28—H28A...O16 ^x | 0.86 | 2.04 | 2.873 (4) | 162 |
| N29—H29A...O1W ^{vii} | 0.86 | 2.07 | 2.876 (4) | 155 |
| N29—H29B...O3W ^{vii} | 0.86 | 1.95 | 2.800 (4) | 168 |
| N70—H70A...O14 ^{xi} | 0.86 | 2.38 | 3.055 (4) | 136 |
| N70—H70B...O3W ^{vii} | 0.86 | 2.47 | 3.264 (5) | 154 |
| N71—H71A...O2W ^{ix} | 0.86 | 2.36 | 3.155 (4) | 154 |
| N71—H71B...O1 ^{ix} | 0.86 | 2.17 | 2.999 (4) | 163 |
| N72—H72B...O1 ^{ix} | 0.86 | 2.33 | 3.153 (4) | 161 |

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINTE* (Bruker, 2000); data reduction: *SAINTE* (Bruker, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2663).

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supplementary materials

Acta Cryst. (2008). E64, m1440-m1441 [doi:10.1107/S1600536808033278]

Tris(oxamide dioxime- κ^2N,N')nickel(II) sulfate pentahydrate

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Comment

We recently reported the Co^{III} complex salt, [Co(H₂oxado)₃]₂(C₂O₄)(SO₄)₂·12H₂O (H₂oxado is oxamide dioxime), which crystallizes with a channelled lattice network encapsulating infinite water tapes (Belombe *et al.*, 2007). This compound was shown to be one of the few well documented examples of solid materials containing water cluster patterns of category T according to the classification of Infantes & Motherwell (2002). Most importantly, such nano-channelled frameworks enclosing infinite water tapes or water filaments (Martin *et al.*, 2007) provide excellent template systems to probe the feasibility of the fascinating prospect of *one dimensional proton conduction in solids (one-dimensional-PCS)* (Bélombé *et al.*, 2006, 2007; Rashid *et al.*, 2001; Akutsu-Sato *et al.*, 2005). Herein we report the crystal structure of the title compound, (I), as yet another example of a closely related solid material encapsulating water cluster patterns that fit into the Infantes–Motherwell classification.

Fig. 1 depicts the ionic constituents of (I). The helical pseudo-octahedral coordination geometry of the complex cation, [Ni(H₂oxado)₃]²⁺ (H₂oxado iso xamide dioxime), is similar to the usual chiral geometries, and the bond lengths and angles compare within experimental error with those reported previously (Endres & Jannack, 1980; Bélombé *et al.*, 2006). The asymmetric unit of (I) contains two complex cations, two sulfate anions and ten lattice water molecules. The skeletal lattice framework of (I) is constructed by the ionic partners, and by those of the crystal waters (dubbed "skeletal" waters), all of which are held together by a three-dimensional network of O—H···O and N—H···O hydrogen bonds as shown in Fig. 2. It is obvious from this figure that the major part of the crystal waters is concentrated along the elliptic nanochannels (*ca* 4.68 Å wide and 14.61 Å long). These "central" water molecules are linked *via* hydrogen bonds (Table 1) into discrete broken-line pentamers (Fig. 3) that fit into category D of the classification of Infantes & Motherwell (2002).

Fig. 2 reveals that all equivalent atoms of the three molecular partners in this crystal structure pile up on top of one another forming rectilinear homoatomic chains parallel to [100]. Thus, the [Ni(H₂oxado)₃]²⁺ complexes generate positively charged, and the SO₄²⁻ anions negatively charged "linear stacks" with a Ni···Ni and an S···S regular spacing of *a* = 12.31 Å. In other words, these lattice components are ordered along the stacking direction strictly in an eclipsed sequence relative to one another, hence leading to an unusually short spacing of 2.0 Å between the O atoms of neighboring water molecules.

The geometric parameters within the coordination spheres of the crystallographically independent [Ni(H₂oxado)₃]²⁺ complexes are closely comparable. So are also those of the sulfate ions, despite the fact that one O atom, *viz.* O2, in the SO₄²⁻ ion, is disordered (apparently along the bonding axis) over two sites. This disorder, obviously, leads to the observation of the two bond lengths, S2—O2A = 1.678 (7) Å and S2—O2B = 1.446 (4) Å, with an average of S2—O2 = 1.562 Å.

As shown in Fig. 2, four of the twenty crystal waters in the unit cell of (I) are lodged inside the "walls" of the host or skeletal lattice, and are involved in O—H···O bridgings with the O atoms of the SO₄²⁻ ions or with the —OH groups of the oxamide dioxime ligands. Hence, these water molecules (O1w and O3w) are called "skeletal" waters. The molecules

supplementary materials

of water containing the atoms O2W, O4W, O5W and O6W are positioned at the periphery of the channel walls, due to their involvement in hydrogen bonding with the "external" O atoms of the sulfate ions and with the amino groups of the organic ligands. They are, therefore, termed "peripheral" waters. Some of the water molecules containing the atoms O7W, O8W, O9W and O10W are lodged around the central axes of the lattice channels and dubbed "central" waters form together with the "skeletal" water molecules discrete linear pentamers and involve the disordered molecules mentioned above. All the water molecules in this structure lie with their molecular planes parallel to the *bc* plane, *i.e.* perpendicular to the [100] stacking direction. Within separate stacks, however, the group orientations of these molecules with respect to the improper axis of rotation ($\bar{2}$) are different.

It is worth noting finally, that compound (**I**) represents a highly promising precursor system in the context of our ongoing metathetic syntheses of nanochannelled metal organic frameworks (MOFs) conceived as potential *one dimensional proton conducting solids (one-dimensional-PCS)* (Bélombé *et al.*, 2006, 2007).

Experimental

Commercial NiSO₄·6H₂O and freshly prepared oxamide dioxime (Ephraim, 1889; Nenwa, 2004) were mixed together in a ratio of 0.53 g (2 mmol): 0.71 g (6 mmol) and dissolved in warm H₂O (323 K, 40 ml) acidified with 1 drop of concentrated H₂SO₄. The resulting indigo-blue solution was stirred for 2 h and filtered. The filtrate collected in an open dish was evaporated completely over a few days in a hood. Prismatic violet crystals were deposited, contaminated with a slight amount of starting NiSO₄ which was washed off with H₂O (3 ml) and separated by filtration. After drying for 48 h between filter papers at ambient temperature, 1.1 g (~92% yield) of crystalline material was obtained and used for X-ray analysis.

Refinement

One of the sulfate O atoms, O2, is disordered over two positions (O2A and O2B), with refined occupancies of 0.621 (5) and 0.379 (5). Two water molecules are disordered over three sites (O9W/O10W/O11W and O12W/O13W/O14W) with refined occupancies of 0.356 (3)/0.324 (5)/0.320 (5) and 0.247 (3)/0.293 (6)/0.460 (6). All water H atoms were first located in a difference Fourier map and then refined with distance restraints of O—H = 0.85 (3) Å and H···H = 1.39 (3) Å, and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. The remaining H atoms were positioned geometrically (O—H = 0.82 Å and N—H = 0.86 Å) and refined as riding on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$ and $1.5U_{\text{eq}}(\text{O})$. The highest peak and deepest hole in the final difference map are 1.47 Å from atom O12W and 1.45 Å from S1, respectively. The H atoms on the disordered water molecules could not be located.

Figures

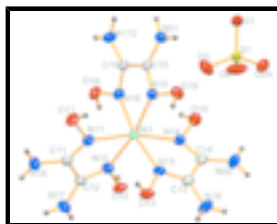


Fig. 1. Ionic constituents of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

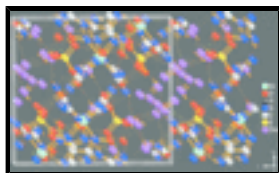


Fig. 2. Crystal structure of the title compound, viewed down the a axis. Hydrogen bonds are shown as dashed lines.

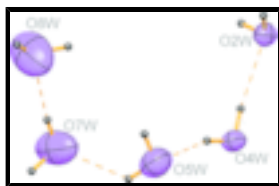


Fig. 3. A view of discrete hydrogen-bonded (dashed lines) water pentamers. Displacement ellipsoids are drawn at the 50% probability level.

Tris(oxamide dioxime- κ^2N,N')nickel(II) sulfate pentahydrate

Crystal data

$[\text{Ni}(\text{C}_2\text{H}_6\text{N}_4\text{O}_2)_3]\text{SO}_4 \cdot 5\text{H}_2\text{O}$

$M_r = 599.17$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 12.3141$ (16) Å

$b = 14.0458$ (17) Å

$c = 14.7734$ (18) Å

$\alpha = 86.077$ (3)°

$\beta = 77.769$ (3)°

$\gamma = 72.868$ (3)°

$V = 2386.4$ (5) Å³

$Z = 4$

$F_{000} = 1248$

$D_x = 1.668$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 9771 reflections

$\theta = 1.4$ – 28.5 °

$\mu = 0.99$ mm⁻¹

$T = 293$ (2) K

Prism, violet

$0.25 \times 0.15 \times 0.10$ mm

Data collection

Bruker APEX CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293$ (2) K

φ and ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2001)

$T_{\min} = 0.789$, $T_{\max} = 0.907$

33235 measured reflections

11834 independent reflections

9771 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.029$

$\theta_{\max} = 28.5$ °

$\theta_{\min} = 1.4$ °

$h = -16 \rightarrow 16$

$k = -18 \rightarrow 18$

$l = -19 \rightarrow 19$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.053$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of

supplementary materials

| | |
|--|--|
| | independent and constrained refinement |
| $wR(F^2) = 0.164$ | $w = 1/[\sigma^2(F_o^2) + (0.085P)^2 + 2.9067P]$ |
| | where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.12$ | $(\Delta/\sigma)_{\max} = 0.001$ |
| 11834 reflections | $\Delta\rho_{\max} = 1.48 \text{ e } \text{\AA}^{-3}$ |
| 707 parameters | $\Delta\rho_{\min} = -1.45 \text{ e } \text{\AA}^{-3}$ |
| 23 restraints | Extinction correction: none |
| Primary atom site location: structure-invariant direct methods | |

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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ | Occ. (<1) |
|------|---------------|--------------|--------------|----------------------------------|-----------|
| Ni1 | 0.22824 (3) | 0.70919 (3) | 0.43918 (3) | 0.01960 (10) | |
| O11 | -0.03779 (18) | 0.75648 (17) | 0.42903 (17) | 0.0302 (5) | |
| H11 | -0.0565 | 0.7732 | 0.4836 | 0.045* | |
| O12 | 0.39957 (17) | 0.53631 (15) | 0.30737 (16) | 0.0258 (4) | |
| H12 | 0.4331 | 0.5629 | 0.2636 | 0.039* | |
| O13 | 0.17174 (19) | 0.53968 (16) | 0.58228 (18) | 0.0300 (5) | |
| H13 | 0.1029 | 0.5709 | 0.5956 | 0.045* | |
| O14 | 0.4687 (2) | 0.75163 (18) | 0.43870 (18) | 0.0330 (5) | |
| H14 | 0.4771 | 0.7611 | 0.3826 | 0.050* | |
| O15 | 0.1369 (2) | 0.84859 (17) | 0.61577 (15) | 0.0293 (5) | |
| H15 | 0.1001 | 0.8111 | 0.6422 | 0.044* | |
| O16 | 0.2531 (2) | 0.82103 (17) | 0.25043 (15) | 0.0288 (5) | |
| H16 | 0.3118 | 0.7757 | 0.2319 | 0.043* | |
| N11 | 0.0759 (2) | 0.69133 (18) | 0.41189 (18) | 0.0235 (5) | |
| N12 | 0.2847 (2) | 0.59940 (18) | 0.33832 (19) | 0.0240 (5) | |
| N13 | 0.2385 (2) | 0.60678 (18) | 0.54913 (18) | 0.0234 (5) | |
| N14 | 0.3927 (2) | 0.69172 (18) | 0.46659 (18) | 0.0231 (5) | |
| N15 | 0.1549 (2) | 0.83731 (18) | 0.51985 (17) | 0.0219 (5) | |
| N16 | 0.2318 (2) | 0.82492 (18) | 0.34758 (17) | 0.0226 (5) | |
| N17 | 0.2259 (2) | 0.4790 (2) | 0.2751 (2) | 0.0325 (6) | |
| H17A | 0.2957 | 0.4438 | 0.2538 | 0.039* | |
| H17B | 0.1683 | 0.4601 | 0.2668 | 0.039* | |
| N18 | -0.0021 (2) | 0.6149 (2) | 0.3162 (2) | 0.0327 (6) | |

| | | | | |
|------|-------------|--------------|--------------|--------------|
| H18A | -0.0712 | 0.6537 | 0.3331 | 0.039* |
| H18B | 0.0113 | 0.5690 | 0.2762 | 0.039* |
| N19 | 0.3688 (3) | 0.5020 (2) | 0.6338 (2) | 0.0380 (7) |
| H19A | 0.3223 | 0.4671 | 0.6561 | 0.046* |
| H19B | 0.4358 | 0.4880 | 0.6483 | 0.046* |
| N50 | 0.5092 (2) | 0.6344 (2) | 0.5760 (2) | 0.0327 (6) |
| H50A | 0.5551 | 0.6697 | 0.5535 | 0.039* |
| H50B | 0.5212 | 0.5966 | 0.6234 | 0.039* |
| N51 | 0.1255 (2) | 1.01000 (19) | 0.51951 (19) | 0.0259 (5) |
| H51A | 0.1094 | 1.0135 | 0.5790 | 0.031* |
| H51B | 0.1250 | 1.0630 | 0.4866 | 0.031* |
| N112 | 0.1564 (3) | 0.9958 (2) | 0.3233 (2) | 0.0320 (6) |
| H11A | 0.1743 | 0.9904 | 0.2639 | 0.038* |
| H11B | 0.1224 | 1.0533 | 0.3482 | 0.038* |
| C11 | 0.0851 (2) | 0.6260 (2) | 0.3521 (2) | 0.0223 (5) |
| C12 | 0.2069 (3) | 0.5620 (2) | 0.3206 (2) | 0.0217 (5) |
| C13 | 0.3367 (2) | 0.5783 (2) | 0.5762 (2) | 0.0235 (6) |
| C14 | 0.4192 (2) | 0.6382 (2) | 0.5373 (2) | 0.0232 (6) |
| C15 | 0.1513 (2) | 0.9220 (2) | 0.4781 (2) | 0.0209 (5) |
| C16 | 0.1813 (2) | 0.9149 (2) | 0.3766 (2) | 0.0213 (5) |
| Ni2 | 0.74507 (3) | 0.93920 (3) | 0.18804 (3) | 0.02347 (11) |
| O21 | 0.7713 (2) | 0.7911 (2) | 0.02902 (16) | 0.0394 (6) |
| H21 | 0.7026 | 0.7956 | 0.0489 | 0.059* |
| O22 | 0.9726 (2) | 0.92640 (18) | 0.25835 (17) | 0.0319 (5) |
| H22 | 0.9709 | 0.9850 | 0.2495 | 0.048* |
| O23 | 0.7535 (2) | 0.74561 (16) | 0.30809 (15) | 0.0278 (5) |
| H23 | 0.7345 | 0.7199 | 0.2681 | 0.042* |
| O24 | 0.6378 (2) | 1.14404 (17) | 0.29771 (19) | 0.0357 (5) |
| H24 | 0.6888 | 1.1691 | 0.2721 | 0.054* |
| O25 | 0.4745 (2) | 0.9706 (2) | 0.20188 (18) | 0.0405 (6) |
| H25 | 0.4820 | 0.9122 | 0.2175 | 0.061* |
| O26 | 0.8624 (2) | 1.0583 (2) | 0.02780 (17) | 0.0379 (6) |
| H26 | 0.9036 | 1.0671 | 0.0615 | 0.057* |
| N21 | 0.8177 (2) | 0.8203 (2) | 0.09796 (18) | 0.0282 (6) |
| N22 | 0.9191 (2) | 0.8971 (2) | 0.19356 (18) | 0.0264 (5) |
| N23 | 0.7122 (2) | 0.85047 (19) | 0.30099 (17) | 0.0244 (5) |
| N24 | 0.6833 (2) | 1.0389 (2) | 0.29737 (19) | 0.0283 (5) |
| N25 | 0.5823 (2) | 0.9807 (2) | 0.15110 (19) | 0.0303 (6) |
| N26 | 0.7602 (2) | 1.0431 (2) | 0.08268 (18) | 0.0282 (5) |
| N27 | 0.9930 (3) | 0.7204 (3) | 0.0169 (2) | 0.0479 (8) |
| H27A | 0.9603 | 0.7005 | -0.0212 | 0.057* |
| H27B | 1.0670 | 0.6991 | 0.0117 | 0.057* |
| N28 | 1.0966 (2) | 0.7732 (2) | 0.1539 (2) | 0.0341 (6) |
| H28A | 1.1294 | 0.7951 | 0.1905 | 0.041* |
| H28B | 1.1346 | 0.7214 | 0.1207 | 0.041* |
| N29 | 0.6902 (2) | 0.8415 (2) | 0.46124 (18) | 0.0279 (5) |
| H29A | 0.7101 | 0.7775 | 0.4619 | 0.034* |
| H29B | 0.6722 | 0.8738 | 0.5123 | 0.034* |
| N70 | 0.5991 (2) | 1.0539 (2) | 0.45455 (19) | 0.0304 (6) |

supplementary materials

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|------|--------------|--------------|---------------|--------------|-----------|
| H70A | 0.5787 | 1.1179 | 0.4525 | 0.037* | |
| H70B | 0.5833 | 1.0235 | 0.5060 | 0.037* | |
| N71 | 0.4611 (3) | 1.1035 (2) | 0.0738 (2) | 0.0366 (7) | |
| H71A | 0.3993 | 1.0897 | 0.1029 | 0.044* | |
| H71B | 0.4566 | 1.1505 | 0.0330 | 0.044* | |
| N72 | 0.6752 (3) | 1.1231 (3) | -0.0394 (2) | 0.0483 (9) | |
| H72A | 0.7380 | 1.1355 | -0.0684 | 0.058* | |
| H72B | 0.6138 | 1.1420 | -0.0627 | 0.058* | |
| C21 | 0.9295 (3) | 0.7833 (2) | 0.0833 (2) | 0.0279 (6) | |
| C22 | 0.9857 (3) | 0.8199 (2) | 0.1486 (2) | 0.0250 (6) | |
| C23 | 0.6871 (2) | 0.8908 (2) | 0.3812 (2) | 0.0241 (6) | |
| C24 | 0.6552 (2) | 1.0017 (2) | 0.3779 (2) | 0.0245 (6) | |
| C25 | 0.5645 (3) | 1.0519 (2) | 0.0922 (2) | 0.0245 (6) | |
| C26 | 0.6730 (3) | 1.0746 (2) | 0.0417 (2) | 0.0270 (6) | |
| S1 | 0.54943 (9) | 0.71047 (11) | 0.18146 (9) | 0.0654 (4) | |
| O1 | 0.5649 (3) | 0.7641 (3) | 0.0930 (2) | 0.0628 (10) | |
| O2B | 0.4535 (4) | 0.6686 (3) | 0.1908 (3) | 0.0363 (8) | 0.621 (5) |
| O2A | 0.5035 (6) | 0.6156 (5) | 0.1573 (5) | 0.0363 (8) | 0.379 (5) |
| O3 | 0.6619 (3) | 0.6507 (2) | 0.2002 (2) | 0.0468 (7) | |
| O4 | 0.4917 (3) | 0.7854 (3) | 0.2578 (3) | 0.0838 (15) | |
| S2 | -0.08243 (7) | 0.72405 (6) | 0.67222 (6) | 0.02780 (17) | |
| O10 | -0.0585 (2) | 0.63057 (16) | 0.62249 (18) | 0.0322 (5) | |
| O20 | -0.1067 (3) | 0.80865 (18) | 0.60729 (19) | 0.0422 (6) | |
| O30 | 0.0196 (2) | 0.72385 (18) | 0.70916 (18) | 0.0352 (5) | |
| O40 | -0.1855 (3) | 0.7347 (2) | 0.7468 (2) | 0.0541 (8) | |
| O1W | 0.2423 (2) | 0.36282 (18) | 0.47889 (18) | 0.0332 (5) | |
| H1W1 | 0.225 (4) | 0.417 (3) | 0.507 (3) | 0.050* | |
| H2W1 | 0.189 (3) | 0.361 (3) | 0.455 (3) | 0.050* | |
| O2W | 0.8027 (2) | 0.8875 (2) | -0.13981 (18) | 0.0373 (6) | |
| H1W2 | 0.804 (4) | 0.843 (3) | -0.177 (2) | 0.056* | |
| H2W2 | 0.788 (4) | 0.866 (3) | -0.0850 (18) | 0.056* | |
| O3W | 0.3647 (3) | 0.0814 (4) | 0.3596 (2) | 0.0728 (12) | |
| H1W3 | 0.410 (5) | 0.053 (5) | 0.311 (3) | 0.109* | |
| H2W3 | 0.302 (4) | 0.118 (5) | 0.344 (5) | 0.109* | |
| O4W | 0.9698 (2) | 0.0965 (2) | 0.1617 (2) | 0.0414 (6) | |
| H1W4 | 1.039 (2) | 0.102 (4) | 0.148 (4) | 0.062* | |
| H2W4 | 0.922 (3) | 0.153 (3) | 0.166 (4) | 0.062* | |
| O5W | 0.7762 (4) | 0.2610 (3) | 0.2056 (3) | 0.0689 (10) | |
| H1W5 | 0.738 (6) | 0.271 (5) | 0.160 (4) | 0.103* | |
| H2W5 | 0.795 (6) | 0.313 (4) | 0.212 (5) | 0.103* | |
| O6W | 0.4198 (3) | 0.2840 (3) | 0.2453 (3) | 0.0759 (12) | |
| H1W6 | 0.417 (6) | 0.308 (5) | 0.193 (3) | 0.114* | |
| H2W6 | 0.475 (5) | 0.236 (4) | 0.253 (5) | 0.114* | |
| O7W | 0.7536 (4) | 0.3573 (3) | 0.0333 (4) | 0.1086 (18) | |
| H7W1 | 0.7706 | 0.4088 | 0.0457 | 0.163* | |
| H7W2 | 0.6893 | 0.3750 | 0.0154 | 0.163* | |
| O8W | 0.8211 (6) | 0.5178 (5) | 0.0779 (5) | 0.131 (2) | |
| H1W8 | 0.860 (9) | 0.483 (7) | 0.124 (6) | 0.197* | |
| H2W8 | 0.788 (9) | 0.576 (4) | 0.109 (6) | 0.197* | |

| | | | | | |
|------|-------------|-------------|--------------|-------------|-----------|
| O9W | 0.5490 (7) | 0.4195 (6) | -0.0320 (5) | 0.0457 (11) | 0.356 (3) |
| O10W | 0.5124 (8) | 0.3663 (7) | 0.0475 (6) | 0.0457 (11) | 0.324 (5) |
| O11W | 0.3927 (8) | 0.3266 (7) | 0.0828 (6) | 0.0457 (11) | 0.320 (5) |
| O12W | 0.9444 (16) | 0.5729 (10) | -0.1176 (11) | 0.0641 (17) | 0.247 (3) |
| O13W | 0.8574 (13) | 0.6098 (9) | -0.0713 (9) | 0.0641 (17) | 0.293 (6) |
| O14W | 1.0291 (8) | 0.5305 (5) | -0.1952 (5) | 0.0641 (17) | 0.460 (6) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|------|--------------|--------------|--------------|---------------|---------------|--------------|
| Ni1 | 0.01604 (18) | 0.01608 (17) | 0.0279 (2) | -0.00461 (13) | -0.00771 (14) | 0.00212 (13) |
| O11 | 0.0170 (10) | 0.0300 (11) | 0.0385 (12) | 0.0027 (8) | -0.0067 (9) | -0.0037 (10) |
| O12 | 0.0168 (10) | 0.0200 (10) | 0.0362 (12) | -0.0023 (8) | -0.0018 (8) | 0.0043 (8) |
| O13 | 0.0192 (10) | 0.0201 (10) | 0.0508 (14) | -0.0084 (8) | -0.0059 (10) | 0.0078 (9) |
| O14 | 0.0314 (12) | 0.0328 (12) | 0.0446 (14) | -0.0214 (10) | -0.0161 (11) | 0.0150 (10) |
| O15 | 0.0381 (13) | 0.0318 (12) | 0.0234 (10) | -0.0187 (10) | -0.0059 (9) | 0.0022 (9) |
| O16 | 0.0266 (11) | 0.0313 (12) | 0.0235 (10) | 0.0019 (9) | -0.0084 (8) | -0.0010 (9) |
| N11 | 0.0131 (11) | 0.0220 (12) | 0.0337 (13) | -0.0013 (9) | -0.0058 (9) | -0.0014 (10) |
| N12 | 0.0149 (11) | 0.0209 (11) | 0.0352 (14) | -0.0037 (9) | -0.0044 (10) | -0.0010 (10) |
| N13 | 0.0186 (11) | 0.0171 (11) | 0.0354 (14) | -0.0075 (9) | -0.0057 (10) | 0.0044 (10) |
| N14 | 0.0179 (11) | 0.0199 (11) | 0.0338 (13) | -0.0082 (9) | -0.0077 (10) | 0.0051 (10) |
| N15 | 0.0238 (12) | 0.0219 (11) | 0.0220 (11) | -0.0090 (9) | -0.0060 (9) | 0.0016 (9) |
| N16 | 0.0221 (12) | 0.0235 (12) | 0.0214 (11) | -0.0044 (9) | -0.0063 (9) | 0.0014 (9) |
| N17 | 0.0261 (13) | 0.0258 (13) | 0.0479 (17) | -0.0073 (11) | -0.0104 (12) | -0.0082 (12) |
| N18 | 0.0245 (13) | 0.0303 (14) | 0.0473 (17) | -0.0067 (11) | -0.0159 (12) | -0.0054 (12) |
| N19 | 0.0282 (14) | 0.0362 (16) | 0.0521 (18) | -0.0121 (12) | -0.0171 (13) | 0.0226 (14) |
| N50 | 0.0284 (14) | 0.0373 (15) | 0.0393 (15) | -0.0151 (12) | -0.0182 (12) | 0.0140 (12) |
| N51 | 0.0300 (13) | 0.0198 (11) | 0.0299 (13) | -0.0077 (10) | -0.0093 (10) | -0.0001 (10) |
| N112 | 0.0444 (16) | 0.0207 (12) | 0.0321 (14) | -0.0069 (11) | -0.0155 (12) | 0.0055 (10) |
| C11 | 0.0196 (13) | 0.0201 (13) | 0.0290 (14) | -0.0083 (10) | -0.0073 (11) | 0.0056 (11) |
| C12 | 0.0232 (14) | 0.0179 (12) | 0.0245 (13) | -0.0069 (10) | -0.0054 (11) | 0.0025 (10) |
| C13 | 0.0201 (13) | 0.0198 (13) | 0.0297 (14) | -0.0041 (10) | -0.0061 (11) | 0.0021 (11) |
| C14 | 0.0187 (13) | 0.0206 (13) | 0.0302 (15) | -0.0049 (10) | -0.0063 (11) | 0.0015 (11) |
| C15 | 0.0151 (12) | 0.0198 (12) | 0.0294 (14) | -0.0045 (10) | -0.0092 (10) | 0.0017 (11) |
| C16 | 0.0183 (13) | 0.0197 (13) | 0.0280 (14) | -0.0062 (10) | -0.0097 (11) | 0.0037 (11) |
| Ni2 | 0.01747 (19) | 0.0306 (2) | 0.02196 (19) | -0.00640 (15) | -0.00600 (14) | 0.00652 (15) |
| O21 | 0.0372 (14) | 0.0701 (18) | 0.0243 (11) | -0.0338 (13) | -0.0104 (10) | 0.0040 (11) |
| O22 | 0.0314 (12) | 0.0339 (12) | 0.0366 (12) | -0.0116 (10) | -0.0172 (10) | -0.0002 (10) |
| O23 | 0.0298 (11) | 0.0237 (10) | 0.0297 (11) | -0.0027 (9) | -0.0135 (9) | 0.0020 (8) |
| O24 | 0.0307 (12) | 0.0252 (11) | 0.0460 (14) | -0.0040 (9) | -0.0049 (10) | 0.0080 (10) |
| O25 | 0.0190 (11) | 0.0626 (17) | 0.0356 (13) | -0.0116 (11) | -0.0021 (9) | 0.0185 (12) |
| O26 | 0.0262 (12) | 0.0592 (16) | 0.0315 (12) | -0.0197 (11) | -0.0066 (9) | 0.0153 (11) |
| N21 | 0.0260 (13) | 0.0424 (15) | 0.0223 (12) | -0.0176 (12) | -0.0076 (10) | 0.0025 (11) |
| N22 | 0.0215 (12) | 0.0339 (14) | 0.0280 (13) | -0.0101 (10) | -0.0113 (10) | 0.0003 (11) |
| N23 | 0.0229 (12) | 0.0233 (12) | 0.0248 (12) | -0.0028 (10) | -0.0067 (10) | 0.0046 (10) |
| N24 | 0.0258 (13) | 0.0240 (12) | 0.0316 (14) | -0.0027 (10) | -0.0062 (10) | 0.0050 (10) |
| N25 | 0.0166 (12) | 0.0442 (16) | 0.0280 (13) | -0.0090 (11) | -0.0038 (10) | 0.0127 (12) |
| N26 | 0.0223 (12) | 0.0377 (14) | 0.0259 (12) | -0.0117 (11) | -0.0056 (10) | 0.0077 (11) |

supplementary materials

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|------|-------------|-------------|-------------|--------------|--------------|--------------|
| N27 | 0.0390 (18) | 0.057 (2) | 0.0458 (19) | -0.0105 (16) | -0.0035 (14) | -0.0215 (16) |
| N28 | 0.0219 (13) | 0.0362 (15) | 0.0429 (16) | -0.0039 (11) | -0.0087 (11) | -0.0038 (12) |
| N29 | 0.0292 (13) | 0.0281 (13) | 0.0235 (12) | -0.0045 (11) | -0.0053 (10) | 0.0036 (10) |
| N70 | 0.0267 (13) | 0.0301 (14) | 0.0303 (14) | -0.0038 (11) | -0.0025 (11) | -0.0014 (11) |
| N71 | 0.0261 (14) | 0.0346 (15) | 0.0498 (18) | -0.0071 (12) | -0.0165 (12) | 0.0163 (13) |
| N72 | 0.0368 (17) | 0.073 (2) | 0.0435 (18) | -0.0267 (17) | -0.0216 (14) | 0.0350 (17) |
| C21 | 0.0264 (15) | 0.0311 (16) | 0.0265 (15) | -0.0116 (12) | -0.0018 (12) | 0.0000 (12) |
| C22 | 0.0200 (13) | 0.0277 (14) | 0.0281 (14) | -0.0093 (11) | -0.0040 (11) | 0.0032 (12) |
| C23 | 0.0149 (12) | 0.0298 (15) | 0.0261 (14) | -0.0040 (11) | -0.0057 (10) | 0.0046 (11) |
| C24 | 0.0151 (12) | 0.0289 (15) | 0.0282 (14) | -0.0029 (11) | -0.0068 (11) | 0.0012 (12) |
| C25 | 0.0221 (14) | 0.0277 (14) | 0.0246 (14) | -0.0065 (11) | -0.0084 (11) | 0.0025 (11) |
| C26 | 0.0278 (15) | 0.0287 (15) | 0.0257 (14) | -0.0095 (12) | -0.0085 (12) | 0.0079 (12) |
| S1 | 0.0390 (5) | 0.1017 (10) | 0.0765 (8) | -0.0486 (6) | -0.0389 (6) | 0.0710 (8) |
| O1 | 0.0446 (16) | 0.096 (3) | 0.068 (2) | -0.0469 (17) | -0.0350 (15) | 0.0597 (19) |
| O2B | 0.032 (2) | 0.037 (2) | 0.045 (2) | -0.0197 (16) | -0.0063 (16) | 0.0074 (16) |
| O2A | 0.032 (2) | 0.037 (2) | 0.045 (2) | -0.0197 (16) | -0.0063 (16) | 0.0074 (16) |
| O3 | 0.0505 (17) | 0.0438 (15) | 0.0553 (17) | -0.0146 (13) | -0.0335 (14) | 0.0150 (13) |
| O4 | 0.0345 (16) | 0.115 (3) | 0.064 (2) | 0.0070 (18) | 0.0118 (15) | 0.060 (2) |
| S2 | 0.0260 (4) | 0.0218 (3) | 0.0372 (4) | -0.0098 (3) | -0.0053 (3) | -0.0005 (3) |
| O10 | 0.0263 (11) | 0.0222 (10) | 0.0496 (14) | -0.0084 (9) | -0.0075 (10) | -0.0039 (10) |
| O20 | 0.0579 (17) | 0.0223 (11) | 0.0469 (15) | -0.0038 (11) | -0.0224 (13) | -0.0006 (10) |
| O30 | 0.0382 (13) | 0.0337 (12) | 0.0410 (13) | -0.0179 (10) | -0.0148 (11) | 0.0058 (10) |
| O40 | 0.0426 (16) | 0.0634 (19) | 0.0584 (18) | -0.0302 (15) | 0.0133 (13) | -0.0214 (15) |
| O1W | 0.0303 (12) | 0.0305 (12) | 0.0419 (14) | -0.0096 (10) | -0.0138 (10) | 0.0021 (10) |
| O2W | 0.0401 (14) | 0.0443 (15) | 0.0294 (12) | -0.0156 (12) | -0.0069 (11) | 0.0021 (11) |
| O3W | 0.0364 (16) | 0.128 (4) | 0.0477 (18) | -0.0053 (19) | -0.0114 (14) | -0.032 (2) |
| O4W | 0.0399 (14) | 0.0454 (15) | 0.0444 (15) | -0.0215 (12) | -0.0095 (12) | 0.0063 (12) |
| O5W | 0.067 (2) | 0.062 (2) | 0.077 (3) | -0.0253 (19) | -0.0048 (19) | 0.0059 (19) |
| O6W | 0.052 (2) | 0.0450 (19) | 0.132 (4) | 0.0006 (16) | -0.037 (2) | -0.016 (2) |
| O7W | 0.059 (3) | 0.063 (3) | 0.188 (6) | -0.005 (2) | -0.004 (3) | -0.021 (3) |
| O8W | 0.122 (5) | 0.086 (4) | 0.185 (7) | -0.003 (3) | -0.056 (5) | -0.038 (4) |
| O9W | 0.055 (3) | 0.047 (3) | 0.031 (2) | -0.002 (2) | -0.016 (2) | -0.0087 (19) |
| O10W | 0.055 (3) | 0.047 (3) | 0.031 (2) | -0.002 (2) | -0.016 (2) | -0.0087 (19) |
| O11W | 0.055 (3) | 0.047 (3) | 0.031 (2) | -0.002 (2) | -0.016 (2) | -0.0087 (19) |
| O12W | 0.099 (5) | 0.047 (3) | 0.062 (4) | -0.024 (3) | -0.052 (3) | 0.019 (3) |
| O13W | 0.099 (5) | 0.047 (3) | 0.062 (4) | -0.024 (3) | -0.052 (3) | 0.019 (3) |
| O14W | 0.099 (5) | 0.047 (3) | 0.062 (4) | -0.024 (3) | -0.052 (3) | 0.019 (3) |

Geometric parameters (Å, °)

| | | | |
|---------|-----------|---------|-----------|
| Ni1—N16 | 2.047 (2) | O24—H24 | 0.82 |
| Ni1—N12 | 2.080 (3) | O25—N25 | 1.422 (3) |
| Ni1—N15 | 2.087 (2) | O25—H25 | 0.82 |
| Ni1—N11 | 2.087 (2) | O26—N26 | 1.411 (3) |
| Ni1—N14 | 2.089 (2) | O26—H26 | 0.82 |
| Ni1—N13 | 2.094 (3) | N21—C21 | 1.296 (4) |
| O11—N11 | 1.410 (3) | N22—C22 | 1.278 (4) |
| O11—H11 | 0.82 | N23—C23 | 1.286 (4) |
| O12—N12 | 1.428 (3) | N24—C24 | 1.287 (4) |

| | | | |
|-----------|-----------|----------|-----------|
| O12—H12 | 0.82 | N25—C25 | 1.280 (4) |
| O13—N13 | 1.424 (3) | N26—C26 | 1.294 (4) |
| O13—H13 | 0.82 | N27—C21 | 1.320 (4) |
| O14—N14 | 1.417 (3) | N27—H27A | 0.86 |
| O14—H14 | 0.82 | N27—H27B | 0.86 |
| O15—N15 | 1.400 (3) | N28—C22 | 1.346 (4) |
| O15—H15 | 0.82 | N28—H28A | 0.86 |
| O16—N16 | 1.405 (3) | N28—H28B | 0.86 |
| O16—H16 | 0.82 | N29—C23 | 1.330 (4) |
| N11—C11 | 1.282 (4) | N29—H29A | 0.86 |
| N12—C12 | 1.297 (4) | N29—H29B | 0.86 |
| N13—C13 | 1.296 (4) | N70—C24 | 1.334 (4) |
| N14—C14 | 1.287 (4) | N70—H70A | 0.86 |
| N15—C15 | 1.295 (4) | N70—H70B | 0.86 |
| N16—C16 | 1.290 (4) | N71—C25 | 1.340 (4) |
| N17—C12 | 1.322 (4) | N71—H71A | 0.86 |
| N17—H17A | 0.86 | N71—H71B | 0.86 |
| N17—H17B | 0.86 | N72—C26 | 1.337 (4) |
| N18—C11 | 1.345 (4) | N72—H72A | 0.86 |
| N18—H18A | 0.86 | N72—H72B | 0.86 |
| N18—H18B | 0.86 | C21—C22 | 1.495 (4) |
| N19—C13 | 1.340 (4) | C23—C24 | 1.491 (4) |
| N19—H19A | 0.86 | C25—C26 | 1.496 (4) |
| N19—H19B | 0.86 | S1—O2B | 1.446 (4) |
| N50—C14 | 1.337 (4) | S1—O3 | 1.465 (3) |
| N50—H50A | 0.86 | S1—O1 | 1.468 (3) |
| N50—H50B | 0.86 | S1—O4 | 1.506 (5) |
| N51—C15 | 1.339 (4) | S1—O2A | 1.678 (7) |
| N51—H51A | 0.86 | S2—O10 | 1.471 (2) |
| N51—H51B | 0.86 | S2—O30 | 1.471 (3) |
| N112—C16 | 1.335 (4) | S2—O40 | 1.472 (3) |
| N112—H11A | 0.86 | S2—O20 | 1.476 (3) |
| N112—H11B | 0.86 | O1W—H1W1 | 0.84 (2) |
| C11—C12 | 1.497 (4) | O1W—H2W1 | 0.82 (2) |
| C13—C14 | 1.503 (4) | O2W—H1W2 | 0.86 (3) |
| C15—C16 | 1.470 (4) | O2W—H2W2 | 0.84 (3) |
| Ni2—N23 | 2.056 (3) | O3W—H1W3 | 0.85 (3) |
| Ni2—N22 | 2.066 (3) | O3W—H2W3 | 0.86 (3) |
| Ni2—N21 | 2.068 (3) | O4W—H1W4 | 0.85 (3) |
| Ni2—N24 | 2.076 (3) | O4W—H2W4 | 0.83 (3) |
| Ni2—N26 | 2.077 (3) | O5W—H1W5 | 0.88 (3) |
| Ni2—N25 | 2.095 (3) | O5W—H2W5 | 0.84 (3) |
| O21—N21 | 1.405 (3) | O6W—H1W6 | 0.83 (3) |
| O21—H21 | 0.82 | O6W—H2W6 | 0.82 (3) |
| O22—N22 | 1.414 (3) | O7W—H7W1 | 0.85 |
| O22—H22 | 0.82 | O7W—H7W2 | 0.85 |
| O23—N23 | 1.414 (3) | O8W—H1W8 | 0.95 (3) |
| O23—H23 | 0.82 | O8W—H2W8 | 0.91 (3) |
| O24—N24 | 1.416 (3) | | |

supplementary materials

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| N16—Ni1—N12 | 95.16 (10) | N21—Ni2—N25 | 95.71 (11) |
| N16—Ni1—N15 | 75.08 (10) | N24—Ni2—N25 | 91.10 (11) |
| N12—Ni1—N15 | 168.23 (10) | N26—Ni2—N25 | 76.44 (10) |
| N16—Ni1—N11 | 94.49 (10) | N21—O21—H21 | 109.5 |
| N12—Ni1—N11 | 75.53 (10) | N22—O22—H22 | 109.5 |
| N15—Ni1—N11 | 98.36 (10) | N23—O23—H23 | 109.5 |
| N16—Ni1—N14 | 95.36 (10) | N24—O24—H24 | 109.5 |
| N12—Ni1—N14 | 95.08 (10) | N25—O25—H25 | 109.5 |
| N15—Ni1—N14 | 92.42 (10) | N26—O26—H26 | 109.5 |
| N11—Ni1—N14 | 166.96 (10) | C21—N21—O21 | 111.2 (3) |
| N16—Ni1—N13 | 168.20 (10) | C21—N21—Ni2 | 117.0 (2) |
| N12—Ni1—N13 | 93.84 (10) | O21—N21—Ni2 | 128.9 (2) |
| N15—Ni1—N13 | 96.75 (10) | C22—N22—O22 | 111.7 (2) |
| N11—Ni1—N13 | 95.14 (10) | C22—N22—Ni2 | 118.3 (2) |
| N14—Ni1—N13 | 76.23 (10) | O22—N22—Ni2 | 128.0 (2) |
| N11—O11—H11 | 109.5 | C23—N23—O23 | 110.7 (2) |
| N12—O12—H12 | 109.5 | C23—N23—Ni2 | 116.9 (2) |
| N13—O13—H13 | 109.5 | O23—N23—Ni2 | 127.93 (18) |
| N14—O14—H14 | 109.5 | C24—N24—O24 | 111.2 (3) |
| N15—O15—H15 | 109.5 | C24—N24—Ni2 | 116.0 (2) |
| N16—O16—H16 | 109.5 | O24—N24—Ni2 | 130.5 (2) |
| C11—N11—O11 | 109.9 (2) | C25—N25—O25 | 109.8 (2) |
| C11—N11—Ni1 | 117.98 (19) | C25—N25—Ni2 | 116.4 (2) |
| O11—N11—Ni1 | 129.75 (19) | O25—N25—Ni2 | 129.53 (19) |
| C12—N12—O12 | 112.0 (2) | C26—N26—O26 | 111.9 (2) |
| C12—N12—Ni1 | 116.5 (2) | C26—N26—Ni2 | 115.9 (2) |
| O12—N12—Ni1 | 128.10 (18) | O26—N26—Ni2 | 128.2 (2) |
| C13—N13—O13 | 110.4 (2) | C21—N27—H27A | 120.0 |
| C13—N13—Ni1 | 116.1 (2) | C21—N27—H27B | 120.0 |
| O13—N13—Ni1 | 130.52 (18) | H27A—N27—H27B | 120.0 |
| C14—N14—O14 | 110.0 (2) | C22—N28—H28A | 120.0 |
| C14—N14—Ni1 | 117.3 (2) | C22—N28—H28B | 120.0 |
| O14—N14—Ni1 | 129.70 (18) | H28A—N28—H28B | 120.0 |
| C15—N15—O15 | 110.4 (2) | C23—N29—H29A | 120.0 |
| C15—N15—Ni1 | 117.2 (2) | C23—N29—H29B | 120.0 |
| O15—N15—Ni1 | 129.94 (18) | H29A—N29—H29B | 120.0 |
| C16—N16—O16 | 111.1 (2) | C24—N70—H70A | 120.0 |
| C16—N16—Ni1 | 118.9 (2) | C24—N70—H70B | 120.0 |
| O16—N16—Ni1 | 127.38 (18) | H70A—N70—H70B | 120.0 |
| C12—N17—H17A | 120.0 | C25—N71—H71A | 120.0 |
| C12—N17—H17B | 120.0 | C25—N71—H71B | 120.0 |
| H17A—N17—H17B | 120.0 | H71A—N71—H71B | 120.0 |
| C11—N18—H18A | 120.0 | C26—N72—H72A | 120.0 |
| C11—N18—H18B | 120.0 | C26—N72—H72B | 120.0 |
| H18A—N18—H18B | 120.0 | H72A—N72—H72B | 120.0 |
| C13—N19—H19A | 120.0 | N21—C21—N27 | 125.6 (3) |
| C13—N19—H19B | 120.0 | N21—C21—C22 | 113.9 (3) |
| H19A—N19—H19B | 120.0 | N27—C21—C22 | 120.4 (3) |
| C14—N50—H50A | 120.0 | N22—C22—N28 | 126.8 (3) |

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| C14—N50—H50B | 120.0 | N22—C22—C21 | 113.2 (3) |
| H50A—N50—H50B | 120.0 | N28—C22—C21 | 120.0 (3) |
| C15—N51—H51A | 120.0 | N23—C23—N29 | 125.3 (3) |
| C15—N51—H51B | 120.0 | N23—C23—C24 | 113.6 (3) |
| H51A—N51—H51B | 120.0 | N29—C23—C24 | 121.1 (3) |
| C16—N112—H11A | 120.0 | N24—C24—N70 | 125.5 (3) |
| C16—N112—H11B | 120.0 | N24—C24—C23 | 114.7 (3) |
| H11A—N112—H11B | 120.0 | N70—C24—C23 | 119.8 (3) |
| N11—C11—N18 | 125.7 (3) | N25—C25—N71 | 125.8 (3) |
| N11—C11—C12 | 113.4 (2) | N25—C25—C26 | 113.6 (3) |
| N18—C11—C12 | 120.9 (3) | N71—C25—C26 | 120.6 (3) |
| N12—C12—N17 | 126.8 (3) | N26—C26—N72 | 124.9 (3) |
| N12—C12—C11 | 113.6 (2) | N26—C26—C25 | 114.6 (3) |
| N17—C12—C11 | 119.5 (3) | N72—C26—C25 | 120.4 (3) |
| N13—C13—N19 | 125.8 (3) | O2B—S1—O3 | 121.3 (2) |
| N13—C13—C14 | 114.9 (3) | O2B—S1—O1 | 110.8 (2) |
| N19—C13—C14 | 119.3 (3) | O3—S1—O1 | 110.49 (19) |
| N14—C14—N50 | 125.5 (3) | O2B—S1—O4 | 95.4 (3) |
| N14—C14—C13 | 113.5 (3) | O3—S1—O4 | 108.7 (2) |
| N50—C14—C13 | 121.0 (3) | O1—S1—O4 | 108.7 (2) |
| N15—C15—N51 | 125.8 (3) | O3—S1—O2A | 97.2 (3) |
| N15—C15—C16 | 113.8 (3) | O1—S1—O2A | 104.2 (3) |
| N51—C15—C16 | 120.4 (3) | O4—S1—O2A | 126.7 (3) |
| N16—C16—N112 | 125.8 (3) | O10—S2—O30 | 109.54 (14) |
| N16—C16—C15 | 113.1 (2) | O10—S2—O40 | 109.32 (16) |
| N112—C16—C15 | 121.1 (3) | O30—S2—O40 | 111.26 (18) |
| N23—Ni2—N22 | 90.48 (10) | O10—S2—O20 | 109.14 (15) |
| N23—Ni2—N21 | 93.75 (10) | O30—S2—O20 | 109.04 (15) |
| N22—Ni2—N21 | 75.89 (10) | O40—S2—O20 | 108.51 (19) |
| N23—Ni2—N24 | 76.68 (10) | H1W1—O1W—H2W1 | 111 (3) |
| N22—Ni2—N24 | 98.66 (11) | H1W2—O2W—H2W2 | 108 (3) |
| N21—Ni2—N24 | 169.08 (10) | H1W3—O3W—H2W3 | 108 (4) |
| N23—Ni2—N26 | 172.62 (11) | H1W4—O4W—H2W4 | 110 (4) |
| N22—Ni2—N26 | 94.45 (10) | H1W5—O5W—H2W5 | 108 (4) |
| N21—Ni2—N26 | 92.77 (11) | H1W6—O6W—H2W6 | 119 (5) |
| N24—Ni2—N26 | 97.12 (11) | H7W1—O7W—H7W2 | 109.5 |
| N23—Ni2—N25 | 99.46 (10) | H1W8—O8W—H2W8 | 97 (3) |
| N22—Ni2—N25 | 167.46 (11) | | |
| N16—Ni1—N11—C11 | 95.2 (2) | N15—C15—C16—N112 | 164.4 (3) |
| N12—Ni1—N11—C11 | 1.0 (2) | N51—C15—C16—N112 | -16.8 (4) |
| N15—Ni1—N11—C11 | 170.7 (2) | N23—Ni2—N21—C21 | -94.2 (2) |
| N14—Ni1—N11—C11 | -43.8 (6) | N22—Ni2—N21—C21 | -4.6 (2) |
| N13—Ni1—N11—C11 | -91.7 (2) | N24—Ni2—N21—C21 | -65.7 (6) |
| N16—Ni1—N11—O11 | -65.5 (3) | N26—Ni2—N21—C21 | 89.3 (2) |
| N12—Ni1—N11—O11 | -159.7 (3) | N25—Ni2—N21—C21 | 165.9 (2) |
| N15—Ni1—N11—O11 | 10.0 (3) | N23—Ni2—N21—O21 | 106.9 (2) |
| N14—Ni1—N11—O11 | 155.5 (4) | N22—Ni2—N21—O21 | -163.5 (3) |
| N13—Ni1—N11—O11 | 107.6 (2) | N24—Ni2—N21—O21 | 135.4 (5) |
| N16—Ni1—N12—C12 | -104.9 (2) | N26—Ni2—N21—O21 | -69.6 (2) |

supplementary materials

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| N15—Ni1—N12—C12 | -71.4 (5) | N25—Ni2—N21—O21 | 7.0 (3) |
| N11—Ni1—N12—C12 | -11.6 (2) | N23—Ni2—N22—C22 | 89.3 (2) |
| N14—Ni1—N12—C12 | 159.2 (2) | N21—Ni2—N22—C22 | -4.5 (2) |
| N13—Ni1—N12—C12 | 82.7 (2) | N24—Ni2—N22—C22 | 165.9 (2) |
| N16—Ni1—N12—O12 | 97.8 (2) | N26—Ni2—N22—C22 | -96.2 (2) |
| N15—Ni1—N12—O12 | 131.3 (4) | N25—Ni2—N22—C22 | -53.4 (6) |
| N11—Ni1—N12—O12 | -168.9 (2) | N23—Ni2—N22—O22 | -73.3 (2) |
| N14—Ni1—N12—O12 | 1.9 (2) | N21—Ni2—N22—O22 | -167.1 (3) |
| N13—Ni1—N12—O12 | -74.6 (2) | N24—Ni2—N22—O22 | 3.3 (3) |
| N16—Ni1—N13—C13 | -49.3 (6) | N26—Ni2—N22—O22 | 101.2 (2) |
| N12—Ni1—N13—C13 | 90.4 (2) | N25—Ni2—N22—O22 | 144.1 (5) |
| N15—Ni1—N13—C13 | -94.8 (2) | N22—Ni2—N23—C23 | 89.8 (2) |
| N11—Ni1—N13—C13 | 166.1 (2) | N21—Ni2—N23—C23 | 165.6 (2) |
| N14—Ni1—N13—C13 | -3.9 (2) | N24—Ni2—N23—C23 | -9.0 (2) |
| N16—Ni1—N13—O13 | 152.2 (4) | N25—Ni2—N23—C23 | -97.9 (2) |
| N12—Ni1—N13—O13 | -68.1 (2) | N22—Ni2—N23—O23 | -64.0 (2) |
| N15—Ni1—N13—O13 | 106.8 (2) | N21—Ni2—N23—O23 | 11.9 (2) |
| N11—Ni1—N13—O13 | 7.7 (2) | N24—Ni2—N23—O23 | -162.8 (2) |
| N14—Ni1—N13—O13 | -162.4 (3) | N25—Ni2—N23—O23 | 108.3 (2) |
| N16—Ni1—N14—C14 | 165.9 (2) | N23—Ni2—N24—C24 | -0.3 (2) |
| N12—Ni1—N14—C14 | -98.4 (2) | N22—Ni2—N24—C24 | -88.7 (2) |
| N15—Ni1—N14—C14 | 90.7 (2) | N21—Ni2—N24—C24 | -29.6 (7) |
| N11—Ni1—N14—C14 | -55.2 (6) | N26—Ni2—N24—C24 | 175.6 (2) |
| N13—Ni1—N14—C14 | -5.7 (2) | N25—Ni2—N24—C24 | 99.2 (2) |
| N16—Ni1—N14—O14 | 7.6 (3) | N23—Ni2—N24—O24 | -161.4 (3) |
| N12—Ni1—N14—O14 | 103.3 (3) | N22—Ni2—N24—O24 | 110.2 (3) |
| N15—Ni1—N14—O14 | -67.7 (3) | N21—Ni2—N24—O24 | 169.3 (4) |
| N11—Ni1—N14—O14 | 146.5 (4) | N26—Ni2—N24—O24 | 14.5 (3) |
| N13—Ni1—N14—O14 | -164.0 (3) | N25—Ni2—N24—O24 | -61.9 (3) |
| N16—Ni1—N15—C15 | -2.7 (2) | N23—Ni2—N25—C25 | 167.6 (2) |
| N12—Ni1—N15—C15 | -37.4 (6) | N22—Ni2—N25—C25 | -50.4 (7) |
| N11—Ni1—N15—C15 | -95.2 (2) | N21—Ni2—N25—C25 | -97.6 (3) |
| N14—Ni1—N15—C15 | 92.2 (2) | N24—Ni2—N25—C25 | 90.9 (3) |
| N13—Ni1—N15—C15 | 168.6 (2) | N26—Ni2—N25—C25 | -6.1 (2) |
| N16—Ni1—N15—O15 | -162.8 (2) | N23—Ni2—N25—O25 | 13.4 (3) |
| N12—Ni1—N15—O15 | 162.5 (4) | N22—Ni2—N25—O25 | 155.4 (4) |
| N11—Ni1—N15—O15 | 104.8 (2) | N21—Ni2—N25—O25 | 108.2 (3) |
| N14—Ni1—N15—O15 | -67.9 (2) | N24—Ni2—N25—O25 | -63.3 (3) |
| N13—Ni1—N15—O15 | 8.5 (2) | N26—Ni2—N25—O25 | -160.4 (3) |
| N12—Ni1—N16—C16 | 166.6 (2) | N22—Ni2—N26—C26 | 165.5 (3) |
| N15—Ni1—N16—C16 | -6.7 (2) | N21—Ni2—N26—C26 | 89.5 (3) |
| N11—Ni1—N16—C16 | 90.8 (2) | N24—Ni2—N26—C26 | -95.2 (3) |
| N14—Ni1—N16—C16 | -97.8 (2) | N25—Ni2—N26—C26 | -5.8 (2) |
| N13—Ni1—N16—C16 | -53.8 (6) | N22—Ni2—N26—O26 | 10.2 (3) |
| N12—Ni1—N16—O16 | 6.7 (2) | N21—Ni2—N26—O26 | -65.8 (3) |
| N15—Ni1—N16—O16 | -166.6 (2) | N24—Ni2—N26—O26 | 109.5 (3) |
| N11—Ni1—N16—O16 | -69.2 (2) | N25—Ni2—N26—O26 | -161.1 (3) |
| N14—Ni1—N16—O16 | 102.3 (2) | O21—N21—C21—N27 | -4.7 (5) |
| N13—Ni1—N16—O16 | 146.2 (4) | Ni2—N21—C21—N27 | -167.2 (3) |

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| O11—N11—C11—N18 | -5.1 (4) | O21—N21—C21—C22 | 174.1 (3) |
| Ni1—N11—C11—N18 | -169.4 (2) | Ni2—N21—C21—C22 | 11.6 (4) |
| O11—N11—C11—C12 | 172.4 (2) | O22—N22—C22—N28 | -4.7 (5) |
| Ni1—N11—C11—C12 | 8.1 (3) | Ni2—N22—C22—N28 | -170.0 (3) |
| O12—N12—C12—N17 | -3.7 (4) | O22—N22—C22—C21 | 176.7 (2) |
| Ni1—N12—C12—N17 | -164.6 (3) | Ni2—N22—C22—C21 | 11.4 (3) |
| O12—N12—C12—C11 | 179.9 (2) | N21—C21—C22—N22 | -15.0 (4) |
| Ni1—N12—C12—C11 | 19.1 (3) | N27—C21—C22—N22 | 163.9 (3) |
| N11—C11—C12—N12 | -17.8 (4) | N21—C21—C22—N28 | 166.3 (3) |
| N18—C11—C12—N12 | 159.9 (3) | N27—C21—C22—N28 | -14.8 (5) |
| N11—C11—C12—N17 | 165.6 (3) | O23—N23—C23—N29 | -5.1 (4) |
| N18—C11—C12—N17 | -16.7 (4) | Ni2—N23—C23—N29 | -163.2 (2) |
| O13—N13—C13—N19 | -5.4 (4) | O23—N23—C23—C24 | 173.7 (2) |
| Ni1—N13—C13—N19 | -168.1 (3) | Ni2—N23—C23—C24 | 15.6 (3) |
| O13—N13—C13—C14 | 174.2 (2) | O24—N24—C24—N70 | -5.4 (4) |
| Ni1—N13—C13—C14 | 11.6 (3) | Ni2—N24—C24—N70 | -170.1 (2) |
| O14—N14—C14—N50 | -3.8 (4) | O24—N24—C24—C23 | 172.9 (2) |
| Ni1—N14—C14—N50 | -166.2 (3) | Ni2—N24—C24—C23 | 8.2 (3) |
| O14—N14—C14—C13 | 175.3 (2) | N23—C23—C24—N24 | -15.7 (4) |
| Ni1—N14—C14—C13 | 12.9 (3) | N29—C23—C24—N24 | 163.2 (3) |
| N13—C13—C14—N14 | -16.2 (4) | N23—C23—C24—N70 | 162.6 (3) |
| N19—C13—C14—N14 | 163.5 (3) | N29—C23—C24—N70 | -18.5 (4) |
| N13—C13—C14—N50 | 162.9 (3) | O25—N25—C25—N71 | -6.0 (5) |
| N19—C13—C14—N50 | -17.4 (5) | Ni2—N25—C25—N71 | -165.1 (3) |
| O15—N15—C15—N51 | -4.7 (4) | O25—N25—C25—C26 | 174.4 (3) |
| Ni1—N15—C15—N51 | -168.5 (2) | Ni2—N25—C25—C26 | 15.3 (4) |
| O15—N15—C15—C16 | 174.1 (2) | O26—N26—C26—N72 | -5.0 (5) |
| Ni1—N15—C15—C16 | 10.3 (3) | Ni2—N26—C26—N72 | -164.3 (3) |
| O16—N16—C16—N112 | -3.1 (4) | O26—N26—C26—C25 | 174.4 (3) |
| Ni1—N16—C16—N112 | -166.1 (2) | Ni2—N26—C26—C25 | 15.1 (4) |
| O16—N16—C16—C15 | 176.7 (2) | N25—C25—C26—N26 | -20.3 (4) |
| Ni1—N16—C16—C15 | 13.7 (3) | N71—C25—C26—N26 | 160.2 (3) |
| N15—C15—C16—N16 | -15.4 (4) | N25—C25—C26—N72 | 159.2 (3) |
| N51—C15—C16—N16 | 163.4 (3) | N71—C25—C26—N72 | -20.4 (5) |

Hydrogen-bond geometry (Å, °)

| <i>D</i> —H... <i>A</i> | <i>D</i> —H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> —H... <i>A</i> |
|----------------------------|-------------|---------------|-----------------------|-------------------------|
| O11—H11...O20 | 0.82 | 1.85 | 2.673 (4) | 177 |
| O12—H12...O2A | 0.82 | 1.85 | 2.663 (7) | 174 |
| O13—H13...O10 | 0.82 | 1.88 | 2.698 (3) | 174 |
| O15—H15...O30 | 0.82 | 1.90 | 2.716 (3) | 177 |
| O16—H16...O2B | 0.82 | 1.95 | 2.770 (5) | 178 |
| O16—H16...O4 | 0.82 | 2.37 | 2.857 (4) | 119 |
| O21—H21...O1 | 0.82 | 1.85 | 2.645 (4) | 163 |
| O23—H23...O3 | 0.82 | 1.94 | 2.744 (4) | 165 |
| O25—H25...O4 | 0.82 | 1.82 | 2.636 (5) | 177 |
| O22—H22...O4W ⁱ | 0.82 | 1.96 | 2.694 (4) | 148 |
| O24—H24...O5W ⁱ | 0.82 | 2.00 | 2.796 (5) | 164 |

supplementary materials

| | | | | |
|-------------------------------|----------|----------|-----------|----------|
| O26—H26…O4W ⁱ | 0.82 | 1.95 | 2.760 (4) | 167 |
| O1W—H1W1…O13 | 0.84 (2) | 1.98 (3) | 2.819 (3) | 174 (5) |
| O2W—H2W2…O21 | 0.84 (3) | 1.93 (3) | 2.764 (4) | 168 (4) |
| O4W—H2W4…O5W | 0.83 (3) | 1.98 (3) | 2.783 (5) | 160 (5) |
| O5W—H1W5…O7W | 0.88 (3) | 2.16 (6) | 2.827 (7) | 132 (6) |
| O7W—H7W1…O8W | 0.85 | 1.93 | 2.782 (8) | 175 |
| O8W—H2W8…O3 | 0.91 (3) | 1.92 (7) | 2.720 (7) | 147 (11) |
| O1W—H2W1…O10 ⁱⁱ | 0.82 (2) | 2.13 (3) | 2.944 (3) | 172 (5) |
| O2W—H1W2…O40 ⁱⁱⁱ | 0.86 (3) | 1.91 (3) | 2.764 (4) | 175 (5) |
| O3W—H2W3…O20 ⁱⁱ | 0.86 (3) | 2.29 (4) | 3.045 (4) | 146 (6) |
| O4W—H1W4…O2W ^{iv} | 0.85 (3) | 1.98 (3) | 2.825 (4) | 170 (5) |
| O6W—H2W6…O24 ^v | 0.82 (3) | 2.25 (4) | 3.038 (4) | 161 (7) |
| N17—H17B…O10 ⁱⁱ | 0.86 | 2.43 | 3.022 (4) | 126 |
| N18—H18A…O23 ^{vi} | 0.86 | 2.26 | 3.052 (3) | 154 |
| N19—H19A…O3 ^{vii} | 0.86 | 2.60 | 3.182 (4) | 125 |
| N19—H19B…O12 ^{vii} | 0.86 | 2.19 | 3.044 (4) | 175 |
| N50—H50A…O1W ^{vii} | 0.86 | 2.35 | 3.006 (4) | 134 |
| N50—H50B…O12 ^{vii} | 0.86 | 2.14 | 2.941 (3) | 155 |
| N51—H51B…O20 ^{viii} | 0.86 | 2.19 | 3.039 (4) | 172 |
| N112—H11A…O2W ^{ix} | 0.86 | 2.45 | 3.096 (4) | 132 |
| N112—H11B…O20 ^{viii} | 0.86 | 2.03 | 2.846 (4) | 158 |
| N28—H28A…O16 ^x | 0.86 | 2.04 | 2.873 (4) | 162 |
| N29—H29A…O1W ^{vii} | 0.86 | 2.07 | 2.876 (4) | 155 |
| N29—H29B…O3W ^{vii} | 0.86 | 1.95 | 2.800 (4) | 168 |
| N70—H70A…O14 ^{xi} | 0.86 | 2.38 | 3.055 (4) | 136 |
| N70—H70B…O3W ^{vii} | 0.86 | 2.47 | 3.264 (5) | 154 |
| N71—H71A…O2W ^{ix} | 0.86 | 2.36 | 3.155 (4) | 154 |
| N71—H71B…O1 ^{ix} | 0.86 | 2.17 | 2.999 (4) | 163 |
| N72—H72B…O1 ^{ix} | 0.86 | 2.33 | 3.153 (4) | 161 |

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

Fig. 1

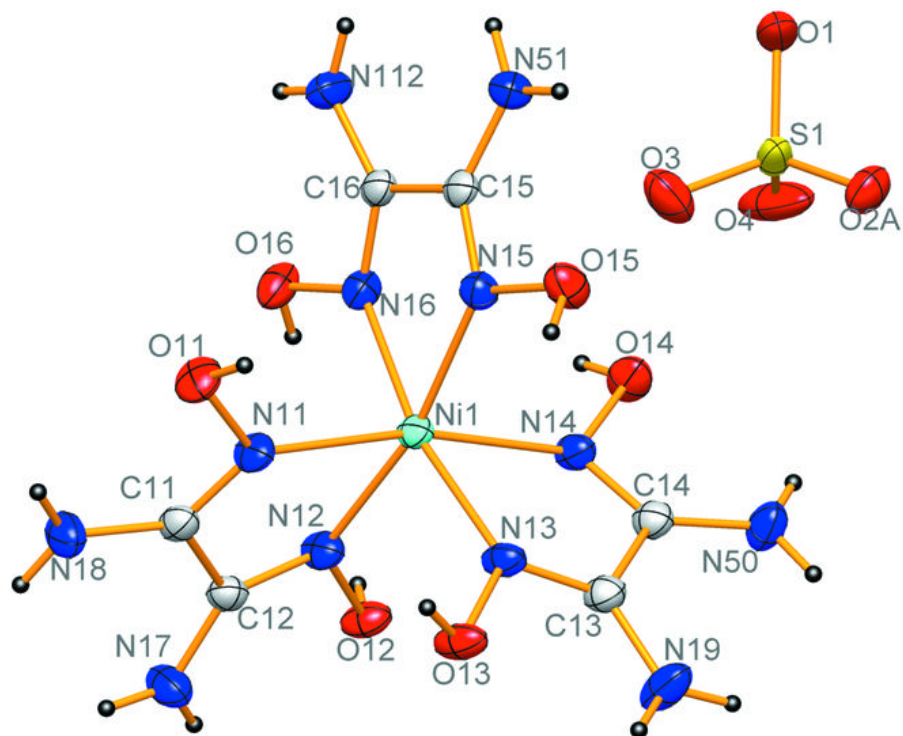


Fig. 2

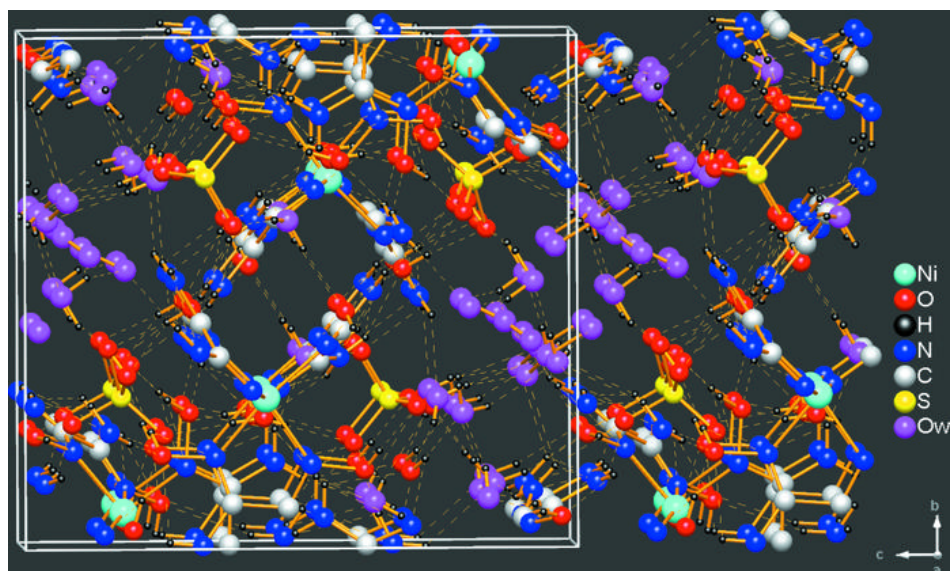


Fig. 3

