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Hexaaquahexakis(μ_2-3,5-diamino-1,2,4-triazole)trinickel(II) trisulfate octadecahydrate

Guo-Fang Zhang,[a] Shu-Min Zhao,[a] Jiang-Bo She[a] and Seik Weng Ng[b]*

[a]Key Laboratory for Macromolecular Science of Shaanxi Province, School of Chemistry and Materials Science, Shaanxi Normal University, Xi'an 710062, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

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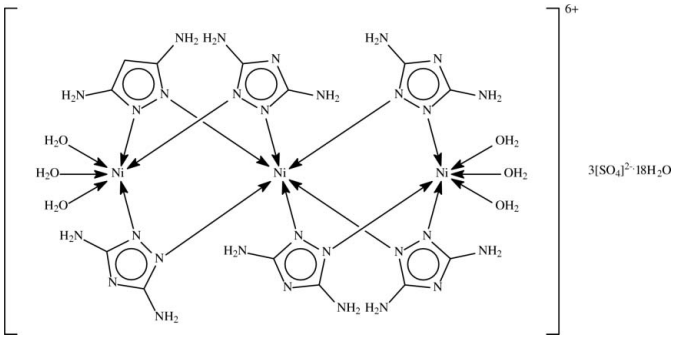
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(S–O) = 0.005 Å; disorder in solvent or counterion; R factor = 0.047; wR factor = 0.180; data-to-parameter ratio = 11.5.

In the centrosymmetric trinuclear cation of the title compound, $[Ni_3(C_2H_5N_5)_6(H_2O)_6](SO_4)_3\cdot 18H_2O$, the six 3,5-diamino-1,2,4-triazole ligands each bridge two metal atoms; the Ni atom in the centre (site symmetry 3 2) of the cluster is coordinated by six N atoms in an octahedral geometry. The other metal atom (site symmetry 3) is connected to three N atoms and three O atoms. The sulfate anion on the $\overline{3}$ site is heavily disordered whereas that on the 3 site is ordered. The hexacation, dianions and uncoordinated water molecules interact through numerous O—H···O and N—H···O hydrogen bonds, forming a three-dimensional network.

Related literature

For the structure of a related cobalt-containing complex, see: Antolini *et al.* (1991).



Experimental

Crystal data

$[Ni_3(C_2H_5N_5)_6(H_2O)_6](SO_4)_3\cdot 18H_2O$
M_r = 1491.35
Trigonal, $R\overline{3}c$
a = 12.664 (2) Å
c = 63.653 (6) Å
V = 8841 (2) Å^3
Z = 6
Mo $K\alpha$ radiation
μ = 1.17 mm^{-1}
T = 295 (2) K
0.43 × 0.32 × 0.23 mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.676, T_{max} = 0.775
24396 measured reflections
2269 independent reflections
1868 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.180
S = 1.33
2269 reflections
197 parameters
66 restraints
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.91 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni1—N2	2.108 (2)	Ni2—O1*w*	2.101 (2)
Ni2—N3	2.065 (2)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H1*w*1···O2w	0.84 (1)	1.89 (1)	2.719 (4)	173 (3)
O1*w*—H1*w*2···O3*w*	0.84 (1)	1.94 (2)	2.754 (3)	162 (4)
N4—H4*n*1···O1*w*^{i}	0.86 (1)	2.33 (3)	2.962 (4)	131 (4)
N4—H4*n*2···O2^{ii}	0.85 (1)	2.41 (3)	3.15 (2)	147 (4)
N5—H5*n*···O6^{iii}	0.85 (1)	2.08 (2)	2.843 (5)	150 (3)
O2*W*—H2*w*1···O3*w*^{iv}	0.85 (1)	2.12 (1)	2.962 (4)	168 (4)
O2*W*—H2*w*2···O4*w*	0.85 (1)	2.01 (2)	2.828 (5)	160 (5)
O3*w*—H3*w*1···O5	0.85 (1)	1.97 (2)	2.787 (5)	162 (4)
O3*w*—H3*w*2···O4*w*^{v}	0.85 (1)	2.10 (2)	2.885 (5)	154 (5)
O4*w*—H4*w*1···O6^{vi}	0.84 (1)	1.98 (2)	2.786 (6)	163 (6)
O4*w*—H4*w*2···O1	0.85 (1)	1.83 (4)	2.57 (2)	145 (6)

Symmetry codes: (i) $-y+1, x-y, z$; (ii) $-x+y+1, -x+1, z$; (iii) $-x+y+\frac{1}{3}, y-\frac{1}{3}, z+\frac{1}{6}$; (iv) $-x+2, -y+1, -z$; (v) $x-y, x-1, -z$; (vi) $-x+y+\frac{4}{3}, y-\frac{1}{3}, z+\frac{1}{6}$.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2392).

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supplementary materials

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Hexaaquahexakis(μ_2-3,5-diamino-1,2,4-triazole)trinickel(II) trisulfate octadecahydrate

G.-F. Zhang, S.-M. Zhao, J.-B. She and S. W. Ng

Comment

3,5-Diamino-1,2,4-triazole ($C_2H_5N_5$) binds to cobalt to yield a centrosymmetric mixed-valence compound in which six of the ligands function as a bridge to a chain of three cobalt centers. The central metal atom is connected to six *N*-donor sites whereas the other two are each connected to three N atoms as well as to three water molecules. The charge of the cation is balanced by chloride ions, and the structure of the salt is stabilized by extensive hydrogen bonds (Antolini *et al.*, 1991).

The title nickel analog displays a similar structure (Fig. 1, Table 1), but the charge of the trinuclear cation is balanced by three sulfate dianions. The cations and anions interact through uncoordinated water molecules to give rise to a three-dimensional, hydrogen bonded network (Table 2).

Experimental

Single crystals of (I) were grown by slowly diffusing 3,5-diamino-1,2,4-triazole (0.020 g, 0.2 mmol) dissolved in methanol (5 ml) into nickel(II) sulfate hexahydrate (0.027 g, 0.1 mmol) dissolved in water (5 ml).

Refinement

The N– and O-bound H atoms were found in difference maps and refined with distance restraints of O–H = N–H = 0.85 (1) Å; for the water molecules, an additional H···H = 1.39±0.01 Å restraint was imposed. The U_{iso} values of the H atoms were tied to those of the parent atoms by a factor of 1.2.

The O atoms of one of the sulfate ions are diordered. For the ordered and disordered sulfate ions, the S–O distance was restrained to 1.45±0.01 Å and the O···O distance to 2.35±0.01 Å; the vibration of the oxygen atoms was restrained to be nearly isotropic.

Figures

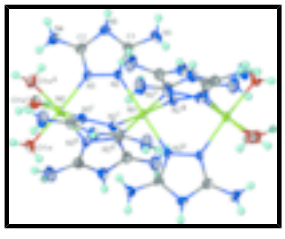


Fig. 1. View of the trinuclear cation in (I) at the 50% ellipsoid probability level. Hydrogen atoms are shown as spheres of arbitrary radius. Symmetry codes: (i) 1 − *y*, *x*-*y*, *z*; (ii) 1 − *x* + *y*, 1 − *x*, *z*; (iii) *x*-*y* + 1/3, 2/3 − *y*, 1/6 − *z*; (iv) 4/3 − *x*, 2/3 − *x* + *y*,1/6 − *z*; (v) 1/3 + *y*,*x* − 1/3,1/6 − *z*.

Hexaaquahexakis(μ$_2$-3,5-diamino-1,2,4-triazole)trinickel(II) trisulfate octadecahydrate

Crystal data

$[Ni_3(C_2H_5N_5)_6(H_2O)_6](SO_4)_3\cdot 18H_2O$	$Z = 6$
$M_r = 1491.35$	$F_{000} = 4680$
Trigonal, $R\bar{3}c$	$D_x = 1.681$ Mg m^{-3}
Hall symbol: -R 3 2"c	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 12.664$ (2) Å	Cell parameters from 7201 reflections
$b = 12.664$ Å	$\theta = 3.2$–28.2°
$c = 63.653$ (6) Å	$\mu = 1.17$ mm^{-1}
$\alpha = 90^\circ$	$T = 295$ (2) K
$\beta = 90^\circ$	Block, blue
$\gamma = 120^\circ$	0.43 × 0.32 × 0.23 mm
$V = 8841$ (2) Å^3	

Data collection

Bruker APEX CCD diffractometer	2269 independent reflections
Radiation source: fine-focus sealed tube	1868 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.026$
$T = 295(2)$ K	$\theta_{max} = 27.5^\circ$
φ and ω scans	$\theta_{min} = 3.2^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -16\rightarrow15$
$T_{min} = 0.676$, $T_{max} = 0.775$	$k = -16\rightarrow16$
24396 measured reflections	$l = -82\rightarrow81$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.047$	All H-atom parameters refined
$wR(F^2) = 0.180$	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 1P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.33$	$(\Delta/\sigma)_{max} = 0.001$
2269 reflections	$\Delta\rho_{max} = 0.91$ e Å^{-3}
197 parameters	$\Delta\rho_{min} = -0.64$ e Å^{-3}
66 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ni1	0.6667	0.3333	0.0833	0.0208 (3)	
Ni2	0.6667	0.3333	0.025169 (9)	0.0238 (2)	
S1	1.0000	0.0000	0.0000	0.0730 (9)	
S2	0.6667	0.3333	−0.08615 (2)	0.0328 (3)	
O1	1.0719 (19)	0.068 (2)	0.0183 (3)	0.118 (14)	0.1666667
O2	0.8739 (9)	−0.0434 (17)	0.0039 (3)	0.071 (7)	0.1666667
O3	1.040 (2)	0.0874 (19)	−0.0174 (3)	0.098 (11)	0.1666667
O4	1.0253 (16)	−0.0949 (13)	−0.0048 (3)	0.065 (6)	0.1666667
O5	0.6667	0.3333	−0.06391 (8)	0.107 (3)	
O6	0.6948 (4)	0.4519 (3)	−0.09445 (7)	0.0967 (12)	
O1w	0.8185 (2)	0.3878 (2)	0.00548 (3)	0.0359 (5)	
H1w1	0.875 (2)	0.390 (3)	0.0128 (4)	0.043*	
H1w2	0.812 (3)	0.352 (3)	−0.0060 (3)	0.043*	
O2W	1.0048 (2)	0.4140 (3)	0.03031 (5)	0.0591 (8)	
H2w1	1.060 (3)	0.4875 (15)	0.0326 (8)	0.071*	
H2w2	1.038 (3)	0.370 (3)	0.0293 (8)	0.071*	
O3w	0.8269 (3)	0.3208 (3)	−0.03537 (4)	0.0596 (7)	
H3w1	0.781 (4)	0.314 (3)	−0.0456 (5)	0.072*	
H3w2	0.818 (4)	0.251 (2)	−0.0324 (6)	0.072*	
O4w	1.1016 (4)	0.2587 (4)	0.03766 (9)	0.0919 (12)	
H4w1	1.099 (6)	0.229 (6)	0.0495 (4)	0.110*	
H4w2	1.111 (7)	0.220 (5)	0.0278 (6)	0.110*	
N1	0.3477 (3)	0.1713 (3)	0.08987 (5)	0.0489 (9)	
H1n1	0.394 (3)	0.157 (4)	0.0974 (6)	0.059*	
H1n2	0.2696 (11)	0.134 (3)	0.0909 (8)	0.059*	
N2	0.5086 (2)	0.2574 (2)	0.06450 (3)	0.0265 (5)	
N3	0.5114 (2)	0.2826 (2)	0.04272 (3)	0.0255 (5)	
N4	0.3585 (3)	0.2501 (3)	0.01736 (4)	0.0492 (8)	
H4n1	0.404 (3)	0.290 (3)	0.0070 (4)	0.059*	
H4n2	0.292 (2)	0.194 (3)	0.0123 (6)	0.059*	
N5	0.3218 (2)	0.1958 (3)	0.05358 (4)	0.0348 (6)	
H5n	0.2477 (13)	0.177 (3)	0.0544 (6)	0.042*	
C1	0.3940 (3)	0.2063 (3)	0.07033 (5)	0.0307 (6)	
C2	0.3987 (2)	0.2440 (3)	0.03683 (4)	0.0308 (6)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0225 (3)	0.0225 (3)	0.0173 (5)	0.01127 (16)	0.000	0.000
Ni2	0.0269 (3)	0.0269 (3)	0.0177 (4)	0.01346 (15)	0.000	0.000
S1	0.0772 (13)	0.0772 (13)	0.0646 (19)	0.0386 (7)	0.000	0.000
S2	0.0295 (4)	0.0295 (4)	0.0392 (7)	0.0148 (2)	0.000	0.000
O1	0.118 (17)	0.127 (16)	0.108 (17)	0.061 (11)	−0.007 (9)	0.000 (10)
O2	0.059 (10)	0.080 (10)	0.080 (10)	0.039 (8)	−0.015 (7)	0.016 (8)

O3	0.108 (13)	0.096 (14)	0.083 (13)	0.045 (9)	0.012 (8)	0.011 (9)
O4	0.069 (9)	0.051 (8)	0.098 (10)	0.047 (7)	−0.024 (8)	−0.001 (7)
O5	0.131 (4)	0.131 (4)	0.058 (4)	0.065 (2)	0.000	0.000
O6	0.092 (3)	0.062 (2)	0.134 (3)	0.037 (2)	−0.002 (3)	0.023 (2)
O1w	0.0364 (12)	0.0448 (12)	0.0269 (10)	0.0205 (10)	0.0055 (9)	0.0021 (9)
O2W	0.0448 (15)	0.0558 (16)	0.0683 (18)	0.0187 (12)	−0.0077 (13)	0.0059 (14)
O3w	0.0704 (19)	0.0721 (18)	0.0478 (14)	0.0442 (16)	−0.0095 (13)	−0.0148 (13)
O4w	0.065 (2)	0.074 (2)	0.139 (3)	0.0363 (19)	0.018 (3)	0.031 (3)
N1	0.0305 (15)	0.077 (2)	0.0313 (15)	0.0208 (14)	0.0076 (12)	0.0115 (13)
N2	0.0267 (12)	0.0321 (12)	0.0191 (11)	0.0135 (9)	0.0011 (9)	0.0009 (8)
N3	0.0267 (11)	0.0309 (11)	0.0199 (10)	0.0153 (9)	−0.0014 (8)	−0.0008 (9)
N4	0.0322 (14)	0.073 (2)	0.0317 (14)	0.0182 (14)	−0.0094 (11)	0.0048 (13)
N5	0.0228 (11)	0.0443 (14)	0.0337 (13)	0.0141 (11)	−0.0003 (10)	0.0005 (11)
C1	0.0249 (14)	0.0370 (15)	0.0267 (14)	0.0128 (11)	0.0016 (11)	0.0001 (10)
C2	0.0293 (14)	0.0344 (15)	0.0287 (13)	0.0159 (12)	−0.0040 (10)	−0.0023 (11)

Geometric parameters (Å, °)

Ni1—N2	2.108 (2)	S2—O5	1.415 (5)
Ni1—N2^{i}	2.108 (2)	S2—O6^{ii}	1.458 (3)
Ni1—N2^{ii}	2.108 (2)	S2—O6^{i}	1.458 (3)
Ni1—N2^{iii}	2.108 (2)	S2—O6	1.458 (3)
Ni1—N2^{iv}	2.108 (2)	O1w—H1w1	0.838 (10)
Ni1—N2^{v}	2.108 (2)	O1w—H1w2	0.841 (10)
Ni2—N3	2.065 (2)	O2W—H2w1	0.853 (10)
Ni2—N3^{i}	2.065 (2)	O2W—H2w2	0.852 (10)
Ni2—N3^{ii}	2.065 (2)	O3w—H3w1	0.848 (10)
Ni2—O1w	2.101 (2)	O3w—H3w2	0.852 (10)
Ni2—O1w^{i}	2.101 (2)	O4w—H4w1	0.838 (10)
Ni2—O1w^{ii}	2.101 (2)	O4w—H4w2	0.845 (10)
S1—O4^{vi}	1.422 (8)	N1—C1	1.352 (4)
S1—O4^{vii}	1.422 (8)	N1—H1n1	0.846 (10)
S1—O4^{viii}	1.422 (8)	N1—H1n2	0.859 (11)
S1—O4	1.422 (8)	N2—C1	1.313 (4)
S1—O4^{ix}	1.422 (8)	N2—N3	1.419 (3)
S1—O4^{x}	1.422 (8)	N3—C2	1.311 (3)
S1—O2^{vii}	1.427 (9)	N4—C2	1.357 (4)
S1—O2^{x}	1.427 (9)	N4—H4n1	0.855 (10)
S1—O2	1.427 (9)	N4—H4n2	0.846 (10)
S1—O2^{viii}	1.427 (9)	N5—C2	1.365 (4)
S1—O2^{vi}	1.427 (9)	N5—C1	1.367 (4)
S1—O2^{ix}	1.427 (9)	N5—H5n	0.847 (10)
N2^{iii}—Ni1—N2^{iv}	90.85 (8)	O2^{vii}—S1—O2^{viii}	117.0 (4)
N2^{iii}—Ni1—N2^{v}	90.85 (8)	O4^{vi}—S1—O2^{vi}	113.1 (8)

N2^{iv}—Ni1—N2^{v}	90.85 (8)	O2^{vii}—S1—O2^{vi}	117.0 (4)
N2^{iii}—Ni1—N2^{i}	177.85 (11)	O2^{viii}—S1—O2^{vi}	117.0 (4)
N2^{iv}—Ni1—N2^{i}	90.70 (12)	O4^{ix}—S1—O2^{ix}	113.1 (8)
N2^{v}—Ni1—N2^{i}	87.63 (12)	O2^{x}—S1—O2^{ix}	117.0 (4)
N2^{iii}—Ni1—N2	87.64 (12)	O2—S1—O2^{ix}	117.0 (4)
N2^{iv}—Ni1—N2	177.85 (11)	O5—S2—O6^{ii}	111.26 (18)
N2^{v}—Ni1—N2	90.70 (12)	O5—S2—O6^{i}	111.26 (19)
N2^{i}—Ni1—N2	90.85 (8)	O6^{ii}—S2—O6^{i}	107.6 (2)
N2^{iii}—Ni1—N2^{ii}	90.70 (12)	O5—S2—O6	111.26 (18)
N2^{iv}—Ni1—N2^{ii}	87.64 (12)	O6^{ii}—S2—O6	107.6 (2)
N2^{v}—Ni1—N2^{ii}	177.85 (11)	O6^{i}—S2—O6	107.6 (2)
N2^{i}—Ni1—N2^{ii}	90.85 (8)	Ni2—O1w—H1w1	108 (2)
N2—Ni1—N2^{ii}	90.85 (8)	Ni2—O1w—H1w2	121 (2)
N3^{i}—Ni2—N3^{ii}	93.50 (8)	H1w1—O1w—H1w2	110.9 (17)
N3^{i}—Ni2—N3	93.50 (8)	H2w1—O2W—H2w2	108.3 (17)
N3^{ii}—Ni2—N3	93.50 (8)	H3w1—O3w—H3w2	109.4 (18)
N3^{i}—Ni2—O1w	90.39 (9)	H4w1—O4w—H4w2	113 (2)
N3^{ii}—Ni2—O1w	87.94 (9)	C1—N1—H1n1	111 (3)
N3—Ni2—O1w	175.77 (8)	C1—N1—H1n2	116 (3)
N3^{i}—Ni2—O1w^{ii}	87.94 (9)	H1n1—N1—H1n2	125 (4)
N3^{ii}—Ni2—O1w^{ii}	175.77 (8)	C1—N2—N3	106.5 (2)
N3—Ni2—O1w^{ii}	90.39 (9)	C1—N2—Ni1	128.87 (19)
O1w—Ni2—O1w^{ii}	88.07 (9)	N3—N2—Ni1	122.82 (17)
N3^{i}—Ni2—O1w^{i}	175.77 (8)	C2—N3—N2	107.2 (2)
N3^{ii}—Ni2—O1w^{i}	90.39 (9)	C2—N3—Ni2	130.62 (18)
N3—Ni2—O1w^{i}	87.94 (9)	N2—N3—Ni2	120.73 (16)
O1w—Ni2—O1w^{i}	88.07 (9)	C2—N4—H4n1	125 (3)
O1w^{ii}—Ni2—O1w^{i}	88.07 (9)	C2—N4—H4n2	123 (3)
O4^{vi}—S1—O4^{vii}	115.6 (5)	H4n1—N4—H4n2	107 (4)
O4^{vi}—S1—O4^{viii}	115.6 (5)	C2—N5—C1	105.8 (2)
O4—S1—O4^{ix}	115.6 (5)	C2—N5—H5n	128 (2)
O4—S1—O4^{x}	115.6 (5)	C1—N5—H5n	125 (2)
O4^{ix}—S1—O4^{x}	115.6 (5)	N2—C1—N1	127.9 (3)
O4^{vii}—S1—O2^{vii}	113.1 (8)	N2—C1—N5	110.4 (3)
O4^{x}—S1—O2^{x}	113.1 (8)	N1—C1—N5	121.7 (3)
O4—S1—O2	113.1 (8)	N3—C2—N4	127.6 (3)
O2^{x}—S1—O2	117.0 (4)	N3—C2—N5	110.1 (2)
O4^{viii}—S1—O2^{viii}	113.1 (8)	N4—C2—N5	122.3 (3)
N2^{iii}—Ni1—N2—C1	−41.1 (2)	N3^{i}—Ni2—N3—N2	32.54 (16)
N2^{v}—Ni1—N2—C1	49.7 (2)	N3^{ii}—Ni2—N3—N2	−61.19 (14)
N2^{i}—Ni1—N2—C1	137.3 (3)	O1w^{ii}—Ni2—N3—N2	120.50 (19)

N2^{ii}—Ni1—N2—C1	−131.8 (3)	O1w^{i}—Ni2—N3—N2	−151.45 (19)
N2^{iii}—Ni1—N2—N3	121.4 (2)	N3—N2—C1—N1	−176.9 (3)
N2^{v}—Ni1—N2—N3	−147.8 (2)	Ni1—N2—C1—N1	−12.1 (4)
N2^{i}—Ni1—N2—N3	−60.12 (14)	N3—N2—C1—N5	0.5 (3)
N2^{ii}—Ni1—N2—N3	30.75 (16)	Ni1—N2—C1—N5	165.2 (2)
C1—N2—N3—C2	−0.7 (3)	C2—N5—C1—N2	−0.1 (3)
Ni1—N2—N3—C2	−166.61 (18)	C2—N5—C1—N1	177.4 (3)
C1—N2—N3—Ni2	−168.31 (18)	N2—N3—C2—N4	179.5 (3)
Ni1—N2—N3—Ni2	25.8 (3)	Ni2—N3—C2—N4	−14.5 (5)
N3^{i}—Ni2—N3—C2	−131.8 (3)	N2—N3—C2—N5	0.7 (3)
N3^{ii}—Ni2—N3—C2	134.5 (3)	Ni2—N3—C2—N5	166.6 (2)
O1w^{ii}—Ni2—N3—C2	−43.8 (3)	C1—N5—C2—N3	−0.4 (3)
O1w^{i}—Ni2—N3—C2	44.2 (3)	C1—N5—C2—N4	−179.3 (3)

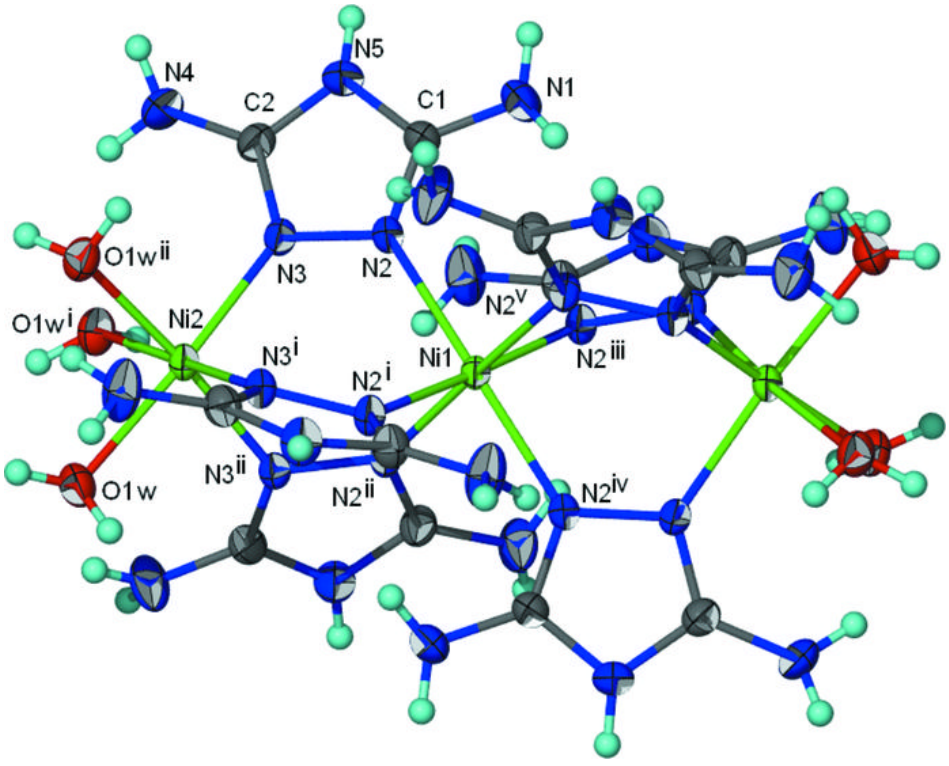
Symmetry codes: (i) −*y*+1, *x*−*y*, *z*; (ii) −*x*+*y*+1, −*x*+1, *z*; (iii) *x*−*y*+1/3, −*y*+2/3, −*z*+1/6; (iv) −*x*+4/3, −*x*+*y*+2/3, −*z*+1/6; (v) *y*+1/3, *x*−1/3, −*z*+1/6; (vi) *y*+1, −*x*+*y*+1, −*z*; (vii) *x*−*y*, *x*−1, −*z*; (viii) −*x*+2, −*y*, −*z*; (ix) −*y*+1, *x*−*y*−1, *z*; (x) −*x*+*y*+2, −*x*+1, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H1w1···O2w	0.84 (1)	1.89 (1)	2.719 (4)	173 (3)
O1w—H1w2···O3w	0.84 (1)	1.94 (2)	2.754 (3)	162 (4)
N4—H4n1···O1w^{i}	0.86 (1)	2.33 (3)	2.962 (4)	131 (4)
N4—H4n2···O2^{ii}	0.85 (1)	2.41 (3)	3.15 (2)	147 (4)
N5—H5n···O6^{xi}	0.85 (1)	2.08 (2)	2.843 (5)	150 (3)
O2W—H2w1···O3w^{xii}	0.85 (1)	2.12 (1)	2.962 (4)	168 (4)
O2W—H2w2···O4w	0.85 (1)	2.01 (2)	2.828 (5)	160 (5)
O3w—H3w1···O5	0.85 (1)	1.97 (2)	2.787 (5)	162 (4)
O3w—H3w2···O4w^{vii}	0.85 (1)	2.10 (2)	2.885 (5)	154 (5)
O4w—H4w1···O6^{xiii}	0.84 (1)	1.98 (2)	2.786 (6)	163 (6)
O4w—H4w2···O1	0.85 (1)	1.83 (4)	2.57 (2)	145 (6)

Symmetry codes: (i) −*y*+1, *x*−*y*, *z*; (ii) −*x*+*y*+1, −*x*+1, *z*; (xi) −*x*+*y*+1/3, *y*−1/3, *z*+1/6; (xii) −*x*+2, −*y*+1, −*z*; (vii) *x*−*y*, *x*−1, −*z*; (xiii) −*x*+*y*+4/3, *y*−1/3, *z*+1/6.

Fig. 1


N5
N4
C2
C1
N1
O1w^{ii}
N3
N2
N2^{v}
O1w^{i}
Ni2
N3^{i}
Ni1
N2^{iii}
N2^{i}
N3^{ii}
O1w
N2^{ii}
N2^{iv}