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Hexaaquahexakis(μ_2-3,5-diamino-4*H*-1,2,4-triazole)trinickel(II) tris(hexafluoridosilicate) icosahydrate

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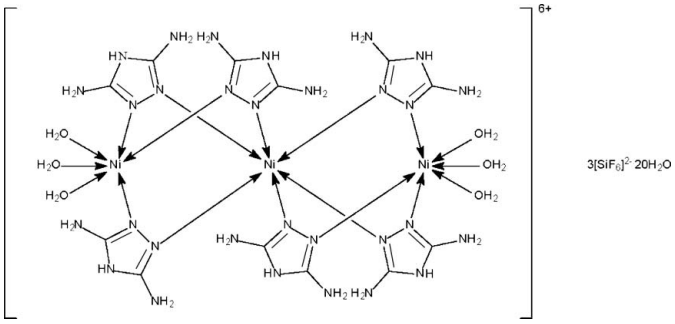
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(Si–F) = 0.003 Å; disorder in solvent or counterion; R factor = 0.033; wR factor = 0.107; data-to-parameter ratio = 13.1.

The trinuclear cation of the title compound, $[Ni_3(C_2H_5N_5)_6(H_2O)_6][SiF_6]_3\cdot 20H_2O$, has the six 3,5-diamino-1,2,4-triazole ligands each bridging two metal atoms; the metal atom in the middle, which lies on a special position (of 32 site symmetry), is connected to six N atoms in an octahedral geometry. The other metal atom, which lies on a special position (of 3 site symmetry), is connected to three N atoms and three O atoms. One hexafluoridosilicate anion lies on a site of 3 symmetry and the other lies on a site of $\overline{3}$ symmetry. The hexacation, dianions and uncoordinated water molecules interact through hydrogen bonds to form a three-dimensional network. One uncoordinated water molecule is disordered, with site occupancy 0.3.

Related literature

For the structure of the title hexacation as the hydrated sulfate salt, see: Zhang *et al.* (2007).



Experimental

Crystal data

$[Ni_3(C_2H_5N_5)_6(H_2O)_6][SiF_6]_3\cdot 20H_2O$
M_r = 1665.48
Trigonal, $R\overline{3}c$
a = 13.024 (1) Å
c = 64.462 (5) Å
V = 9469.8 (9) Å^3
Z = 6
Mo $K\alpha$ radiation
μ = 1.09 mm^{-1}
T = 293 (2) K
0.49 × 0.46 × 0.44 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.560, T_{max} = 0.646
25347 measured reflections
2420 independent reflections
2093 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.106
S = 1.06
2420 reflections
185 parameters
23 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni1—N1	2.062 (2)	Ni2—N2	2.111 (2)
Ni1—O1	2.104 (2)		

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2084).

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Zhang, G.-F., Zhao, S.-M., She, J.-B. & Ng, S. W. (2007). *Acta Cryst.* E**63**, m1517–m1518.

supporting information

Acta Cryst. (2008). E**64**, m802 [doi:10.1107/S1600536808013329]

Hexaaquahexakis(μ_2-3,5-diamino-4*H*-1,2,4-triazole)trinickel(II) tris-(hexafluoridosilicate) icosahydrate

Li-Ping Wu, Shu-Ming Zhao, Guo-Fang Zhang and Seik Weng Ng

S1. Comment

A recent study reported the nickel sulfate complex of 3,5-diamino-1,2,4-triazole. The cation is a centrosymmetric trinuclear hexacation $[Ni_3(C_2H_5N_5)_6(H_2O)_6]^{6+}$, whose charge is balanced by the sulfate anions. The *N*-heterocyclic ligands each bridge two nickel atoms (Zhang *et al.*, 2007). The corresponding synthesis with nickel hexafluoridosilicate in place of nickel sulfate gave the analogous cluster cation (Scheme I, Fig. 1). The cation and anions interact through the coordinated and free water molecules to give rise to a three-dimensional, hydrogen bonded network.

S2. Experimental

Single crystal of the compound were grown by diffusing 3,5-diamino-1,2,4-triazole (0.020 g, 0.2 mmol) dissolved in methanol (5 ml) into nickle(II) hexafluorosilicate (0.027 g, 0.1 mmol) dissolved in water (5 ml).

S3. Refinement

As one of the five water molecules (O5) lies on a special position of *2* site symmetry, the occupancy would be 0.5. However, the refinement of this atom at the default occupancy lead to a large temperature factor. The refinement of the occupancy factor led to a value of about 0.3; this atom was then allowed to refine off the symmetry element. As the occupancy was nearly 0.3, the occupancy was arbitrarily fixed as 0.3333 so that the formula unit has 20 lattice water molecules.

The N– and O–bound H atoms (other than those of the diordered water molecule) were found in difference maps and were refined with distance restraints of O–H = N–H = O.85±0.01 Å; for the water molecules, an additional H···H = 1.39±0.01 Å restraint was imposed. The U_{iso}(H) values were tied to those of the parent atoms by a factor of 1.5. The H atoms of the disordered water molecule were placed in chemically sensible positions but were not refined.

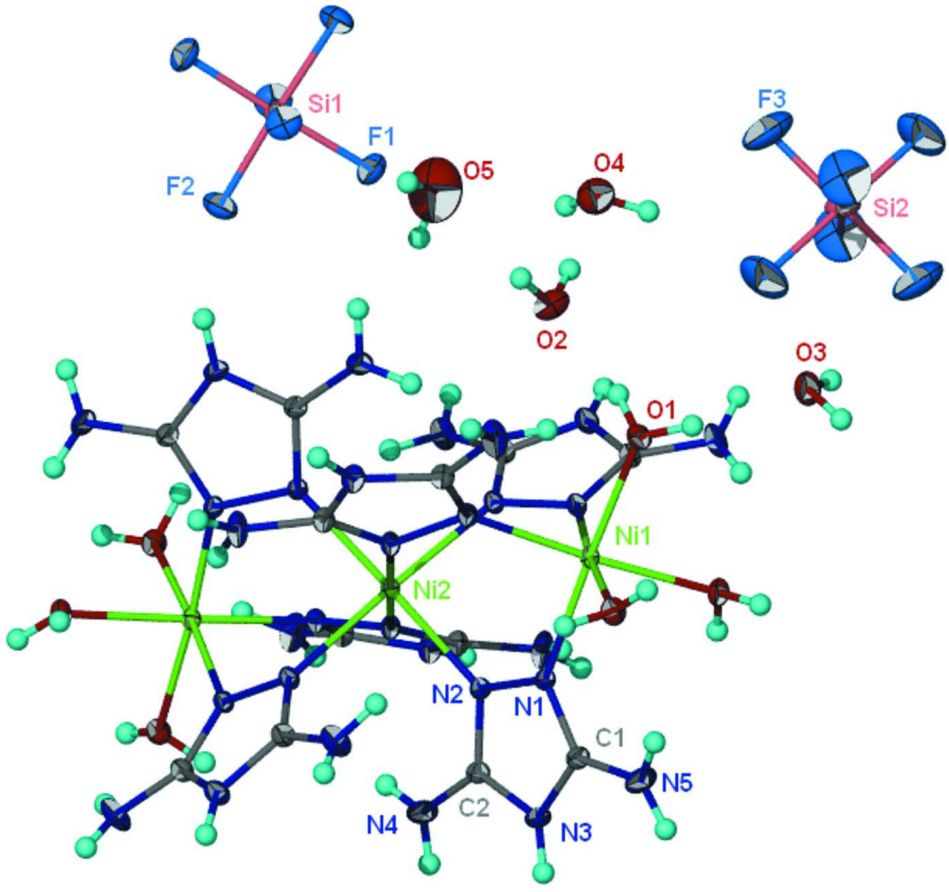

Figure 1

Thermal ellipsoid plot of the title compound. Displacement ellipsoids are drawn at the 25% probability level.

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Crystal data

$[Ni_3(C_2H_5N_5)_6(H_2O)_6][SiF_6]_3\cdot 20H_2O$
$M_r = 1665.48$
Trigonal, $R\bar{3}c$
Hall symbol: -R 3 2"c
$a = 13.024\ (1)$ Å
$c = 64.462\ (5)$ Å
$V = 9469.8\ (9)$ Å^3
$Z = 6$
$F(000) = 5160$
$D_x = 1.752$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5839 reflections
$\theta = 3.1–28.2°$
$\mu = 1.09$ mm^{-1}
$T = 293$ K
Block, blue
0.49 × 0.46 × 0.44 mm

Data collection

Bruker APEX area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.560$, $T_{max} = 0.646$
25347 measured reflections
2420 independent reflections
2093 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -16\rightarrow16$
$k = -16\rightarrow16$
$l = -79\rightarrow83$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.106$
$S = 1.06$
2420 reflections
185 parameters
23 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0612P)^2 + 17.0807P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.43$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ni1	0.6667	0.3333	0.140787 (6)	0.02689 (14)	
Ni2	0.6667	0.3333	0.0833	0.02377 (16)	
Si1	1.0000	0.0000	0.083802 (16)	0.0331 (2)	
Si2	0.3333	−0.3333	0.1667	0.0552 (5)	
F1	0.89685 (14)	0.00226 (15)	0.09960 (2)	0.0623 (4)	
F2	1.00168 (16)	0.10635 (14)	0.06943 (3)	0.0648 (4)	
F3	0.3983 (3)	−0.3868 (3)	0.15169 (5)	0.1399 (12)	
O1	0.72286 (15)	0.24063 (14)	0.16010 (2)	0.0398 (3)	
H11	0.723 (3)	0.1843 (18)	0.1533 (3)	0.060*	
H12	0.699 (3)	0.217 (2)	0.1724 (2)	0.060*	
O2	0.7536 (2)	0.0854 (2)	0.13625 (4)	0.0660 (5)	
H21	0.713 (2)	0.0108 (10)	0.1358 (6)	0.099*	
H22	0.8267 (10)	0.108 (3)	0.1361 (7)	0.099*	
O3	0.65459 (19)	0.15616 (17)	0.19955 (3)	0.0599 (5)	
H31	0.5874 (17)	0.094 (2)	0.1978 (5)	0.090*	
H32	0.650 (3)	0.197 (2)	0.2092 (4)	0.090*	
O4	0.6041 (2)	−0.1661 (3)	0.12859 (4)	0.0796 (6)	
H41	0.576 (3)	−0.184 (4)	0.1164 (3)	0.119*	
H42	0.551 (3)	−0.182 (4)	0.1374 (4)	0.119*	
O5	0.664 (3)	−0.1549 (17)	0.0893 (3)	0.185 (7)	0.3333
H51	0.7382	−0.1072	0.0905	0.278*	0.3333
H52	0.6338	−0.1239	0.0816	0.278*	0.3333
N1	0.61588 (14)	0.43372 (14)	0.12352 (2)	0.0290 (3)	
N2	0.59282 (14)	0.41343 (14)	0.10195 (2)	0.0293 (3)	
N3	0.52872 (17)	0.53100 (17)	0.11289 (3)	0.0381 (4)	
H3	0.500 (2)	0.576 (2)	0.1117 (4)	0.057*	
N4	0.5100 (2)	0.4865 (2)	0.07683 (3)	0.0508 (5)	
H4A	0.514 (3)	0.449 (3)	0.0663 (4)	0.076*	
H4B	0.468 (2)	0.517 (3)	0.0744 (6)	0.076*	
N5	0.5810 (2)	0.5478 (2)	0.14862 (3)	0.0556 (6)	
H5A	0.625 (3)	0.540 (3)	0.1574 (4)	0.083*	
H5B	0.535 (3)	0.575 (3)	0.1509 (5)	0.083*	
C1	0.57611 (18)	0.50413 (18)	0.12943 (3)	0.0343 (4)	

C2	0.54160 (17)	0.47436 (17)	0.09630 (3)	0.0336 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.02997 (17)	0.02997 (17)	0.0207 (2)	0.01499 (9)	0.000	0.000
Ni2	0.0253 (2)	0.0253 (2)	0.0207 (3)	0.01265 (10)	0.000	0.000
Si1	0.0300 (3)	0.0300 (3)	0.0394 (5)	0.01500 (15)	0.000	0.000
Si2	0.0333 (5)	0.0333 (5)	0.0992 (15)	0.0166 (2)	0.000	0.000
F1	0.0555 (9)	0.0683 (10)	0.0701 (10)	0.0363 (8)	0.0170 (7)	0.0016 (8)
F2	0.0710 (10)	0.0574 (9)	0.0741 (10)	0.0382 (8)	−0.0004 (8)	0.0199 (8)
F3	0.146 (3)	0.176 (3)	0.163 (3)	0.129 (3)	0.0160 (19)	−0.025 (2)
O1	0.0497 (8)	0.0454 (8)	0.0292 (7)	0.0274 (7)	−0.0020 (6)	0.0041 (6)
O2	0.0624 (12)	0.0722 (13)	0.0750 (13)	0.0424 (11)	−0.0019 (10)	−0.0133 (11)
O3	0.0764 (13)	0.0541 (11)	0.0436 (9)	0.0283 (10)	0.0132 (9)	−0.0001 (8)
O4	0.0709 (15)	0.0812 (15)	0.0871 (16)	0.0383 (13)	−0.0030 (12)	−0.0025 (14)
O5	0.119 (7)	0.216 (10)	0.178 (13)	0.051 (7)	−0.015 (9)	−0.010 (8)
N1	0.0349 (8)	0.0329 (8)	0.0226 (7)	0.0194 (6)	0.0006 (6)	−0.0010 (6)
N2	0.0352 (8)	0.0355 (8)	0.0219 (7)	0.0213 (7)	−0.0009 (6)	−0.0005 (6)
N3	0.0476 (10)	0.0440 (10)	0.0366 (9)	0.0334 (8)	−0.0010 (7)	−0.0015 (7)
N4	0.0743 (15)	0.0720 (14)	0.0343 (10)	0.0578 (13)	−0.0109 (9)	−0.0043 (9)
N5	0.0821 (16)	0.0803 (15)	0.0348 (10)	0.0635 (14)	−0.0071 (10)	−0.0157 (10)
C1	0.0390 (10)	0.0367 (10)	0.0319 (9)	0.0224 (9)	0.0008 (8)	−0.0023 (8)
C2	0.0377 (10)	0.0374 (10)	0.0312 (9)	0.0229 (9)	−0.0009 (7)	0.0006 (7)

Geometric parameters (Å, º)

Ni1—N1	2.062 (2)	Si2—F3	1.649 (3)
Ni1—N1^{i}	2.062 (2)	O1—H11	0.86 (3)
Ni1—N1^{ii}	2.062 (2)	O1—H12	0.85 (3)
Ni1—O1	2.104 (2)	O2—H21	0.84 (3)
Ni1—O1^{i}	2.104 (2)	O2—H22	0.84 (3)
Ni1—O1^{ii}	2.104 (2)	O3—H31	0.85 (3)
Ni2—N2^{iii}	2.111 (2)	O3—H32	0.84 (3)
Ni2—N2^{iv}	2.111 (2)	O4—H41	0.85 (3)
Ni2—N2^{v}	2.111 (2)	O4—H42	0.84 (3)
Ni2—N2^{ii}	2.111 (2)	O5—H51	0.85
Ni2—N2^{i}	2.111 (2)	O5—H52	0.85
Ni2—N2	2.111 (2)	N1—C1	1.315 (2)
Si1—F2	1.6574 (15)	N1—N2	1.419 (2)
Si1—F2^{vi}	1.6574 (15)	N2—C2	1.318 (3)
Si1—F2^{vii}	1.6574 (15)	N3—C2	1.356 (3)
Si1—F1^{vii}	1.6976 (15)	N3—C1	1.362 (3)
Si1—F1^{vi}	1.6976 (15)	N3—H3	0.85 (1)
Si1—F1	1.6976 (15)	N4—C2	1.354 (3)
Si2—F3^{viii}	1.649 (3)	N4—H4A	0.85 (3)
Si2—F3^{ix}	1.649 (3)	N4—H4B	0.84 (3)
Si2—F3^{x}	1.649 (3)	N5—C1	1.350 (3)

Si2—F3^{xi}	1.649 (3)	N5—H5A	0.84 (3)
Si2—F3^{xii}	1.649 (3)	N5—H5B	0.85 (3)
N1^{ii}—Ni1—N1^{i}	93.61 (6)	F1^{vi}—Si1—F1	87.74 (9)
N1^{ii}—Ni1—N1	93.61 (6)	F3^{viii}—Si2—F3^{ix}	89.21 (17)
N1^{i}—Ni1—N1	93.61 (6)	F3^{viii}—Si2—F3^{x}	89.21 (17)
N1^{ii}—Ni1—O1	87.31 (6)	F3^{ix}—Si2—F3^{x}	89.21 (17)
N1^{i}—Ni1—O1	90.45 (6)	F3^{viii}—Si2—F3^{xi}	90.79 (17)
N1—Ni1—O1	175.77 (6)	F3^{ix}—Si2—F3^{xi}	90.79 (17)
N1^{ii}—Ni1—O1^{i}	90.45 (6)	F3^{x}—Si2—F3^{xi}	179.995 (1)
N1^{i}—Ni1—O1^{i}	175.77 (6)	F3^{viii}—Si2—F3^{xii}	90.79 (17)
N1—Ni1—O1^{i}	87.31 (6)	F3^{ix}—Si2—F3^{xii}	179.995 (1)
O1—Ni1—O1^{i}	88.56 (6)	F3^{x}—Si2—F3^{xii}	90.79 (17)
N1^{ii}—Ni1—O1^{ii}	175.78 (6)	F3^{xi}—Si2—F3^{xii}	89.21 (17)
N1^{i}—Ni1—O1^{ii}	87.31 (6)	F3^{viii}—Si2—F3	179.997 (1)
N1—Ni1—O1^{ii}	90.45 (6)	F3^{ix}—Si2—F3	90.79 (17)
O1—Ni1—O1^{ii}	88.56 (6)	F3^{x}—Si2—F3	90.79 (17)
O1^{i}—Ni1—O1^{ii}	88.56 (6)	F3^{xi}—Si2—F3	89.21 (17)
N2^{iii}—Ni2—N2^{iv}	90.87 (6)	F3^{xii}—Si2—F3	89.21 (17)
N2^{iii}—Ni2—N2^{v}	90.87 (6)	Ni1—O1—H11	110 (2)
N2^{iv}—Ni2—N2^{v}	90.87 (6)	Ni1—O1—H12	126 (2)
N2^{iii}—Ni2—N2^{ii}	87.57 (8)	H11—O1—H12	109 (2)
N2^{iv}—Ni2—N2^{ii}	177.79 (8)	H21—O2—H22	111 (2)
N2^{v}—Ni2—N2^{ii}	90.72 (8)	H31—O3—H32	110 (2)
N2^{iii}—Ni2—N2^{i}	90.72 (8)	H41—O4—H42	111 (2)
N2^{iv}—Ni2—N2^{i}	87.57 (8)	H51—O5—H52	109.4
N2^{v}—Ni2—N2^{i}	177.79 (8)	C1—N1—N2	107.04 (15)
N2^{ii}—Ni2—N2^{i}	90.88 (6)	C1—N1—Ni1	130.48 (12)
N2^{iii}—Ni2—N2	177.79 (8)	N2—N1—Ni1	121.05 (11)
N2^{iv}—Ni2—N2	90.72 (8)	C2—N2—N1	106.38 (15)
N2^{v}—Ni2—N2	87.57 (8)	C2—N2—Ni2	129.31 (13)
N2^{ii}—Ni2—N2	90.88 (6)	N1—N2—Ni2	122.87 (12)
N2^{i}—Ni2—N2	90.88 (6)	C2—N3—C1	106.38 (16)
F2—Si1—F2^{vi}	91.80 (9)	C2—N3—H3	122 (2)
F2—Si1—F2^{vii}	91.80 (9)	C1—N3—H3	132 (2)
F2^{vi}—Si1—F2^{vii}	91.80 (9)	C2—N4—H4A	125 (2)
F2—Si1—F1^{vii}	90.36 (8)	C2—N4—H4B	122 (3)
F2^{vi}—Si1—F1^{vii}	177.12 (10)	H4A—N4—H4B	111 (3)
F2^{vii}—Si1—F1^{vii}	90.03 (8)	C1—N5—H5A	117 (2)
F2—Si1—F1^{vi}	177.12 (10)	C1—N5—H5B	116 (2)
F2^{vi}—Si1—F1^{vi}	90.03 (8)	H5A—N5—H5B	126 (3)
F2^{vii}—Si1—F1^{vi}	90.36 (8)	N1—C1—N5	127.37 (19)
F1^{vii}—Si1—F1^{vi}	87.74 (9)	N1—C1—N3	109.86 (16)
F2—Si1—F1	90.03 (8)	N5—C1—N3	122.76 (18)
F2^{vi}—Si1—F1	90.36 (8)	N2—C2—N4	126.92 (19)
F2^{vii}—Si1—F1	177.12 (10)	N2—C2—N3	110.33 (17)
F1^{vii}—Si1—F1	87.74 (9)	N4—C2—N3	122.67 (19)

N1^{ii}—Ni1—N1—C1	−135.1 (2)	N2^{iv}—Ni2—N2—N1	146.76 (16)
N1^{i}—Ni1—N1—C1	131.1 (2)	N2^{v}—Ni2—N2—N1	−122.40 (15)
O1^{i}—Ni1—N1—C1	−44.81 (19)	N2^{ii}—Ni2—N2—N1	−31.71 (12)
O1^{ii}—Ni1—N1—C1	43.72 (19)	N2^{i}—Ni2—N2—N1	59.18 (10)
N1^{ii}—Ni1—N1—N2	60.39 (10)	N2—N1—C1—N5	−179.0 (2)
N1^{i}—Ni1—N1—N2	−33.46 (12)	Ni1—N1—C1—N5	14.9 (3)
O1^{i}—Ni1—N1—N2	150.67 (13)	N2—N1—C1—N3	−0.1 (2)
O1^{ii}—Ni1—N1—N2	−120.79 (13)	Ni1—N1—C1—N3	−166.30 (14)
C1—N1—N2—C2	0.6 (2)	C2—N3—C1—N1	−0.4 (2)
Ni1—N1—N2—C2	168.37 (13)	C2—N3—C1—N5	178.5 (2)
C1—N1—N2—Ni2	168.09 (13)	N1—N2—C2—N4	176.0 (2)
Ni1—N1—N2—Ni2	−24.17 (18)	Ni2—N2—C2—N4	9.6 (3)
N2^{iv}—Ni2—N2—C2	−48.86 (15)	N1—N2—C2—N3	−0.9 (2)
N2^{v}—Ni2—N2—C2	41.98 (14)	Ni2—N2—C2—N3	−167.25 (14)
N2^{ii}—Ni2—N2—C2	132.67 (18)	C1—N3—C2—N2	0.8 (2)
N2^{i}—Ni2—N2—C2	−136.44 (18)	C1—N3—C2—N4	−176.2 (2)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H11···O2	0.86 (3)	1.88 (3)	2.724 (3)	168 (3)
O1—H12···O3	0.85 (3)	1.89 (3)	2.737 (2)	174 (3)
O2—H21···O4	0.84 (3)	2.07 (3)	2.896 (4)	168 (4)
O2—H22···O3^{xiii}	0.84 (3)	2.12 (3)	2.961 (3)	175 (4)
O3—H31···O4^{ix}	0.85 (3)	2.05 (3)	2.861 (3)	159 (3)
O3—H32···F1^{ix}	0.84 (3)	2.13 (3)	2.904 (2)	153 (3)
O4—H41···F2^{xiv}	0.85 (3)	2.23 (3)	2.950 (3)	143 (4)
O4—H42···F3^{xi}	0.84 (3)	2.16 (3)	2.973 (4)	162 (4)
O4—H41···O5	0.85 (3)	2.03 (3)	2.64 (2)	128 (4)
O5—H51···F1	0.85	1.92	2.76 (3)	167
N3—H3···F2^{iii}	0.85 (3)	1.97 (3)	2.764 (2)	157 (3)
N4—H4b···F1^{iii}	0.84 (3)	2.14 (3)	2.974 (3)	170 (3)
N5—H5a···O1^{i}	0.84 (3)	2.23 (3)	2.942 (3)	142 (3)
N5—H5b···F3^{xv}	0.85 (3)	2.08 (3)	2.909 (3)	167 (3)

Symmetry codes: (i) −*y*+1, *x*−*y*, *z*; (iii) *y*+1/3, *x*−1/3, −*z*+1/6; (ix) *x*−*y*−1/3, *x*−2/3, −*z*+1/3; (xi) −*y*, *x*−*y*−1, *z*; (xiii) −*x*+5/3, −*y*+1/3, −*z*+1/3; (xiv) *y*+1/3, *x*−4/3, −*z*+1/6; (xv) *x*, *y*+1, *z*.