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Hydrogen bonding in cocrystals of *trans*-$Ni^{II}(hfac)_2(H_2O)_2$

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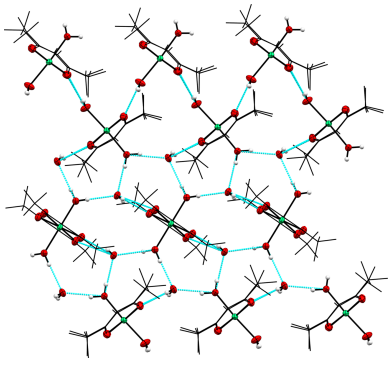


Chemical vapor deposition (CVD) precursors often employ fluorinated β-diketonate ligands bonded to metal atoms; however, these are prone to the formation of hydrates under ambient conditions and form hydrogen-bond networks which hinder the CVD process. This work investigated the use of 1,2-dimethoxybenzene (DMB) as a ligand to prevent the formation of hydrogen-bonding networks. The single-crystal structures of two complexes of diaquabis(1,1,1,5,5,5-hexafluoro-4-oxopent-2-en-2-olato-κ^2O,O')nickel(II), *trans*-$Ni^{II}(hfac)_2(H_2O)_2$, were determined, one as a 4/3 hydrate, $[Ni(C_5HF_6O_2)_2(H_2O)_2]_3\cdot 4H_2O$, and one as a 1,2-dimethoxybenzene (DMB) pentasolvate, $[Ni(C_5HF_6O_2)_2(H_2O)_2]\cdot 5C_8H_{10}O_2$. The hydrogen-bond networks of these two materials were compared to previously reported hydrogen-bond networks seen in $Ni^{II}(hfac)_2(H_2O)_2$. DMB was found to disrupt the formation of an extended hydrogen-bond network without coordinating to the Ni center.

1. Introduction

The drive for improved microelectronic circuits requires the development of methods to fabricate materials with finely tuned films of metal compounds. Chemical vapor deposition (CVD) has been used for decades in the production of microelectronics. For CVD precursors, ensuring thermal stability while allowing for low-temperature volatilization are ideal. A common strategy has been to employ fluorinated β-diketonate ligands, such as 1,1,1,5,5,5-hexafluoroacetylacetonate (hfac) (Mishra & Daniele, 2015). Under ambient conditions, these transition-metal and lanthanide complexes form hydrate adducts to the metal center (Binnemans, 2005; Malandrino *et al.*, 1996; Malandrino *et al.*, 2006; Zhang *et al.*, 2008). These hydrates hinder the sublimation process, presumably through the formation of strong intermolecular hydrogen-bonding networks. Neutral bidentate ligands such as dimethoxyethane (DME) are capable of displacing coordinated water molecules (Malandrino *et al.*, 1996; Fatila *et al.*, 2012) and are capable of forming volatile mononuclear complexes, making them amenable to acting as CVD precursors. We sought to determine whether the 1,2-dimethoxybenzene (DMB) ligand could successfully displace the aqua ligands in *trans*-$Ni(hfac)_2(H_2O)_2$. While the $Ni(hfac)_2(DME)$ and $Mn(hfac)_2(DME)$ complexes have been prepared (Ibrahim *et al.*, 2025; Gray *et al.*, 2026), to the best of our knowledge, analogous compounds containing the DMB ligand have not been isolated. Based on its reduced flexibility and the reduced donating ability of the methoxy group, we did not expect it to coordinate as strongly as DME. We were interested in the possibility that DMB could disrupt the hydrogen-bond

Table 1
Experimental details.

Experiments were carried out at 153 K with Mo *Kα* radiation using a Bruker D8 VENTURE diffractometer. H atoms were treated by a mixture of independent and constrained refinement.

	1	**2**
Crystal data		
Chemical formula	$[Ni(C_5HF_6O_2)_2(H_2O)_2]_3{\cdot}4H_2O$	$[Ni(C_5HF_6O_2)_2(H_2O)_2]{\cdot}5C_8H_{10}O_2$
M_r	1598.64	1199.65
Crystal system, space group	Monoclinic, $P2_1/n$	Monoclinic, $P2_1/c$
a, b, c (Å)	24.3968 (14), 7.2381 (4), 31.5461 (17)	11.9278 (5), 15.7842 (6), 15.0115 (6)
β (°)	106.300 (2)	93.887 (1)
V (Å^3)	5346.7 (5)	2819.7 (2)
Z	4	2
μ (mm^{-1})	1.25	0.45
Crystal size (mm)	0.27 × 0.25 × 0.08	0.34 × 0.26 × 0.08
Data collection		
Absorption correction	Multi-scan (*TWINABS*; Sevvana *et al.*, 2019; Sheldrick, 2012)	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.603, 0.745	0.679, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11657, 11657, 10792	66877, 7928, 5947
R_{int}	Not applicable	0.060
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.629	0.695
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.065, 0.147, 1.16	0.038, 0.106, 1.02
No. of reflections	11657	7928
No. of parameters	1020	558
No. of restraints	566	267
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.98, −0.69	0.40, −0.42

Computer programs: *APEX6* (Bruker, 2024), *SAINT* (Bruker, 2019), *ShelXle* (Hübschle *et al.*, 2011), *SHELXT2018* (Sheldrick, 2015*a*), *SHELXL2019* (Sheldrick, 2015*b*), and *Mercury* (Macrae *et al.*, 2020).

network around the $Ni(hfac)_2(H_2O)_2$ complex and what structural changes the DMB ligand could facilitate.

2. Experimental

2.1. Chemicals and materials

$NaHCO_3$ (99.9%) and $NiCl_2{\cdot}6H_2O$ (99.5%) were purchased from Mallinckrodt Chemical Works. 1,1,1,5,5,5-Hexafluoropentane-2,4-dione (H-hfac) (98%) and *n*-heptane were obtained from Thermo Scientific Chemicals. 1,2-Dimethoxybenzene (DMB) (veratrole) was purchased from Acros Organics (99%). Ultrapure water (18 MΩ) was used as solvent.

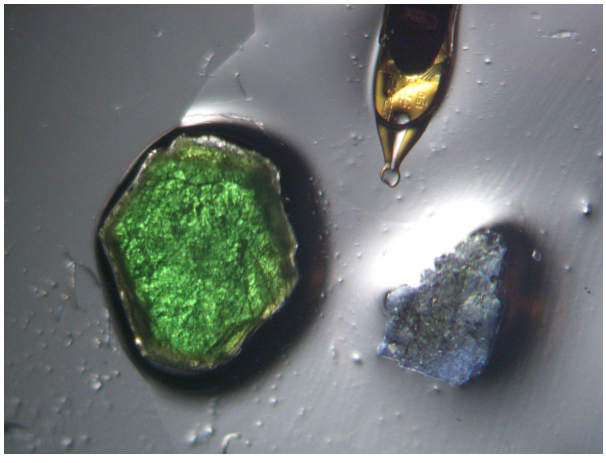


Figure 1
Crystals of **1** (green, left) and **2** (colorless, right). A 150 µm MiTeGen loop is shown for scale. The specimens shown in this image are not the crystals used for the data collection.

2.2. Synthetic procedure

$NaHCO_3$ (0.5934 g, 7.063 mmol) was dissolved in water (50 ml). An equimolar amount of H-hfac (1 ml, 7 mmol) was then added. The pH was measured to be approximately 6. To this solution, 0.1 g of $NaHCO_3$ was added to raise the pH to approximately 7. $NiCl_2{\cdot}6H_2O$ (0.8397 g, 3.533 mmol) was added to the solution. A precipitate immediately formed. The precipitate was filtered off under vacuum. The crude yield was 0.6052 g [33%, 1.189 mmol, assuming a formula of $Ni^{II}(hfac)_2(H_2O)_2$]. The green solid was immediately suspended in *n*-heptane (10 ml) and reacted with 1,2-dimethoxybenzene (0.9 ml, 7 mmol). Recrystallization *via* slow evaporation yielded colorless and green crystals in the same pot (the yield was not obtained). Throughout this article, the green crystals are referred to as **1** and the colorless crystals as **2** (see Scheme 1 and Fig. 1).

2.3. Crystallographic data collection

Crystal data, data collection and structure refinement details are summarized in Table 1. H atoms of water molecules were located in the difference map and refined freely with relative isotropic displacement parameters, with the exception of H3*OA*_2 and H3*OB*_2. These atoms were placed *via* the

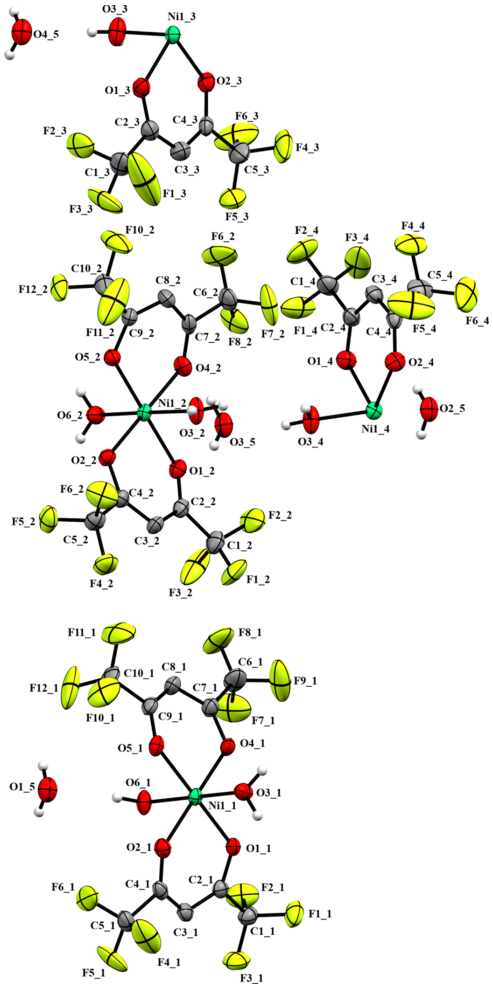


Figure 2
The asymmetric unit of **1**. Only the majorly occupied parts of disordered CF_3 groups are shown. H atoms not bonded to water have been hidden for clarity. Unless otherwise stated, the following applies to all images of crystal structures in this article: non-H atoms are drawn as displacement ellipsoids at the 50% probability level and H atoms are drawn as fixed size spheres.

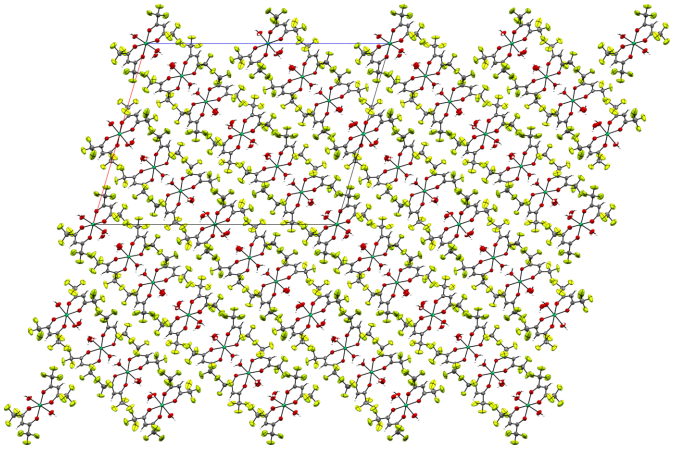


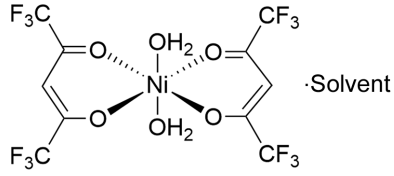
Figure 3
A 2 × 2 × 2 supercell of **1**, viewed along the crystallographic *b* axis, highlighting the alternating layers of hydrogen-bond networks and $CF_3\cdots CF_3$ contacts. The red and blue axes of the displayed unit cell are the *a* and *c* axes, respectively. Only the majorly occupied parts of disordered CF_3 groups are shown.

Table 2
Hydrogen-bond geometry (Å, °) for **1**.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3_1—H3*OB*_1···O1_1^{i}	0.81 (2)	2.11 (4)	2.824 (5)	147 (6)
O3_1—H3*OA*_1···O4_1^{i}	0.81 (2)	2.21 (4)	2.879 (5)	141 (6)
O6_1—H6*OA*_1···O1_5	0.80 (2)	2.00 (2)	2.796 (6)	172 (6)
O6_1—H6*OB*_1···O4_5^{ii}	0.80 (2)	1.94 (2)	2.728 (6)	166 (7)
O3_2—H3*OA*_2···O2_5^{iii}	0.78*	2.01*	2.786 (6)*	173*
O3_2—H3*OB*_2···O3_5^{iv}	0.88*	1.87*	2.733 (6)*	167*
O6_2—H6*OB*_2···O2_2^{ii}	0.81 (2)	2.13 (4)	2.837 (5)	145 (6)
O6_2—H6*OA*_2···O5_2^{ii}	0.81 (2)	2.18 (4)	2.876 (5)	145 (6)
O3_3—H3*OA*_3···O4_5	0.78 (5)	2.07 (5)	2.842 (6)	173 (9)
O3_3—H3*OB*_3···O1_5^{ii}	0.78 (5)	1.99 (5)	2.766 (6)	173 (8)
O3_4—H3*OB*_4···O3_5	0.81 (2)	2.05 (2)	2.842 (6)	168 (8)
O3_4—H3*OA*_4···O2_5^{iii}	0.81 (2)	1.97 (2)	2.769 (6)	171 (8)
O1_5—H1*OA*_5···O2_3^{v}	0.81 (2)	2.05 (3)	2.835 (6)	161 (6)
O1_5—H1*OB*_5···O1_3^{ii}	0.81 (2)	2.31 (5)	2.943 (6)	135 (6)
O2_5—H2*OB*_5···O1_4^{vi}	0.81 (2)	2.34 (5)	2.965 (6)	135 (6)
O2_5—H2*OA*_5···O2_4	0.81 (2)	2.09 (4)	2.845 (6)	154 (6)
O3_5—H3*OA*_5···O4_2	0.81 (2)	2.16 (5)	2.823 (6)	139 (6)
O3_5—H3*OB*_5···O1_2	0.81 (2)	2.12 (4)	2.848 (6)	150 (6)
O4_5—H4*OA*_5···O2_1^{ii}	0.82 (2)	2.09 (4)	2.835 (6)	152 (8)
O4_5—H4*OB*_5···O5_1^{ii}	0.81 (2)	2.10 (5)	2.823 (6)	147 (8)

Symmetry codes: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (iii) $-x+1, -y, -z+1$; (iv) $x, y-1, z$; (v) $x-\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$; (vi) $-x+1, -y+1, -z+1$. Note: (*) these H atoms were initially placed *via* the difference map. They were refined using fixed positions, as otherwise H3*OB*_2 would refine to an unrealistic position.

difference map but their positions were not allowed to refine, as otherwise H3*OB*_2 would refine to an unrealistic position. All other H atoms were placed in computed locations and refined as riding atoms with relative isotropic displacement parameters. Hirshfeld surface compositions were calculated using the *CrystalExplorer* software package (Spackman *et al.*, 2021). The crystal of *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ and water, crystal **1**, for which the data are reported, was found to be a 2-component non-merohedral twin with an approximate domain ratio of 89:11. The minor domain was rotated from the first domain by 179.9° about an axis in reciprocal space given by the following vector [0.484 0.000 1.000] and an axis in direct space given by the following vector [0.996 0.001 1.000]. The twin law relating the two domains is (in line format): [−0.350 0.004 0.653] [0.000 −1.000 0.000] [1.345 −0.002 0.350].



1 Solvent = ·1.33H_2O
2 Solvent = ·5DMB
Scheme 1

3. Results and discussion

3.1. Crystal structure analysis

The crystal structure of **1** is a cocrystal of *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ and water, and it crystallized in the space group $P2_1/n$. The asymmetric unit contains two molecules of the complex, as well as two half-molecules in which the Ni atom is located on a crystallographic inversion center (Fig. 2). There are four

Table 3
Hydrogen-bond geometry (Å, °) for **2**.

D—H···A	D—H	H···A	D···A	D—H···A
O3_1—H1_1···O1_2	0.80 (2)	2.17 (2)	2.8978 (17)	152 (2)
O3_1—H1_1···O2_2	0.80 (2)	2.33 (2)	2.9854 (17)	140 (2)
O3_1—H2_1···O1_3	0.84 (2)	2.31 (2)	2.9100 (16)	128.8 (19)
O3_1—H2_1···O2_3	0.84 (2)	2.23 (3)	3.0377 (17)	161 (2)

cocrystallized water molecules, resulting in a *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ to water stoichiometry of 3:4. Eight of the twelve trifluoromethyl (CF_3) groups in the asymmetric unit are disordered and modeled in two partially occupied parts. Geometric and rigid bond restraints were applied to both parts of all of the disordered CF_3 groups to ensure reasonable geometries and anisotropic displacement parameters (ADPs). When necessary, ADP constraints were applied to the F atoms to prevent the refinement of prolate, oblate, or non-positive definite ADPs. Bond distance restraints were applied to the O—H and H···H distances for all of the aqua ligands to ensure similar bond lengths and angles between all of the ligands. Similar restraints were applied to the cocrystallized water molecules in the structure. The packing of crystal **1** consists of alternating layers parallel to the [101] direction featuring hydrogen-bonding interactions between the aqua ligands and free water molecules, and sheets of $CF_3\cdots CF_3$ interactions (Fig. 3 and Table 2). There are two primary hydrogen-bonding motifs that make up the hydrogen-bonding layers, which will be categorized using graph-set notation (Etter *et al.*, 1990). In the first type (Fig. 4, **a**), one of the aqua ligands on the *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ complex forms an

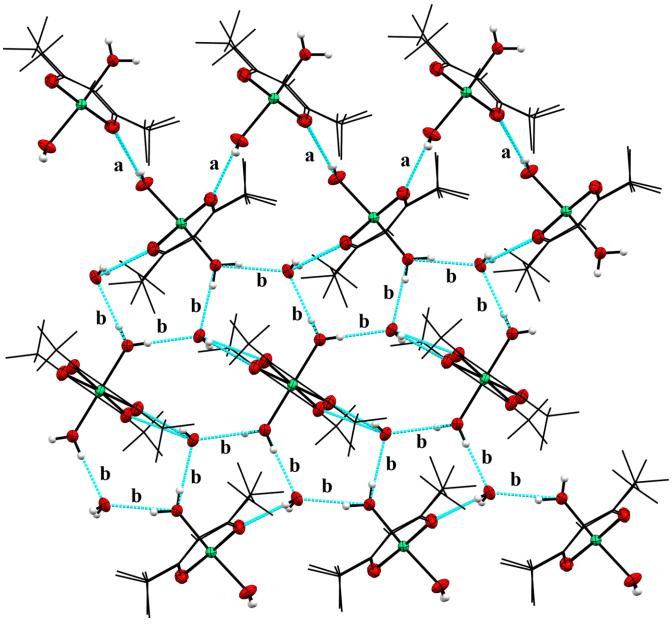


Figure 4
A layer of the hydrogen-bonding network present in **1**, viewed in the [101] direction. In this figure and subsequent figures, hydrogen bonds are represented by dashed blue lines. Hydrogen bonds labeled '**a**' involve an aqua ligand donor and hfac acceptors, while hydrogen bonds labeled '**b**' involve aqua ligand donors and water acceptors. Portions of the hfac ligands are drawn in wireframe for clarity.

$R_2^2(6)$ hydrogen-bonded ring with the two O atoms of a hfac ligand on an adjacent $Ni^{II}(hfac)_2(H_2O)_2$ complex. The aqua ligand at the other end of the complex donates a hydrogen bond to two of the cocrystallized water molecules. In the second type of hydrogen-bond motif, both of the aqua ligands on a *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ unit act as hydrogen-bond donors to cocrystallized water molecules, forming $C_4^4(6)$ hydrogen-bond chains (Fig. 4, **b**). The cocrystallized water molecules in this layer also form $R_2^2(6)$ hydrogen-bonded rings with the O atoms of adjacent hfac ligands. This leads to a general packing scheme in which one layer of an aqua–hfac $R_2^2(6)$ hydrogen-bond network is followed by two layers of $C_4^4(6)$ aqua–water hydrogen-bond networks. All cocrystallized water molecules act as hydrogen-bond donors to the O atoms of hfac ligands and as acceptors from aqua ligands. This complex hydrogen-bonding network explains the large number of molecules in the asymmetric unit of the crystal. As shown in Fig. 1, crystals of **1** were large and it was necessary to cut the crystals for data collection. Obtaining a high-quality single crystal of a suitable size proved to be difficult, as the crystals tended to slip rather than split cleanly when being cut. This resulted in streaks in the diffraction pattern, and also made it difficult to select a quality single crystal. Data collection was attempted on several crystals before a satisfactory structure solution could be obtained. The crystal packing offers a possible explanation for the macroscopic slipping behavior of the crystals. Based on the weak intermolecular forces of $CF_3\cdots CF_3$ contacts, it can be speculated that when the crystals were being cut for mounting the slipping occurred along the areas of $CF_3\cdots CF_3$ interactions, although this was not confirmed by experiment.

Crystal **2** is a cocrystal of *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ and DMB, and crystallized in the space group $P2_1/c$. The Ni atom is situated on a crystallographic inversion center, leading to half

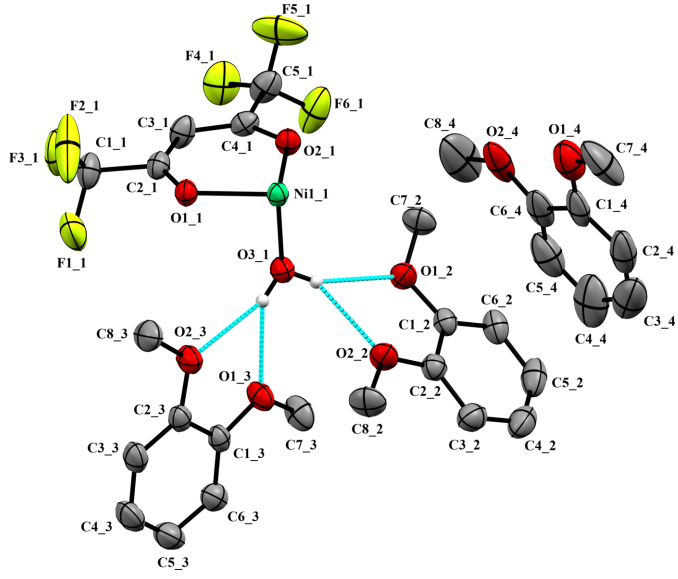


Figure 5
The asymmetric unit of **2**. The DMB molecule in Residue 4 is disordered. Only the majorly occupied disordered parts are shown. H atoms not bonded to water have been hidden for clarity.

Table 4
Contributions (%) of different contact types to the Hirshfeld surfaces of each of the four *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ complexes in **1**, the average values in **1**, and for the *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ complex in **2**.

All contacts include reciprocal contacts. Minor contributions have been omitted, leading to a sum of less than 100% for each complex.

Hirshfeld surface contact type	**1**, Residue 1	**1**, Residue 2	**1**, Residue 3	**1**, Residue 4	**1**, Average	**2**
F···F	43.8	42.6	45.0	45.1	44.1	0.7
F···H/H···F	28.9	27.2	28.3	30.2	28.7	61.5
F···C/C···F	7.3	9.9	6.3	6.0	7.4	2.7
F···O/O···F	2.2	1.7	2.4	2.6	2.2	1.7
C···H/H···C	0	0	0	0	0	4.4
H···H	3.4	3.5	3.9	3.9	3.7	10.9
O···H/H···O	12.9	12.4	11.8	12.1	12.3	16.7

of the molecule being crystallographically unique. Within the asymmetric unit, the aqua ligand acts as a hydrogen-bond donor to two cocrystallized DMB molecules, with both of the O atoms on the DMB acting as acceptors to one of the H atoms of the aqua ligand in an $R_1^2(5)$ manner (Fig. 5 and Table 3). Each of the CF_3 groups of the complex are disordered and were modeled in two partially occupied parts using geometric and rigid bond restraints to ensure realistic geometries and ADPs. An ADP constraint was used to prevent atom F3′_1 from having prolate ADPs. There is an additional cocrystallized DMB molecule that is located in a cavity on a crystallographic inversion center and is only half occupied within the asymmetric unit, giving a *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ to DMB stoichiometry of 1:5. The DMB molecule located on the inversion center is disordered and was modeled in two partially occupied general positions, with occupancies that add up to 50%. The two disordered parts were modeled using a geometric restraints based on the ordered DMB molecule in Residue 3. A rigid bond restraint was applied to both parts of the disordered DMB molecule. In the unit cell, the Ni atoms of the *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ complexes sit on the inversion centers located at $\frac{1}{2}$, 0, 0 and $\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$, with all of the Ni atoms in a plane. The disordered free DMB molecule sits on the inversion centers between the metal complexes at $\frac{1}{2}$, $\frac{1}{2}$, 0 and $\frac{1}{2}$, 0, $\frac{1}{2}$ (Fig. 6). In the packing of the crystal, the *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ complexes and associated hydrogen-bonded DMB molecules form contacts with the free DMB molecule in the crystallographic *b* and *c* directions, and contact adjacent complexes in the *a*, [011], and [0$\bar{1}$1] directions (Fig. 6).

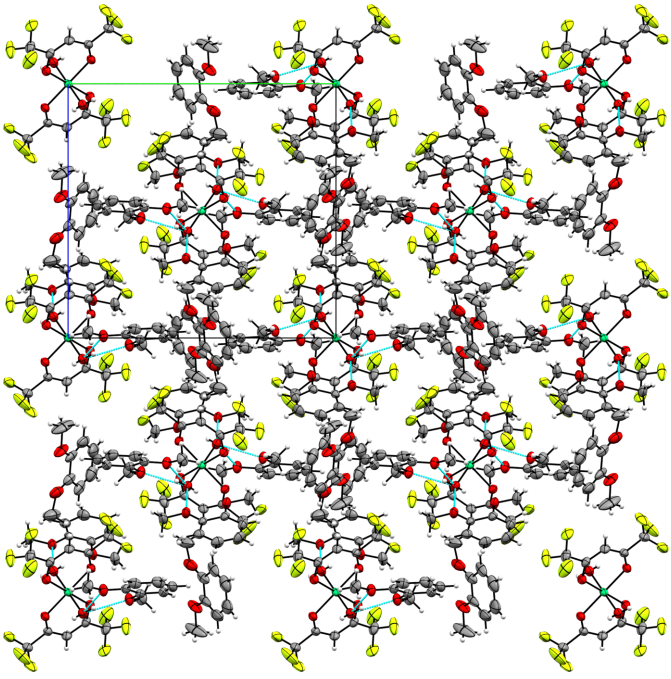


Figure 6
A 2 × 2 × 2 supercell of **2**, viewed along the crystallographic *a* axis. The *b* and *c* axes are shown in green and blue, respectively. Minorly occupied portions of disordered parts have been hidden for clarity.

Like with **1**, crystals of **2** were large and needed to be cut to obtain an appropriate size for data collection. Contrary to **1**, the crystals of **2** cleaved cleanly, likely because the crystal structure lacks the layers of $CF_3\cdots CF_3$ interactions present in compound **1**. In fact, there are no F···F short contacts (defined as a distance less than the sum of the van der Waals radii of the two atoms) in the crystal packing of **2**, and all of the close contacts to the *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ complex are with DMB molecules. The chemical environments of the metal complexes in the two crystal structures were investigated using Hirshfeld surface analysis, a useful method for enumerating the differences in packing environments between different molecules in crystal structures (Spackman & Jayatilaka, 2009). Hirshfeld surfaces were computed for the *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ complexes in **1** and **2**. Table 4 gives the surface compositions for the metal complexes in each of the structures. Each of the four *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ molecules in the structure of **1** have very similar surface compositions, with F···F contacts being the largest contributor to the Hirshfeld surface. In contrast, the *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ complex in **2** has almost no F···F contacts, making up less than 1% of the Hirshfeld surface. The complex in **2** has about double the F···H/H···F contacts of the complexes in **1**, and about triple the contribution from H···H contacts. Notably, there are no C···H/H···C contacts for any of the *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ complexes in **1**, while the complex in **2** has a 4.4% contribution of these contacts to the Hirshfeld surface.

3.2. Comparison to literature structures

A search of the Cambridge Structural Database (CSD; Version 6.01, including May 2026 updates) (Groom *et al.*, 2016) reveals only four crystal structures containing $Ni^{II}(hfac)_2(H_2O)_2$ complexes: VOXRAB (Romero *et al.*, 1992), KUM-

BEZ (Luneau *et al.*, 1992), TUKPEU (Burdukov *et al.*, 1996), and ECOJAI (Maekawa *et al.*, 2006). VOXRAB is a neat form of the *cis*-$Ni^{II}(hfac)_2(H_2O)_2$ complex, in which the two aqua ligands are *cis* rather than *trans* across the nickel center. The crystal packing of VOXRAB bears some similarities to that of **1**, with $R_2^2(6)$ hydrogen-bonded rings between the aqua ligands and hfac ligands leading to chains of metal complexes in which the hydrogen-bonded rings are separated by Ni atoms [Fig. 7(*a*)]. Unlike in crystal **1**, in which the hydrogen-bond network forms two-dimensional sheets separated by F···F contacts, the hydrogen-bond chains of metal complexes in VOXRAB are one-dimensional, and contacts between chains include F···F contacts, as well as F···H contacts. An examination of the Hirshfeld surface compositions between **1** and VOXRAB shows that VOXRAB has significantly more F···O contacts compared to **1**, while having fewer H···O contacts (Table 5).

Table 5
A comparison of Hirshfeld surface compositions (%) between **1** and VOXRAB.

Hirshfeld surface contact	**1**, average	VOXRAB
F···F	44.1	46.6
F···H/H···F	28.7	25.1
F···C/C···F	7.4	8.1
F···O/O···F	2.2	9.8
C···H/H···C	0	0
H···H	3.7	1.8
O···H/H···O	12.3	8.6

The structures of KUMBEZ, TUKPEU, and ECOJAI are all cocrystals of *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ with 2,5-dihydroimidazole nitroxide-based coformers. For crystals KUMBEZ and TUKPEU, each H atom on the aqua ligands acts as a donor to a coformer, giving a *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ to coformer ratio of 1:4, similar to what is seen in crystal **2**. Unlike in **2**, the coformers in KUMBEZ and TUKPEU have multiple hydrogen-bond-accepting sites, resulting in the formation of hydrogen-bond networks. In TUKPEU, the hydrogen bonding forms $R_4^4(14)$ rings in which the aqua ligand acts as a hydrogen-bond donor to an imidazole N atom and a methoxy O atom of two separate coformers [Fig. 7(*b*)]. Similar to **1**, the hydrogen-bond networks in KUMBEZ form two-dimensional hydrogen-bonded sheets parallel to the [101] direction [Fig. 7(*c*)]. Each *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ complex participates in two $R_4^4(14)$ hydrogen-bonded rings, and each hydrogen-bonded ring is separated from the next by the Ni atom of the metal complex.

ECOJAI includes a coformer that contains a *trans*-$Ni^{II}(hfac)_2$ center, with a symmetric 2,5-dihydroimidazole nitroxide dimer acting as a bidentate ligand on the metal center. This ligand has two hydrogen-bond-accepting sites. Contrary to **2**, in which each H atom of the aqua ligand acts as a donor to both acceptor atoms on the DMB coformer, each acceptor of the coformer in ECOJAI is hydrogen bonded to only one H atom from the aqua ligand. The crystal packing and hydrogen-bond network are quite different from crystal **1**, consisting of $R_4^4(18)$ hydrogen-bonded rings in which each H

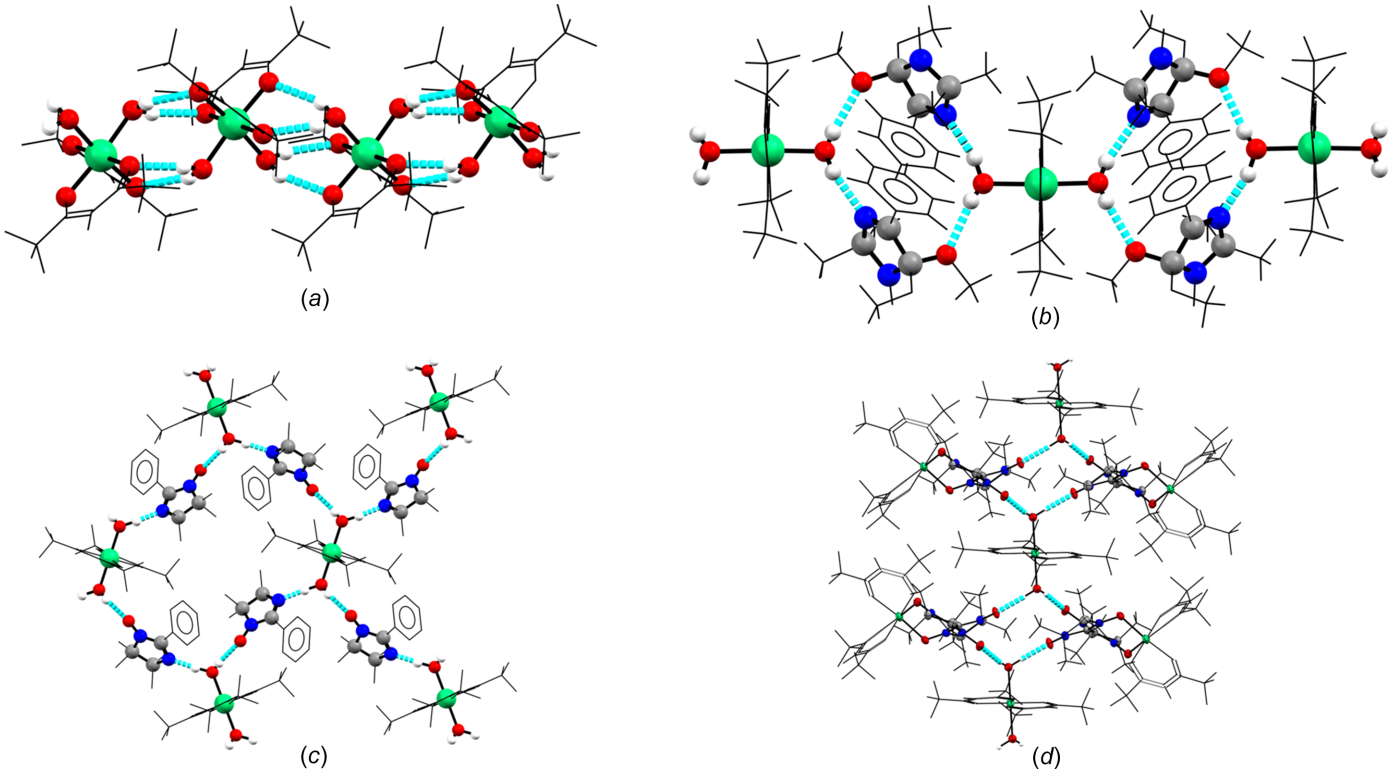


Figure 7
(*a*) Hydrogen bonding between *cis*-$Ni^{II}(hfac)_2(H_2O)_2$ complexes in VOXRAB. (*b*) $R_4^4(14)$ hydrogen-bonded rings in TUKPEU. (*c*) A view of the hydrogen-bond sheet in KUMBEZ. (*d*) $R_4^4(18)$ hydrogen-bonded rings in ECOJAI. The CIF files deposited in the CSD for structures VOXRAB, KUMBEZ, and TUKPEU do not contain displacement ellipsoid information, so the atoms are drawn as fixed size spheres.

atom of the aqua ligand of the *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ complex forms a hydrogen bond with the *N*-oxide O atom of the other complex, with a crystallographic inversion center located in the center of the hydrogen-bond network [Fig. 7(*d*)]. Similarly to TUKPEU, the *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ complex participates in two $R_4^4(18)$ hydrogen-bonded rings, and each hydrogen-bonded ring is separated frem the next by the Ni atom of $Ni^{II}(hfac)_2$. While the sample size is small, it is observed that cocrystals of *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ are capable of forming different hydrogen-bond motifs depending on the identity of the coformer. Coformers which have two accepting sites on different ends of the molecule can form hydrogen-bonded sheets or rings linked by Ni centers. Water, a coformer with two donating sites and two accepting sites, enabled the formation of sheets which contained both ring and chain hydrogen-bond motifs. Notably, the crystal structure of **2** demonstrates that DMB, a coformer with two accepting sites located on the same side of the molecule, prevents the formation of a hydrogen-bond network, even when the DMB molecule itself does not coordinate to the metal center. This provides insight into methods by which cocrystal design can be used to manipulate the hydrogen-bond networks in *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ and structurally related compounds.

4. Conclusion

In this work, the crystal structures of two solvates of *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ are reported. The crystal structure containing water as a coformer formed layers of hydrogen-bond networks separated by layers of $CF_3\cdots CF_3$ contacts, a packing motif that potentially results in the macroscopic tendency of the crystals to slip rather than break cleanly when cut. The DMB cocrystal formed discrete units of *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ hydrogen bonded to four DMB molecules, with the DMB molecules occupying all hydrogen-bond-accepting sites of the aqua ligands, preventing the formation of an extended hydrogen-bond network. These new structures increased the amount of reported $Ni^{II}(hfac)_2(H_2O)_2$ crystal structures, with only four such structures having been reported previously. An examination of the hydrogen-bonding motifs in each of the structures revealed that despite the small sample size, *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ cocrystals can form a variety of hydrogen-bond network motifs, and that DMB is capable of disrupting the formation of a hydrogen-bond network in *trans*-$Ni^{II}(hfac)_2(H_2O)_2$ without needing to coordinate to the metal center.

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Conflict of interest

The authors declare no conflicts of interest.

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Hydrogen bonding in cocrystals of *trans*-$Ni^{II}(hfac)_2(H_2O)_2$

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Computing details

Diaquabis(1,1,1,5,5,5-hexafluoro-4-oxopent-2-en-2-olato-κ^2O,O')nickel(II) 1.33-hydrate (26169twin5revised)

Crystal data

$[Ni(C_5HF_6O_2)_2(H_2O)_2]\cdot 1.33H_2O$
M_r = 1598.64
Monoclinic, $P2_1/n$
a = 24.3968 (14) Å
b = 7.2381 (4) Å
c = 31.5461 (17) Å
β = 106.300 (2)°
V = 5346.7 (5) Å^3
Z = 4
$F(000)$ = 3160
D_x = 1.986 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9824 reflections
θ = 3.1–26.4°
μ = 1.25 mm^{-1}
T = 153 K
Plate, green
0.27 × 0.25 × 0.08 mm

Data collection

Bruker D8 VENTURE diffractometer
Radiation source: microfocus sealed tube, Incoatec IμS 3.0
Multilayer mirror monochromator
Detector resolution: 7.3910 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (TWINABS; Sevvana *et al.*, 2019; Sheldrick, 2012)
T_{min} = 0.603, T_{max} = 0.745
11657 measured reflections
11657 independent reflections
10792 reflections with $I > 2\sigma(I)$
θ_{max} = 26.6°, θ_{min} = 2.0°
h = −30→29
k = 0→9
l = 0→39

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.147
S = 1.16
11657 reflections
1020 parameters
566 restraints
Primary atom site location: intrinsic phasing
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0153P)^2 + 34.3181P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.98 e Å^{-3}
$\Delta\rho_{min}$ = −0.69 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Data was collected on a Bruker D8 Venture diffractometer equipped with a Photon-III CPAD detector and an Incoatec IμS 3.0 Mo microfocus X-ray source. Data collection strategies were computed using the APEX 6 software package (Bruker Analytical X-ray Systems, 2023), data was integrated using SAINT (Bruker Analytical X-ray Systems, 2016), and scaled using TWINABS (Sevvana *et al.*, 2019) for crystal **1** and SADABS (Krause *et al.*, 2015) for crystal **2**. Structures were solved using SHELXT (Sheldrick, 2015) and refined using SHELXL (Sheldrick, 2015*a*) within the ShelXle program (Hübschle *et al.*, 2011).

Refined as a 2-component non-merohedral twin with an approximate domain ratio of 89:11. The twin law relating the two domains is given below: -0.350 0.004 0.653 0.000 -1.000 0.000 1.345 -0.002 0.350

The reflections -4 1 1, -2 0 2, -3 1 1, -2 1 1, -1 1 1, -1 1 2, 1 1 1, and 0 1 1 were omitted due to suspected interference from the beam stop.

The H atoms H5OA_1 and H5OB_1 were located in a reasonable location in the difference map, but upon refinement H5OB_1 would move to alocation that gave a small Ni-O-H angle. These two H atoms were placed via the difference map, then their locations fixed using an AFIX 3 command.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ni1_1	0.31584 (3)	0.44806 (10)	0.81859 (2)	0.02094 (16)	
F1_1	0.14168 (17)	0.7763 (6)	0.79353 (13)	0.0517 (11)	
F2_1	0.2089 (2)	0.9486 (6)	0.83071 (17)	0.0577 (12)	
F3_1	0.15241 (17)	0.8167 (6)	0.86263 (14)	0.0521 (11)	
C10_1	0.4849 (3)	0.2365 (9)	0.8331 (2)	0.0428 (14)	0.365 (6)
F10_1	0.4817 (7)	0.090 (2)	0.8103 (6)	0.085 (6)	0.365 (6)
F11_1	0.5315 (5)	0.329 (2)	0.8276 (5)	0.056 (3)	0.365 (6)
F12_1	0.4963 (8)	0.215 (3)	0.8744 (5)	0.070 (6)	0.365 (6)
C10′_1	0.4849 (3)	0.2365 (9)	0.8331 (2)	0.0428 (14)	0.635 (6)
F10′_1	0.4700 (4)	0.0605 (10)	0.8418 (4)	0.075 (3)	0.635 (6)
F11′_1	0.5150 (5)	0.208 (2)	0.8064 (4)	0.109 (5)	0.635 (6)
F12′_1	0.5120 (6)	0.2927 (18)	0.8718 (4)	0.088 (4)	0.635 (6)
O1_1	0.24621 (15)	0.6102 (6)	0.81176 (12)	0.0261 (8)	
O2_1	0.29368 (16)	0.3025 (5)	0.86651 (12)	0.0272 (8)	
O3_1	0.27152 (17)	0.2594 (7)	0.77374 (13)	0.0328 (10)	
H3OB_1	0.276 (2)	0.251 (11)	0.7494 (10)	0.049*	
H3OA_1	0.2383 (11)	0.240 (11)	0.7718 (19)	0.049*	
O4_1	0.33738 (15)	0.6014 (6)	0.77180 (12)	0.0254 (8)	
O5_1	0.38786 (15)	0.2962 (5)	0.82605 (12)	0.0271 (8)	
O6_1	0.36174 (18)	0.6194 (6)	0.86612 (13)	0.0309 (9)	
H6OA_1	0.388 (2)	0.582 (7)	0.8860 (16)	0.046*	
H6OB_1	0.364 (3)	0.730 (3)	0.865 (2)	0.046*	
C1_1	0.1805 (3)	0.7922 (10)	0.8326 (2)	0.0355 (14)	
C2_1	0.2211 (2)	0.6312 (8)	0.84127 (17)	0.0256 (11)	
C3_1	0.2270 (2)	0.5224 (8)	0.87933 (17)	0.0273 (12)	

H3_1	0.206632	0.556800	0.899694	0.033*	
C4_1	0.2616 (2)	0.3671 (9)	0.88812 (17)	0.0278 (12)	
C5_1	0.2598 (2)	0.2494 (9)	0.92837 (18)	0.0338 (12)	0.825 (9)
F4_1	0.2239 (3)	0.1145 (10)	0.91650 (18)	0.077 (3)	0.825 (9)
F5_1	0.2427 (3)	0.3488 (9)	0.95796 (18)	0.0654 (18)	0.825 (9)
F6_1	0.3104 (3)	0.1883 (12)	0.9495 (2)	0.070 (2)	0.825 (9)
C5′_1	0.2598 (2)	0.2494 (9)	0.92837 (18)	0.0338 (12)	0.175 (9)
F4′_1	0.2730 (16)	0.078 (3)	0.9207 (8)	0.0654 (18)	0.175 (9)
F5′_1	0.2165 (11)	0.245 (6)	0.9434 (11)	0.080 (10)	0.175 (9)
F6′_1	0.3030 (13)	0.293 (6)	0.9623 (9)	0.081 (11)	0.175 (9)
C6_1	0.3956 (3)	0.7664 (11)	0.7384 (2)	0.0503 (16)	0.365 (6)
F7_1	0.3536 (7)	0.827 (3)	0.7108 (7)	0.067 (6)	0.365 (6)
F8_1	0.4342 (7)	0.877 (2)	0.7558 (5)	0.076 (4)	0.365 (6)
F9_1	0.4216 (8)	0.6818 (19)	0.7096 (5)	0.084 (2)	0.365 (6)
C6′_1	0.3956 (3)	0.7664 (11)	0.7384 (2)	0.0503 (16)	0.635 (6)
F7′_1	0.3823 (5)	0.9359 (10)	0.7567 (3)	0.084 (2)	0.635 (6)
F8′_1	0.4454 (3)	0.7977 (16)	0.7348 (4)	0.080 (3)	0.635 (6)
F9′_1	0.3558 (6)	0.769 (2)	0.7018 (4)	0.076 (4)	0.635 (6)
C7_1	0.3873 (2)	0.6127 (9)	0.76900 (19)	0.0297 (13)	
C8_1	0.4343 (2)	0.5048 (9)	0.78890 (19)	0.0324 (13)	
H8_1	0.470323	0.535696	0.784755	0.039*	
C9_1	0.4304 (2)	0.3531 (9)	0.81472 (19)	0.0306 (13)	
Ni1_2	0.67842 (3)	0.04941 (10)	0.68460 (2)	0.02003 (16)	
F4_2	0.56524 (16)	−0.3162 (6)	0.77868 (14)	0.0514 (11)	
F5_2	0.65514 (16)	−0.2863 (6)	0.80655 (13)	0.0489 (10)	
F6_2	0.6235 (2)	−0.4529 (6)	0.74887 (16)	0.0579 (12)	
O1_2	0.60623 (16)	0.1958 (5)	0.68402 (12)	0.0264 (8)	
O2_2	0.66495 (15)	−0.1120 (5)	0.73287 (12)	0.0253 (8)	
O3_2	0.62867 (18)	−0.1210 (6)	0.63839 (13)	0.0345 (10)	
H3OA_2	0.610797	−0.102940	0.613967	0.052*	
H3OB_2	0.627797	−0.241739	0.640169	0.052*	
O4_2	0.69150 (17)	0.2028 (5)	0.63436 (12)	0.0277 (8)	
O5_2	0.74780 (15)	−0.1038 (6)	0.68460 (12)	0.0254 (8)	
O6_2	0.72526 (17)	0.2350 (7)	0.72866 (13)	0.0346 (10)	
H6OB_2	0.7590 (10)	0.249 (11)	0.732 (2)	0.052*	
H6OA_2	0.720 (2)	0.254 (11)	0.7526 (11)	0.052*	
C1_2	0.5122 (3)	0.2480 (9)	0.68636 (19)	0.0395 (13)	0.685 (8)
F1_2	0.4661 (3)	0.1419 (11)	0.6829 (3)	0.0601 (18)	0.685 (8)
F2_2	0.5011 (4)	0.3175 (14)	0.6463 (3)	0.072 (2)	0.685 (8)
F3_2	0.5133 (4)	0.3713 (14)	0.7153 (3)	0.089 (3)	0.685 (8)
C1′_2	0.5122 (3)	0.2480 (9)	0.68636 (19)	0.0395 (13)	0.315 (8)
F1′_2	0.4680 (7)	0.170 (3)	0.6612 (8)	0.089 (3)	0.315 (8)
F2′_2	0.5190 (6)	0.412 (2)	0.6676 (6)	0.0601 (18)	0.315 (8)
F3′_2	0.4967 (8)	0.306 (3)	0.7211 (5)	0.072 (2)	0.315 (8)
C2_2	0.5669 (2)	0.1341 (8)	0.69786 (18)	0.0272 (12)	
C3_2	0.5683 (2)	−0.0228 (9)	0.72437 (18)	0.0286 (12)	
H3_2	0.534750	−0.055924	0.732243	0.034*	
C4_2	0.6162 (2)	−0.1297 (8)	0.73929 (17)	0.0247 (11)	

C5_2	0.6133 (3)	−0.2948 (9)	0.7683 (2)	0.0340 (13)	
C6_2	0.7132 (2)	0.2675 (9)	0.56807 (19)	0.0382 (13)	0.685 (8)
F7_2	0.6710 (5)	0.2057 (18)	0.5355 (4)	0.078 (4)	0.685 (8)
F8_2	0.6957 (4)	0.4406 (10)	0.5746 (3)	0.0572 (17)	0.685 (8)
F9_2	0.7594 (3)	0.2917 (15)	0.5563 (3)	0.085 (3)	0.685 (8)
C6′_2	0.7132 (2)	0.2675 (9)	0.56807 (19)	0.0382 (13)	0.315 (8)
F7′_2	0.7416 (8)	0.187 (2)	0.5423 (5)	0.0572 (17)	0.315 (8)
F8′_2	0.6610 (7)	0.269 (4)	0.5447 (10)	0.076 (8)	0.315 (8)
F9′_2	0.7352 (12)	0.426 (2)	0.5779 (6)	0.100 (8)	0.315 (8)
C7_2	0.7207 (2)	0.1485 (8)	0.60971 (17)	0.0277 (12)	
C8_2	0.7564 (2)	−0.0033 (9)	0.61489 (18)	0.0324 (13)	
H8_2	0.773790	−0.031921	0.592250	0.039*	
C9_2	0.7677 (2)	−0.1151 (9)	0.65210 (18)	0.0271 (12)	
C10_2	0.8103 (3)	−0.2800 (10)	0.65625 (19)	0.0465 (15)	0.685 (8)
F10_2	0.8383 (5)	−0.284 (2)	0.6278 (3)	0.127 (6)	0.685 (8)
F11_2	0.7826 (6)	−0.4372 (16)	0.6531 (5)	0.111 (4)	0.685 (8)
F12_2	0.8467 (3)	−0.2879 (10)	0.69478 (19)	0.0494 (16)	0.685 (8)
C10′_2	0.8103 (3)	−0.2800 (10)	0.65625 (19)	0.0465 (15)	0.315 (8)
F10′_2	0.8177 (8)	−0.311 (3)	0.6177 (5)	0.0494 (16)	0.315 (8)
F11′_2	0.7896 (10)	−0.433 (3)	0.6681 (6)	0.058 (5)	0.315 (8)
F12′_2	0.8566 (9)	−0.221 (3)	0.6839 (8)	0.111 (4)	0.315 (8)
Ni1_3	1.000000	0.500000	0.500000	0.0224 (2)	
F4_3	0.8190 (2)	0.7787 (10)	0.46200 (16)	0.092 (2)	
F5_3	0.81937 (18)	0.8353 (7)	0.52766 (14)	0.0589 (12)	
F6_3	0.8754 (3)	0.9841 (8)	0.4993 (2)	0.096 (2)	
O1_3	0.97546 (17)	0.3572 (6)	0.54747 (13)	0.0317 (9)	
O2_3	0.93715 (16)	0.6880 (5)	0.49586 (13)	0.0285 (9)	
O3_3	1.0565 (2)	0.6498 (6)	0.54673 (15)	0.0379 (11)	
H3OA_3	1.076 (3)	0.599 (11)	0.567 (2)	0.057*	
H3OB_3	1.051 (3)	0.754 (8)	0.550 (3)	0.057*	
C1_3	0.9234 (3)	0.2726 (10)	0.5968 (2)	0.0473 (15)	0.365 (6)
F1_3	0.9449 (9)	0.105 (2)	0.5918 (6)	0.086 (3)	0.365 (6)
F2_3	0.9439 (11)	0.323 (3)	0.6357 (5)	0.145 (6)	0.365 (6)
F3_3	0.8695 (6)	0.229 (3)	0.5898 (7)	0.061 (4)	0.365 (6)
C1′_3	0.9234 (3)	0.2726 (10)	0.5968 (2)	0.0473 (15)	0.635 (6)
F1′_3	0.8827 (7)	0.161 (2)	0.5833 (5)	0.145 (6)	0.635 (6)
F2′_3	0.9695 (4)	0.1944 (15)	0.6203 (3)	0.087 (4)	0.635 (6)
F3′_3	0.9098 (4)	0.3765 (14)	0.6282 (3)	0.086 (3)	0.635 (6)
C2_3	0.9327 (3)	0.3979 (9)	0.55988 (19)	0.0321 (13)	
C3_3	0.8938 (3)	0.5412 (10)	0.5458 (2)	0.0377 (14)	
H3_3	0.862251	0.549698	0.557746	0.045*	
C4_3	0.8989 (2)	0.6712 (8)	0.51518 (18)	0.0287 (12)	
C5_3	0.8528 (3)	0.8230 (11)	0.5019 (2)	0.0452 (17)	
Ni1_4	0.500000	0.500000	0.500000	0.0217 (2)	
C5_4	0.5532 (3)	0.1863 (11)	0.4031 (2)	0.0477 (18)	
F4_4	0.5998 (2)	0.1713 (7)	0.39114 (16)	0.0686 (15)	
F5_4	0.5409 (3)	0.0211 (7)	0.4155 (2)	0.098 (2)	
F6_4	0.5109 (2)	0.2266 (10)	0.36829 (17)	0.093 (2)	

O1_4	0.57316 (17)	0.6378 (6)	0.50245 (13)	0.0296 (9)	
O2_4	0.51705 (17)	0.3122 (6)	0.45797 (13)	0.0303 (9)	
O3_4	0.5402 (2)	0.3491 (6)	0.55400 (14)	0.0369 (10)	
H3OB_4	0.558 (3)	0.394 (8)	0.5773 (13)	0.055*	
H3OA_4	0.551 (3)	0.244 (4)	0.554 (2)	0.055*	
C1_4	0.6574 (3)	0.7266 (9)	0.48577 (19)	0.0413 (14)	0.711 (10)
F1_4	0.6682 (4)	0.8145 (16)	0.5221 (3)	0.082 (3)	0.711 (10)
F2_4	0.7054 (2)	0.6186 (11)	0.4903 (3)	0.071 (2)	0.711 (10)
F3_4	0.6552 (4)	0.8298 (16)	0.4522 (3)	0.084 (3)	0.711 (10)
C1′_4	0.6574 (3)	0.7266 (9)	0.48577 (19)	0.0413 (14)	0.289 (10)
F1′_4	0.6857 (10)	0.764 (4)	0.5260 (5)	0.084 (3)	0.289 (10)
F2′_4	0.6898 (9)	0.714 (4)	0.4604 (7)	0.082 (3)	0.289 (10)
F3′_4	0.6347 (8)	0.902 (2)	0.4744 (9)	0.080 (6)	0.289 (10)
C2_4	0.6048 (2)	0.6000 (9)	0.47858 (18)	0.0299 (13)	
C3_4	0.5990 (3)	0.4621 (9)	0.44747 (18)	0.0324 (13)	
H3_4	0.625674	0.456976	0.430589	0.039*	
C4_4	0.5559 (2)	0.3302 (9)	0.43973 (18)	0.0303 (13)	
O1_5	0.45239 (19)	0.5244 (6)	0.93922 (14)	0.0361 (10)	
H1OA_5	0.443 (3)	0.589 (8)	0.957 (2)	0.054*	
H1OB_5	0.480 (2)	0.574 (9)	0.935 (2)	0.054*	
O2_5	0.43493 (18)	0.0239 (6)	0.44663 (14)	0.0322 (9)	
H2OB_5	0.420 (2)	0.073 (9)	0.4635 (19)	0.048*	
H2OA_5	0.4648 (17)	0.078 (9)	0.449 (2)	0.048*	
O3_5	0.6168 (2)	0.5040 (6)	0.63077 (14)	0.0343 (9)	
H3OA_5	0.6483 (15)	0.465 (9)	0.632 (2)	0.051*	
H3OB_5	0.605 (2)	0.443 (9)	0.647 (2)	0.051*	
O4_5	1.1323 (2)	0.4939 (6)	0.62378 (15)	0.0374 (10)	
H4OA_5	1.159 (2)	0.558 (9)	0.622 (3)	0.056*	
H4OB_5	1.124 (3)	0.545 (10)	0.6440 (18)	0.056*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1_1	0.0210 (3)	0.0200 (4)	0.0198 (3)	−0.0001 (3)	0.0025 (3)	0.0021 (3)
F1_1	0.042 (2)	0.059 (3)	0.044 (2)	0.021 (2)	−0.0033 (17)	0.002 (2)
F2_1	0.068 (3)	0.029 (2)	0.086 (3)	0.000 (2)	0.040 (3)	−0.001 (2)
F3_1	0.050 (2)	0.058 (3)	0.059 (2)	0.018 (2)	0.032 (2)	0.003 (2)
C10_1	0.029 (3)	0.046 (4)	0.048 (3)	0.019 (3)	0.002 (2)	0.006 (3)
F10_1	0.071 (11)	0.063 (9)	0.094 (11)	0.047 (7)	−0.024 (9)	−0.022 (9)
F11_1	0.023 (5)	0.081 (9)	0.065 (8)	0.027 (5)	0.013 (5)	0.024 (7)
F12_1	0.043 (10)	0.119 (19)	0.049 (6)	0.043 (11)	0.015 (6)	0.041 (8)
C10′_1	0.029 (3)	0.046 (4)	0.048 (3)	0.019 (3)	0.002 (2)	0.006 (3)
F10′_1	0.065 (5)	0.036 (4)	0.125 (8)	0.028 (3)	0.030 (5)	0.019 (4)
F11′_1	0.083 (8)	0.158 (13)	0.109 (8)	0.090 (9)	0.064 (7)	0.072 (8)
F12′_1	0.070 (9)	0.072 (8)	0.084 (6)	0.026 (5)	−0.044 (6)	−0.010 (6)
O1_1	0.0231 (18)	0.032 (2)	0.0216 (18)	0.0053 (16)	0.0036 (15)	0.0066 (16)
O2_1	0.031 (2)	0.024 (2)	0.0252 (19)	−0.0005 (16)	0.0053 (16)	0.0031 (16)
O3_1	0.028 (2)	0.045 (3)	0.026 (2)	−0.015 (2)	0.0087 (16)	−0.0134 (19)

O4_1	0.0186 (17)	0.030 (2)	0.0252 (18)	0.0007 (16)	0.0018 (14)	0.0063 (16)
O5_1	0.0243 (19)	0.024 (2)	0.0281 (19)	0.0026 (16)	−0.0008 (15)	0.0004 (16)
O6_1	0.036 (2)	0.020 (2)	0.027 (2)	0.0039 (18)	−0.0052 (17)	0.0046 (17)
C1_1	0.029 (3)	0.042 (4)	0.036 (3)	−0.003 (3)	0.009 (3)	−0.012 (3)
C2_1	0.024 (3)	0.026 (3)	0.025 (3)	−0.003 (2)	0.004 (2)	−0.005 (2)
C3_1	0.028 (3)	0.032 (3)	0.021 (3)	−0.004 (2)	0.006 (2)	−0.004 (2)
C4_1	0.028 (3)	0.034 (3)	0.019 (2)	−0.010 (2)	0.003 (2)	−0.002 (2)
C5_1	0.037 (3)	0.039 (3)	0.023 (3)	−0.008 (2)	0.005 (2)	0.005 (2)
F4_1	0.106 (6)	0.073 (4)	0.049 (3)	−0.063 (4)	0.017 (3)	0.005 (3)
F5_1	0.121 (5)	0.055 (3)	0.034 (3)	0.012 (3)	0.045 (3)	0.012 (2)
F6_1	0.051 (3)	0.108 (6)	0.053 (4)	0.024 (4)	0.016 (3)	0.055 (4)
C5′_1	0.037 (3)	0.039 (3)	0.023 (3)	−0.008 (2)	0.005 (2)	0.005 (2)
F4′_1	0.121 (5)	0.055 (3)	0.034 (3)	0.012 (3)	0.045 (3)	0.012 (2)
F5′_1	0.065 (12)	0.11 (3)	0.08 (2)	0.005 (16)	0.046 (14)	0.03 (2)
F6′_1	0.070 (15)	0.11 (2)	0.043 (13)	−0.012 (18)	−0.016 (11)	−0.008 (15)
C6_1	0.035 (3)	0.061 (4)	0.053 (4)	−0.009 (3)	0.010 (3)	0.022 (3)
F7_1	0.031 (6)	0.071 (15)	0.096 (13)	0.004 (7)	0.012 (5)	0.061 (11)
F8_1	0.081 (6)	0.071 (7)	0.056 (4)	−0.037 (5)	−0.016 (4)	0.037 (4)
F9_1	0.123 (7)	0.039 (4)	0.107 (6)	0.009 (4)	0.061 (5)	0.028 (3)
C6′_1	0.035 (3)	0.061 (4)	0.053 (4)	−0.009 (3)	0.010 (3)	0.022 (3)
F7′_1	0.123 (7)	0.039 (4)	0.107 (6)	0.009 (4)	0.061 (5)	0.028 (3)
F8′_1	0.034 (3)	0.092 (8)	0.119 (8)	−0.002 (4)	0.030 (4)	0.065 (7)
F9′_1	0.081 (6)	0.071 (7)	0.056 (4)	−0.037 (5)	−0.016 (4)	0.037 (4)
C7_1	0.027 (3)	0.034 (3)	0.027 (3)	−0.005 (2)	0.004 (2)	0.004 (2)
C8_1	0.020 (3)	0.046 (4)	0.029 (3)	−0.002 (3)	0.003 (2)	0.001 (3)
C9_1	0.022 (3)	0.039 (4)	0.028 (3)	0.008 (3)	0.002 (2)	−0.004 (3)
Ni1_2	0.0197 (3)	0.0173 (4)	0.0207 (3)	0.0001 (3)	0.0018 (3)	−0.0003 (3)
F4_2	0.0328 (19)	0.066 (3)	0.058 (2)	−0.0016 (19)	0.0185 (18)	0.022 (2)
F5_2	0.043 (2)	0.053 (3)	0.042 (2)	−0.0015 (19)	−0.0014 (17)	0.0226 (19)
F6_2	0.081 (3)	0.027 (2)	0.073 (3)	−0.007 (2)	0.035 (3)	−0.002 (2)
O1_2	0.0269 (19)	0.021 (2)	0.030 (2)	0.0042 (16)	0.0058 (16)	0.0019 (16)
O2_2	0.0218 (18)	0.025 (2)	0.0280 (19)	0.0017 (16)	0.0060 (15)	0.0032 (16)
O3_2	0.044 (2)	0.019 (2)	0.030 (2)	−0.0022 (18)	−0.0073 (18)	−0.0012 (17)
O4_2	0.035 (2)	0.021 (2)	0.0258 (19)	−0.0028 (17)	0.0072 (16)	0.0021 (16)
O5_2	0.0263 (19)	0.027 (2)	0.0230 (18)	0.0023 (16)	0.0069 (15)	0.0003 (16)
O6_2	0.027 (2)	0.048 (3)	0.029 (2)	−0.011 (2)	0.0077 (17)	−0.015 (2)
C1_2	0.034 (3)	0.038 (3)	0.041 (3)	0.010 (3)	0.001 (2)	−0.001 (2)
F1_2	0.024 (2)	0.066 (4)	0.085 (5)	0.012 (2)	0.005 (3)	0.021 (4)
F2_2	0.058 (4)	0.096 (6)	0.064 (3)	0.048 (4)	0.023 (3)	0.036 (4)
F3_2	0.051 (4)	0.077 (5)	0.114 (6)	0.028 (3)	−0.015 (4)	−0.066 (5)
C1′_2	0.034 (3)	0.038 (3)	0.041 (3)	0.010 (3)	0.001 (2)	−0.001 (2)
F1′_2	0.051 (4)	0.077 (5)	0.114 (6)	0.028 (3)	−0.015 (4)	−0.066 (5)
F2′_2	0.024 (2)	0.066 (4)	0.085 (5)	0.012 (2)	0.005 (3)	0.021 (4)
F3′_2	0.058 (4)	0.096 (6)	0.064 (3)	0.048 (4)	0.023 (3)	0.036 (4)
C2_2	0.022 (3)	0.027 (3)	0.030 (3)	0.002 (2)	0.003 (2)	−0.009 (2)
C3_2	0.018 (2)	0.035 (3)	0.031 (3)	0.000 (2)	0.004 (2)	0.001 (2)
C4_2	0.021 (3)	0.026 (3)	0.025 (3)	−0.004 (2)	0.003 (2)	−0.003 (2)
C5_2	0.030 (3)	0.031 (3)	0.041 (3)	−0.004 (3)	0.010 (3)	0.006 (3)

C6_2	0.044 (3)	0.040 (3)	0.028 (3)	−0.004 (3)	0.006 (2)	0.012 (3)
F7_2	0.110 (7)	0.064 (7)	0.032 (4)	−0.016 (6)	−0.025 (5)	0.018 (4)
F8_2	0.087 (5)	0.042 (3)	0.050 (3)	0.011 (3)	0.031 (4)	0.028 (3)
F9_2	0.074 (5)	0.099 (8)	0.103 (7)	0.027 (5)	0.061 (5)	0.072 (6)
C6′_2	0.044 (3)	0.040 (3)	0.028 (3)	−0.004 (3)	0.006 (2)	0.012 (3)
F7′_2	0.087 (5)	0.042 (3)	0.050 (3)	0.011 (3)	0.031 (4)	0.028 (3)
F8′_2	0.042 (6)	0.12 (2)	0.065 (16)	0.012 (8)	0.004 (6)	0.047 (13)
F9′_2	0.20 (2)	0.056 (9)	0.053 (10)	−0.065 (13)	0.043 (14)	−0.009 (8)
C7_2	0.027 (3)	0.030 (3)	0.021 (3)	−0.007 (2)	−0.001 (2)	0.007 (2)
C8_2	0.032 (3)	0.046 (4)	0.019 (3)	0.002 (3)	0.007 (2)	0.000 (2)
C9_2	0.021 (3)	0.033 (3)	0.024 (3)	0.004 (2)	0.003 (2)	0.001 (2)
C10_2	0.050 (4)	0.053 (4)	0.034 (3)	0.022 (3)	0.009 (2)	−0.006 (3)
F10_2	0.128 (9)	0.215 (13)	0.061 (6)	0.133 (9)	0.064 (6)	0.056 (7)
F11_2	0.089 (6)	0.053 (5)	0.148 (9)	0.017 (4)	−0.036 (6)	−0.049 (6)
F12_2	0.057 (3)	0.051 (4)	0.033 (2)	0.036 (3)	0.000 (2)	0.003 (2)
C10′_2	0.050 (4)	0.053 (4)	0.034 (3)	0.022 (3)	0.009 (2)	−0.006 (3)
F10′_2	0.057 (3)	0.051 (4)	0.033 (2)	0.036 (3)	0.000 (2)	0.003 (2)
F11′_2	0.095 (13)	0.045 (8)	0.047 (9)	0.038 (6)	0.040 (9)	0.019 (7)
F12′_2	0.089 (6)	0.053 (5)	0.148 (9)	0.017 (4)	−0.036 (6)	−0.049 (6)
Ni1_3	0.0246 (5)	0.0183 (5)	0.0226 (5)	0.0022 (4)	0.0039 (4)	0.0023 (4)
F4_3	0.074 (3)	0.135 (5)	0.048 (3)	0.069 (4)	−0.013 (2)	0.000 (3)
F5_3	0.051 (2)	0.072 (3)	0.059 (3)	0.025 (2)	0.023 (2)	0.001 (2)
F6_3	0.090 (4)	0.049 (3)	0.173 (6)	0.036 (3)	0.073 (4)	0.032 (4)
O1_3	0.029 (2)	0.032 (2)	0.032 (2)	0.0008 (18)	0.0065 (17)	0.0100 (18)
O2_3	0.032 (2)	0.023 (2)	0.030 (2)	0.0073 (17)	0.0060 (16)	0.0027 (16)
O3_3	0.042 (3)	0.019 (2)	0.039 (2)	0.0019 (19)	−0.011 (2)	−0.0022 (19)
C1_3	0.045 (3)	0.051 (4)	0.045 (3)	−0.008 (3)	0.012 (3)	0.016 (3)
F1_3	0.122 (7)	0.094 (5)	0.061 (4)	0.053 (5)	0.059 (5)	0.050 (4)
F2_3	0.204 (11)	0.144 (11)	0.060 (5)	−0.141 (10)	−0.006 (7)	0.015 (6)
F3_3	0.042 (5)	0.072 (11)	0.078 (10)	−0.011 (5)	0.032 (5)	0.027 (8)
C1′_3	0.045 (3)	0.051 (4)	0.045 (3)	−0.008 (3)	0.012 (3)	0.016 (3)
F1′_3	0.204 (11)	0.144 (11)	0.060 (5)	−0.141 (10)	−0.006 (7)	0.015 (6)
F2′_3	0.098 (6)	0.117 (8)	0.063 (5)	0.067 (6)	0.052 (4)	0.074 (6)
F3′_3	0.122 (7)	0.094 (5)	0.061 (4)	0.053 (5)	0.059 (5)	0.050 (4)
C2_3	0.034 (3)	0.034 (3)	0.028 (3)	−0.009 (3)	0.008 (2)	0.000 (3)
C3_3	0.031 (3)	0.046 (4)	0.037 (3)	0.002 (3)	0.012 (3)	0.002 (3)
C4_3	0.028 (3)	0.031 (3)	0.021 (3)	0.006 (2)	−0.003 (2)	−0.004 (2)
C5_3	0.045 (4)	0.047 (4)	0.044 (4)	0.021 (3)	0.011 (3)	0.007 (3)
Ni1_4	0.0236 (5)	0.0155 (5)	0.0250 (5)	−0.0025 (4)	0.0053 (4)	−0.0037 (4)
C5_4	0.057 (4)	0.048 (4)	0.045 (4)	−0.012 (4)	0.024 (3)	−0.028 (3)
F4_4	0.063 (3)	0.081 (4)	0.072 (3)	−0.013 (3)	0.036 (2)	−0.048 (3)
F5_4	0.148 (6)	0.039 (3)	0.140 (5)	−0.022 (3)	0.097 (5)	−0.043 (3)
F6_4	0.078 (4)	0.123 (5)	0.057 (3)	0.021 (4)	−0.014 (3)	−0.054 (3)
O1_4	0.033 (2)	0.025 (2)	0.032 (2)	−0.0065 (17)	0.0107 (17)	−0.0075 (17)
O2_4	0.031 (2)	0.025 (2)	0.035 (2)	−0.0015 (17)	0.0100 (17)	−0.0069 (17)
O3_4	0.045 (3)	0.020 (2)	0.033 (2)	0.0019 (19)	−0.0079 (19)	−0.0020 (18)
C1_4	0.040 (3)	0.048 (4)	0.038 (3)	−0.016 (3)	0.015 (3)	−0.002 (3)
F1_4	0.061 (5)	0.121 (8)	0.077 (4)	−0.060 (5)	0.040 (4)	−0.065 (5)

F2_4	0.030 (3)	0.074 (5)	0.107 (7)	−0.013 (3)	0.014 (3)	−0.020 (4)
F3_4	0.071 (5)	0.117 (7)	0.054 (3)	−0.046 (5)	0.001 (3)	0.048 (4)
C1′_4	0.040 (3)	0.048 (4)	0.038 (3)	−0.016 (3)	0.015 (3)	−0.002 (3)
F1′_4	0.071 (5)	0.117 (7)	0.054 (3)	−0.046 (5)	0.001 (3)	0.048 (4)
F2′_4	0.061 (5)	0.121 (8)	0.077 (4)	−0.060 (5)	0.040 (4)	−0.065 (5)
F3′_4	0.066 (11)	0.046 (8)	0.111 (16)	−0.025 (6)	−0.002 (9)	0.033 (9)
C2_4	0.031 (3)	0.034 (3)	0.025 (3)	−0.008 (3)	0.007 (2)	0.000 (2)
C3_4	0.033 (3)	0.042 (4)	0.024 (3)	−0.003 (3)	0.010 (2)	−0.008 (3)
C4_4	0.034 (3)	0.030 (3)	0.022 (3)	0.008 (2)	−0.001 (2)	−0.006 (2)
O1_5	0.039 (2)	0.026 (2)	0.037 (2)	−0.0016 (19)	0.0000 (19)	−0.0017 (18)
O2_5	0.038 (2)	0.019 (2)	0.033 (2)	−0.0049 (18)	−0.0001 (18)	−0.0067 (17)
O3_5	0.045 (2)	0.018 (2)	0.034 (2)	0.0036 (18)	0.0028 (19)	0.0062 (17)
O4_5	0.042 (3)	0.025 (2)	0.038 (2)	0.0003 (19)	0.000 (2)	−0.0020 (19)

Geometric parameters (Å, º)

Ni1_1—O6_1	2.024 (4)	C6_2—F9_2	1.294 (8)
Ni1_1—O1_1	2.026 (4)	C6_2—F7_2	1.312 (10)
Ni1_1—O5_1	2.029 (4)	C6_2—F8_2	1.358 (9)
Ni1_1—O4_1	2.030 (4)	C6_2—C7_2	1.538 (8)
Ni1_1—O2_1	2.036 (4)	C6′_2—F9′_2	1.268 (14)
Ni1_1—O3_1	2.044 (4)	C6′_2—F8′_2	1.278 (16)
F1_1—C1_1	1.333 (7)	C6′_2—F7′_2	1.340 (14)
F2_1—C1_1	1.337 (8)	C6′_2—C7_2	1.538 (8)
F3_1—C1_1	1.326 (7)	C7_2—C8_2	1.383 (9)
C10_1—F12_1	1.262 (14)	C8_2—C9_2	1.388 (8)
C10_1—F10_1	1.271 (13)	C8_2—H8_2	0.9500
C10_1—F11_1	1.370 (13)	C9_2—C10′_2	1.564 (9)
C10_1—C9_1	1.544 (8)	C9_2—C10_2	1.564 (9)
C10′_1—F11′_1	1.279 (9)	C10_2—F10_2	1.271 (9)
C10′_1—F12′_1	1.280 (11)	C10_2—F12_2	1.289 (8)
C10′_1—F10′_1	1.373 (9)	C10_2—F11_2	1.313 (12)
C10′_1—C9_1	1.544 (8)	C10′_2—F12′_2	1.289 (16)
O1_1—C2_1	1.259 (6)	C10′_2—F10′_2	1.298 (16)
O2_1—C4_1	1.263 (7)	C10′_2—F11′_2	1.312 (16)
O3_1—H3OB_1	0.806 (16)	Ni1_3—O3_3	2.026 (4)
O3_1—H3OA_1	0.808 (17)	Ni1_3—O3_3^{i}	2.026 (4)
O4_1—C7_1	1.247 (7)	Ni1_3—O2_3	2.027 (4)
O5_1—C9_1	1.258 (7)	Ni1_3—O2_3^{i}	2.027 (4)
O6_1—H6OA_1	0.801 (17)	Ni1_3—O1_3	2.043 (4)
O6_1—H6OB_1	0.802 (17)	Ni1_3—O1_3^{i}	2.043 (4)
C1_1—C2_1	1.504 (9)	F4_3—C5_3	1.337 (9)
C2_1—C3_1	1.409 (8)	F5_3—C5_3	1.306 (8)
C3_1—C4_1	1.386 (8)	F6_3—C5_3	1.303 (9)
C3_1—H3_1	0.9500	O1_3—C2_3	1.249 (7)
C4_1—C5′_1	1.540 (8)	O2_3—C4_3	1.256 (7)
C4_1—C5_1	1.540 (8)	O3_3—H3OA_3	0.78 (5)
C5_1—F4_1	1.294 (7)	O3_3—H3OB_3	0.78 (5)

C5_1—F6_1	1.306 (7)	C1_3—F2_3	1.243 (14)
C5_1—F5_1	1.334 (7)	C1_3—F3_3	1.309 (14)
C5′_1—F5′_1	1.273 (19)	C1_3—F1_3	1.345 (14)
C5′_1—F6′_1	1.31 (2)	C1_3—C2_3	1.541 (9)
C5′_1—F4′_1	1.32 (2)	C1′_3—F1′_3	1.259 (11)
C6_1—F7_1	1.225 (15)	C1′_3—F2′_3	1.292 (9)
C6_1—F8_1	1.240 (13)	C1′_3—F3′_3	1.358 (10)
C6_1—F9_1	1.390 (14)	C1′_3—C2_3	1.541 (9)
C6_1—C7_1	1.522 (9)	C2_3—C3_3	1.391 (9)
C6′_1—F8′_1	1.272 (8)	C3_3—C4_3	1.378 (9)
C6′_1—F9′_1	1.284 (11)	C3_3—H3_3	0.9500
C6′_1—F7′_1	1.431 (10)	C4_3—C5_3	1.543 (8)
C6′_1—C7_1	1.522 (9)	Ni1_4—O2_4^{ii}	2.022 (4)
C7_1—C8_1	1.385 (8)	Ni1_4—O2_4	2.022 (4)
C8_1—C9_1	1.387 (9)	Ni1_4—O1_4	2.027 (4)
C8_1—H8_1	0.9500	Ni1_4—O1_4^{ii}	2.027 (4)
Ni1_2—O2_2	2.018 (4)	Ni1_4—O3_4^{ii}	2.030 (4)
Ni1_2—O5_2	2.023 (4)	Ni1_4—O3_4	2.030 (4)
Ni1_2—O3_2	2.032 (4)	C5_4—F4_4	1.300 (8)
Ni1_2—O4_2	2.032 (4)	C5_4—F6_4	1.312 (9)
Ni1_2—O6_2	2.037 (4)	C5_4—F5_4	1.319 (9)
Ni1_2—O1_2	2.051 (4)	C5_4—C4_4	1.543 (8)
F4_2—C5_2	1.311 (7)	O1_4—C2_4	1.250 (7)
F5_2—C5_2	1.346 (7)	O2_4—C4_4	1.247 (7)
F6_2—C5_2	1.355 (8)	O3_4—H3OB_4	0.807 (17)
O1_2—C2_2	1.243 (7)	O3_4—H3OA_4	0.806 (17)
O2_2—C4_2	1.268 (6)	C1_4—F1_4	1.273 (9)
O3_2—H3OA_2	0.7825	C1_4—F3_4	1.285 (8)
O3_2—H3OB_2	0.8761	C1_4—F2_4	1.383 (8)
O4_2—C7_2	1.256 (7)	C1_4—C2_4	1.540 (8)
O5_2—C9_2	1.255 (6)	C1′_4—F2′_4	1.277 (14)
O6_2—H6OB_2	0.809 (17)	C1′_4—F1′_4	1.291 (17)
O6_2—H6OA_2	0.811 (16)	C1′_4—F3′_4	1.390 (15)
C1_2—F3_2	1.271 (9)	C1′_4—C2_4	1.540 (8)
C1_2—F2_2	1.315 (8)	C2_4—C3_4	1.379 (8)
C1_2—F1_2	1.340 (9)	C3_4—C4_4	1.389 (9)
C1_2—C2_2	1.524 (8)	C3_4—H3_4	0.9500
C1′_2—F1′_2	1.276 (14)	O1_5—H1OA_5	0.813 (17)
C1′_2—F3′_2	1.323 (15)	O1_5—H1OB_5	0.814 (17)
C1′_2—F2′_2	1.354 (14)	O2_5—H2OB_5	0.809 (17)
C1′_2—C2_2	1.524 (8)	O2_5—H2OA_5	0.811 (17)
C2_2—C3_2	1.405 (8)	O3_5—H3OA_5	0.809 (17)
C3_2—C4_2	1.370 (8)	O3_5—H3OB_5	0.806 (17)
C3_2—H3_2	0.9500	O4_5—H4OA_5	0.816 (17)
C4_2—C5_2	1.519 (8)	O4_5—H4OB_5	0.814 (17)

O6_1—Ni1_1—O1_1	89.82 (17)	F4_2—C5_2—C4_2	116.1 (5)
O6_1—Ni1_1—O5_1	88.00 (17)	F5_2—C5_2—C4_2	110.6 (5)

O1_1—Ni1_1—O5_1	177.36 (17)	F6_2—C5_2—C4_2	110.2 (5)
O6_1—Ni1_1—O4_1	90.07 (17)	F9_2—C6_2—F7_2	112.2 (9)
O1_1—Ni1_1—O4_1	89.21 (15)	F9_2—C6_2—F8_2	104.7 (7)
O5_1—Ni1_1—O4_1	89.32 (15)	F7_2—C6_2—F8_2	102.9 (8)
O6_1—Ni1_1—O2_1	88.53 (17)	F9_2—C6_2—C7_2	114.5 (6)
O1_1—Ni1_1—O2_1	89.39 (15)	F7_2—C6_2—C7_2	111.0 (8)
O5_1—Ni1_1—O2_1	92.02 (16)	F8_2—C6_2—C7_2	110.8 (5)
O4_1—Ni1_1—O2_1	178.02 (16)	F9′_2—C6′_2—F8′_2	114.8 (17)
O6_1—Ni1_1—O3_1	175.82 (18)	F9′_2—C6′_2—F7′_2	106.4 (12)
O1_1—Ni1_1—O3_1	92.77 (17)	F8′_2—C6′_2—F7′_2	104.8 (13)
O5_1—Ni1_1—O3_1	89.50 (17)	F9′_2—C6′_2—C7_2	110.8 (10)
O4_1—Ni1_1—O3_1	93.24 (17)	F8′_2—C6′_2—C7_2	111.0 (17)
O2_1—Ni1_1—O3_1	88.22 (17)	F7′_2—C6′_2—C7_2	108.6 (8)
F12_1—C10_1—F10_1	116.1 (13)	O4_2—C7_2—C8_2	128.6 (5)
F12_1—C10_1—F11_1	103.9 (11)	O4_2—C7_2—C6_2	113.6 (5)
F10_1—C10_1—F11_1	104.9 (12)	C8_2—C7_2—C6_2	117.8 (5)
F12_1—C10_1—C9_1	111.9 (11)	O4_2—C7_2—C6′_2	113.6 (5)
F10_1—C10_1—C9_1	109.5 (8)	C8_2—C7_2—C6′_2	117.8 (5)
F11_1—C10_1—C9_1	110.1 (7)	C7_2—C8_2—C9_2	122.2 (5)
F11′_1—C10′_1—F12′_1	116.2 (10)	C7_2—C8_2—H8_2	118.9
F11′_1—C10′_1—F10′_1	102.5 (9)	C9_2—C8_2—H8_2	118.9
F12′_1—C10′_1—F10′_1	101.5 (8)	O5_2—C9_2—C8_2	128.5 (5)
F11′_1—C10′_1—C9_1	115.6 (6)	O5_2—C9_2—C10′_2	112.5 (5)
F12′_1—C10′_1—C9_1	110.1 (8)	C8_2—C9_2—C10′_2	119.0 (5)
F10′_1—C10′_1—C9_1	109.5 (6)	O5_2—C9_2—C10_2	112.5 (5)
C2_1—O1_1—Ni1_1	123.9 (4)	C8_2—C9_2—C10_2	119.0 (5)
C4_1—O2_1—Ni1_1	122.9 (4)	F10_2—C10_2—F12_2	107.5 (7)
Ni1_1—O3_1—H3OB_1	122 (5)	F10_2—C10_2—F11_2	107.0 (11)
Ni1_1—O3_1—H3OA_1	120 (5)	F12_2—C10_2—F11_2	103.7 (8)
H3OB_1—O3_1—H3OA_1	108 (3)	F10_2—C10_2—C9_2	115.8 (7)
C7_1—O4_1—Ni1_1	123.0 (4)	F12_2—C10_2—C9_2	112.2 (5)
C9_1—O5_1—Ni1_1	123.1 (4)	F11_2—C10_2—C9_2	109.8 (8)
Ni1_1—O6_1—H6OA_1	121 (4)	F12′_2—C10′_2—F10′_2	111.5 (14)
Ni1_1—O6_1—H6OB_1	127 (4)	F12′_2—C10′_2—F11′_2	114.8 (14)
H6OA_1—O6_1—H6OB_1	109 (3)	F10′_2—C10′_2—F11′_2	106.6 (12)
F3_1—C1_1—F1_1	107.3 (5)	F12′_2—C10′_2—C9_2	103.8 (11)
F3_1—C1_1—F2_1	107.3 (5)	F10′_2—C10′_2—C9_2	108.5 (9)
F1_1—C1_1—F2_1	105.9 (6)	F11′_2—C10′_2—C9_2	111.5 (12)
F3_1—C1_1—C2_1	114.9 (6)	O3_3—Ni1_3—O3_3^{i}	180.0
F1_1—C1_1—C2_1	111.2 (5)	O3_3—Ni1_3—O2_3	92.02 (17)
F2_1—C1_1—C2_1	109.9 (5)	O3_3^{i}—Ni1_3—O2_3	87.98 (17)
O1_1—C2_1—C3_1	127.4 (5)	O3_3—Ni1_3—O2_3^{i}	87.98 (17)
O1_1—C2_1—C1_1	113.1 (5)	O3_3^{i}—Ni1_3—O2_3^{i}	92.02 (17)
C3_1—C2_1—C1_1	119.5 (5)	O2_3—Ni1_3—O2_3^{i}	180.0
C4_1—C3_1—C2_1	122.4 (5)	O3_3—Ni1_3—O1_3	90.96 (19)
C4_1—C3_1—H3_1	118.8	O3_3^{i}—Ni1_3—O1_3	89.04 (19)
C2_1—C3_1—H3_1	118.8	O2_3—Ni1_3—O1_3	90.86 (16)
O2_1—C4_1—C3_1	128.8 (5)	O2_3^{i}—Ni1_3—O1_3	89.15 (16)

O2_1—C4_1—C5′_1	114.0 (5)	O3_3—Ni1_3—O1_3^{i}	89.04 (19)
C3_1—C4_1—C5′_1	117.2 (5)	O3_3^{i}—Ni1_3—O1_3^{i}	90.96 (19)
O2_1—C4_1—C5_1	114.0 (5)	O2_3—Ni1_3—O1_3^{i}	89.15 (16)
C3_1—C4_1—C5_1	117.2 (5)	O2_3^{i}—Ni1_3—O1_3^{i}	90.85 (16)
F4_1—C5_1—F6_1	110.9 (7)	O1_3—Ni1_3—O1_3^{i}	180.0 (3)
F4_1—C5_1—F5_1	107.0 (6)	C2_3—O1_3—Ni1_3	123.6 (4)
F6_1—C5_1—F5_1	105.2 (6)	C4_3—O2_3—Ni1_3	123.8 (4)
F4_1—C5_1—C4_1	110.6 (5)	Ni1_3—O3_3—H3OA_3	119 (6)
F6_1—C5_1—C4_1	111.4 (5)	Ni1_3—O3_3—H3OB_3	120 (6)
F5_1—C5_1—C4_1	111.4 (5)	H3OA_3—O3_3—H3OB_3	116 (8)
F5′_1—C5′_1—F6′_1	105.2 (18)	F2_3—C1_3—F3_3	110.0 (13)
F5′_1—C5′_1—F4′_1	108.4 (18)	F2_3—C1_3—F1_3	108.3 (14)
F6′_1—C5′_1—F4′_1	101.1 (18)	F3_3—C1_3—F1_3	99.9 (11)
F5′_1—C5′_1—C4_1	122.7 (16)	F2_3—C1_3—C2_3	118.1 (10)
F6′_1—C5′_1—C4_1	109.7 (19)	F3_3—C1_3—C2_3	111.6 (11)
F4′_1—C5′_1—C4_1	107.6 (10)	F1_3—C1_3—C2_3	107.3 (8)
F7_1—C6_1—F8_1	117.5 (14)	F1′_3—C1′_3—F2′_3	112.9 (11)
F7_1—C6_1—F9_1	97.9 (13)	F1′_3—C1′_3—F3′_3	105.7 (10)
F8_1—C6_1—F9_1	98.2 (11)	F2′_3—C1′_3—F3′_3	100.1 (7)
F7_1—C6_1—C7_1	118.8 (13)	F1′_3—C1′_3—C2_3	113.2 (9)
F8_1—C6_1—C7_1	114.2 (8)	F2′_3—C1′_3—C2_3	113.8 (6)
F9_1—C6_1—C7_1	105.0 (8)	F3′_3—C1′_3—C2_3	110.1 (6)
F8′_1—C6′_1—F9′_1	114.5 (10)	O1_3—C2_3—C3_3	129.1 (6)
F8′_1—C6′_1—F7′_1	102.3 (8)	O1_3—C2_3—C1_3	114.2 (6)
F9′_1—C6′_1—F7′_1	98.7 (9)	C3_3—C2_3—C1_3	116.7 (5)
F8′_1—C6′_1—C7_1	119.1 (7)	O1_3—C2_3—C1′_3	114.2 (6)
F9′_1—C6′_1—C7_1	112.4 (9)	C3_3—C2_3—C1′_3	116.7 (5)
F7′_1—C6′_1—C7_1	106.6 (6)	C4_3—C3_3—C2_3	123.1 (6)
O4_1—C7_1—C8_1	129.2 (6)	C4_3—C3_3—H3_3	118.5
O4_1—C7_1—C6_1	113.5 (5)	C2_3—C3_3—H3_3	118.5
C8_1—C7_1—C6_1	117.3 (5)	O2_3—C4_3—C3_3	129.1 (5)
O4_1—C7_1—C6′_1	113.5 (5)	O2_3—C4_3—C5_3	112.6 (5)
C8_1—C7_1—C6′_1	117.3 (5)	C3_3—C4_3—C5_3	118.3 (6)
C7_1—C8_1—C9_1	121.9 (5)	F6_3—C5_3—F5_3	109.2 (6)
C7_1—C8_1—H8_1	119.1	F6_3—C5_3—F4_3	108.4 (7)
C9_1—C8_1—H8_1	119.1	F5_3—C5_3—F4_3	105.9 (6)
O5_1—C9_1—C8_1	128.6 (5)	F6_3—C5_3—C4_3	111.4 (6)
O5_1—C9_1—C10′_1	114.0 (5)	F5_3—C5_3—C4_3	114.5 (6)
C8_1—C9_1—C10′_1	117.3 (5)	F4_3—C5_3—C4_3	107.2 (6)
O5_1—C9_1—C10_1	114.0 (5)	O2_4^{ii}—Ni1_4—O2_4	180.0
C8_1—C9_1—C10_1	117.3 (5)	O2_4^{ii}—Ni1_4—O1_4	89.16 (16)
O2_2—Ni1_2—O5_2	89.78 (15)	O2_4—Ni1_4—O1_4	90.85 (16)
O2_2—Ni1_2—O3_2	89.93 (17)	O2_4^{ii}—Ni1_4—O1_4^{ii}	90.84 (16)
O5_2—Ni1_2—O3_2	89.91 (17)	O2_4—Ni1_4—O1_4^{ii}	89.15 (16)
O2_2—Ni1_2—O4_2	177.67 (16)	O1_4—Ni1_4—O1_4^{ii}	180.0
O5_2—Ni1_2—O4_2	89.13 (16)	O2_4^{ii}—Ni1_4—O3_4^{ii}	92.79 (18)
O3_2—Ni1_2—O4_2	88.00 (16)	O2_4—Ni1_4—O3_4^{ii}	87.21 (18)
O2_2—Ni1_2—O6_2	92.63 (17)	O1_4—Ni1_4—O3_4^{ii}	88.87 (18)

O5_2—Ni1_2—O6_2	92.99 (17)	O1_4^{ii}—Ni1_4—O3_4^{ii}	91.13 (18)
O3_2—Ni1_2—O6_2	176.13 (19)	O2_4^{ii}—Ni1_4—O3_4	87.21 (18)
O4_2—Ni1_2—O6_2	89.48 (17)	O2_4—Ni1_4—O3_4	92.79 (18)
O2_2—Ni1_2—O1_2	89.12 (15)	O1_4—Ni1_4—O3_4	91.13 (18)
O5_2—Ni1_2—O1_2	177.82 (16)	O1_4^{ii}—Ni1_4—O3_4	88.87 (18)
O3_2—Ni1_2—O1_2	88.21 (16)	O3_4^{ii}—Ni1_4—O3_4	180.0 (3)
O4_2—Ni1_2—O1_2	91.90 (16)	F4_4—C5_4—F6_4	108.8 (6)
O6_2—Ni1_2—O1_2	88.94 (17)	F4_4—C5_4—F5_4	107.6 (7)
C2_2—O1_2—Ni1_2	123.8 (4)	F6_4—C5_4—F5_4	105.0 (7)
C4_2—O2_2—Ni1_2	122.5 (4)	F4_4—C5_4—C4_4	114.6 (6)
Ni1_2—O3_2—H3OA_2	131.3	F6_4—C5_4—C4_4	109.6 (6)
Ni1_2—O3_2—H3OB_2	125.5	F5_4—C5_4—C4_4	110.8 (6)
H3OA_2—O3_2—H3OB_2	102.3	C2_4—O1_4—Ni1_4	123.7 (4)
C7_2—O4_2—Ni1_2	123.5 (4)	C4_4—O2_4—Ni1_4	123.8 (4)
C9_2—O5_2—Ni1_2	123.5 (4)	Ni1_4—O3_4—H3OB_4	124 (5)
Ni1_2—O6_2—H6OB_2	121 (5)	Ni1_4—O3_4—H3OA_4	125 (5)
Ni1_2—O6_2—H6OA_2	123 (5)	H3OB_4—O3_4—H3OA_4	108 (3)
H6OB_2—O6_2—H6OA_2	107 (3)	F1_4—C1_4—F3_4	113.8 (8)
F3_2—C1_2—F2_2	112.2 (8)	F1_4—C1_4—F2_4	103.5 (7)
F3_2—C1_2—F1_2	108.0 (7)	F3_4—C1_4—F2_4	104.5 (7)
F2_2—C1_2—F1_2	101.5 (6)	F1_4—C1_4—C2_4	112.6 (6)
F3_2—C1_2—C2_2	111.6 (6)	F3_4—C1_4—C2_4	112.7 (6)
F2_2—C1_2—C2_2	111.4 (5)	F2_4—C1_4—C2_4	109.0 (6)
F1_2—C1_2—C2_2	111.6 (6)	F2′_4—C1′_4—F1′_4	112.0 (13)
F1′_2—C1′_2—F3′_2	105.5 (12)	F2′_4—C1′_4—F3′_4	100.1 (14)
F1′_2—C1′_2—F2′_2	107.5 (13)	F1′_4—C1′_4—F3′_4	97.4 (14)
F3′_2—C1′_2—F2′_2	100.4 (11)	F2′_4—C1′_4—C2_4	120.2 (9)
F1′_2—C1′_2—C2_2	116.1 (9)	F1′_4—C1′_4—C2_4	117.5 (11)
F3′_2—C1′_2—C2_2	114.2 (9)	F3′_4—C1′_4—C2_4	104.5 (9)
F2′_2—C1′_2—C2_2	111.7 (8)	O1_4—C2_4—C3_4	129.0 (6)
O1_2—C2_2—C3_2	127.4 (5)	O1_4—C2_4—C1_4	114.2 (5)
O1_2—C2_2—C1_2	115.7 (5)	C3_4—C2_4—C1_4	116.7 (5)
C3_2—C2_2—C1_2	116.8 (5)	O1_4—C2_4—C1′_4	114.2 (5)
O1_2—C2_2—C1′_2	115.7 (5)	C3_4—C2_4—C1′_4	116.7 (5)
C3_2—C2_2—C1′_2	116.8 (5)	C2_4—C3_4—C4_4	122.9 (5)
C4_2—C3_2—C2_2	122.4 (5)	C2_4—C3_4—H3_4	118.5
C4_2—C3_2—H3_2	118.8	C4_4—C3_4—H3_4	118.5
C2_2—C3_2—H3_2	118.8	O2_4—C4_4—C3_4	128.8 (5)
O2_2—C4_2—C3_2	129.5 (5)	O2_4—C4_4—C5_4	113.4 (5)
O2_2—C4_2—C5_2	112.3 (5)	C3_4—C4_4—C5_4	117.8 (5)
C3_2—C4_2—C5_2	118.1 (5)	H1OA_5—O1_5—H1OB_5	106 (3)
F4_2—C5_2—F5_2	106.8 (5)	H2OB_5—O2_5—H2OA_5	107 (3)
F4_2—C5_2—F6_2	107.7 (5)	H3OA_5—O3_5—H3OB_5	108 (3)
F5_2—C5_2—F6_2	104.7 (5)	H4OA_5—O4_5—H4OB_5	101 (8)
Ni1_1—O1_1—C2_1—C3_1	−14.9 (8)	Ni1_2—O4_2—C7_2—C8_2	−11.5 (8)
Ni1_1—O1_1—C2_1—C1_1	165.6 (4)	Ni1_2—O4_2—C7_2—C6_2	166.7 (3)
F3_1—C1_1—C2_1—O1_1	178.8 (5)	Ni1_2—O4_2—C7_2—C6′_2	166.7 (3)

F1_1—C1_1—C2_1—O1_1	56.8 (7)
F2_1—C1_1—C2_1—O1_1	−60.1 (7)
F3_1—C1_1—C2_1—C3_1	−0.7 (8)
F1_1—C1_1—C2_1—C3_1	−122.8 (6)
F2_1—C1_1—C2_1—C3_1	120.3 (6)
O1_1—C2_1—C3_1—C4_1	−2.6 (9)
C1_1—C2_1—C3_1—C4_1	176.8 (5)
Ni1_1—O2_1—C4_1—C3_1	13.9 (8)
Ni1_1—O2_1—C4_1—C5′_1	−168.9 (3)
Ni1_1—O2_1—C4_1—C5_1	−168.9 (3)
C2_1—C3_1—C4_1—O2_1	3.0 (9)
C2_1—C3_1—C4_1—C5′_1	−174.1 (5)
C2_1—C3_1—C4_1—C5_1	−174.1 (5)
O2_1—C4_1—C5_1—F4_1	−82.7 (7)
C3_1—C4_1—C5_1—F4_1	94.8 (7)
O2_1—C4_1—C5_1—F6_1	41.2 (8)
C3_1—C4_1—C5_1—F6_1	−141.2 (7)
O2_1—C4_1—C5_1—F5_1	158.4 (6)
C3_1—C4_1—C5_1—F5_1	−24.0 (8)
O2_1—C4_1—C5′_1—F5′_1	−152 (2)
C3_1—C4_1—C5′_1—F5′_1	26 (2)
O2_1—C4_1—C5′_1—F6′_1	84.3 (19)
C3_1—C4_1—C5′_1—F6′_1	−98.1 (19)
O2_1—C4_1—C5′_1—F4′_1	−24.9 (18)
C3_1—C4_1—C5′_1—F4′_1	152.7 (18)
Ni1_1—O4_1—C7_1—C8_1	13.9 (9)
Ni1_1—O4_1—C7_1—C6_1	−167.3 (4)
Ni1_1—O4_1—C7_1—C6′_1	−167.3 (4)
F7_1—C6_1—C7_1—O4_1	−20.3 (16)
F8_1—C6_1—C7_1—O4_1	125.2 (13)
F9_1—C6_1—C7_1—O4_1	−128.3 (10)
F7_1—C6_1—C7_1—C8_1	158.7 (14)
F8_1—C6_1—C7_1—C8_1	−55.8 (14)
F9_1—C6_1—C7_1—C8_1	50.7 (11)
F8′_1—C6′_1—C7_1—O4_1	176.2 (9)
F9′_1—C6′_1—C7_1—O4_1	−45.8 (11)
F7′_1—C6′_1—C7_1—O4_1	61.3 (8)
F8′_1—C6′_1—C7_1—C8_1	−4.8 (12)
F9′_1—C6′_1—C7_1—C8_1	133.2 (10)
F7′_1—C6′_1—C7_1—C8_1	−119.7 (7)
O4_1—C7_1—C8_1—C9_1	3.6 (11)
C6_1—C7_1—C8_1—C9_1	−175.2 (6)
C6′_1—C7_1—C8_1—C9_1	−175.2 (6)
Ni1_1—O5_1—C9_1—C8_1	−12.7 (9)
Ni1_1—O5_1—C9_1—C10′_1	166.4 (4)
Ni1_1—O5_1—C9_1—C10_1	166.4 (4)
C7_1—C8_1—C9_1—O5_1	−4.3 (10)
C7_1—C8_1—C9_1—C10′_1	176.6 (6)
F9_2—C6_2—C7_2—O4_2	142.3 (8)
F7_2—C6_2—C7_2—O4_2	−89.4 (9)
F8_2—C6_2—C7_2—O4_2	24.2 (8)
F9_2—C6_2—C7_2—C8_2	−39.3 (10)
F7_2—C6_2—C7_2—C8_2	89.0 (9)
F8_2—C6_2—C7_2—C8_2	−157.4 (6)
F9′_2—C6′_2—C7_2—O4_2	69.4 (16)
F8′_2—C6′_2—C7_2—O4_2	−59.5 (15)
F7′_2—C6′_2—C7_2—O4_2	−174.1 (10)
F9′_2—C6′_2—C7_2—C8_2	−112.3 (16)
F8′_2—C6′_2—C7_2—C8_2	118.9 (14)
F7′_2—C6′_2—C7_2—C8_2	4.3 (11)
O4_2—C7_2—C8_2—C9_2	−4.4 (10)
C6_2—C7_2—C8_2—C9_2	177.5 (5)
C6′_2—C7_2—C8_2—C9_2	177.5 (5)
Ni1_2—O5_2—C9_2—C8_2	15.0 (9)
Ni1_2—O5_2—C9_2—C10′_2	−164.8 (4)
Ni1_2—O5_2—C9_2—C10_2	−164.8 (4)
C7_2—C8_2—C9_2—O5_2	2.4 (10)
C7_2—C8_2—C9_2—C10′_2	−177.8 (6)
C7_2—C8_2—C9_2—C10_2	−177.8 (6)
O5_2—C9_2—C10_2—F10_2	−170.4 (9)
C8_2—C9_2—C10_2—F10_2	9.8 (12)
O5_2—C9_2—C10_2—F12_2	−46.4 (8)
C8_2—C9_2—C10_2—F12_2	133.8 (7)
O5_2—C9_2—C10_2—F11_2	68.3 (9)
C8_2—C9_2—C10_2—F11_2	−111.4 (9)
O5_2—C9_2—C10′_2—F12′_2	−77.2 (15)
C8_2—C9_2—C10′_2—F12′_2	103.0 (15)
O5_2—C9_2—C10′_2—F10′_2	164.1 (10)
C8_2—C9_2—C10′_2—F10′_2	−15.7 (12)
O5_2—C9_2—C10′_2—F11′_2	47.0 (11)
C8_2—C9_2—C10′_2—F11′_2	−132.8 (10)
Ni1_3—O1_3—C2_3—C3_3	−0.3 (9)
Ni1_3—O1_3—C2_3—C1_3	−178.8 (4)
Ni1_3—O1_3—C2_3—C1′_3	−178.8 (4)
F2_3—C1_3—C2_3—O1_3	93.2 (18)
F3_3—C1_3—C2_3—O1_3	−137.8 (10)
F1_3—C1_3—C2_3—O1_3	−29.4 (12)
F2_3—C1_3—C2_3—C3_3	−85.5 (18)
F3_3—C1_3—C2_3—C3_3	43.5 (12)
F1_3—C1_3—C2_3—C3_3	151.9 (11)
F1′_3—C1′_3—C2_3—O1_3	−106.0 (12)
F2′_3—C1′_3—C2_3—O1_3	24.6 (10)
F3′_3—C1′_3—C2_3—O1_3	136.0 (7)
F1′_3—C1′_3—C2_3—C3_3	75.4 (13)
F2′_3—C1′_3—C2_3—C3_3	−154.0 (8)
F3′_3—C1′_3—C2_3—C3_3	−42.7 (9)

C7_1—C8_1—C9_1—C10_1	176.6 (6)	O1_3—C2_3—C3_3—C4_3	−2.9 (11)
F11′_1—C10′_1—C9_1—O5_1	139.9 (11)	C1_3—C2_3—C3_3—C4_3	175.6 (6)
F12′_1—C10′_1—C9_1—O5_1	−85.9 (9)	C1′_3—C2_3—C3_3—C4_3	175.6 (6)
F10′_1—C10′_1—C9_1—O5_1	24.8 (9)	Ni1_3—O2_3—C4_3—C3_3	7.6 (9)
F11′_1—C10′_1—C9_1—C8_1	−40.9 (12)	Ni1_3—O2_3—C4_3—C5_3	−173.4 (4)
F12′_1—C10′_1—C9_1—C8_1	93.3 (9)	C2_3—C3_3—C4_3—O2_3	−1.3 (11)
F10′_1—C10′_1—C9_1—C8_1	−156.0 (7)	C2_3—C3_3—C4_3—C5_3	179.7 (6)
F12_1—C10_1—C9_1—O5_1	−51.8 (13)	O2_3—C4_3—C5_3—F6_3	−41.5 (8)
F10_1—C10_1—C9_1—O5_1	78.4 (14)	C3_3—C4_3—C5_3—F6_3	137.6 (7)
F11_1—C10_1—C9_1—O5_1	−166.7 (8)	O2_3—C4_3—C5_3—F5_3	−166.0 (6)
F12_1—C10_1—C9_1—C8_1	127.5 (12)	C3_3—C4_3—C5_3—F5_3	13.2 (9)
F10_1—C10_1—C9_1—C8_1	−102.4 (14)	O2_3—C4_3—C5_3—F4_3	76.9 (7)
F11_1—C10_1—C9_1—C8_1	12.5 (10)	C3_3—C4_3—C5_3—F4_3	−103.9 (7)
Ni1_2—O1_2—C2_2—C3_2	14.8 (8)	Ni1_4—O1_4—C2_4—C3_4	−1.5 (9)
Ni1_2—O1_2—C2_2—C1_2	−168.3 (3)	Ni1_4—O1_4—C2_4—C1_4	178.8 (4)
Ni1_2—O1_2—C2_2—C1′_2	−168.3 (3)	Ni1_4—O1_4—C2_4—C1′_4	178.8 (4)
F3_2—C1_2—C2_2—O1_2	−88.4 (9)	F1_4—C1_4—C2_4—O1_4	17.8 (10)
F2_2—C1_2—C2_2—O1_2	37.9 (9)	F3_4—C1_4—C2_4—O1_4	−112.5 (9)
F1_2—C1_2—C2_2—O1_2	150.6 (6)	F2_4—C1_4—C2_4—O1_4	132.0 (7)
F3_2—C1_2—C2_2—C3_2	88.8 (9)	F1_4—C1_4—C2_4—C3_4	−162.0 (8)
F2_2—C1_2—C2_2—C3_2	−144.9 (7)	F3_4—C1_4—C2_4—C3_4	67.8 (10)
F1_2—C1_2—C2_2—C3_2	−32.2 (8)	F2_4—C1_4—C2_4—C3_4	−47.7 (8)
F1′_2—C1′_2—C2_2—O1_2	115.6 (15)	F2′_4—C1′_4—C2_4—O1_4	−173.0 (18)
F3′_2—C1′_2—C2_2—O1_2	−121.3 (12)	F1′_4—C1′_4—C2_4—O1_4	44.6 (17)
F2′_2—C1′_2—C2_2—O1_2	−8.2 (12)	F3′_4—C1′_4—C2_4—O1_4	−61.9 (13)
F1′_2—C1′_2—C2_2—C3_2	−67.2 (16)	F2′_4—C1′_4—C2_4—C3_4	7.3 (19)
F3′_2—C1′_2—C2_2—C3_2	55.9 (13)	F1′_4—C1′_4—C2_4—C3_4	−135.1 (16)
F2′_2—C1′_2—C2_2—C3_2	169.1 (11)	F3′_4—C1′_4—C2_4—C3_4	118.4 (13)
O1_2—C2_2—C3_2—C4_2	1.1 (10)	O1_4—C2_4—C3_4—C4_4	−4.2 (11)
C1_2—C2_2—C3_2—C4_2	−175.8 (5)	C1_4—C2_4—C3_4—C4_4	175.5 (6)
C1′_2—C2_2—C3_2—C4_2	−175.8 (5)	C1′_4—C2_4—C3_4—C4_4	175.5 (6)
Ni1_2—O2_2—C4_2—C3_2	−16.3 (8)	Ni1_4—O2_4—C4_4—C3_4	8.7 (9)
Ni1_2—O2_2—C4_2—C5_2	164.3 (4)	Ni1_4—O2_4—C4_4—C5_4	−169.7 (4)
C2_2—C3_2—C4_2—O2_2	−0.2 (10)	C2_4—C3_4—C4_4—O2_4	0.0 (11)
C2_2—C3_2—C4_2—C5_2	179.1 (5)	C2_4—C3_4—C4_4—C5_4	178.4 (6)
O2_2—C4_2—C5_2—F4_2	176.1 (5)	F4_4—C5_4—C4_4—O2_4	−163.8 (6)
C3_2—C4_2—C5_2—F4_2	−3.4 (8)	F6_4—C5_4—C4_4—O2_4	73.5 (8)
O2_2—C4_2—C5_2—F5_2	54.3 (7)	F5_4—C5_4—C4_4—O2_4	−41.9 (9)
C3_2—C4_2—C5_2—F5_2	−125.2 (6)	F4_4—C5_4—C4_4—C3_4	17.6 (10)
O2_2—C4_2—C5_2—F6_2	−61.1 (6)	F6_4—C5_4—C4_4—C3_4	−105.1 (7)
C3_2—C4_2—C5_2—F6_2	119.4 (6)	F5_4—C5_4—C4_4—C3_4	139.5 (7)

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3_1—H3*OB*_1···O1_1^{iii}	0.81 (2)	2.11 (4)	2.824 (5)	147 (6)

O3_1—H3*OA*_1···O4_1^{iii}	0.81 (2)	2.21 (4)	2.879 (5)	141 (6)
O6_1—H6*OA*_1···O1_5	0.80 (2)	2.00 (2)	2.796 (6)	172 (6)
O6_1—H6*OB*_1···O4_5^{iv}	0.80 (2)	1.94 (2)	2.728 (6)	166 (7)
O3_2—H3*OA*_2···O2_5^{v}	0.78	2.01	2.786 (6)	173
O3_2—H3*OB*_2···O3_5^{vi}	0.88	1.87	2.733 (6)	167
O6_2—H6*OB*_2···O2_2^{iv}	0.81 (2)	2.13 (4)	2.837 (5)	145 (6)
O6_2—H6*OA*_2···O5_2^{iv}	0.81 (2)	2.18 (4)	2.876 (5)	145 (6)
O3_3—H3*OA*_3···O4_5	0.78 (5)	2.07 (5)	2.842 (6)	173 (9)
O3_3—H3*OB*_3···O1_5^{iv}	0.78 (5)	1.99 (5)	2.766 (6)	173 (8)
O3_4—H3*OB*_4···O3_5	0.81 (2)	2.05 (2)	2.842 (6)	168 (8)
O3_4—H3*OA*_4···O2_5^{v}	0.81 (2)	1.97 (2)	2.769 (6)	171 (8)
O1_5—H1*OA*_5···O2_3^{vii}	0.81 (2)	2.05 (3)	2.835 (6)	161 (6)
O1_5—H1*OB*_5···O1_3^{iv}	0.81 (2)	2.31 (5)	2.943 (6)	135 (6)
O2_5—H2*OB*_5···O1_4^{ii}	0.81 (2)	2.34 (5)	2.965 (6)	135 (6)
O2_5—H2*OA*_5···O2_4	0.81 (2)	2.09 (4)	2.845 (6)	154 (6)
O3_5—H3*OA*_5···O4_2	0.81 (2)	2.16 (5)	2.823 (6)	139 (6)
O3_5—H3*OB*_5···O1_2	0.81 (2)	2.12 (4)	2.848 (6)	150 (6)
O4_5—H4*OA*_5···O2_1^{iv}	0.82 (2)	2.09 (4)	2.835 (6)	152 (8)
O4_5—H4*OB*_5···O5_1^{iv}	0.81 (2)	2.10 (5)	2.823 (6)	147 (8)

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

Diaquabis(1,1,1,5,5,5-hexafluoro-4-oxopent-2-en-2-olato-κ^2O,O')nickel(II) 1,2-dimethoxybenzene pentasolvate (26164revised)

Crystal data

$[Ni(C_5HF_6O_2)_2(H_2O)_2]\cdot 5C_8H_{10}O_2$
M_r = 1199.65
Monoclinic, $P2_1/c$
a = 11.9278 (5) Å
b = 15.7842 (6) Å
c = 15.0115 (6) Å
β = 93.887 (1)°
V = 2819.7 (2) Å^3
Z = 2
$F(000)$ = 1240
D_x = 1.413 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9886 reflections
θ = 2.5–26.4°
μ = 0.45 mm^{-1}
T = 153 K
Plate, colorless
0.34 × 0.26 × 0.08 mm

Data collection

Bruker D8 VENTURE diffractometer
Radiation source: microfocus sealed tube, Incoatec IμS 3.0
Multilayer mirror monochromator
ω and φ scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.679, T_{max} = 0.746
66877 measured reflections
7928 independent reflections
5947 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
θ_{max} = 29.6°, θ_{min} = 1.9°
h = −16→16
k = −21→21
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.106$
$S = 1.02$
7928 reflections
558 parameters
267 restraints
Primary atom site location: instrinsic phasing
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2 + 1.0764P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Data was collected on a Bruker D8 Venture diffractometer equipped with a Photon-III CPAD detector and an Incoatec IμS 3.0 Mo microfocus X-ray source. Data collection strategies were computed using the APEX 6 software package (Bruker Analytical X-ray Systems, 2023), data was integrated using SAINT (Bruker Analytical X-ray Systems, 2016), and scaled using TWINABS (Sevvana *et al.*, 2019) for crystal **1** and SADABS (Krause *et al.*, 2015) for crystal **2**. Structures were solved using SHELXT (Sheldrick, 2015) and refined using SHELXL (Sheldrick, 2015*a*) within the ShelXle program (Hübschle *et al.*, 2011).

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ni1_1	0.500000	0.500000	0.500000	0.02710 (8)	
O3_1	0.60985 (10)	0.55398 (8)	0.41693 (8)	0.0358 (2)	
H1_1	0.6423 (19)	0.5948 (15)	0.4369 (15)	0.054*	
H2_1	0.6602 (19)	0.5229 (15)	0.3978 (15)	0.054*	
O2_1	0.38160 (9)	0.58169 (7)	0.44955 (7)	0.0339 (2)	
O1_1	0.45486 (9)	0.41404 (7)	0.40504 (7)	0.0321 (2)	
C1_1	0.36040 (17)	0.34842 (12)	0.28312 (11)	0.0458 (4)	0.705 (4)
F1_1	0.46100 (19)	0.3272 (2)	0.2492 (2)	0.0932 (10)	0.705 (4)
F2_1	0.3335 (5)	0.2811 (2)	0.32449 (18)	0.1213 (17)	0.705 (4)
F3_1	0.2955 (2)	0.35904 (17)	0.21228 (16)	0.0740 (8)	0.705 (4)
C1′_1	0.36040 (17)	0.34842 (12)	0.28312 (11)	0.0458 (4)	0.295 (4)
F1′_1	0.4039 (8)	0.2845 (4)	0.3055 (5)	0.084 (3)	0.295 (4)
F2′_1	0.2451 (4)	0.3269 (4)	0.2851 (6)	0.097 (3)	0.295 (4)
F3′_1	0.3666 (12)	0.3705 (4)	0.2059 (4)	0.1213 (17)	0.295 (4)
C2_1	0.37824 (14)	0.42448 (10)	0.34565 (10)	0.0328 (3)	
C3_1	0.30970 (15)	0.49522 (11)	0.32892 (11)	0.0405 (4)	
H3_1	0.255353	0.493871	0.279659	0.049*	
C4_1	0.31819 (13)	0.56737 (10)	0.38169 (11)	0.0337 (3)	
C5_1	0.23950 (16)	0.64149 (11)	0.35642 (14)	0.0473 (4)	0.67 (4)
F4_1	0.1967 (8)	0.6359 (5)	0.2710 (4)	0.0661 (14)	0.67 (4)
F5_1	0.1548 (6)	0.6413 (7)	0.4096 (7)	0.0889 (17)	0.67 (4)
F6_1	0.2898 (8)	0.7157 (4)	0.3658 (8)	0.0751 (17)	0.67 (4)
C5′_1	0.23950 (16)	0.64149 (11)	0.35642 (14)	0.0473 (4)	0.33 (4)

F4′_1	0.172 (2)	0.662 (2)	0.4151 (13)	0.116 (6)	0.33 (4)
F5′_1	0.172 (2)	0.6357 (11)	0.2868 (18)	0.085 (5)	0.33 (4)
F6′_1	0.2989 (16)	0.7089 (12)	0.345 (2)	0.083 (5)	0.33 (4)
O1_2	0.64963 (9)	0.72811 (7)	0.47148 (8)	0.0397 (3)	
O2_2	0.81529 (10)	0.63148 (7)	0.50792 (9)	0.0411 (3)	
C1_2	0.74786 (14)	0.76918 (10)	0.49456 (10)	0.0332 (3)	
C2_2	0.84016 (14)	0.71572 (10)	0.51330 (10)	0.0350 (3)	
C3_2	0.94530 (16)	0.74947 (13)	0.53471 (12)	0.0476 (4)	
H3_2	1.008169	0.713247	0.546476	0.057*	
C4_2	0.95838 (19)	0.83695 (15)	0.53890 (14)	0.0569 (5)	
H4_2	1.030565	0.860505	0.553614	0.068*	
C5_2	0.8683 (2)	0.88927 (13)	0.52202 (12)	0.0545 (5)	
H5_2	0.878122	0.948921	0.525580	0.065*	
C6_2	0.76200 (17)	0.85588 (11)	0.49964 (11)	0.0424 (4)	
H6_2	0.699592	0.892566	0.487937	0.051*	
C7_2	0.54760 (15)	0.77499 (12)	0.47392 (13)	0.0469 (4)	
H7A_2	0.545349	0.819136	0.427926	0.070*	
H7B_2	0.543911	0.801294	0.532786	0.070*	
H7C_2	0.483466	0.736749	0.462724	0.070*	
C8_2	0.90531 (16)	0.57284 (13)	0.52226 (15)	0.0528 (5)	
H8A_2	0.877353	0.515188	0.510934	0.079*	
H8B_2	0.936684	0.577207	0.584131	0.079*	
H8C_2	0.963897	0.585726	0.481581	0.079*	
C1_3	0.87129 (13)	0.49747 (9)	0.27944 (9)	0.0311 (3)	
C2_3	0.83857 (13)	0.41464 (10)	0.29912 (10)	0.0332 (3)	
C3_3	0.89692 (15)	0.34720 (11)	0.26642 (12)	0.0426 (4)	
H3_3	0.875186	0.290837	0.279246	0.051*	
C4_3	0.98769 (17)	0.36163 (13)	0.21459 (14)	0.0531 (5)	
H4_3	1.027246	0.315036	0.191795	0.064*	
C5_3	1.01997 (16)	0.44247 (13)	0.19646 (13)	0.0496 (4)	
H5_3	1.082392	0.451828	0.161628	0.059*	
C6_3	0.96191 (14)	0.51125 (11)	0.22875 (11)	0.0390 (4)	
H6_3	0.984543	0.567412	0.215960	0.047*	
O1_3	0.80672 (10)	0.55966 (7)	0.31271 (8)	0.0406 (3)	
C7_3	0.83227 (18)	0.64502 (10)	0.29028 (13)	0.0487 (5)	
H7A_3	0.828929	0.651133	0.225190	0.073*	
H7B_3	0.907933	0.659335	0.315284	0.073*	
H7C_3	0.777515	0.683223	0.314970	0.073*	
O2_3	0.74832 (10)	0.40845 (7)	0.35033 (8)	0.0413 (3)	
C8_3	0.70853 (17)	0.32513 (11)	0.36825 (15)	0.0502 (5)	
H8A_3	0.686782	0.296488	0.311777	0.075*	
H8B_3	0.643273	0.328969	0.404349	0.075*	
H8C_3	0.768254	0.292821	0.400892	0.075*	
C1_4	0.5620 (14)	1.0048 (13)	0.5537 (6)	0.057 (4)	0.300 (14)
C2_4	0.5252 (13)	1.0124 (12)	0.4634 (6)	0.063 (3)	0.300 (14)
C3_4	0.5908 (15)	1.0577 (10)	0.4077 (6)	0.078 (4)	0.300 (14)
H3_4	0.566057	1.064047	0.346582	0.093*	0.300 (14)
C4_4	0.6928 (16)	1.0944 (8)	0.4392 (9)	0.096 (4)	0.300 (14)

H4_4	0.738981	1.122367	0.399316	0.115*	0.300 (14)
C5_4	0.7247 (12)	1.0894 (9)	0.5278 (9)	0.093 (4)	0.300 (14)
H5_4	0.791808	1.116456	0.550456	0.111*	0.300 (14)
C6_4	0.6594 (14)	1.0448 (15)	0.5856 (7)	0.077 (4)	0.300 (14)
H6_4	0.682235	1.042026	0.647379	0.092*	0.300 (14)
O1_4	0.4927 (18)	0.960 (2)	0.6055 (10)	0.073 (5)	0.300 (14)
C7_4	0.5356 (17)	0.9424 (13)	0.6948 (8)	0.096 (5)	0.300 (14)
H7A_4	0.607483	0.912588	0.693488	0.144*	0.300 (14)
H7B_4	0.481859	0.906815	0.724278	0.144*	0.300 (14)
H7C_4	0.546680	0.995648	0.727820	0.144*	0.300 (14)
O2_4	0.4255 (16)	0.9729 (17)	0.4401 (10)	0.073 (5)	0.300 (14)
C8_4	0.3800 (16)	0.9814 (16)	0.3498 (11)	0.127 (10)	0.300 (14)
H8A_4	0.441514	0.986353	0.309967	0.190*	0.300 (14)
H8B_4	0.332856	1.032225	0.344350	0.190*	0.300 (14)
H8C_4	0.334553	0.931414	0.333156	0.190*	0.300 (14)
C1′_4	0.549 (3)	1.009 (3)	0.5540 (10)	0.049 (7)	0.200 (14)
C2′_4	0.4944 (14)	1.0023 (12)	0.4685 (7)	0.039 (3)	0.200 (14)
C3′_4	0.542 (2)	1.042 (2)	0.3981 (10)	0.060 (6)	0.200 (14)
H3′_4	0.505351	1.038337	0.339927	0.073*	0.200 (14)
C4′_4	0.6416 (18)	1.0882 (12)	0.4110 (14)	0.076 (6)	0.200 (14)
H4′_4	0.673201	1.114941	0.361804	0.092*	0.200 (14)
C5′_4	0.6934 (14)	1.0944 (11)	0.4942 (16)	0.078 (5)	0.200 (14)
H5′_4	0.760615	1.126394	0.503452	0.093*	0.200 (14)
C6′_4	0.6479 (16)	1.0539 (19)	0.5661 (13)	0.066 (5)	0.200 (14)
H6′_4	0.685580	1.057040	0.623766	0.079*	0.200 (14)
O1′_4	0.499 (2)	0.966 (3)	0.6196 (10)	0.055 (4)	0.200 (14)
C7′_4	0.563 (3)	0.957 (2)	0.7030 (11)	0.115 (12)	0.200 (14)
H7′A_4	0.632147	0.925914	0.693811	0.172*	0.200 (14)
H7′B_4	0.518515	0.925429	0.744700	0.172*	0.200 (14)
H7′C_4	0.581172	1.013023	0.727708	0.172*	0.200 (14)
O2′_4	0.3969 (15)	0.9565 (14)	0.4646 (9)	0.046 (3)	0.200 (14)
C8′_4	0.3351 (17)	0.9498 (15)	0.3796 (10)	0.064 (5)	0.200 (14)
H8′A_4	0.308572	1.006017	0.360262	0.096*	0.200 (14)
H8′B_4	0.270533	0.912134	0.384879	0.096*	0.200 (14)
H8′C_4	0.383901	0.926565	0.335688	0.096*	0.200 (14)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1_1	0.02699 (13)	0.02611 (13)	0.02750 (13)	0.00305 (10)	−0.00321 (9)	−0.00338 (10)
O3_1	0.0363 (6)	0.0313 (6)	0.0402 (6)	0.0000 (5)	0.0063 (5)	−0.0050 (5)
O2_1	0.0327 (5)	0.0321 (5)	0.0360 (6)	0.0059 (4)	−0.0047 (4)	−0.0022 (4)
O1_1	0.0342 (5)	0.0306 (5)	0.0308 (5)	0.0011 (4)	−0.0028 (4)	−0.0053 (4)
C1_1	0.0631 (12)	0.0419 (9)	0.0312 (8)	−0.0080 (9)	−0.0061 (8)	−0.0050 (7)
F1_1	0.0715 (14)	0.114 (2)	0.0936 (19)	0.0114 (14)	−0.0005 (13)	−0.0713 (17)
F2_1	0.264 (5)	0.0608 (16)	0.0405 (10)	−0.075 (3)	0.023 (2)	−0.0144 (10)
F3_1	0.0862 (18)	0.0763 (15)	0.0533 (12)	0.0161 (13)	−0.0398 (12)	−0.0295 (11)
C1′_1	0.0631 (12)	0.0419 (9)	0.0312 (8)	−0.0080 (9)	−0.0061 (8)	−0.0050 (7)

F1′_1	0.129 (6)	0.041 (3)	0.075 (5)	0.051 (4)	−0.058 (5)	−0.034 (3)
F2′_1	0.066 (3)	0.062 (3)	0.161 (7)	−0.021 (3)	0.003 (4)	−0.063 (4)
F3′_1	0.264 (5)	0.0608 (16)	0.0405 (10)	−0.075 (3)	0.023 (2)	−0.0144 (10)
C2_1	0.0384 (8)	0.0323 (7)	0.0272 (7)	−0.0055 (6)	−0.0011 (6)	−0.0007 (6)
C3_1	0.0446 (9)	0.0377 (8)	0.0369 (8)	−0.0014 (7)	−0.0147 (7)	0.0023 (7)
C4_1	0.0299 (7)	0.0327 (8)	0.0377 (8)	0.0007 (6)	−0.0028 (6)	0.0073 (6)
C5_1	0.0437 (10)	0.0382 (9)	0.0577 (11)	0.0031 (8)	−0.0143 (8)	0.0078 (8)
F4_1	0.077 (3)	0.058 (2)	0.059 (2)	0.0178 (18)	−0.0303 (18)	0.0130 (15)
F5_1	0.058 (3)	0.081 (3)	0.131 (4)	0.042 (2)	0.0332 (18)	0.040 (2)
F6_1	0.072 (2)	0.0313 (15)	0.115 (4)	0.0066 (15)	−0.048 (2)	−0.001 (2)
C5′_1	0.0437 (10)	0.0382 (9)	0.0577 (11)	0.0031 (8)	−0.0143 (8)	0.0078 (8)
F4′_1	0.135 (11)	0.113 (13)	0.104 (7)	0.088 (9)	0.044 (7)	0.046 (6)
F5′_1	0.072 (8)	0.052 (4)	0.121 (8)	0.013 (4)	−0.064 (7)	−0.012 (6)
F6′_1	0.089 (6)	0.042 (6)	0.111 (10)	−0.017 (5)	−0.040 (5)	0.041 (6)
O1_2	0.0326 (6)	0.0302 (5)	0.0558 (7)	0.0069 (5)	−0.0016 (5)	−0.0045 (5)
O2_2	0.0347 (6)	0.0328 (6)	0.0551 (7)	0.0099 (5)	−0.0024 (5)	−0.0014 (5)
C1_2	0.0400 (8)	0.0315 (7)	0.0283 (7)	0.0007 (6)	0.0037 (6)	−0.0011 (6)
C2_2	0.0367 (8)	0.0368 (8)	0.0315 (7)	0.0002 (7)	0.0020 (6)	−0.0017 (6)
C3_2	0.0384 (9)	0.0610 (12)	0.0431 (9)	−0.0045 (8)	0.0012 (7)	−0.0039 (8)
C4_2	0.0562 (12)	0.0678 (13)	0.0468 (11)	−0.0258 (11)	0.0054 (9)	−0.0086 (9)
C5_2	0.0831 (15)	0.0417 (10)	0.0392 (9)	−0.0229 (10)	0.0085 (10)	−0.0041 (8)
C6_2	0.0625 (11)	0.0327 (8)	0.0324 (8)	−0.0001 (8)	0.0049 (8)	−0.0011 (6)
C7_2	0.0397 (9)	0.0437 (10)	0.0572 (11)	0.0163 (8)	0.0027 (8)	0.0032 (8)
C8_2	0.0419 (10)	0.0496 (11)	0.0663 (13)	0.0198 (8)	0.0000 (9)	0.0084 (9)
C1_3	0.0342 (7)	0.0317 (7)	0.0266 (6)	0.0062 (6)	−0.0045 (5)	−0.0044 (6)
C2_3	0.0333 (8)	0.0344 (8)	0.0310 (7)	0.0038 (6)	−0.0046 (6)	−0.0059 (6)
C3_3	0.0456 (9)	0.0338 (8)	0.0478 (10)	0.0074 (7)	−0.0028 (8)	−0.0106 (7)
C4_3	0.0515 (11)	0.0515 (11)	0.0569 (12)	0.0173 (9)	0.0075 (9)	−0.0159 (9)
C5_3	0.0421 (10)	0.0595 (12)	0.0479 (10)	0.0091 (9)	0.0091 (8)	−0.0056 (9)
C6_3	0.0380 (8)	0.0453 (9)	0.0332 (8)	0.0028 (7)	−0.0014 (6)	−0.0005 (7)
O1_3	0.0496 (7)	0.0273 (5)	0.0458 (7)	0.0077 (5)	0.0104 (5)	−0.0014 (5)
C7_3	0.0696 (13)	0.0284 (8)	0.0494 (10)	0.0080 (8)	0.0124 (9)	0.0053 (7)
O2_3	0.0456 (7)	0.0285 (5)	0.0507 (7)	0.0010 (5)	0.0109 (6)	−0.0052 (5)
C8_3	0.0528 (11)	0.0314 (8)	0.0674 (12)	−0.0041 (8)	0.0121 (10)	−0.0044 (8)
C1_4	0.070 (11)	0.042 (8)	0.058 (7)	0.029 (6)	−0.015 (7)	−0.026 (6)
C2_4	0.059 (8)	0.065 (8)	0.062 (7)	0.040 (5)	−0.023 (5)	−0.029 (5)
C3_4	0.107 (14)	0.066 (12)	0.060 (6)	0.041 (8)	−0.001 (6)	−0.012 (5)
C4_4	0.128 (11)	0.044 (5)	0.111 (8)	0.031 (6)	−0.029 (8)	−0.011 (6)
C5_4	0.065 (7)	0.065 (6)	0.143 (9)	0.021 (5)	−0.028 (6)	−0.034 (6)
C6_4	0.078 (10)	0.068 (8)	0.080 (8)	0.034 (6)	−0.035 (6)	−0.043 (8)
O1_4	0.076 (9)	0.081 (9)	0.060 (9)	0.024 (7)	−0.015 (7)	−0.023 (9)
C7_4	0.120 (11)	0.122 (11)	0.047 (6)	0.061 (10)	0.011 (7)	−0.015 (7)
O2_4	0.069 (11)	0.091 (14)	0.055 (7)	0.054 (8)	−0.029 (7)	−0.036 (8)
C8_4	0.098 (12)	0.21 (2)	0.066 (9)	0.072 (14)	−0.055 (9)	−0.057 (12)
C1′_4	0.024 (8)	0.076 (19)	0.043 (9)	0.024 (8)	−0.017 (6)	−0.017 (9)
C2′_4	0.043 (10)	0.039 (6)	0.032 (6)	0.027 (7)	−0.012 (5)	−0.015 (6)
C3′_4	0.085 (17)	0.051 (10)	0.045 (10)	0.015 (12)	0.004 (8)	−0.010 (8)
C4′_4	0.076 (12)	0.055 (10)	0.102 (12)	0.020 (8)	0.031 (8)	−0.007 (9)

C5′_4	0.042 (8)	0.057 (8)	0.133 (14)	0.018 (6)	0.000 (8)	−0.036 (10)
C6′_4	0.029 (8)	0.064 (11)	0.102 (11)	0.026 (7)	−0.015 (7)	−0.043 (11)
O1′_4	0.050 (8)	0.082 (11)	0.031 (5)	0.028 (6)	−0.012 (4)	−0.021 (5)
C7′_4	0.14 (2)	0.15 (3)	0.048 (9)	0.036 (17)	−0.060 (12)	−0.007 (11)
O2′_4	0.044 (8)	0.053 (6)	0.038 (5)	0.020 (5)	−0.024 (5)	−0.020 (5)
C8′_4	0.064 (10)	0.080 (11)	0.045 (8)	0.031 (7)	−0.020 (7)	−0.032 (8)

Geometric parameters (Å, º)

Ni1_1—O1_1	2.0146 (10)	C3_3—H3_3	0.9500
Ni1_1—O1_1^{i}	2.0147 (10)	C4_3—C5_3	1.365 (3)
Ni1_1—O2_1	2.0213 (10)	C4_3—H4_3	0.9500
Ni1_1—O2_1^{i}	2.0213 (10)	C5_3—C6_3	1.392 (2)
Ni1_1—O3_1	2.0541 (12)	C5_3—H5_3	0.9500
Ni1_1—O3_1^{i}	2.0541 (12)	C6_3—H6_3	0.9500
O3_1—H1_1	0.80 (2)	O1_3—C7_3	1.427 (2)
O3_1—H2_1	0.84 (2)	C7_3—H7A_3	0.9800
O2_1—C4_1	1.2475 (18)	C7_3—H7B_3	0.9800
O1_1—C2_1	1.2437 (18)	C7_3—H7C_3	0.9800
C1_1—F2_1	1.283 (3)	O2_3—C8_3	1.430 (2)
C1_1—F3_1	1.283 (2)	C8_3—H8A_3	0.9800
C1_1—F1_1	1.376 (3)	C8_3—H8B_3	0.9800
C1_1—C2_1	1.530 (2)	C8_3—H8C_3	0.9800
C1′_1—F1′_1	1.173 (5)	C1_4—O1_4	1.367 (5)
C1′_1—F3′_1	1.218 (6)	C1_4—C6_4	1.380 (5)
C1′_1—F2′_1	1.419 (5)	C1_4—C2_4	1.401 (5)
C1′_1—C2_1	1.530 (2)	C2_4—O2_4	1.367 (5)
C2_1—C3_1	1.396 (2)	C2_4—C3_4	1.382 (5)
C3_1—C4_1	1.387 (2)	C3_4—C4_4	1.400 (5)
C3_1—H3_1	0.9500	C3_4—H3_4	0.9500
C4_1—C5′_1	1.531 (2)	C4_4—C5_4	1.361 (5)
C4_1—C5_1	1.531 (2)	C4_4—H4_4	0.9500
C5_1—F6_1	1.320 (7)	C5_4—C6_4	1.394 (5)
C5_1—F5_1	1.330 (6)	C5_4—H5_4	0.9500
C5_1—F4_1	1.351 (5)	C6_4—H6_4	0.9500
C5′_1—F5′_1	1.275 (13)	O1_4—C7_4	1.430 (5)
C5′_1—F4′_1	1.276 (14)	C7_4—H7A_4	0.9800
C5′_1—F6′_1	1.296 (12)	C7_4—H7B_4	0.9800
O1_2—C1_2	1.363 (2)	C7_4—H7C_4	0.9800
O1_2—C7_2	1.4270 (19)	O2_4—C8_4	1.433 (5)
O2_2—C2_2	1.364 (2)	C8_4—H8A_4	0.9800
O2_2—C8_2	1.423 (2)	C8_4—H8B_4	0.9800
C1_2—C6_2	1.380 (2)	C8_4—H8C_4	0.9800
C1_2—C2_2	1.400 (2)	C1′_4—O1′_4	1.366 (5)
C2_2—C3_2	1.380 (2)	C1′_4—C6′_4	1.379 (5)
C3_2—C4_2	1.391 (3)	C1′_4—C2′_4	1.401 (5)
C3_2—H3_2	0.9500	C2′_4—O2′_4	1.367 (5)
C4_2—C5_2	1.366 (3)	C2′_4—C3′_4	1.382 (5)

C4_2—H4_2	0.9500	C3′_4—C4′_4	1.399 (5)
C5_2—C6_2	1.393 (3)	C3′_4—H3′_4	0.9500
C5_2—H5_2	0.9500	C4′_4—C5′_4	1.359 (5)
C6_2—H6_2	0.9500	C4′_4—H4′_4	0.9500
C7_2—H7A_2	0.9800	C5′_4—C6′_4	1.395 (5)
C7_2—H7B_2	0.9800	C5′_4—H5′_4	0.9500
C7_2—H7C_2	0.9800	C6′_4—H6′_4	0.9500
C8_2—H8A_2	0.9800	O1′_4—C7′_4	1.428 (5)
C8_2—H8B_2	0.9800	C7′_4—H7′A_4	0.9800
C8_2—H8C_2	0.9800	C7′_4—H7′B_4	0.9800
C1_3—O1_3	1.3632 (18)	C7′_4—H7′C_4	0.9800
C1_3—C6_3	1.381 (2)	O2′_4—C8′_4	1.433 (5)
C1_3—C2_3	1.402 (2)	C8′_4—H8′A_4	0.9800
C2_3—O2_3	1.368 (2)	C8′_4—H8′B_4	0.9800
C2_3—C3_3	1.380 (2)	C8′_4—H8′C_4	0.9800
C3_3—C4_3	1.394 (3)		

O1_1—Ni1_1—O1_1^{i}	180.0	O2_3—C2_3—C1_3	115.22 (13)
O1_1—Ni1_1—O2_1	91.04 (4)	C3_3—C2_3—C1_3	119.35 (15)
O1_1^{i}—Ni1_1—O2_1	88.96 (4)	C2_3—C3_3—C4_3	120.13 (17)
O1_1—Ni1_1—O2_1^{i}	88.97 (4)	C2_3—C3_3—H3_3	119.9
O1_1^{i}—Ni1_1—O2_1^{i}	91.04 (4)	C4_3—C3_3—H3_3	119.9
O2_1—Ni1_1—O2_1^{i}	180.0	C5_3—C4_3—C3_3	120.27 (17)
O1_1—Ni1_1—O3_1	90.04 (5)	C5_3—C4_3—H4_3	119.9
O1_1^{i}—Ni1_1—O3_1	89.96 (5)	C3_3—C4_3—H4_3	119.9
O2_1—Ni1_1—O3_1	88.06 (5)	C4_3—C5_3—C6_3	120.37 (18)
O2_1^{i}—Ni1_1—O3_1	91.94 (5)	C4_3—C5_3—H5_3	119.8
O1_1—Ni1_1—O3_1^{i}	89.96 (5)	C6_3—C5_3—H5_3	119.8
O1_1^{i}—Ni1_1—O3_1^{i}	90.04 (5)	C1_3—C6_3—C5_3	119.69 (17)
O2_1—Ni1_1—O3_1^{i}	91.94 (5)	C1_3—C6_3—H6_3	120.2
O2_1^{i}—Ni1_1—O3_1^{i}	88.06 (5)	C5_3—C6_3—H6_3	120.2
O3_1—Ni1_1—O3_1^{i}	180.0	C1_3—O1_3—C7_3	117.29 (13)
Ni1_1—O3_1—H1_1	114.8 (16)	O1_3—C7_3—H7A_3	109.5
Ni1_1—O3_1—H2_1	117.7 (15)	O1_3—C7_3—H7B_3	109.5
H1_1—O3_1—H2_1	105 (2)	H7A_3—C7_3—H7B_3	109.5
C4_1—O2_1—Ni1_1	124.05 (10)	O1_3—C7_3—H7C_3	109.5
C2_1—O1_1—Ni1_1	124.48 (10)	H7A_3—C7_3—H7C_3	109.5
F2_1—C1_1—F3_1	110.7 (3)	H7B_3—C7_3—H7C_3	109.5
F2_1—C1_1—F1_1	103.3 (3)	C2_3—O2_3—C8_3	117.08 (13)
F3_1—C1_1—F1_1	102.6 (2)	O2_3—C8_3—H8A_3	109.5
F2_1—C1_1—C2_1	112.47 (18)	O2_3—C8_3—H8B_3	109.5
F3_1—C1_1—C2_1	117.19 (18)	H8A_3—C8_3—H8B_3	109.5
F1_1—C1_1—C2_1	109.25 (17)	O2_3—C8_3—H8C_3	109.5
F1′_1—C1′_1—F3′_1	117.7 (6)	H8A_3—C8_3—H8C_3	109.5
F1′_1—C1′_1—F2′_1	101.5 (5)	H8B_3—C8_3—H8C_3	109.5
F3′_1—C1′_1—F2′_1	102.1 (6)	O1_4—C1_4—C6_4	124.5 (6)
F1′_1—C1′_1—C2_1	117.3 (3)	O1_4—C1_4—C2_4	115.6 (5)
F3′_1—C1′_1—C2_1	110.2 (3)	C6_4—C1_4—C2_4	119.8 (5)

F2′_1—C1′_1—C2_1	105.7 (2)	O2_4—C2_4—C3_4	126.8 (5)
O1_1—C2_1—C3_1	128.88 (14)	O2_4—C2_4—C1_4	114.7 (5)
O1_1—C2_1—C1_1	113.62 (14)	C3_4—C2_4—C1_4	118.5 (5)
C3_1—C2_1—C1_1	117.49 (14)	C2_4—C3_4—C4_4	121.6 (6)
O1_1—C2_1—C1′_1	113.62 (14)	C2_4—C3_4—H3_4	119.2
C3_1—C2_1—C1′_1	117.49 (14)	C4_4—C3_4—H3_4	119.2
C4_1—C3_1—C2_1	122.31 (15)	C5_4—C4_4—C3_4	119.0 (6)
C4_1—C3_1—H3_1	118.8	C5_4—C4_4—H4_4	120.5
C2_1—C3_1—H3_1	118.8	C3_4—C4_4—H4_4	120.5
O2_1—C4_1—C3_1	129.19 (14)	C4_4—C5_4—C6_4	120.4 (6)
O2_1—C4_1—C5′_1	113.04 (14)	C4_4—C5_4—H5_4	119.8
C3_1—C4_1—C5′_1	117.77 (14)	C6_4—C5_4—H5_4	119.8
O2_1—C4_1—C5_1	113.04 (14)	C1_4—C6_4—C5_4	120.5 (6)
C3_1—C4_1—C5_1	117.77 (14)	C1_4—C6_4—H6_4	119.7
F6_1—C5_1—F5_1	107.3 (6)	C5_4—C6_4—H6_4	119.7
F6_1—C5_1—F4_1	107.4 (5)	C1_4—O1_4—C7_4	116.3 (7)
F5_1—C5_1—F4_1	108.4 (5)	O1_4—C7_4—H7A_4	109.5
F6_1—C5_1—C4_1	112.7 (4)	O1_4—C7_4—H7B_4	109.5
F5_1—C5_1—C4_1	109.1 (4)	H7A_4—C7_4—H7B_4	109.5
F4_1—C5_1—C4_1	111.8 (4)	O1_4—C7_4—H7C_4	109.5
F5′_1—C5′_1—F4′_1	101.1 (13)	H7A_4—C7_4—H7C_4	109.5
F5′_1—C5′_1—F6′_1	105.8 (10)	H7B_4—C7_4—H7C_4	109.5
F4′_1—C5′_1—F6′_1	105.1 (13)	C2_4—O2_4—C8_4	117.8 (7)
F5′_1—C5′_1—C4_1	119.2 (10)	O2_4—C8_4—H8A_4	109.5
F4′_1—C5′_1—C4_1	115.3 (11)	O2_4—C8_4—H8B_4	109.5
F6′_1—C5′_1—C4_1	109.1 (9)	H8A_4—C8_4—H8B_4	109.5
C1_2—O1_2—C7_2	117.82 (13)	O2_4—C8_4—H8C_4	109.5
C2_2—O2_2—C8_2	117.81 (14)	H8A_4—C8_4—H8C_4	109.5
O1_2—C1_2—C6_2	125.82 (16)	H8B_4—C8_4—H8C_4	109.5
O1_2—C1_2—C2_2	114.51 (14)	O1′_4—C1′_4—C6′_4	124.9 (6)
C6_2—C1_2—C2_2	119.66 (16)	O1′_4—C1′_4—C2′_4	115.1 (6)
O2_2—C2_2—C3_2	125.50 (16)	C6′_4—C1′_4—C2′_4	119.9 (5)
O2_2—C2_2—C1_2	114.26 (14)	O2′_4—C2′_4—C3′_4	126.7 (6)
C3_2—C2_2—C1_2	120.25 (16)	O2′_4—C2′_4—C1′_4	114.8 (5)
C2_2—C3_2—C4_2	119.42 (19)	C3′_4—C2′_4—C1′_4	118.6 (5)
C2_2—C3_2—H3_2	120.3	C2′_4—C3′_4—C4′_4	121.3 (6)
C4_2—C3_2—H3_2	120.3	C2′_4—C3′_4—H3′_4	119.4
C5_2—C4_2—C3_2	120.50 (19)	C4′_4—C3′_4—H3′_4	119.4
C5_2—C4_2—H4_2	119.8	C5′_4—C4′_4—C3′_4	119.6 (6)
C3_2—C4_2—H4_2	119.8	C5′_4—C4′_4—H4′_4	120.2
C4_2—C5_2—C6_2	120.54 (18)	C3′_4—C4′_4—H4′_4	120.2
C4_2—C5_2—H5_2	119.7	C4′_4—C5′_4—C6′_4	120.1 (6)
C6_2—C5_2—H5_2	119.7	C4′_4—C5′_4—H5′_4	120.0
C1_2—C6_2—C5_2	119.62 (18)	C6′_4—C5′_4—H5′_4	120.0
C1_2—C6_2—H6_2	120.2	C1′_4—C6′_4—C5′_4	120.5 (6)
C5_2—C6_2—H6_2	120.2	C1′_4—C6′_4—H6′_4	119.7
O1_2—C7_2—H7A_2	109.5	C5′_4—C6′_4—H6′_4	119.7
O1_2—C7_2—H7B_2	109.5	C1′_4—O1′_4—C7′_4	116.7 (8)

H7A_2—C7_2—H7B_2	109.5	O1′_4—C7′_4—H7′A_4	109.5
O1_2—C7_2—H7C_2	109.5	O1′_4—C7′_4—H7′B_4	109.5
H7A_2—C7_2—H7C_2	109.5	H7′A_4—C7′_4—H7′B_4	109.5
H7B_2—C7_2—H7C_2	109.5	O1′_4—C7′_4—H7′C_4	109.5
O2_2—C8_2—H8A_2	109.5	H7′A_4—C7′_4—H7′C_4	109.5
O2_2—C8_2—H8B_2	109.5	H7′B_4—C7′_4—H7′C_4	109.5
H8A_2—C8_2—H8B_2	109.5	C2′_4—O2′_4—C8′_4	117.6 (7)
O2_2—C8_2—H8C_2	109.5	O2′_4—C8′_4—H8′A_4	109.5
H8A_2—C8_2—H8C_2	109.5	O2′_4—C8′_4—H8′B_4	109.5
H8B_2—C8_2—H8C_2	109.5	H8′A_4—C8′_4—H8′B_4	109.5
O1_3—C1_3—C6_3	124.84 (14)	O2′_4—C8′_4—H8′C_4	109.5
O1_3—C1_3—C2_3	114.97 (14)	H8′A_4—C8′_4—H8′C_4	109.5
C6_3—C1_3—C2_3	120.19 (14)	H8′B_4—C8′_4—H8′C_4	109.5
O2_3—C2_3—C3_3	125.43 (15)		

Ni1_1—O1_1—C2_1—C3_1	1.8 (2)	O1_2—C1_2—C6_2—C5_2	−178.37 (15)
Ni1_1—O1_1—C2_1—C1_1	−179.05 (10)	C2_2—C1_2—C6_2—C5_2	1.0 (2)
Ni1_1—O1_1—C2_1—C1′_1	−179.05 (10)	C4_2—C5_2—C6_2—C1_2	0.0 (3)
F2_1—C1_1—C2_1—O1_1	60.7 (4)	O1_3—C1_3—C2_3—O2_3	−1.3 (2)
F3_1—C1_1—C2_1—O1_1	−169.4 (2)	C6_3—C1_3—C2_3—O2_3	179.53 (14)
F1_1—C1_1—C2_1—O1_1	−53.4 (3)	O1_3—C1_3—C2_3—C3_3	178.33 (14)
F2_1—C1_1—C2_1—C3_1	−120.1 (3)	C6_3—C1_3—C2_3—C3_3	−0.8 (2)
F3_1—C1_1—C2_1—C3_1	9.9 (3)	O2_3—C2_3—C3_3—C4_3	179.85 (16)
F1_1—C1_1—C2_1—C3_1	125.9 (3)	C1_3—C2_3—C3_3—C4_3	0.2 (3)
F1′_1—C1′_1—C2_1—O1_1	13.3 (7)	C2_3—C3_3—C4_3—C5_3	0.5 (3)
F3′_1—C1′_1—C2_1—O1_1	−125.0 (7)	C3_3—C4_3—C5_3—C6_3	−0.7 (3)
F2′_1—C1′_1—C2_1—O1_1	125.4 (5)	O1_3—C1_3—C6_3—C5_3	−178.37 (16)
F1′_1—C1′_1—C2_1—C3_1	−167.5 (7)	C2_3—C1_3—C6_3—C5_3	0.7 (2)
F3′_1—C1′_1—C2_1—C3_1	54.2 (8)	C4_3—C5_3—C6_3—C1_3	0.1 (3)
F2′_1—C1′_1—C2_1—C3_1	−55.3 (5)	C6_3—C1_3—O1_3—C7_3	2.6 (2)
O1_1—C2_1—C3_1—C4_1	−1.3 (3)	C2_3—C1_3—O1_3—C7_3	−176.44 (15)
C1_1—C2_1—C3_1—C4_1	179.59 (16)	C3_3—C2_3—O2_3—C8_3	−2.7 (2)
C1′_1—C2_1—C3_1—C4_1	179.59 (16)	C1_3—C2_3—O2_3—C8_3	176.93 (15)
Ni1_1—O2_1—C4_1—C3_1	2.8 (2)	O1_4—C1_4—C2_4—O2_4	−1 (3)
Ni1_1—O2_1—C4_1—C5′_1	−177.85 (11)	C6_4—C1_4—C2_4—O2_4	−178 (2)
Ni1_1—O2_1—C4_1—C5_1	−177.85 (11)	O1_4—C1_4—C2_4—C3_4	179 (3)
C2_1—C3_1—C4_1—O2_1	−1.4 (3)	C6_4—C1_4—C2_4—C3_4	2.4 (19)
C2_1—C3_1—C4_1—C5′_1	179.35 (17)	O2_4—C2_4—C3_4—C4_4	−179 (2)
C2_1—C3_1—C4_1—C5_1	179.35 (17)	C1_4—C2_4—C3_4—C4_4	1.0 (15)
O2_1—C4_1—C5_1—F6_1	40.6 (6)	C2_4—C3_4—C4_4—C5_4	−4 (2)
C3_1—C4_1—C5_1—F6_1	−140.0 (6)	C3_4—C4_4—C5_4—C6_4	3 (2)
O2_1—C4_1—C5_1—F5_1	−78.4 (5)	O1_4—C1_4—C6_4—C5_4	−180 (3)
C3_1—C4_1—C5_1—F5_1	101.0 (6)	C2_4—C1_4—C6_4—C5_4	−3 (3)
O2_1—C4_1—C5_1—F4_1	161.7 (5)	C4_4—C5_4—C6_4—C1_4	0 (3)
C3_1—C4_1—C5_1—F4_1	−18.9 (5)	C6_4—C1_4—O1_4—C7_4	−11 (5)
O2_1—C4_1—C5′_1—F5′_1	178.1 (18)	C2_4—C1_4—O1_4—C7_4	172 (2)
C3_1—C4_1—C5′_1—F5′_1	−2.4 (18)	C3_4—C2_4—O2_4—C8_4	−3 (3)
O2_1—C4_1—C5′_1—F4′_1	−61 (2)	C1_4—C2_4—O2_4—C8_4	177.1 (18)

C3_1—C4_1—C5′_1—F4′_1	118 (2)	O1′_4—C1′_4—C2′_4—O2′_4	3 (5)
O2_1—C4_1—C5′_1—F6′_1	56.6 (16)	C6′_4—C1′_4—C2′_4—O2′_4	180 (3)
C3_1—C4_1—C5′_1—F6′_1	−124.0 (16)	O1′_4—C1′_4—C2′_4—C3′_4	−178 (3)
C7_2—O1_2—C1_2—C6_2	−16.5 (2)	C6′_4—C1′_4—C2′_4—C3′_4	−1 (6)
C7_2—O1_2—C1_2—C2_2	164.10 (15)	O2′_4—C2′_4—C3′_4—C4′_4	179 (3)
C8_2—O2_2—C2_2—C3_2	−2.4 (3)	C1′_4—C2′_4—C3′_4—C4′_4	0 (5)
C8_2—O2_2—C2_2—C1_2	177.37 (15)	C2′_4—C3′_4—C4′_4—C5′_4	0 (5)
O1_2—C1_2—C2_2—O2_2	−1.9 (2)	C3′_4—C4′_4—C5′_4—C6′_4	1 (4)
C6_2—C1_2—C2_2—O2_2	178.67 (15)	O1′_4—C1′_4—C6′_4—C5′_4	179 (4)
O1_2—C1_2—C2_2—C3_2	177.90 (15)	C2′_4—C1′_4—C6′_4—C5′_4	2 (6)
C6_2—C1_2—C2_2—C3_2	−1.5 (2)	C4′_4—C5′_4—C6′_4—C1′_4	−2 (4)
O2_2—C2_2—C3_2—C4_2	−179.18 (17)	C6′_4—C1′_4—O1′_4—C7′_4	−9 (7)
C1_2—C2_2—C3_2—C4_2	1.0 (3)	C2′_4—C1′_4—O1′_4—C7′_4	167 (4)
C2_2—C3_2—C4_2—C5_2	0.0 (3)	C3′_4—C2′_4—O2′_4—C8′_4	−1 (4)
C3_2—C4_2—C5_2—C6_2	−0.5 (3)	C1′_4—C2′_4—O2′_4—C8′_4	178 (3)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3_1—H1_1···O1_2	0.80 (2)	2.17 (2)	2.8978 (17)	152 (2)
O3_1—H1_1···O2_2	0.80 (2)	2.33 (2)	2.9854 (17)	140 (2)
O3_1—H2_1···O1_3	0.84 (2)	2.31 (2)	2.9100 (16)	128.8 (19)
O3_1—H2_1···O2_3	0.84 (2)	2.23 (3)	3.0377 (17)	161 (2)