Syntheses, Structures and Magnetic Properties of A Molecular Pair of [$LnNi_3$] (Ln=Ce, Pr, Gd) Tetrahedra Bridged by Water Molecules

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Chapter 1

Introduction

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Introduction

The synthesis of transition metal clusters with relevance in molecular magnetism has been a very prolific area of coordination chemistry,[1-3] and has become of primary importance since the compound $[Mn_{12}O_{12}(O_2CCH_3)_{16}(H_2O)_4] \cdot 4H_2O \cdot 2CH_3COOH$ (Mn12) was discovered as the first single molecular magnet (SMM) in 1993.[4] As a result, a high level of understanding has been achieved of the nature and mechanism of the magnetic super exchange between 3d metals.[5-7] Indeed, the vast majority of SMMs known to date are made of transition metals such as manganese,[8] iron,[9] nickel,[10] cobalt,[11] and vanadium.[12] This chemistry is extensible to the lanthanides. The first investigation of the magnetic properties of a 3d-4f heterometallic complex is due to Gatteschi et al., who observed and characterized the ferromagnetic interaction between Cu^{II} and Gd^{III}.[13] The first mixed-metal 3d-4f SMM to exhibit hysteresis loops and quantum tunneling of the magnetization, $[Mn_{11}Dy_4O_8(OH)_6(OCH_3)_2(O_2CPh)_{16}(NO_3)_5(H_2O)_3] \cdot 15CH_3CN$ was reported by Christou and co-workers in 2004.[14] The combination of 3d and 4f elements to form large cluster aggregates has produced several novel SMMs with attractive blocking temperatures and thus a slow relaxation of magnetization.[14-18] The immediate advantage of the 4f elements are large number of unpaired electrons, *i.e.*, large spin and pronounced spin-orbit coupling resulting in large Ising type anisotropy. In the case of Gd^{III} ions, the absence of anisotropy is also very appealing, because Gd^{III}－3d molecules

represent excellent magnetic coolers for low-temperature applications.[19] The topic of magnetic refrigeration constitutes one of the potential applications envisioned for polymetallic molecules.[20] The magnetocaloric effect (MCE) is based on the change of magnetic entropy upon application of a magnetic field and is of great technological importance since it can be used for cooling applications[21-23] according to a process known as adiabatic demagnetization.[24, 25] This energy-efficient and environmentally friendly technique is particularly promising for refrigeration in the ultra-low-temperature region, providing, for example, a valid alternative to the use of ^{3}He, which is becoming rare and expensive.[26] Recent studies have demonstrated that the MCE of selected molecular cluster compounds can be much larger than found in the best, and conventionally studied, intermetallic and lanthanide alloys and magnetic nanoparticles. This undoubtedly represents an exciting prospect for these heterometallic molecular clusters, maintaining them in the forefront of investigation in the context of molecular magnetism.

As mentioned above, syntheses and characterization of hetero- and poly-nuclear complexes have attracted special attention in recent years. By choosing suitable chelating ligands, complexes containing both 3d and 4f metal ions may be formed although the metal ions have distinct differences in the chemical nature. An amino acid is one of suitable ligands for construction of heterometallic compounds containing transition and rare earth metals simultaneously. From the point of view of coordination chemistry, an amino acid, which is safe and easily obtained, can be regarded

as a typical multidentate ligand. The exploration of this potential is, in part, motivated by the desire to model metal active sites embedded within naturally occurring enzymes. This group of ligands displays a carboxylate moiety adjacent to an amino group, thus exhibiting the potential of coordinating and/or bridging metals in a variety of modes (for example, see Figure 1, right). In this context, preparations of aggregates involving a variety of different metals, such as Cu, Co, or Fe[27-30] are descrived. For example, the combination of Cu^{II} and Ln^{III} salts with amino acids has led to the formation of an impressive series of architectures based on the presence of capped, superoctahedral, triacontanuclear [Ln_6Cu_{24}] clusters, organized as 1D, 2D, or 3D arrays, as well as in form of discrete clusters.[31-34] Other combinations of Cu^{II}, Ln^{III}, and amino acids in water have led to another family of clusters with a [$LnCu_6$] core showing with a very regular trigonal prism of Cu^{II} ions centered by the Ln^{III} metal.[35] This arrangement is also accessible with Ni^{II} or Co^{II} in aqueous media, although these metals have also unveiled a related topology of centered [LnM_6] regular octahedron.[36, 37] Interestingly, the use of nonaqueous media, such as acetonitrile, also leads to octahedral clusters, but does not produce the prism. [38] These conditions have also opened the way to other new topologies just by changing the counter anion, solvent and the nature of the amino acid. For example, recently, Yukawa and co-workers have reported [Gd_2Ni_2] complex constructed by L-prolinato ligands (Figure 3), which features a cyclic architecture and have an S=9 spin ground state.[39]

The author reports herein a remarkable new addition to this growing family;

it is an octanuclear Ln_2Ni_6 mixed-metal complex cation, exhibits two tetrahedral [$LnNi_3$] (Ln=Ce, Pr, and Gd) fragments linked through coordination of three molecules of water.

Chapter 2

Syntheses and Structures of Water-Bridged Molecular Pair of [$LnNi_3$] (Ln=Ce, Pr) Tetrahedra

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Syntheses and Structures of Water-Bridged Molecular Pair of [$LnNi_3$] (Ln=Ce, Pr) Tetrahedra

2-1 Experimental

2-1-1 Reagents

$NiSO_4 \cdot 6H_2O$, $KHCO_3$, L-valine, acetone, and acetonitrile were purchased from Wako Pure Chemicals Co.

$Ce(NO_3)_3 \cdot 6H_2O$ and $Pr(NO_3)_3 \cdot 6H_2O$ were purchased from KANTO CHEMCAL CO., INC.

$Ni(val)_2 \cdot 2H_2O$ was prepared as follows:

An aqueous solution of $NiSO_4 \cdot 6H_2O$ (30 mmol / 60 ml) and that of $KHCO_3$ (90 mmol / 90ml) were prepared. To the $NiSO_4 \cdot 6H_2O$ solution the $KHCO_3$ solution was added. The pale green mixed suspension was stood at room temperature for a day and was filtered to obtain powder of $NiCO_3$.

To a colorless suspended aqueous solution (90 ml) of L-valine (30 mmol) fresh $NiCO_3$ was added and stirred with heating. The color of the suspension changed from pale green to light blue. The suspension was concentrated to yield light blue powder of $Ni(val)_2 \cdot 2H_2O$. The powder was washed with acetone (50 ml) and dried.

2-1-2 Preparations

*Synthesis of $[Ln_2\{Ni(val)_2\}_6(H_2O)_3(MeCN)_6][Ln(NO_3)_6]_2 \cdot nH_2O$ (Ln=Ce(**1**), Pr(**2**))*

To an acetonitrile solution of $Ln(NO_3)_3 \cdot 6H_2O$ (Ln=Ce, Pr) (3 mmol / 50 ml) $Ni(val)_2 \cdot 2H_2O$ (3 mmol) was added. After heating and stirring the violet suspension was obtained. The suspension was kept at room temperature for few hours and then a colorless powder of starting material was removed by decantation.

Violet prismatic crystals were obtained from the mixed solution by keeping it for a day at room temperature.

2-1-3 Measurements

Infrared spectra

Infrared spectra were measured by means of reflection method on a JASCO FT/IR-4100 Fourier Transform Infrared Spectrophotometer equipped with a Model DR PRO410-M Powder Reflection Unit using silicon powder for the standard and a diluent.

Crystal Structure Determination

A violet prism crystal of $[Ln_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6][Ln(NO_3)_6]_2 \cdot nH_2O$ (Ln=Ce(**1**), Pr(**2**)) having approximate dimensions of 0.40 x 0.20 x 0.20 mm was mounted and shielded in a glass capillary with mother solution since the crystal was unstable in the air. All measurements were made on a Rigaku R-AXIS Ⅳ Imaging Plate diffractometer with graphite monochromated Mo-Kα radiation. The crystal-to-detector distance was 120.00 mm with the detector at the zero swing position. The data were collected at a temperature of 23 ± 1 ℃ to a maximum 2θ value of 51.4° . The structure was solved by heavy-atom Patterson methods and expanded using Fourier techniques. Some non-hydrogen atoms were refined anisotropically, while the rest were refined isotropically. Hydrogen atoms were included but not refined. All calculations were performed using the teXsan (crystallographic software package of Molecular Structure Corporation).

2-2 Results and Discussion

The reaction of $Ln(NO_3)_3 \cdot 6H_2O$ (Ln=Ce, Pr) with $Ni(val)_2 \cdot 2H_2O$ in a molar ratio of 1 to 1 using CH_3CN as a solvent produces the octanuclear complex salt $[Ln_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6][Ln(NO_3)_6]_2 \cdot nH_2O$ (Ln=Ce (**1**), Pr (**2**)). The molecular structures of complexes **1** and **2** were determined by single-crystal X-ray diffraction analysis at room temperature. The crystal data are summarized in Table 1. The compounds **1** and **2** are isomorphous and they crystallized in the same orthorhombic space group $P2_12_12_1$. The lattice parameters of **1** were a = 22.2518(9) Å, b = 25.6730(9) Å, c = 30.025(1) Å, and Z = 4, and of **2** were a = 22.2061(3) Å, b = 25.6527(4) Å, c = 30.0171(3) Å, and Z = 4, respectively.

IR spectra of compounds **1** and **2** are shown in Figure 4 together with that of $Ni(val)_2 \cdot 2H_2O$ for comparison. The spectra of **1** and **2** are almost the same and thus two compounds expected to have the identical structure, these results are correspondence with those of the X-ray diffraction analysis. Both complexes exhibit two ν_s(N−H) peaks at about 3300 cm^{-1}. The spectra also show a strong peak at *ca.* 1600 cm^{-1} which is assigned to stretching vibration of the carboxylate group ν_{asym}(COO) of valinato ligand. This peak split into two peaks, suggesting that two oxygen atoms of a carboxylate group have different coordination environment. The peak at about 2300~2400 cm^{-1} of ν(−C≡N) is the evidence of the presence of acetonitrile molecules.

The crystal lattice of the octanuclear complex salt contains the cluster cation

$[Ln_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6]^{6+}$ (Figure 5) and its large positive charge being compensated by two $[Ln(NO_3)_6]^{3-}$ anions (Figure 6). The structure and atomic labels of the octanuclear cluster cation $[Ln_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6]^{6+}$ (Ln=Ce, Pr) are shown in Figure 5, and selected bond lengths and bond angles are given in Table 2.

In the structure of the clustster cation $[Ln_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6]^{6+}$, each Ni(Ⅱ) ion is chelated in the equatorial plane by two val^- ligands in mutual *cis* configuration so as to forms $[Ni(val)_2]$ moiety. Of the two val^- ligands of the $[Ni(val)_2]$ moiety, one terminally coordinates to Ln(Ⅲ) and Ni(Ⅱ) simultaneously through a carboxylate oxygen atom, whereas the other bridges second Ni(Ⅱ) ion using the rest carboxylate oxygen atom in addition to the coordination of the first one(Figure 7). In other words, by means of the Ni···Ni bridge of *syn,anti* carboxylate, a carboxylate oxygen atom of one valinato ligand of a $[Ni(val)_2]$ molecule coordinates to Ni(Ⅱ) of neighboring $[Ni(val)_2]$ from one axial position. The distorted octahedral coordination of each Ni(Ⅱ) ion is completed by coordination of one molecule of CH_3CN which occupies the remaining axial site. Meanwhile each Ln(Ⅲ) ion is coordinated to three $[Ni(val)_2]$ molecules by virtue of a total of six oxygen atoms from the carboxylate groups of valinato ligands to form a $[Ln\{Ni(val)_2\}_3]^{3+}$ unit. Then two $[Ln\{Ni(val)_2\}_3]^{3+}$ units are connected through Ln(Ⅲ) ions by three bridging water molecules. Consequently, Ln(Ⅲ) ion has nine-coordination geometry including six carboxylato oxygen atoms from six valinato ligands and three oxygen atoms from three water molecules. The nine oxygen donors surrounding each Ln(Ⅲ) atom lead to a remarkably regular coordination

geometry, close to a perfect, spherical, tricapped, trigonal prism (Figure 8), that is, with identical vertex-to-center distances and D_{3h} symmetry. Its metric parameters are found in Table 2.

In the $[Ln\{Ni(val)_2\}_3]^{3+}$ unit, four metals (*i.e.* one lanthanide ion and three nickel ions) are considered to construct a $[LnNi_3]$ trigonal pyramid. The whole structure of complex cation $[Ln_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6]^{6+}$ could be regarded as follows: two $[LnNi_3]$ trigonal pyramids linked through their vertices by means of three molecules of water acting as bridging ligands between two Ln(Ⅲ) metals, to form an unprecedented $[Ln(\mu\text{-}H_2O)_3Ln]$ coordination moiety (Figure 9). The identity of the bridging ligands as H_2O molecules is confirmed by charge considerations. It is remarkable that two positively charged Ln(Ⅲ) ions are connected with the power of three neutral water molecules and this framework makes the cluster cation very unique. Actually, these water molecules and carboxylato oxygens of val^- ligands, which do not coordinate to the axial site of neighboring $[Ni(val)_2]$, form hydrogen bonding. The structures of these hydrogen bonds are shown in Figure 10, and hydrogen bond distances are given in Table 3. As shown in the Figure 10, a total of six hydrogen bonds are formed. These hydrogen bonds are regard to be relatively strong and it seems to permit construction of the cluster cation having unprecedented $[Ln(\mu\text{-}H_2O)_3Ln]$ coordination moiety and stabilize the whole structure.

Crystals of compounds **1** and **2** contain many solvent molecules. These solvent molecules are considered to be loosely trapped in the crystal lattice

and give rise to immediate decomposing of crystals after filtering.

The other lanthanide series, except for the metals described here, of the octanuclear cluster cation $[Ln_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6]^{6+}$ was not obtained by means of the same synthesis methods.

Chapter 3

Syntheses and Structures of Water-Bridged Molecular Pair of [$LnNi_3$] (Ln=Gd) Tetrahedra with Different Counter Anions

Chapter 3

Syntheses and Structures of Water-Bridged Molecular Pair of [$LnNi_3$] (Ln=Gd) Tetrahedra with Different Counter Anions

3-1 Experimental

3-1-1 Reagents

$Gd(NO_3)_3 \cdot 6H_2O$ was purchased from KANTO CHEMCAL CO., INC.

$TEAClO_4$ (tetraethylammonium perchlorate) was purchased from Nacalai Tesque Co.

Diethylether was purchased from Wako Pure Chemicals Co.

Other reagents are the same as ones used in chapter 2.

3-1-2 Preparations

Crystals of $TEA[Gd_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6][Gd(NO_3)_5](ClO_4)_5 \cdot 7CH_3CN \cdot 2H_2O$ (3) and $TEA[Gd_2\{Ni(val)_2\}_6(H_2O)_3(NO_3)_3(CH_3CN)_3](ClO_4)_4$ (4) were prepared by just the identical synthetic method.

Solid $Ni(val)_2 \cdot 2H_2O$ (3 mmol) was added to a solution of $Gd(NO_3)_3 \cdot 6H_2O$ (3 mmol) in MeCN (50 ml) and the resulting light-blue mixture was stirred and heated. When the color became darker, tetraethylammonium perchlorate $TEAClO_4$ (1.37 g, 6 mmol) was added to the system while stirring and heating for a few minutes. The system was then cooled to room temperature and white powdered precipitates were removed by filtration.

The resulting filtrate was layered with Et_2O (50 ml) and kept at room temperature for a few days. Two types of crystals, large violet block crystals of $TEA[Gd_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6][Gd(NO_3)_5](ClO_4)_5 \cdot 7CH_3CN \cdot 2H_2O$ (3) and small blue-violet cubic crystals of $TEA[Gd_2\{Ni(val)_2\}_6(H_2O)_3(NO_3)_3(CH_3CN)_3](ClO_4)_4$ (4) were obtained.

3-1-3 Measurements

Infrared spectra

Infrared spectra were measured by means of reflection method on a JASCO FT/IR-4100 Fourier Transform Infrared Spectrophotometer equipped with a Model DR PRO410-M Powder Reflection Unit using silicon powder for the standard and a diluent.

Crystal Structure Determination

$TEA[Gd_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6][Gd(NO_3)_5](ClO_4)_5 \cdot 7CH_3CN \cdot 2H_2O$ (3)

Data for compound $TEA[Gd_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6][Gd(NO_3)_5](ClO_4)_5 \cdot 7CH_3CN \cdot 2H_2O$ (3) were collected on a blue block on a Bruker APEX Ⅱ CCD diffractometer on Advanced Light Source beamline 11.3.1 at Lawrence Berkeley National Laboratory, from a silicon 111 monochromator (T=100 K, λ=0.7749 Å). Because a single crystal could not be found, the data were collected on a twin. CELL_NOW[40] was used to determine the orientation matrices and the domains were related by a 180° rotation around the reciprocal axis 0 0 1. The integration was performed with both matrices. TWINABS[40] was used to produce a merged HKLF4 file, for structure solution and initial refinement, and HKLF5 file for final structure refinement. The HKLF5 file contained the merged reflections of the first component and those that overlapped with the second component were split into 2 reflections. The twin relative fractions as refined by TWINABS were 0.7242 / 0.2758. The structure was solved by direct methods and the refinement on F^2 and all further calculations were carried out using

SHELX-TL suite.[40.41] All non-hydrogen atoms were refined anisotropically, except the tetraethyl ammonium moiety that present strong disorder and could only be satisfactorily refined as isotropic. Hydrogen atoms were placed geometrically on their carrier atom and refined with a riding model where possible. Hydrogen atoms on the lattice water molecules O1W and O2W could not be found nor fixed and are omitted in the structural model. The participation of these oxygen atoms in hydrogen bonds, however, clearly indicates the presence of these hydrogen atoms. Perchlorate groups and lattice acetonitrile molecules were also refined with distance and displacement parameters restraints, due to disorder.

$TEA[Gd_2\{Ni(val)_2\}_6(H_2O)_3(NO_3)_3(CH_3CN)_3](ClO_4)_4$ (**4**)

A blue-violet cubic crystal of $TEA[Gd_2\{Ni(val)_2\}_6(H_2O)_3(NO_3)_3(CH_3CN)_3](ClO_4)_4$ (**4**) having approximate dimensions of 0.50 x 0.30 x 0.25 mm was manicure-coated and mounted on a glass fiber. All measurements were made on a Rigaku R-AXIS Ⅳ Imaging Plate diffractometer with graphite monochromated Mo-K_α radiation. The crystal-to-detector distance was 100.00 mm with the detector at the zero swing position. The data were collected at a temperature of 23 ± 1 ℃ to a maximum 2θ value of 55.0° . The structure was solved by heavy-atom Patterson methods and expanded using Fourier techniques. Some non-hydrogen atoms were refined anisotropically, while the rest were refined isotropically. Hydrogen atoms were included but not refined. All calculations were performed using the teXsan (crystallographic software package of Molecular Structure Corporation).

3-2 Result and Discussion

The reaction of $Gd(NO_3)_3 \cdot 6H_2O$ with $Ni(val)_2 \cdot 2H_2O$ in molar a ratio of 1 to 1 in the presence of $TEAClO_4$ (tetraethylammonium perchlorate), with CH_3CN as a solvent produces two forms of complex salt containing the octanuclear cation when the system is layered with Et_2O. The first form of the complex salt is $TEA[Gd_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6][Gd(NO_3)_5](ClO_4)_5 \cdot 7CH_3CN \cdot 2H_2O$ (**3**) and the second form is $TEA[Gd_2\{Ni(val)_2\}_6(H_2O)_3(NO_3)_3(CH_3CN)_3](ClO_4)_4$ (**4**). Both of the compounds **3** and **4** were synthesized by just the identical procedure. The molecular structure of each complex was determined by single-crystal X-ray diffraction analysis. It may be noted that the X-ray diffraction of **3** were measured at 100 K whereas that of **4** were measured at room temperature. The crystal data of **3** and **4** are summarized in Table 4 and 5, respectively. The compound **3** crystallized in the orthorhombic space group $P2_12_12_1$, likewise the compounds **1** and **2**, and lattice parameters were a = 22.178(3) Å, b = 22.767(3) Å, c = 31.708(4) Å, and Z = 4. The compound **4** crystallized in the cubic space group $P2_13$ and lattice parameters were a = 24.0192(3) Å and Z = 4.

IR spectra of compounds **3** and **4** are shown in Figure 11. The spectra of **3** and **4** are almost the identical and essentially the same as those of **1** and **2** (Figure 4) except a peak at about 1100 cm^{-1}, which may be assigned to the vibration of ClO_4^-.

The crystal lattice of compound 3 contains the cluster cation $[Gd_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6]^{6+}$ (Figure 12); its structure is the same as those of 1 and 2 (see the chapter 1) replacing Ce or Pr instead of Gd. The structure and atomic labels of the octanuclear cluster cation $[Gd_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6]^{6+}$ of complex salt 3 are shown in Figure 12, and selected bond lengths and bond angles are given in Table 6. The structure may be best described as two $[GdNi_3]$ trigonal pyramids linked through their vertices by means of three molecules of water acting as bridging ligands, as mentioned in chapter 1. Both $[GdNi_3]$ fragments are chemically equivalent. The identity of the bridging ligands as H_2O molecules is confirmed by charge considerations. This bridging of water molecules enables construction of an very unique and unprecedented $[Gd(\mu\text{-}H_2O)_3Gd]$ coordination moiety. Similar to the compounds 1 and 2, hydrogen bonds are formed between bridging water molecules and carboxylato oxygen atoms of val^- ligands and these hydrogen bondings stabilize the framework of the cluster cation. The structures of these hydrogen bonds are shown in Figure 13, and hydrogen bond distances are given in Table 7. The charge of the cluster cation $[Gd_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6]^{6+}$ is compensated by four ClO_4^- groups and the complex anion $[Gd(NO_3)_5]^{2-}$ (Figure 14). In addition, one more ClO_4^- anion together with a TEA^+ (tetraethylammonium) cation exists in the lattice. Crystals of compound 3 also contain many solvent molecules which are loosely trapped in the crystal lattice and evaporate immediately upon filtering, consequently they considered to cause decomposition of crystals.

The crystal lattice of compound **4** contains the cluster cation $[Gd_2\{Ni(val)_2\}_6(H_2O)_3(NO_3)_3(CH_3CN)_3]^{3+}$. The structure and atomic labels of the octanuclear cluster cation $[Gd_2\{Ni(val)_2\}_6(H_2O)_3(NO_3)_3(CH_3CN)_3]^{3+}$ of complex salt **4** are shown in Figure 15. The selected bond lengths and bond angles are given in Table 8. The structure is essentially the same as that of cluster cation of **1~3** but three CH_3CN molecules of one $[GdNi_3]$ moiety, which terminally coordinate to an axial position of each Ni(Ⅱ), were replaced by three NO_3^- anions carrying −1 charge. Coordination of these nitrate anions reduces positive charge of the octanuclear cluseter cation +6 to +3, and this +3 charge being compensated by three symmetry equivalent ClO_4^- anions. In addition, one more ClO_4^- anion together with a TEA^+ cation exists in the lattice; both, ClO_4^- and TEA^+, are in special crystallographic positions. The structure of the cluster cation is regard to linked two $[GdNi_3]$ trigonal pyramids by means of bridging water molecules likewise the compounds **1~3**, and the hydrogen bonds between water molecules and carboxylato oxygen atoms of val^- ligands are also observed. The structures of these hydrogen bonds are shown in Figure 16, and hydrogen bond distances are given in Table 9. Both $[GdNi_3]$ pyramids exhibit crystallographic C_3 symmetry, with a threefold axis running through the gadolinium metals. The two $[GdNi_3]$ fragments are not identical since, as mentioned above, the distorted octahedral coordination of each Ni(Ⅱ) ion is completed by one terminal NO_3^- anion in one pyramid or by one molecule of MeCN in the other pyramid. It is notable that crystals of **4** have no solvent molecule and stable in the air meanwhile crystals of **1~3** decompose upon filtering because of many solvent molecules loosely trapped in the lattice.

The compound **4** crystallize in the cubic space group $P2_13$ different from the compounds **1**~**3** which form crystals having the orthorhombic space group $P2_12_12_1$. It is considered that decrease of positive charge of the cluster cation preclude a packing of rather large counter anions $[Ln(NO_3)_6]^{3-}$ (Ln=Ce, Pr) or $[Gd(NO_3)_5]^{2-}$ and give rise to the replacement of these counter anions by smaller perchlorate anions: By the replacement the crystal packing could be tight in the system. This change of counter anions seems to make crystal packing denser and get rid of the space for solvent molecules, as a result, the crystals are considered to become stable.

The compounds **3** and **4** are simultaneously synthesized under the same synthetic conditions. The factor of what determines either crystal is formed is not known for now.

The other lanthanide series, except for the metals described here, of the octanuclear cluster cation was not obtained by means of the above synthesis methods.

Chapter 4

Magnetic Properties of Water-Bridged Molecular Pair of $[LnNi_3]$ (Ln=Gd) Tetrahedra

Chapter 4

Magnetic Properties of Water-Bridged Molecular Pair of [$LnNi_3$] (Ln=Gd) Tetrahedra

4-1 Experimental

4-1-1 Measurements

Variable-temperature magnetic-susceptibility data were obtained with either a Quantum Design MPMS5 (Barcelona) or an XL (Zaragoza) SQUID magnetometer. The field applied for temperature-dependent measurements was in the range of the linear dependence of M versus B. The measured values were corrected for the experimentally determined contribution of the sample holder, whereas Pascal's constants were utilized to estimate diamagnetic corrections to the molar paramagnetic susceptibility.

4-1-2 Computational details

DFT calculations have been done with the SIESTA[42] computer code using the PBE[43] functional. Pseudopotentials have been used for all the atoms, specifically for the gadolinium atom we have used the pseudopotential proposed by Pollet *et al.*[44] together with a TZV basis. To calculate the exchange coupling values six calculations have been performed, a high-spin solution (S=13), an S=6 solution with negative spin at {Gd1}, an S=5 solution with negative spin at {Ni1, Ni2, Ni4, Ni5}, an S=2 solution with negative spin at {Gd1, Ni1, Ni5} and two S=0 solutions with negative spin at {Gd2, Ni1, Ni2, Ni3} and {Gd1, Ni1, Ni2, Ni3}. A detailed description of that procedure can be found in previous publications.[45-47]

4-2 Results and Discussion

The intramolecular magnetic exchange within the complex $TEA[Gd_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6][Gd(NO_3)_5](ClO_4)_5 \cdot 7CH_3CN \cdot 2H_2O$ (3) was investigated through variable-temperature magnetic susceptibility measurements on polycrystalline samples. Figure 17 shows a plot of $\chi_M T$ versus T in the 2-300 K temperature range, measured under a constant magnetic field of 3 kG. At 300 K, the curve lies at 28.7 cm^3 K mol^{-1}, which is close the expected value (29.6 cm^3 K mol^{-1}) for six Ni^{II} ions (S=1) and three Gd^{III} centers (S=7/2), all magnetically dilute and with g=2. The $\chi_M T$ value remains almost constant until 100 K, where it starts to increase at a growing rate with decreasing temperatures until a maximum of 32.5 cm^3 K mol^{-1} is reached at 5 K. A sharp decrease is then observed upon further cooling to a value of 29 cm^3 K mol^{-1} at 2 K. This behavior indicates the presence of weak ferromagnetic interactions within the cluster added to the Curie-like contribution from the isolated $[Gd(NO_3)_5]^{2-}$ anion. The low-temperature behavior is certainly affected by the effects from magnetoanisotropy terms and/or (antiferromagnetic) intermolecular interactions. The energy of the exchange interaction within the cluster is represented by the Heisenberg spin Hamiltonian in Equation (1), with S_i=1 (i=1-6), S_7=S_8=7/2 (following the numbering scheme in Figure 18), for which neither the magnetoanisotropy, nor intermolecular interactions are included.

$$H = -2J_1(S_1S_2+S_1S_3+S_2S_3+S_4S_5+S_4S_6+S_5S_6) - 2J_2(S_1S_7+S_2S_7+S_3S_7+S_4S_8+S_5S_8+S_6S_8) - 2J_3S_7S_8 \quad (1)$$

The coupling constants in this Hamiltonian, as well as the cluster g value may be obtained by diagonalizing the energy matrix resulting from the interaction of the system with an external magnetic field. This was realized after extracting the contribution of an isolated Gd^{III} spin carrier (S=7/2 and g=1.98)[48] from the data and by using the program CLUMAG.[49] Because the decline at low temperature must be, completely or partially, due to factors not included in the model for the fit (see above), the fit was performed with only the data obtained at temperatures above that of the maximum. The results from this fit (J_1=−2.14 cm^{-1}, J_2=+0.43 cm^{-1}, J_3=+0.07 cm^{-1} and g=2.14; Figure 17) led to a spin ground state of S=7. Drastic differences of the ground state may be caused, however, by small changes to the fitting conditions or resulting parameters, as the natural consequence of very small energies involved in the interactions. Indeed the results from this fit locates just above the ground state two spin states (an S=6 and an S=8) within an energy range of less than 1 cm^{-1}.

The uncertainty with regard to the possible influence of the magnetic anisotropy and intermolecular interactions prompted us to analyze the exchange coupling within the cluster cation of 3, that is $[Gd_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6]^{6+}$, through DFT methods which avoids these factors.[50] To the best of our knowledge, this is the first time that such a computational study is undertaken for a system involving a polynuclear compound containing gadolinium. The calculations yielded J_1=−0.6 cm^{-1}, J_2=+0.7 cm^{-1}, J_3=+0.01 cm^{-1}, in reasonable agreement with those obtained

for the fit, predicting now a ground state of S=13 and a $\chi_M T$-versus-T curve with no maximum at low temperature. The differences must be attributed, to a large extent, to the influence of terms not included in the model used for the fit. This highlights the possibility of the maximum to be caused by magnetic anisotropy or intermolecular interactions. Because of this, and the consistency with previously published exchange-coupling data (see below), we attribute more credibility to the values obtained from the DFT calculations.

The Ni···Ni coupling through a *syn,anti* carboxylate was indeed expected to be feeble.[38,50] There is no precedent of a [Gd(μ-H_2O)$_3$Gd] magnetic-exchanged moiety to which the present system can be compared. Most of the Gd···Gd pathways that occur thorough three monoatomic bridge involve alkoxide or phenolate ligands and are weakly antiferromagnetic ($|J| < 1$ cm^{-1}),[48, 51-53] with some rare exceptions.[54] On the other hand, heterometallic Ni···Gd pairs are very common in the literature. However, the bridging motif in the cluster cation of 3, that is, two single-bridging O atoms and a *syn,syn* carboxylate, is almost unprecedented and has only been studied by us for the magnetic exchange on a [GdNi$_6$] cluster,[38] for which a J constant of +0.13 cm^{-1} was found. In any case, in the sixteen reports involving Ni···Gd exchange that we have identified, the interaction has always been found to be ferromagnetic.[17, 19, 38, 55-67]

The weakness of the magnetic coupling between spin carriers throughout the compound 3 precludes the strict use of the giant spin approximation, because

considerable mixing of the various spin states is expected. The reduced magnetization M measured at constant temperatures in the 2-11 K range under a variable magnetic field B (Figure 17, inset) indeed increases only slowly with B, instead of growing quickly towards saturation as would be expected for a well-isolated ground state. This reflects the fact that the various spin states are nested over a narrow range of energies. The value reached by M at the highest field and lowest temperatures (32.3 μ_B) agrees well with the expected value of 33 μ_B for either a well-isolated S=13 ground state together with an independent Gd^{III} ion, or a very weakly coupled system, overall with g=2.

The presence of many low-lying excited spin-states often results in increased magnetic entropy, which in turn yields an enhancement of the field-dependence of the magnetocaloric effect.[68] We thus made a preliminary evaluation of the potential of the compound 3 for magnetic refrigeration through the determination of the magnetic entropy change ΔS_m from the magnetization data as previously described.[19] The results are represented in Figure 19 for selected field changes ΔB and show that $-\Delta S_m$ increases gradually as ΔB increases and T decrease to reach a value of 17.6 J kg^{-1} K^{-1} at T=3 K and ΔB=5 T. This value is among the highest reported for such temperatures, and can be interpreted as the entropy expected from two S=13/2 and one S=7/2 noninteracting spins, that is, R[2ln(13+1)+ln(7+1)]=17.9 J kg^{-1} K^{-1}. This is in good agreement with the set of exchange coupling interactions obtained experimentally and from DFT calculations, because the central, very weak, ferromagnetic interaction

would be largely overcome by the applied fields used herein; thus, besides the isolated $[Gd(NO_3)_5]^{2-}$ ion, the two $[GdNi_3]$ units are also magnetically decoupled. Conformation of the potential of the compound 3 as a magnetic refrigerant, as well as ascertaining the influence of low-lying, excited, spin states and of the isolated $[Gd(NO_3)_5]^{2-}$ anion, would require deeper magnetothermal studies,[56] which is beyond the scope of the present thesis.

Chapter 5

Summary

Chapter 5

Summary

Syntheses and characterization of hetero- and poly-nuclear complexes with lanthanide and transition metals have attracted special attention in the region of the molecular magnetism which has been inspired by potential functional materials such as SMMs and magnetic refrigerators. In this study, taking advantage of the properties of the amino acid ligands, syntheses of new heterometal complexes with lanthanide(Ⅲ) ion using an amino acidato transition metal complex, $[Ni(val)_2]$, as a ligand were attempted.

The reaction of $Ln(NO_3)_3 \cdot 6H_2O$ (Ln=Ce, Pr) with $Ni(val)_2 \cdot 2H_2O$ in a molar ratio of 1 to 1 using CH_3CN as a solvent produces a new octanuclear complex salt $[Ln_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6][Ln(NO_3)_6]_2 \cdot nH_2O$ (Ln=Ce (**1**), Pr (**2**)). Moreover, addition of $TEAClO_4$ (tetraethylammonium perchlorate) to the system enables the syntheses of two forms of the octanuclear complex salt of another lanthanide when Gd is used, $TEA[Gd_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6][Gd(NO_3)_5](ClO_4)_5 \cdot 7CH_3CN \cdot 2H_2O$ (**3**) and $TEA[Gd_2\{Ni(val)_2\}_6(H_2O)_3(NO_3)_3(CH_3CN)_3](ClO_4)_4$ (**4**). All the molecular structure of complexes was determined by single-crystal X-ray diffraction analysis. The frameworks of octanuclear complex cation $[Ln_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6]^{6+}$ of **1~3** are the identical and have +6 positive charge; whereas in that of 4, three of six neutral CH_3CN ligands are replaced by NO_3^- anions and for that reason the complex cation has +3 charge. The structure of all of the octanuclear complex cation of **1~4** could be

regarded as two [$LnNi_3$] trigonal pyramids linked through their vertices by means of three molecules of water acting as bridging ligands between two Ln(Ⅲ) metals, to form of an unprecedented [$Ln(\mu\text{-}H_2O)_3Ln$] coordination moiety. The bridging water molecules and carboxylato oxygens of val^- ligands form hydrogen bonding. These hydrogen bonds are regard to be relatively strong and considered to permit the construction of a very unique [$Ln(\mu\text{-}H_2O)_3Ln$] moiety. Crystals of compounds **1**~**3** contain many solvent molecules. These solvent molecules are considered to be loosely trapped in the crystal lattice and seem to give rise to immediate decomposing of crystals after filtering. It is notable that crystals of **4** have no solvent molecule and stable in the air. The change of the charge of the cluster cation (from 6+ to 3+) leads to change of anionic charge: Huge anions $[Ln(NO_3)_6]^{3-}$ (Ln=Ce and Pr) or $[Gd(NO_3)_5]^{2-}$ (compounds **1**~**3**) change to small ClO_4^- (compound **4**). The change of cationic and anionic charges causes change of space group of the crystals and therefore, in compound **4**, dense crystal packing precluding solvent is formed instead of loose one including many solvent molecules. Both of the compounds **3** and **4** were synthesized by just the identical procedure. The factor of what determines either crystal is formed is not known for now. The other lanthanide series, except for the metals described here, of the octanuclear cluster cation was not obtained by means of the above synthesis methods.

The intramolecular magnetic exchange within the complex **3** was investigated through variable-temperature magnetic susceptibility measurements on polycrystalline samples. The water-bridged $Gd^{Ⅲ}$ ions

exhibit weak ferromagnetic coupling through a magnetic path never observed before, and the ensemble shows a dense accumulation of spin states within a narrow energy range. Nevertheless, the system allows an evaluation of the intramolecular magnetic-exchange interactions through DFT calculations. The calculations yielded J_1=−0.6 cm^{-1}, J_2=+0.7 cm^{-1}, J_3=+0.01 cm^{-1}, in reasonable agreement with those obtained for the fit to the magnetic susceptibility data, predicting a ground state of S=13 and a $\chi_M T$-versus-T curve with no maximum at low temperature. Because of this, and the consistency with previously published exchange-coupling data, we attribute more credibility to the values obtained from the DFT calculations. Next, we made a preliminary evaluation of the potential of the compound 3 for magnetic refrigeration through the determination of the magnetic entropy change ΔS_m from the magnetization data. The obtained value of ΔS_m of 17.6 J kg^{-1} K^{-1} is among the highest reported which indicate that 3 would be a good magnetic refrigerant for low-temperature applications.

Figures and Tables

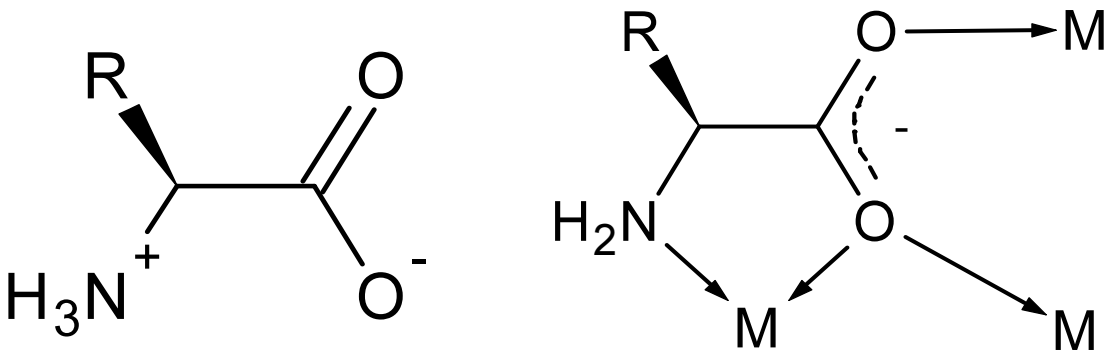
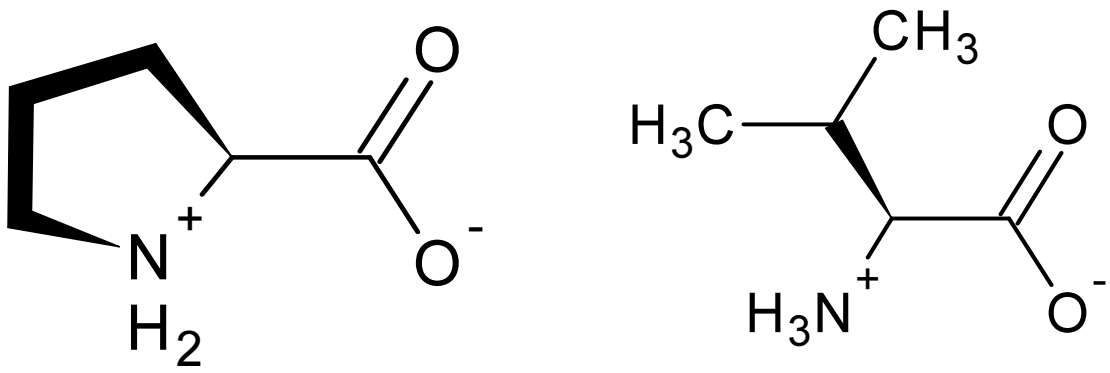


Figure 1. Structure and coordination mode of amino acid.



L-proline L-valine

Figure 2. Structure of L-proline and L-valine.

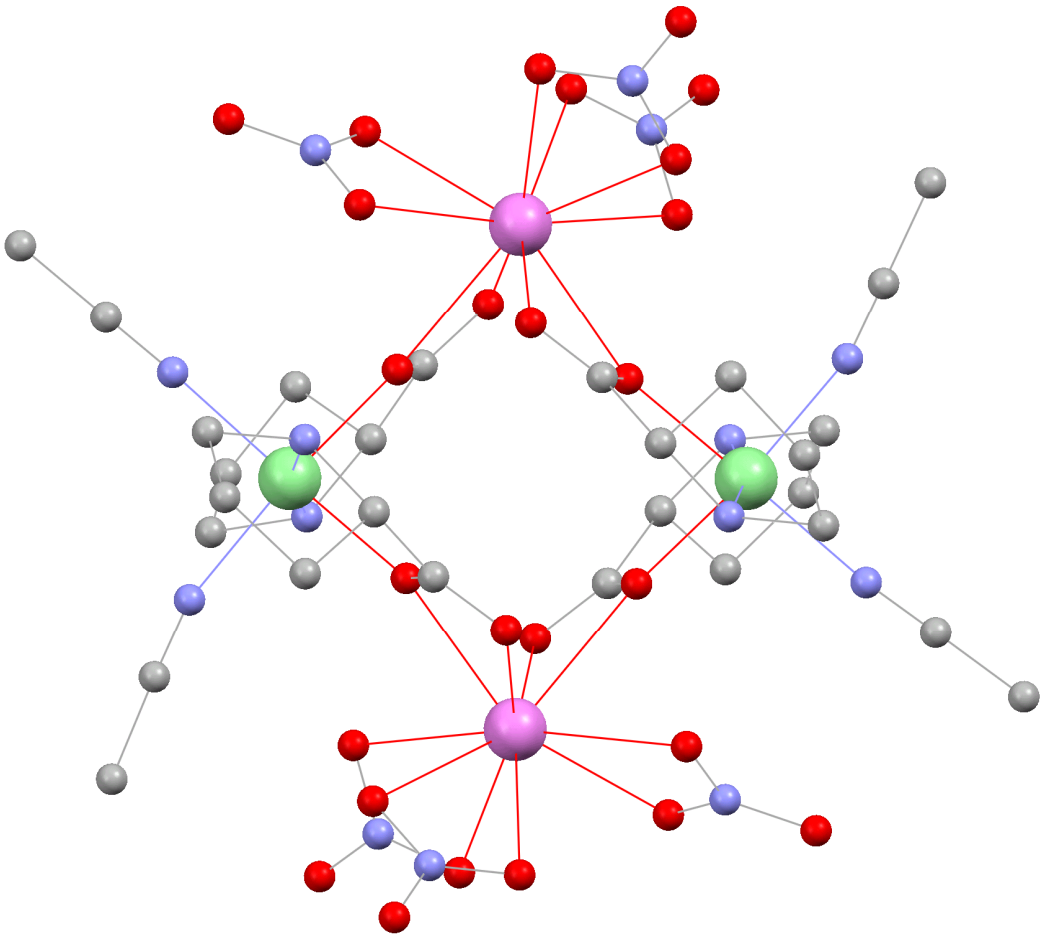


Figure 3. Structure of $[Gd_2Ni_2(pro)_4(NO_3)_6(CH_3CN)_4]$. Hydrogen atoms are omitted for clarity.

Ball color; lanthanide, nickel, oxygen, nitrogen, carbon.

Table 1. Crystal data for $[Ln_2\{Ni(val)_2\}_6(OH_2)_3(CH_3CN)_6][Ln(NO_3)_6]_2 \cdot nH_2O$ (Ln=Ce(**1**), Pr(**2**)).

Empirical Formula	$Ce_4Ni_6O_{75}N_{30}C_{72}H_{168}$	$Pr_4Ni_6O_{75}N_{30}C_{72}H_{168}$
Formula Weight	3566.96	3570.11
Crystal System	Orthorhombic	Orthorhombic
Space Group	$P2_12_12_1$	$P2_12_12_1$
a / Å	22.2518(9)	22.2061(3)
b / Å	25.6730(9)	25.6527(4)
c / Å	30.025(1)	30.0171(3)
V / Å^3	17152(1)	17099.1(4)
Z value	4	4
D_{calcu} / g cm^{-3}	1.381	1.387
F(000)	7240.00	7256.00
μ (Mo-Kα) / cm^{-1}	17.67	18.44
R	0.094	0.076
R_w	0.112	0.088
S	2.33	1.85

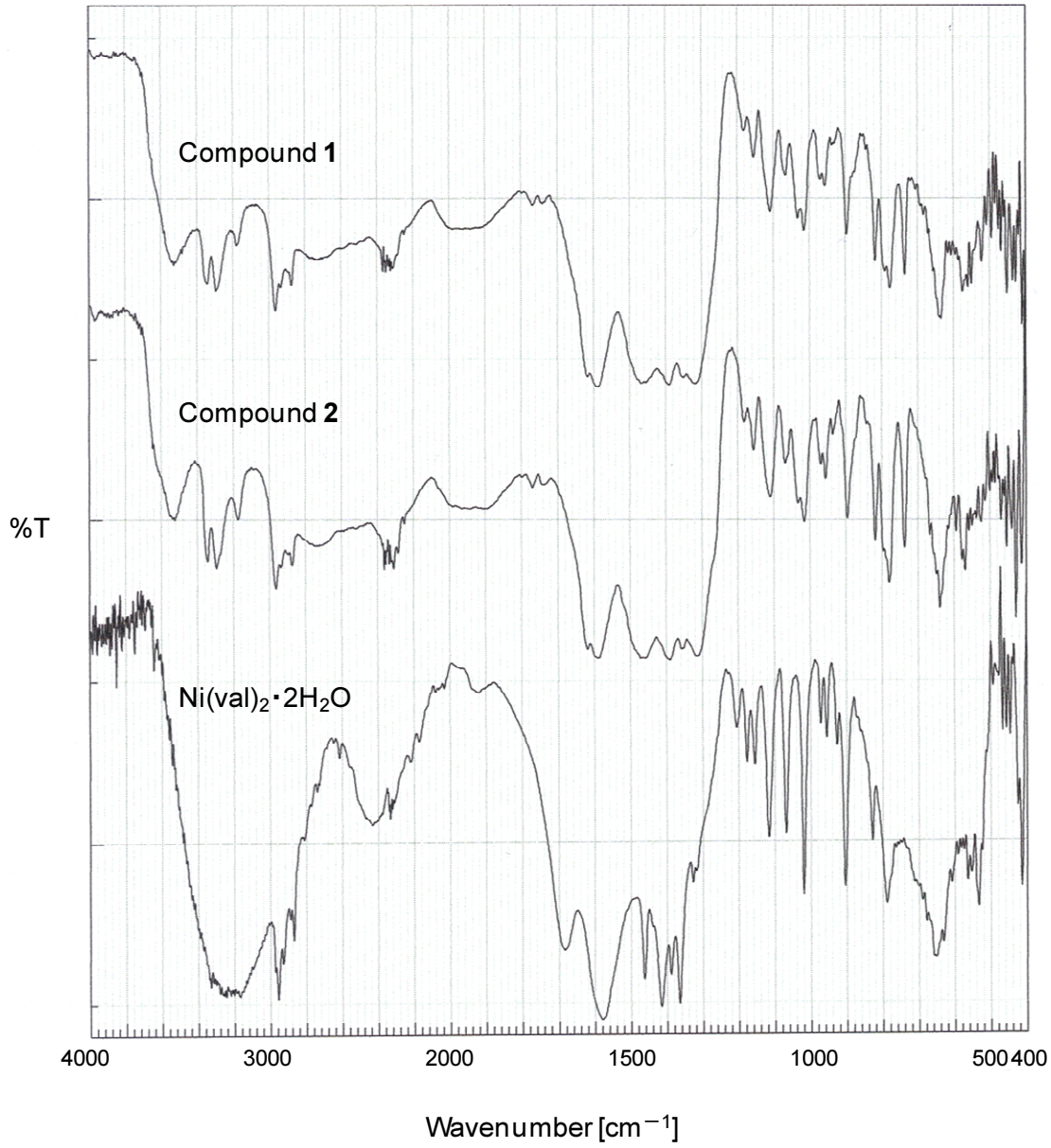


Figure 4. IR spectra of compounds **1**, **2** and $Ni(val)_2 \cdot 2H_2O$

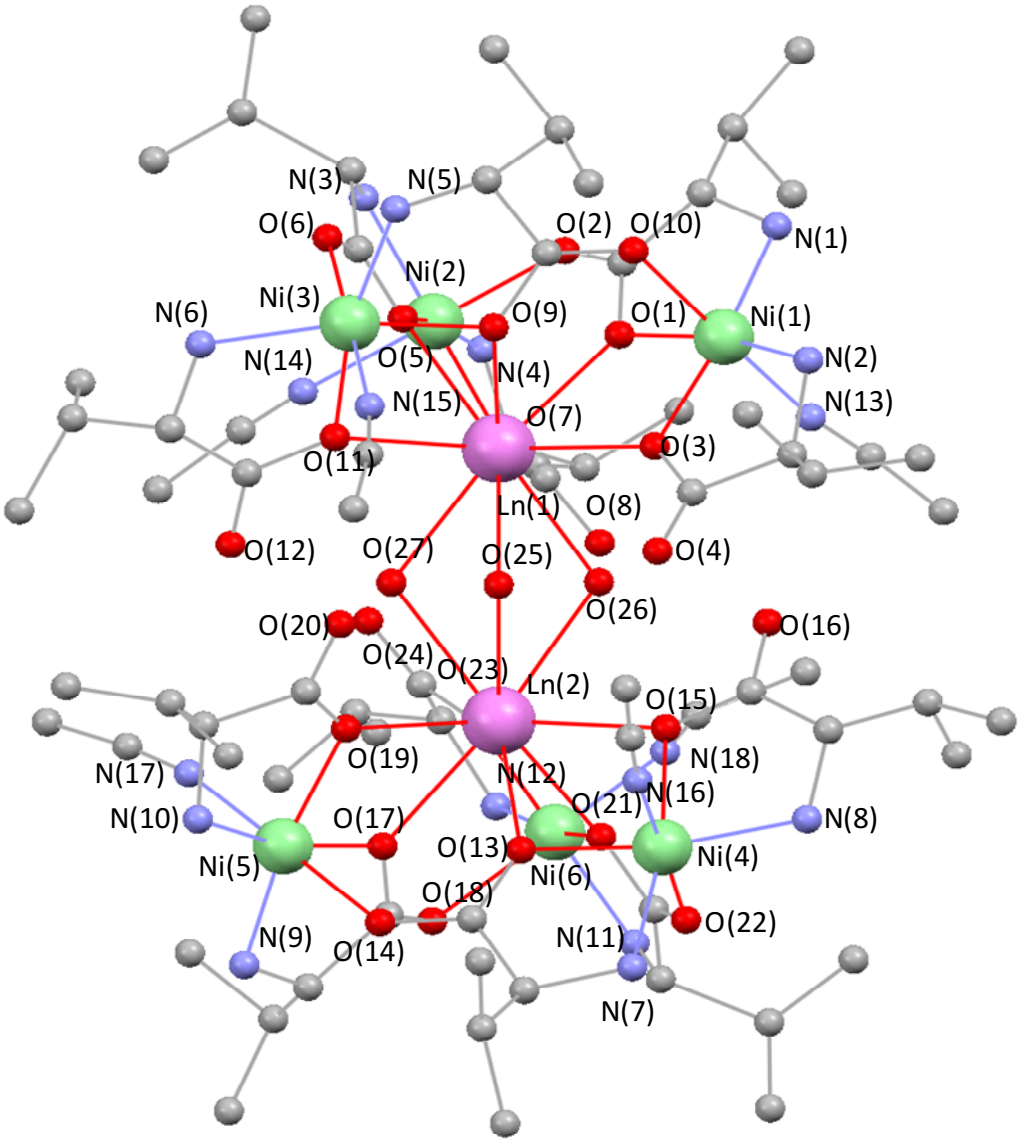


Figure 5. Structure and atomic labels of cluster cation $[Ln\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6]^{6+}$ (Ln=Ce(1), Pr(2)). Hydrogen atoms are omitted for clarity.

Ball color; ●lanthanide, ●nickel, ●oxygen, ●nitrogen, ●carbon.

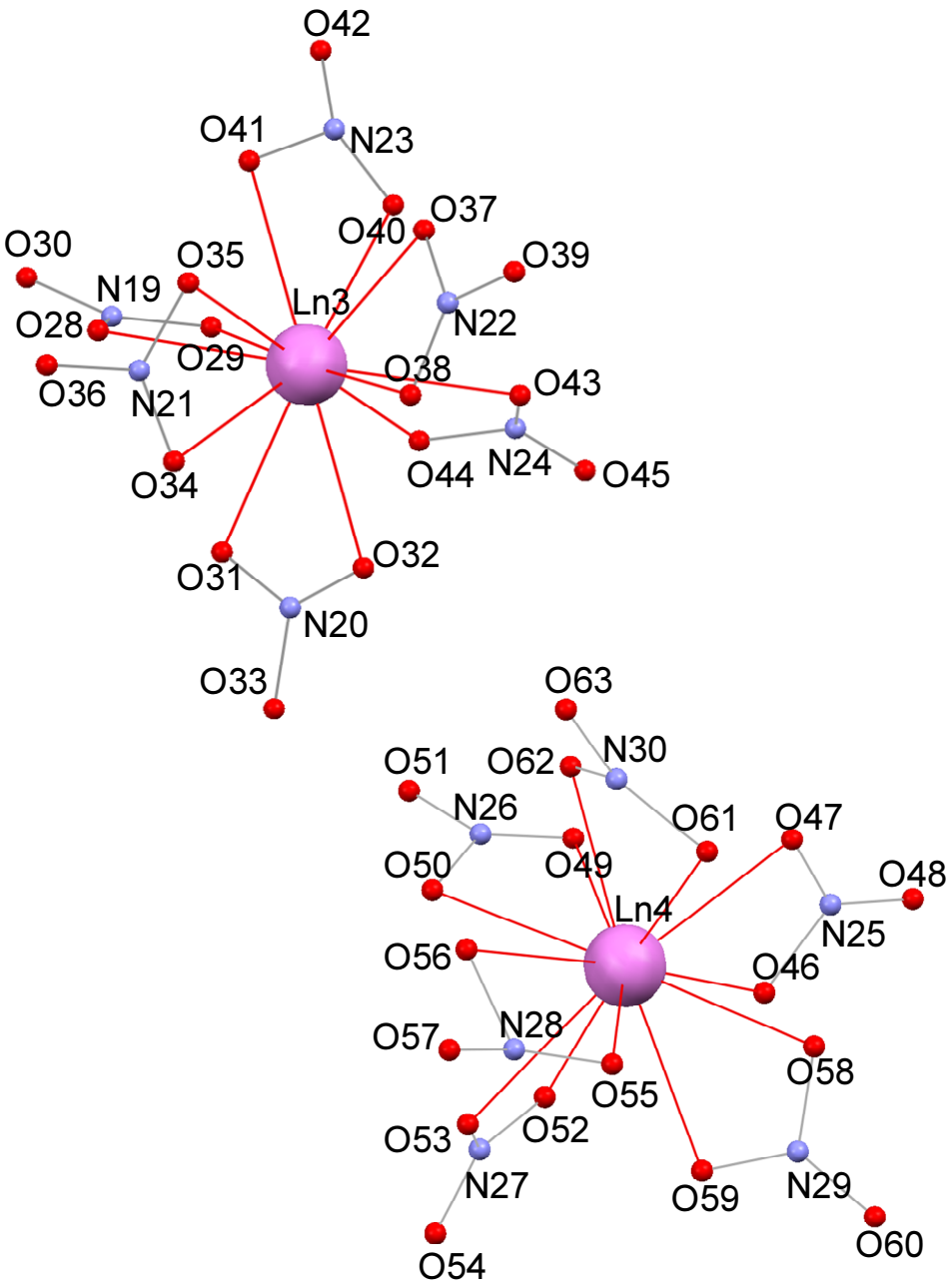


Figure 6. Structure and atomic labels of counter anions $[Ln(NO_3)_6]^{3-}$.

Ball color; lanthanide, oxygen, nitrogen.

Table 2. Selected interatomic distances (Å), including intermetallic separations, and angles (°) in compound $[Ln_2\{Ni(val)_2\}_6(OH_2)_3(CH_3CN)_6][Ln(NO_3)_6]_2 \cdot nH_2O$ (Ln=Ce(**1**), Pr(**2**)).

	Ce_2Ni_6-cluster	Pr_2Ni_6-cluster
Ln1－O1	2.52(1)	2.507(9)
Ln1－O3	2.519(10)	2.504(7)
Ln1－O5	2.47(1)	2.472(8)
Ln1－O7	2.53(1)	2.499(8)
Ln1－O9	2.51(1)	2.498(9)
Ln1－O11	2.50(1)	2.500(8)
Ln1－O25	2.59(1)	2.567(8)
Ln1－O26	2.59(1)	2.588(8)
Ln1－O27	2.55(1)	2.578(8)
Ln1…Ni1	3.572(2)	3.566(2)
Ln1…Ni2	3.551(2)	3.544(2)
Ln1…Ni3	3.570(3)	3.566(2)
Ln2－O13	2.55(1)	2.54(1)
Ln2－O15	2.516(10)	2.512(8)
Ln2－O17	2.49(1)	2.493(10)
Ln2－O19	2.54(1)	2.537(8)
Ln2－O21	2.56(1)	2.510(10)
Ln2－O23	2.51(1)	2.498(8)
Ln2－O25	2.61(1)	2.594(8)
Ln2－O26	2.62(1)	2.605(8)
Ln2－O27	2.59(1)	2.567(8)

Ln2···Ni4	3.560(3)	3.557(2)
Ln2···Ni5	3.544(3)	3.539(2)
Ln2···Ni6	3.591(3)	3.587(2)
Ln3−O28	2.67(2)	2.62(1)
Ln3−O29	2.66(2)	2.68(1)
Ln3−O31	2.68(2)	2.62(1)
Ln3−O32	2.59(1)	2.58(1)
Ln3−O34	2.64(1)	2.62(1)
Ln3−O35	2.61(1)	2.609(10)
Ln3−O37	2.63(2)	2.63(1)
Ln3−O38	2.57(2)	2.56(1)
Ln3−O40	2.66(1)	2.66(1)
Ln3−O41	2.64(1)	2.63(1)
Ln3−O43	2.65(2)	2.65(1)
Ln3−O44	2.64(1)	2.61(1)
Ln4−O46	2.64(1)	2.626(10)
Ln4−O47	2.68(2)	2.64(1)
Ln4−O49	2.73(2)	2.64(2)
Ln4−O50	2.64(2)	2.59(1)
Ln4−O52	2.63(1)	2.63(1)
Ln4−O53	2.68(2)	2.65(1)
Ln4−O55	2.53(3)	2.56(2)
Ln4−O56	2.67(2)	2.66(2)
Ln4−O58	2.59(2)	2.61(1)
Ln4−O59	2.64(1)	2.607(10)

Ln4－O61	2.71(2)	2.63(2)
Ln4－O62	2.56(2)	2.50(2)
Ni1－O1	2.02(1)	2.020(8)
Ni1－O3	2.04(1)	2.045(9)
Ni1－O10	2.07(1)	2.096(10)
Ni1－N1	2.04(2)	2.03(1)
Ni1－N2	2.06(1)	2.05(1)
Ni1－N13	2.13(2)	2.13(1)
Ni2－O5	2.04(1)	2.049(8)
Ni2－O2	2.12(1)	2.136(10)
Ni2－O7	1.98(1)	2.015(8)
Ni2－N3	2.04(2)	2.03(1)
Ni2－N4	2.03(1)	2.07(1)
Ni2－N14	2.04(1)	2.08(1)
Ni3－O9	2.01(1)	2.023(9)
Ni3－O6	2.11(1)	2.099(10)
Ni3－O11	1.99(1)	2.031(9)
Ni3－N5	2.06(2)	2.05(1)
Ni3－N6	2.03(1)	2.05(1)
Ni3－N15	2.09(2)	2.08(1)
Ni4－O13	2.03(1)	2.028(9)
Ni4－O15	2.04(1)	2.040(9)
Ni4－O22	2.08(1)	2.07(1)
Ni4－N7	2.06(2)	2.04(2)
Ni4－N8	2.08(2)	2.11(1)

Ni4－N16	2.08(2)	2.13(2)
Ni5－O14	2.21(1)	2.21(1)
Ni5－O17	2.01(1)	2.01(1)
Ni5－O19	2.01(1)	2.007(8)
Ni5－N9	1.98(2)	1.97(2)
Ni5－N10	2.01(2)	2.00(1)
Ni5－N17	1.97(2)	1.92(1)
Ni6－O18	2.07(1)	2.06(1)
Ni6－O21	1.97(1)	2.015(10)
Ni6－O23	2.05(1)	2.045(8)
Ni6－N11	2.01(2)	2.04(1)
Ni6－N12	2.02(1)	2.03(1)
Ni6－N18	2.07(2)	2.08(1)
Ni1…Ni2	5.340(3)	5.346(2)
Ni1…Ni3	5.307(3)	5.346(2)
Ni2…Ni3	5.354(3)	5.351(3)
Ni4…Ni5	5.322(4)	5.324(3)
Ni4…Ni6	5.333(3)	5.331(3)
Ni5…Ni6	5.350(3)	5.351(3)
Ln1…Ln2	4.028(1)	4.0016(8)
Ln1－O25－Ln2	101.5(3)	101.7(3)
Ln1－O26－Ln2	101.2(3)	100.8(3)
Ln1－O27－Ln2	103.2(3)	102.1(3)
Ni1－O1－Ln1	103.2(5)	103.4(4)
Ni1－O3－Ln1	102.6(4)	102.8(3)

Ni2－O5－Ln1	103.3(4)	102.9(3)
Ni2－O7－Ln1	103.2(5)	102.9(3)
Ni3－O9－Ln1	104.0(4)	103.7(3)
Ni3－O11－Ln1	104.5(4)	103.4(3)
Ni4－O13－Ln2	101.5(5)	101.8(4)
Ni4－O15－Ln2	102.3(4)	102.3(3)
Ni5－O17－Ln2	103.5(5)	103.0(4)
Ni5－O19－Ln2	101.5(5)	101.6(3)
Ni6－O21－Ln2	104.0(5)	104.4(4)
Ni6－O23－Ln2	103.4(4)	103.8(3)

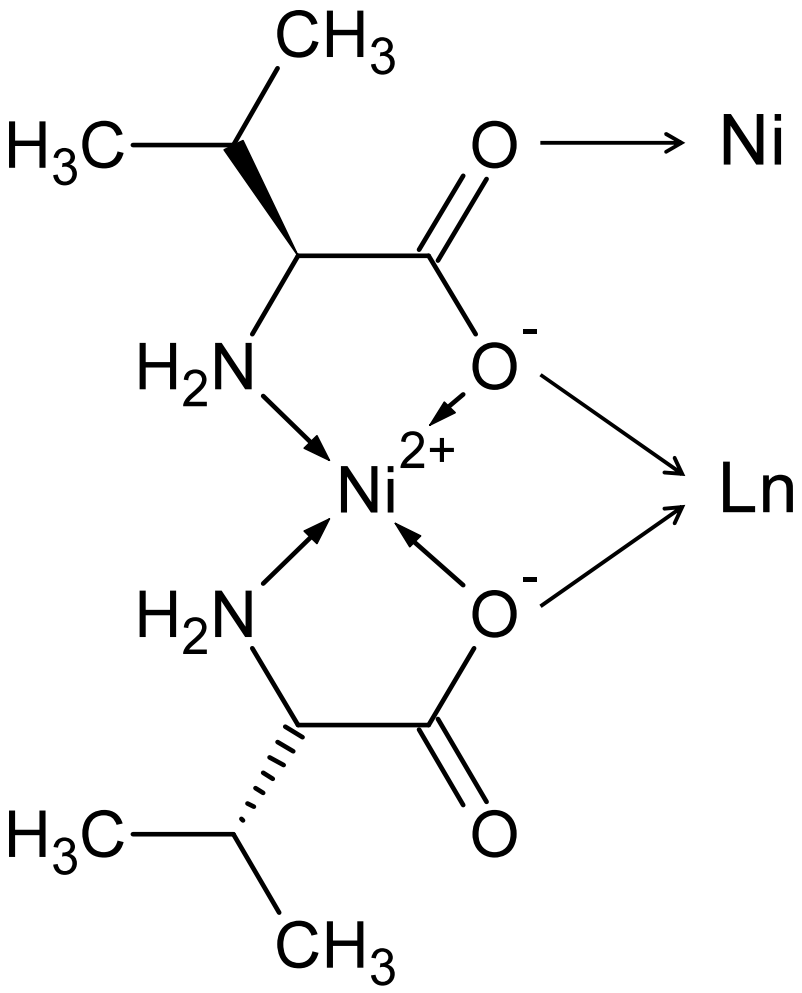


Figure 7. Structure of [Ni(val)$_2$] (val$^-$=L-valinato ion).

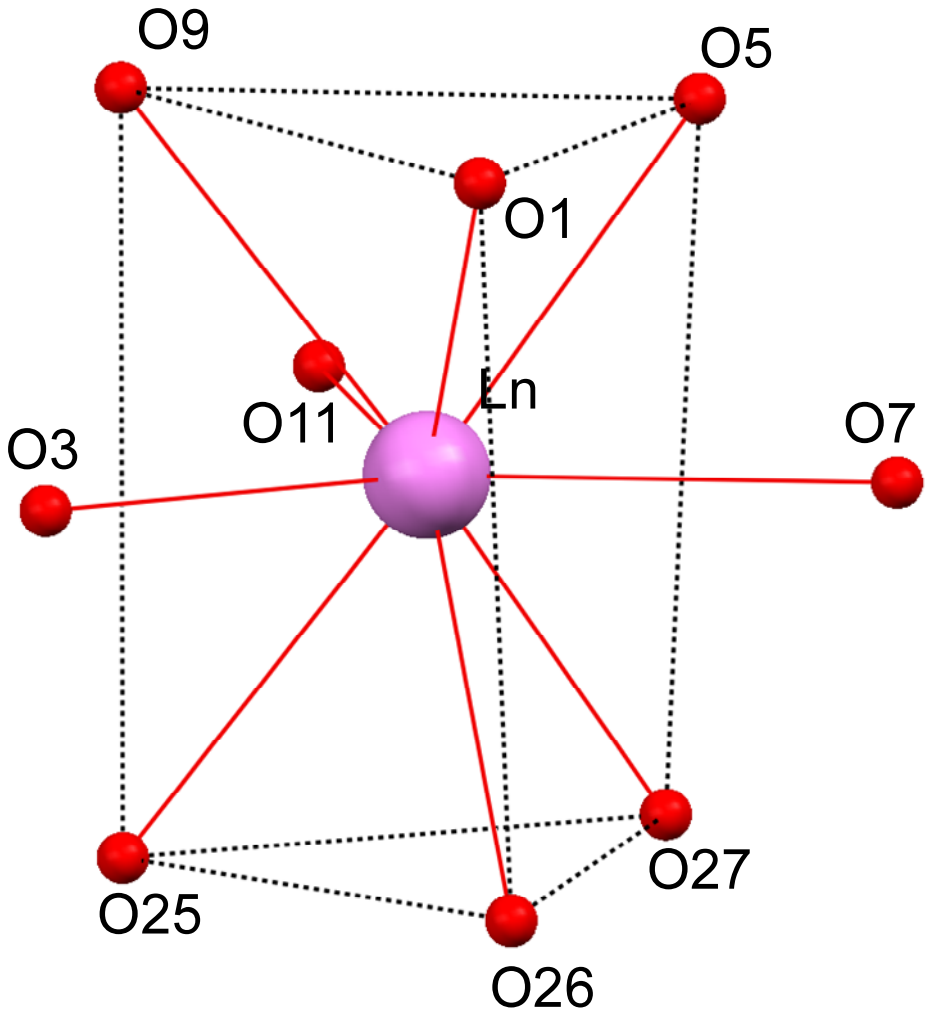


Figure 8. Coordination environment around Ln(Ⅲ) ion.

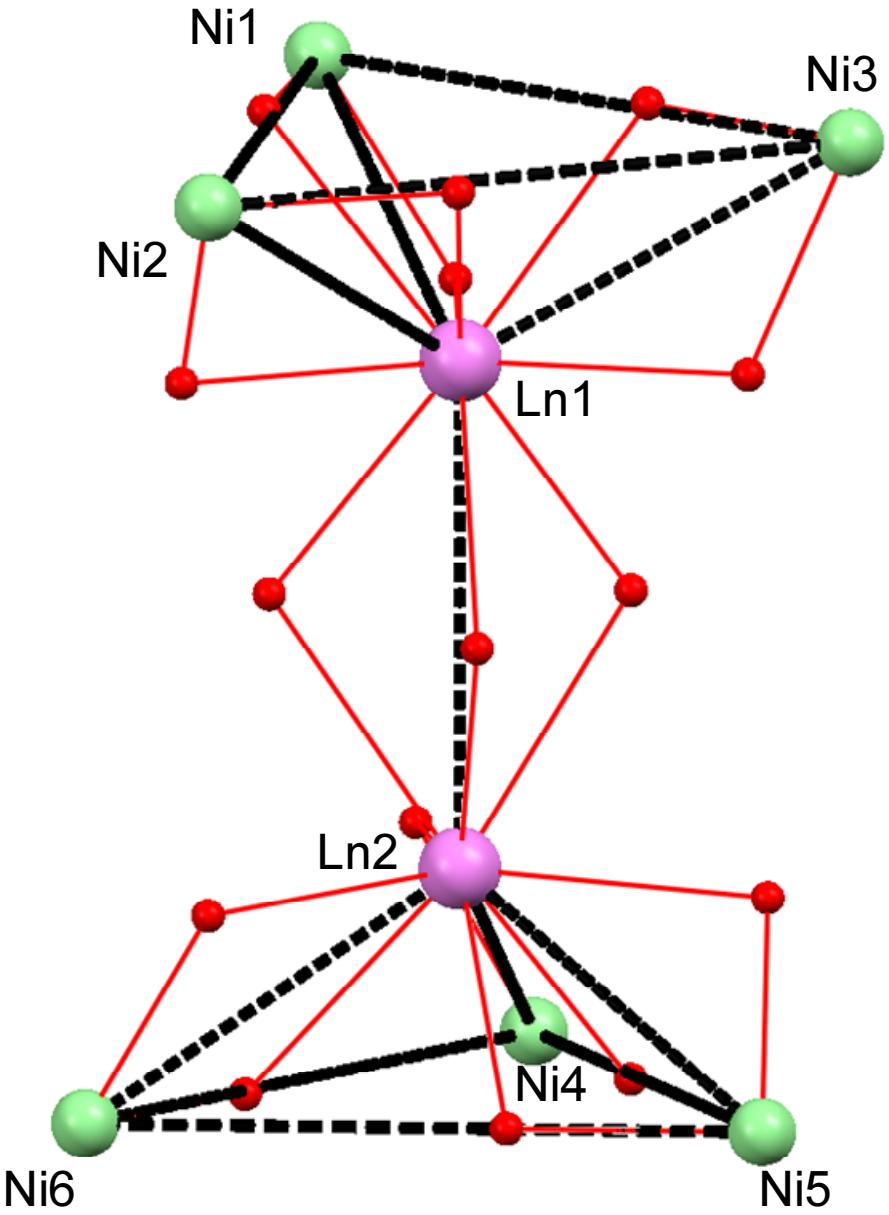


Figure 9. Metal framework of the octahedral cluster cation $[Ln_2Ni_6]$.

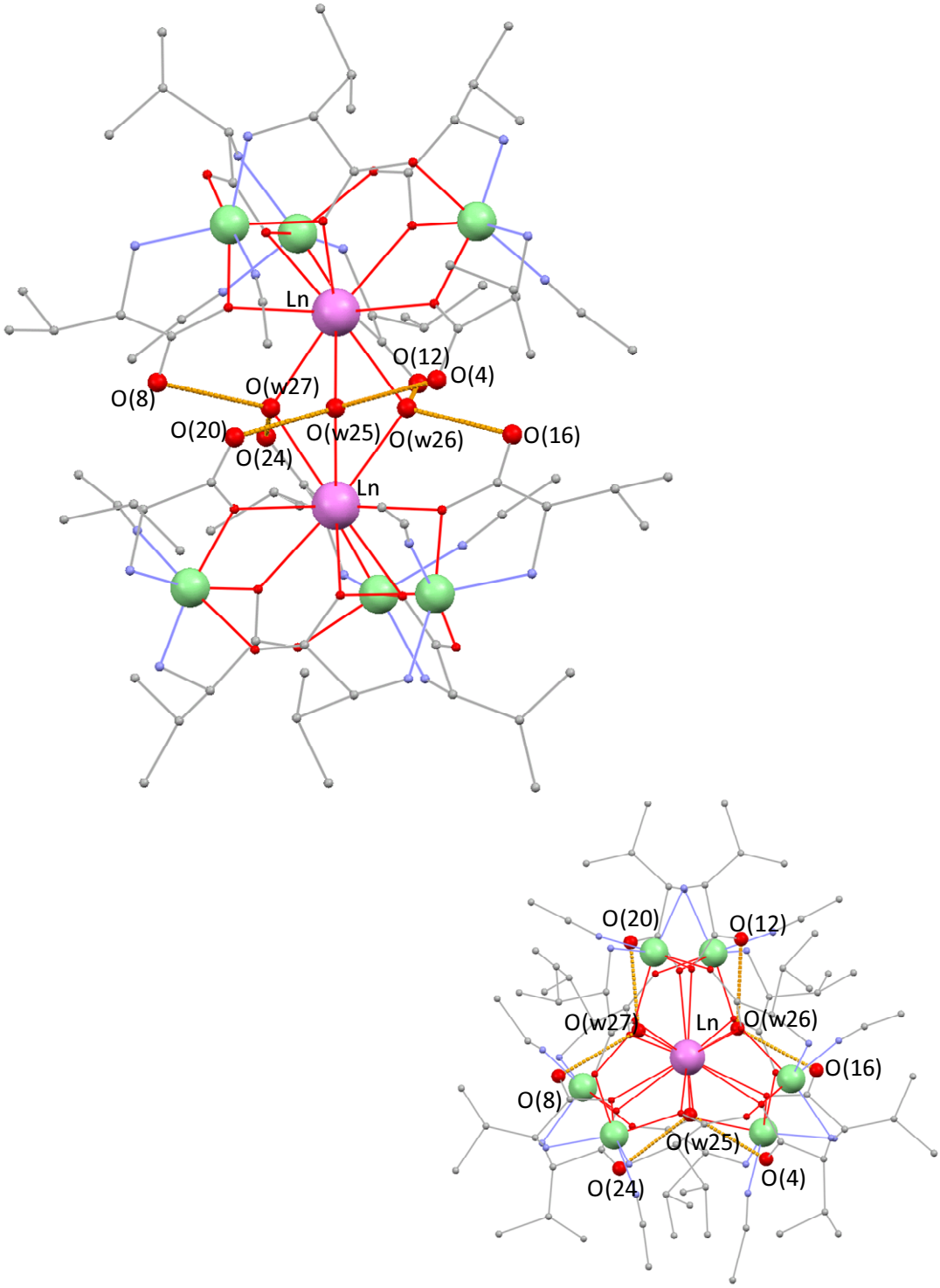


Figure 10. The intramolecular hydrogen bonds between the central water ligands and carboxylate moieties in $[Ln\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6]^{6+}$ (Ln=Ce(**1**), Pr(**2**)).

Table 3. Hydrogen bond distances for the cluster cation $[Ln_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6]^{6+}$ (Ln=Ce(**1**), Pr(**2**)).

	Ce_2Ni_6-cluster	Pr_2Ni_6-cluster
O(w25)-O(4)	2.587	2.574
O(w25)-O(20)	2.608	2.630
O(w26)-O(8)	2.614	2.592
O(w26)-O(16)	2.611	2.602
O(w27)-O(12)	2.686	2.650
O(w27)-O(24)	2.602	2.575
Average	2.618	2.604

Table 4.

Crystal data for TEA[$Gd_2\{Ni(val)_2\}_6(OH_2)_3(CH_3CN)_6$][$Gd(NO_3)_5$]($ClO_4$)$_5$ ・ 7MeCN ・ $2H_2O$ (compound 3).

Empirical Formula	$Gd_3Ni_6O_{64}N_{31}C_{94}H_{189}Cl_5$
Formula Weight	3779.01
Crystal System	Orthorhombic
Space Group	$P2_12_12_1$
a / Å	22.178(3)
b / Å	22.767(3)
c / Å	31.708(4)
V / Å^3	16010(4)
Z value	4
D_{calcu} / g cm^{-3}	1.568
F(000)	7699.00
μ / mm^{-1}	2.677
Temperature / K	100
R	0.0908
wR2	0.1593
S	1.017

Table 5. Crystal data for TEA[$Gd_2\{Ni(val)_2\}_6(OH_2)_3(NO_3)_3(CH_3CN)_3](ClO_4)_4$ (compound **4**).

Empirical Formula	$Gd_2Ni_6O_{52}N_{19}C_{74}H_{155}Cl_4$
Formula Weight	2951.65
Crystal System	Cubic
Space Group	$P2_13$
a / Å	24.0192(3)
V / Å^3	13857.3(4)
Z value	4
D_{calcu} / g cm^{-3}	1.415
F(000)	6048.00
μ (Mo-Kα) / cm^{-1}	19.00
Temperature / ℃	23.0
R	0.041
R_w	0.055
S	1.15

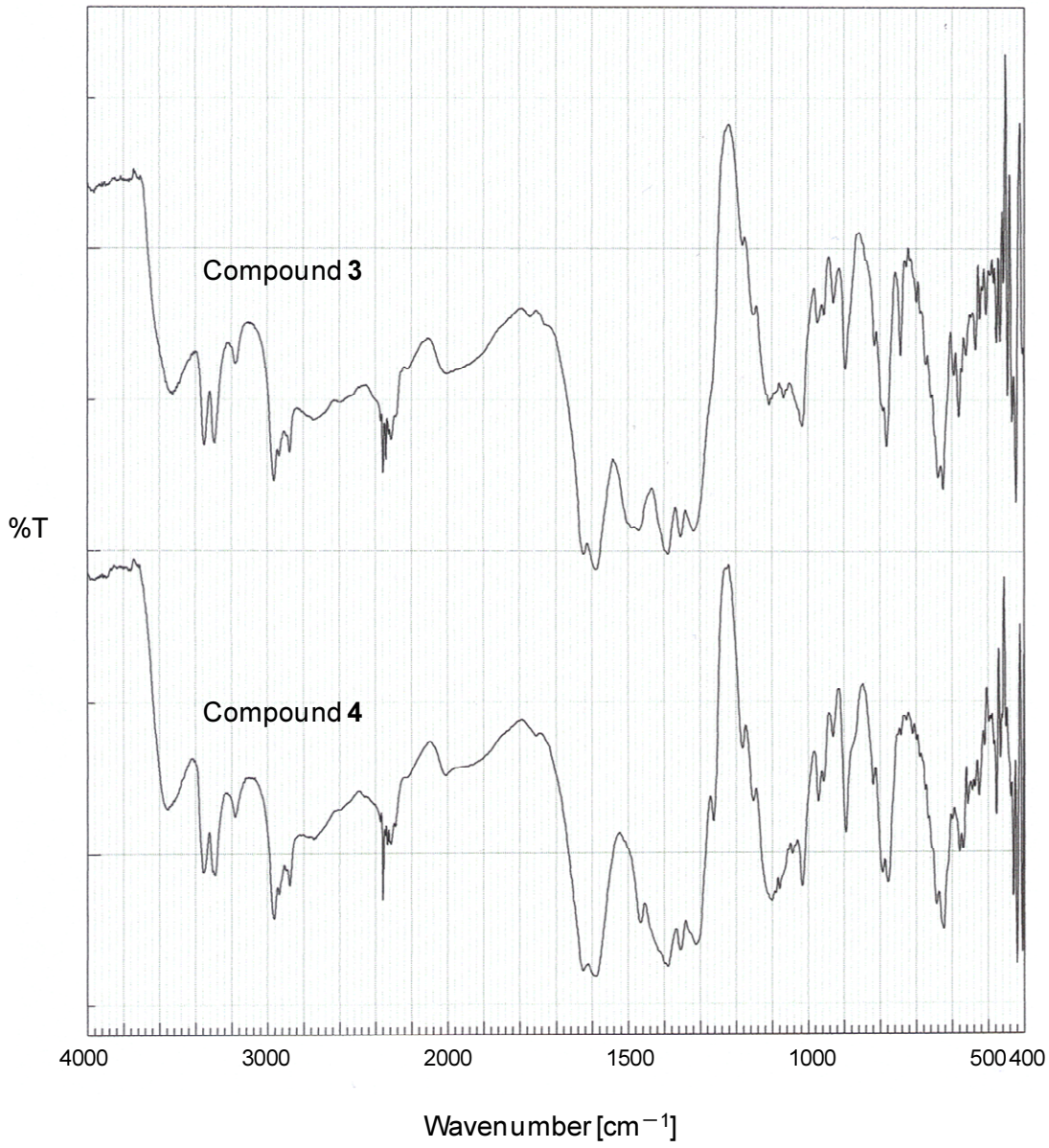


Figure 11. IR spectra of compounds 3 and 4.

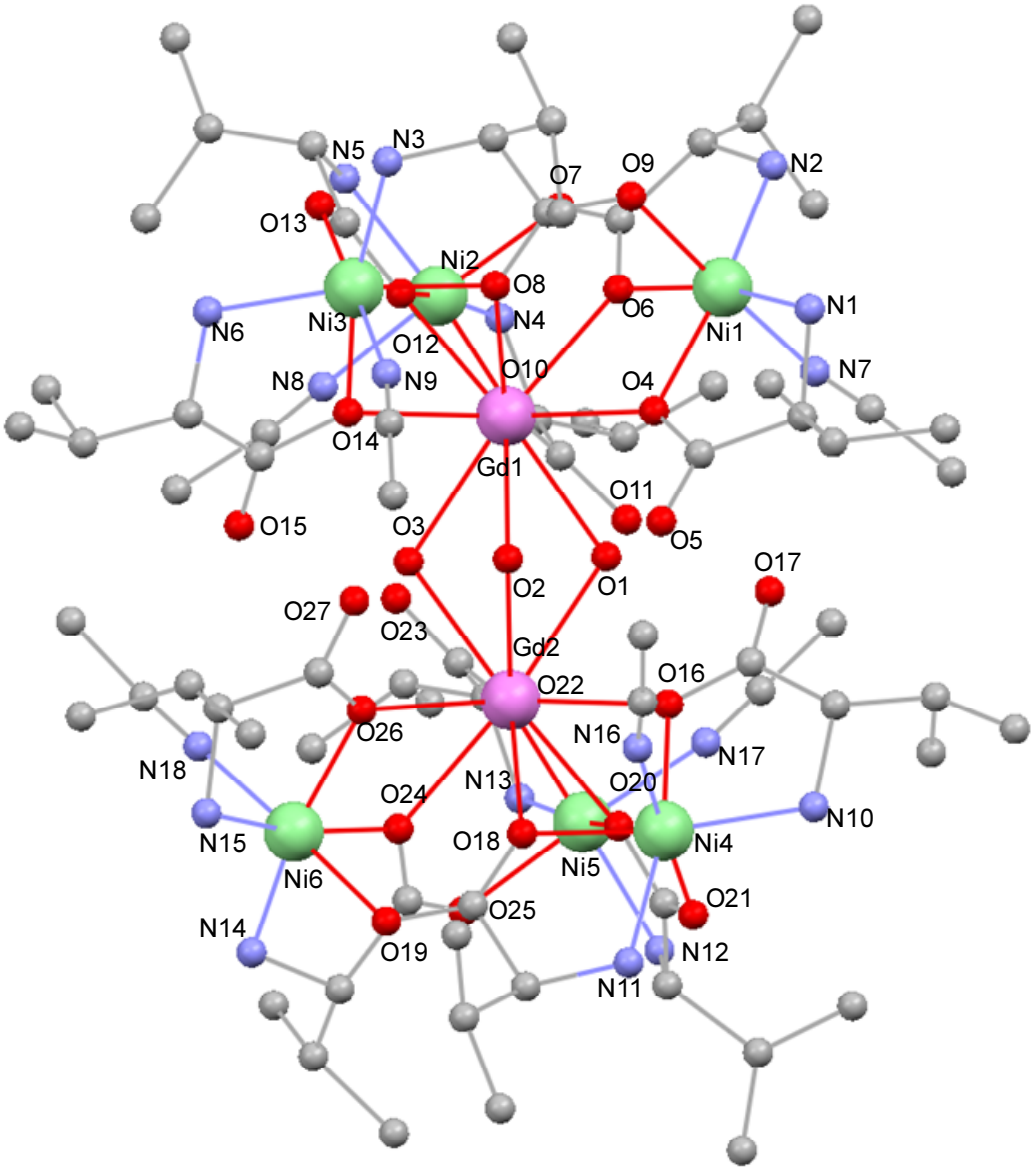


Figure 12. Structure and atomic labels of cluster cation of compound 3, $[Gd_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6]^{6+}$. Hydrogen atoms are omitted for clarity.

Table 6. Selected interatomic distances (Å), including intermetallic separations, and angles (°) in compound TEA[Gd_2{$Ni(val)_2$}$_6(OH_2)_3(CH_3CN)_6$][$Gd(NO_3)_5$]$(ClO_4)_5$ · 7MeCN · $2H_2O$ (3).

Gd1–O1	2491(11)	Ni3－O8	2.022(11)
Gd1－O2	2.502(13)	Ni3－O13	2.095(13)
Gd1－O3	2.528(10)	Ni3–O14	2.047(11)
Gd1－O4	2.447(12)	Ni3–N3	2.039(14)
Gd1－O6	2.443(12)	Ni3–N6	2.051(14)
Gd1－O8	2.437(12)	Ni3–N9	2.093(16)
Gd1－O10	2.431(11)	Ni4–O16	2.045(11)
Gd1－O12	2.416(11)	Ni4–O18	2.025(11)
Gd1－O14	2.430(12)	Ni4–O21	2.112(12)
Gd1⋯Ni1	3.513(2)	Ni4–N10	2.094(14)
Gd1⋯Ni2	3.513(3)	Ni4–N11	2.070(13)
Gd1⋯Ni3	3.522(2)	Ni4–N16	2.109(15)
Gd2–O1	2.473(10)	Ni5–O20	2.049(11)
Gd2–O2	2.505(11)	Ni5–O22	2.016(11)
Gd2–O3	2.472(10)	Ni5–O25	2.084(11)
Gd2–O16	2.450(11)	Ni5–N12	2.042(15)
Gd2–O18	2.468(11)	Ni5–N13	2.057(13)
Gd2–O20	2.474(13)	Ni5–N17	2.074(17)
Gd2–O22	2.482(11)	Ni6–O19	2.110(12)
Gd2–O24	2.485(11)	Ni6–O24	2.034(11)
Gd2–O26	2.422(11)	Ni6–O26	2.039(11)
Gd2⋯Ni4	3.548(2)	Ni6–N14	2.055(12)

Gd2···Ni5	3.541(2)	Ni6–N15	2.106(13)
Gd2···Ni6	3.530(2)	Ni6–N18	2.08(2)
Gd3–O30	2.491(11)	Ni1···Ni2	5.319(4)
Gd3–O31	2.519(12)	Ni1···Ni3	5.297(3)
Gd3–O40	2.504(11)	Ni2···Ni3	5.314(4)
Gd3–O41	2.436(11)	Ni4···Ni5	5.307(3)
Gd3–O50	2.432(11)	Ni4···Ni6	5.329(4)
Gd3–O51	2.511(12)	Ni5···Ni6	5.328(4)
Gd3–O60	2.466(12)	Gd1···Gd2	5.886(2)
Gd3–O61	2.409(11)	Gd1–O1–Gd2	103.0(4)
Gd3–O70	2.427(11)	Gd1–O2–Gd2	101.8(4)
Gd3–O71	2.425(12)	Gd1–O3–Gd2	102.0(4)
Ni1–O4	2.062(10)	Ni1–O4–Gd1	102.0(5)
Ni1–O6	2.015(11)	Ni1–O6–Gd1	103.6(5)
Ni1–O9	2.109(13)	Ni2–O10–Gd1	103.5(5)
Ni1–N1	2.073(14)	Ni2–O12–Gd1	103.8(5)
Ni1–N2	2.061(13)	Ni3–O8–Gd1	103.9(5)
Ni1–N7	2.041(17)	Ni3–O14–Gd1	103.4(5)
Ni2–O7	2.116(11)	Ni4–O16–Gd2	103.9(4)
Ni2–O10	2.032(12)	Ni4–O18–Gd2	103.9(4)
Ni2–O12	2.037(12)	Ni5–O20–Gd2	102.7(5)
Ni2–N4	2.069(16)	Ni5–O22–Gd2	103.4(5)
Ni2–N5	2.050(16)	Ni6–O24–Gd2	102.3(4)
Ni2–N8	2.063(16)	Ni6–O26–Gd2	104.3(5)

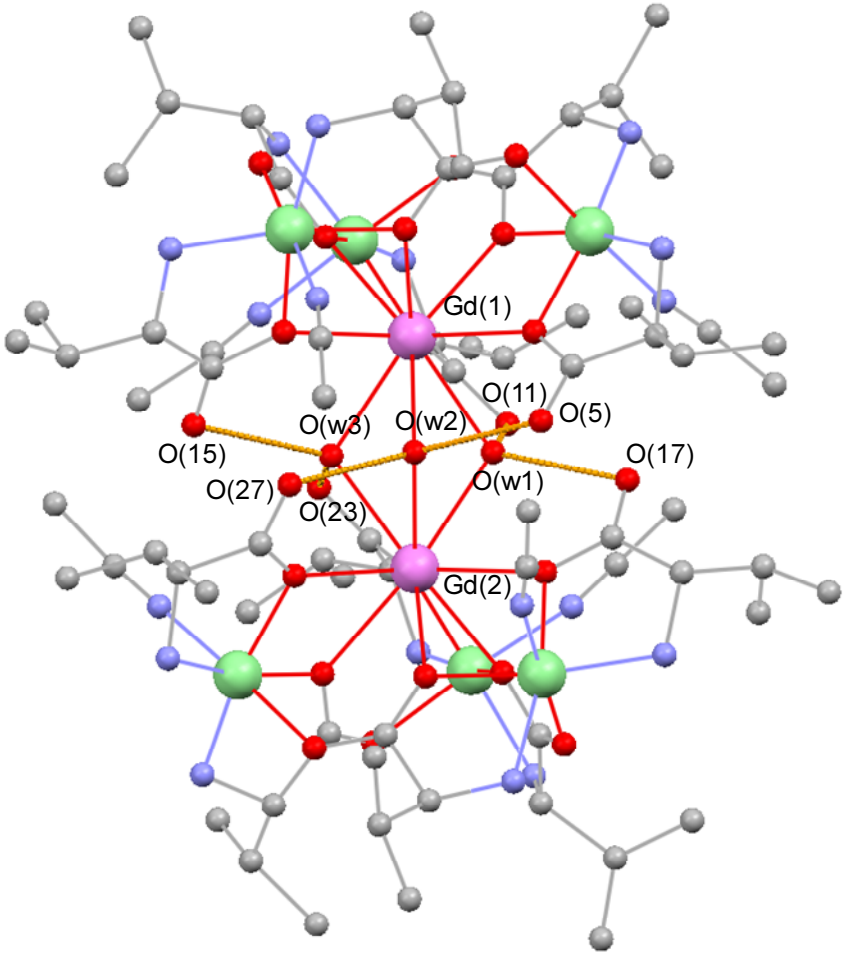


Figure 13. Hydrogen bonding of $[Gd_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6]^{6+}$ (the cluster cation of compound 3). Hydrogen atoms are omitted for clarity.

Table 7. Hydrogen bond distances for the cluster cation of 3, $[Gd_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6]^{3+}$.

O(w1)-O(11)	2.581	O(w2)-O(27)	2.586
O(w1)-O(17)	2.561	O(w3)-O(15)	2.639
O(w2)-O(5)	2.581	O(w3)-O(23)	2.558
Average		2.584	

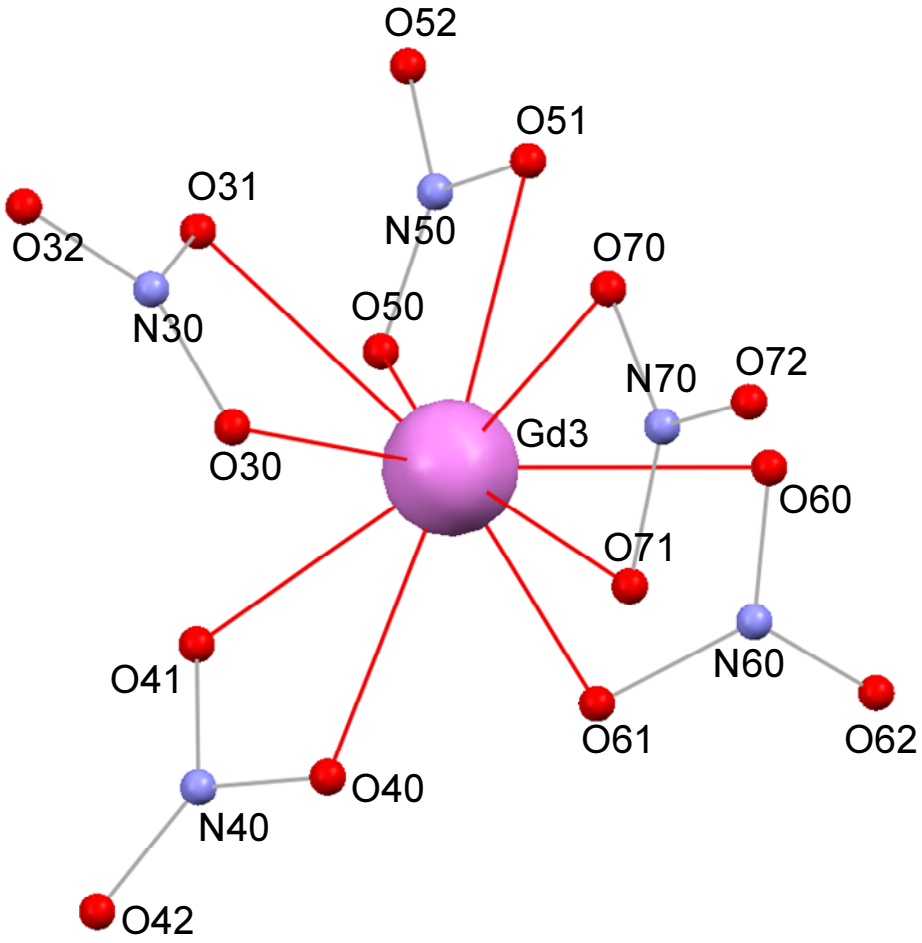


Figure 14. Structure and atomic labels of counter anions $[Gd(NO_3)_5]^{2-}$.

Ball color; lanthanide, oxygen, nitrogen.

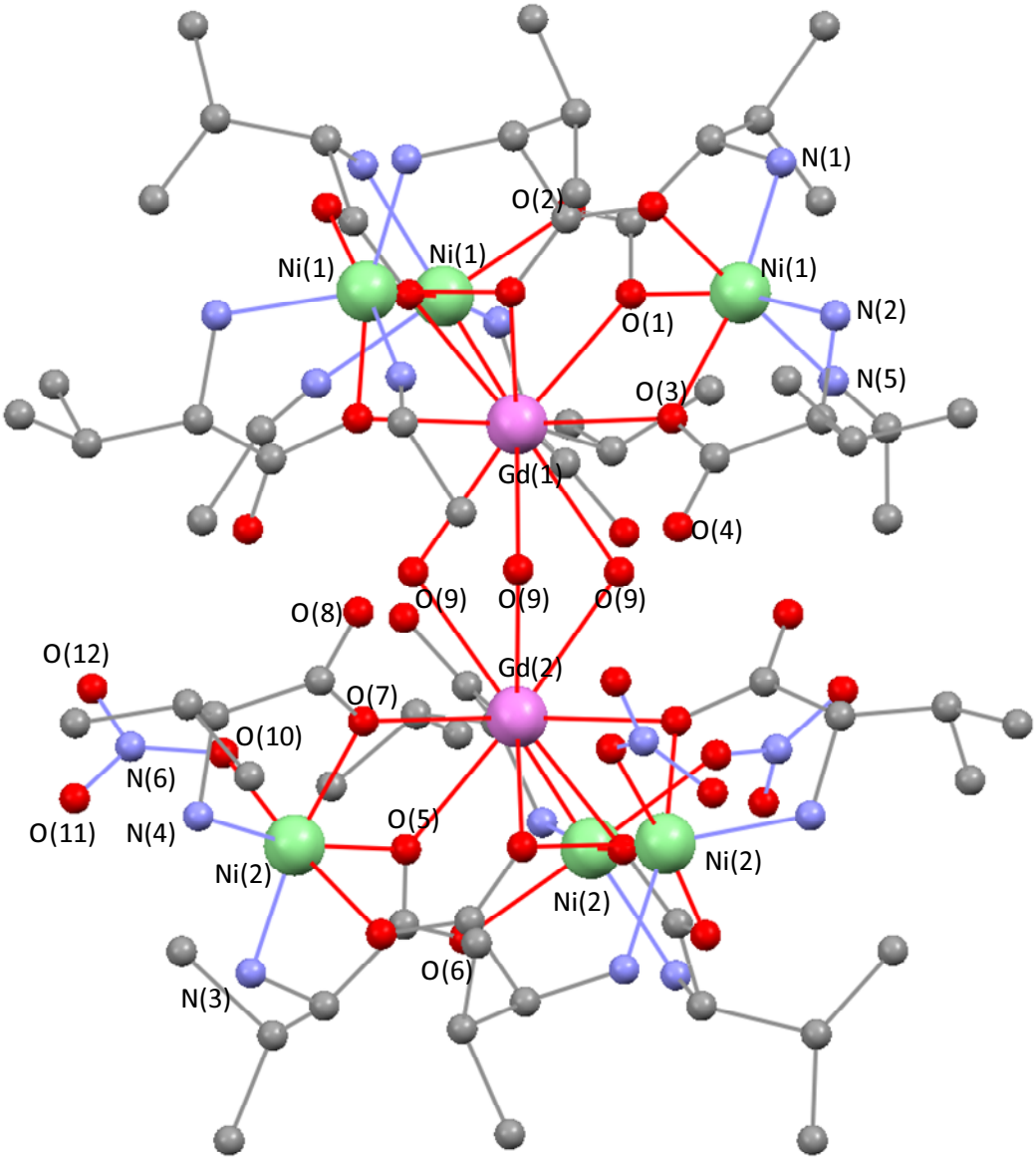


Figure 15.

Atomic labels of $[Gd_2\{Ni(val)_2\}_6(H_2O)_3(NO_3)_3(CH_3CN)_3]^{3+}$ (the cluster cation of compound 4). Hydrogen atoms are omitted for clarity.

Ball color; ●lanthanide, ●nickel, ●oxygen, ●nitrogen, ●carbon.

Table 8. Selected interatomic distances (Å), including intermetallic separations, and angles (°) in compound TEA[$Gd_2\{Ni(val)_2\}_6(OH_2)_3(NO_3)_3(CH_3CN)_3](ClO_4)_4$ (**4**).

Gd1－O1	2.457(6)	Ni2－O5	2.020(6)
Gd1－O3	2.442(5)	Ni2－O6	2.128(7)
Gd1－O9	2.542(5)	Ni2－O7	2.029(6)
Gd1···Ni1	3.530(1)	Ni2－O10	2.103(7)
Gd2－O5	2.446(6)	Ni2－N3	2.047(9)
Gd2－O7	2.431(5)	Ni2－N4	2.020(8)
Gd2－O9	2.532(6)	Ni1···Ni1$^{2)}$	5.304(2)
Gd···Ni2	3.503(1)	Ni2···Ni2$^{2)}$	5.275(2)
Ni1－O1	2.016(6)	Gd1···Gd2	3.937(1)
Ni1－O2	2.098(7)	Gd1－O9－Gd2	101.8(2)
Ni1－O3	2.043(6)	Ni1－O1－Gd1	103.8(2)
Ni1－N1	2.069(8)	Ni1－O3－Gd1	103.4(2)
Ni1－N2	2.066(9)	Ni2－O5－Gd2	102.9(2)
Ni1－N5	2.12(1)	Ni2－O7－Gd2	103.2(2)

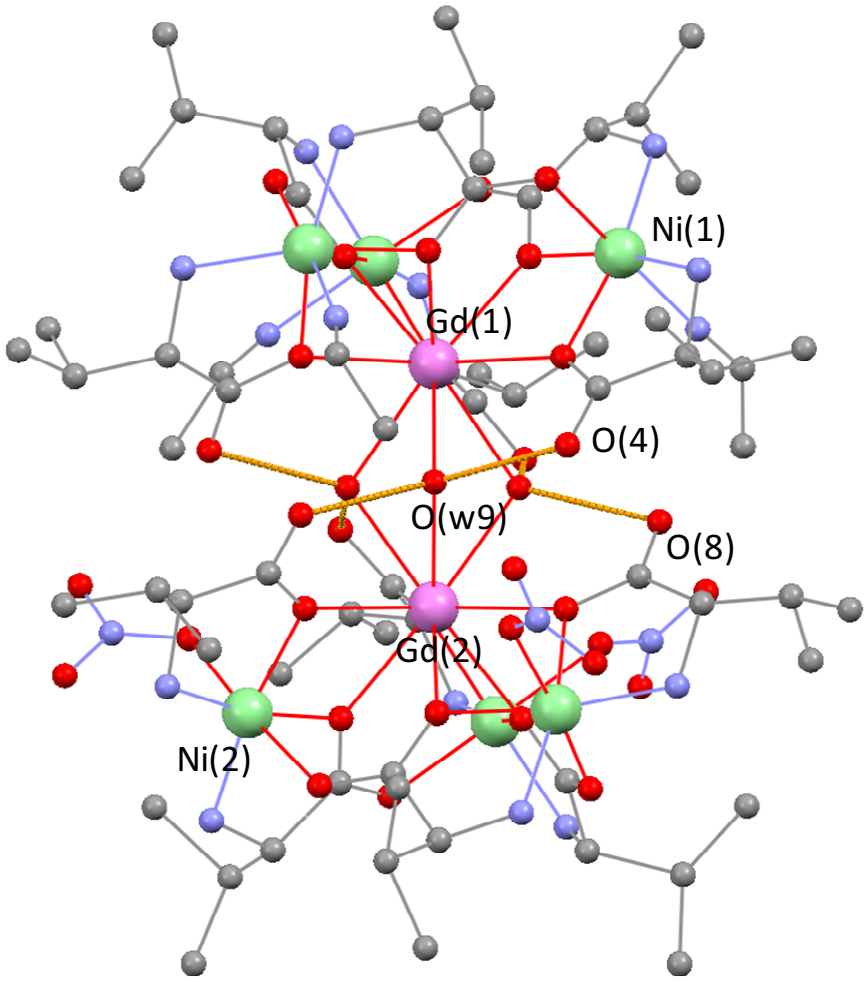


Figure 16. Hydrogen bonding of $[Gd_2\{Ni(val)_2\}_6(H_2O)_3(NO_3)_3(CH_3CN)_3]^{3+}$ (the cluster cation of **4**). Hydrogen atoms are omitted for clarity.

Table 9. Hydrogen bond distances for the cluster cation of **4**, $[Gd_2\{Ni(val)_2\}_6(H_2O)_3(NO_3)_3(CH_3CN)_3]^{3+}$.

O(w9)-O(4)	2.587
O(w9)-O(8)	2.619
Average	2.603

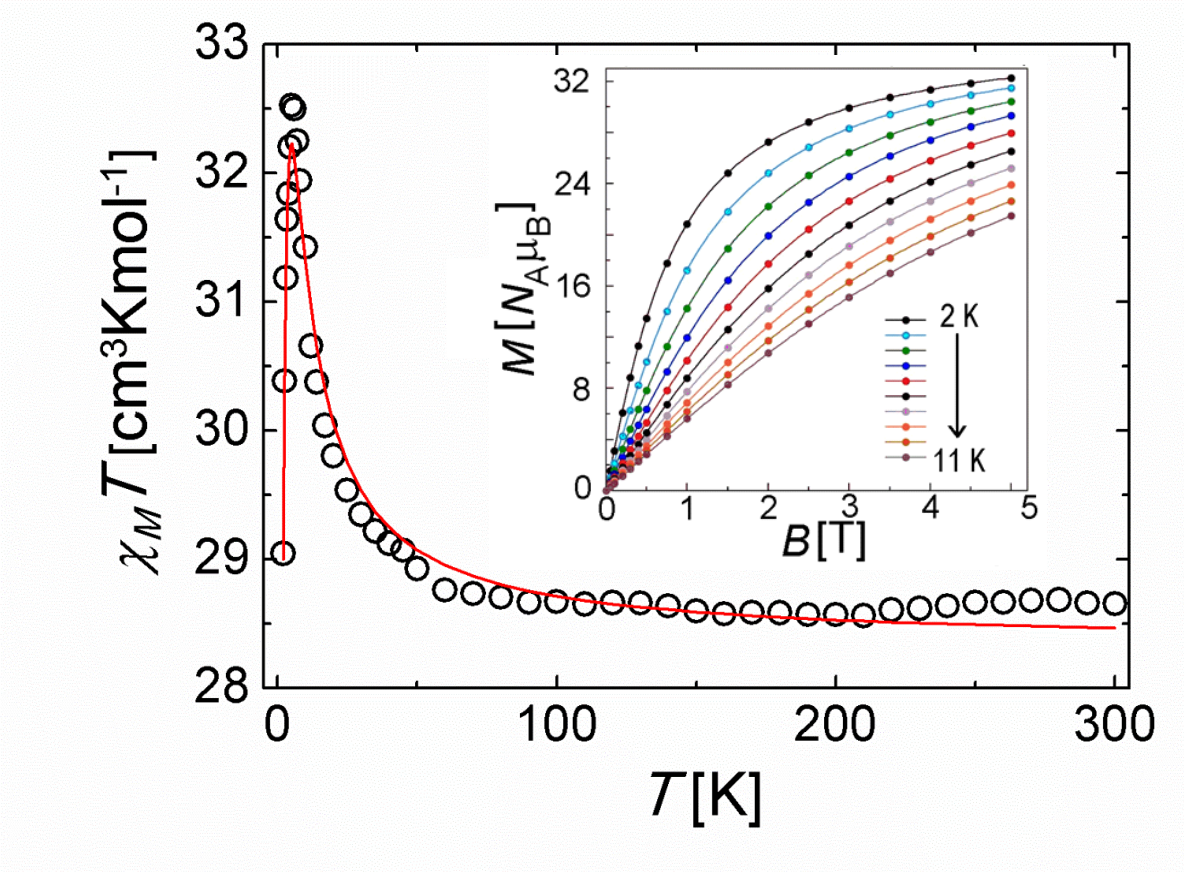


Figure 17. Plot of $\chi_M T$ versus T for compound TEA[Gd_2{$Ni(val)_2$}$_6(H_2O)_3(CH_3CN)_6$][$Gd(NO_3)_5$]$(ClO_4)_5$ (**3**). The red solid line is the best fit to the data above 2 K. The inset shows M (reduced magnetization) versus B (magnetic field) plots at different constant temperatures in the 2-11 K range (the solid lines are guides for the eye).

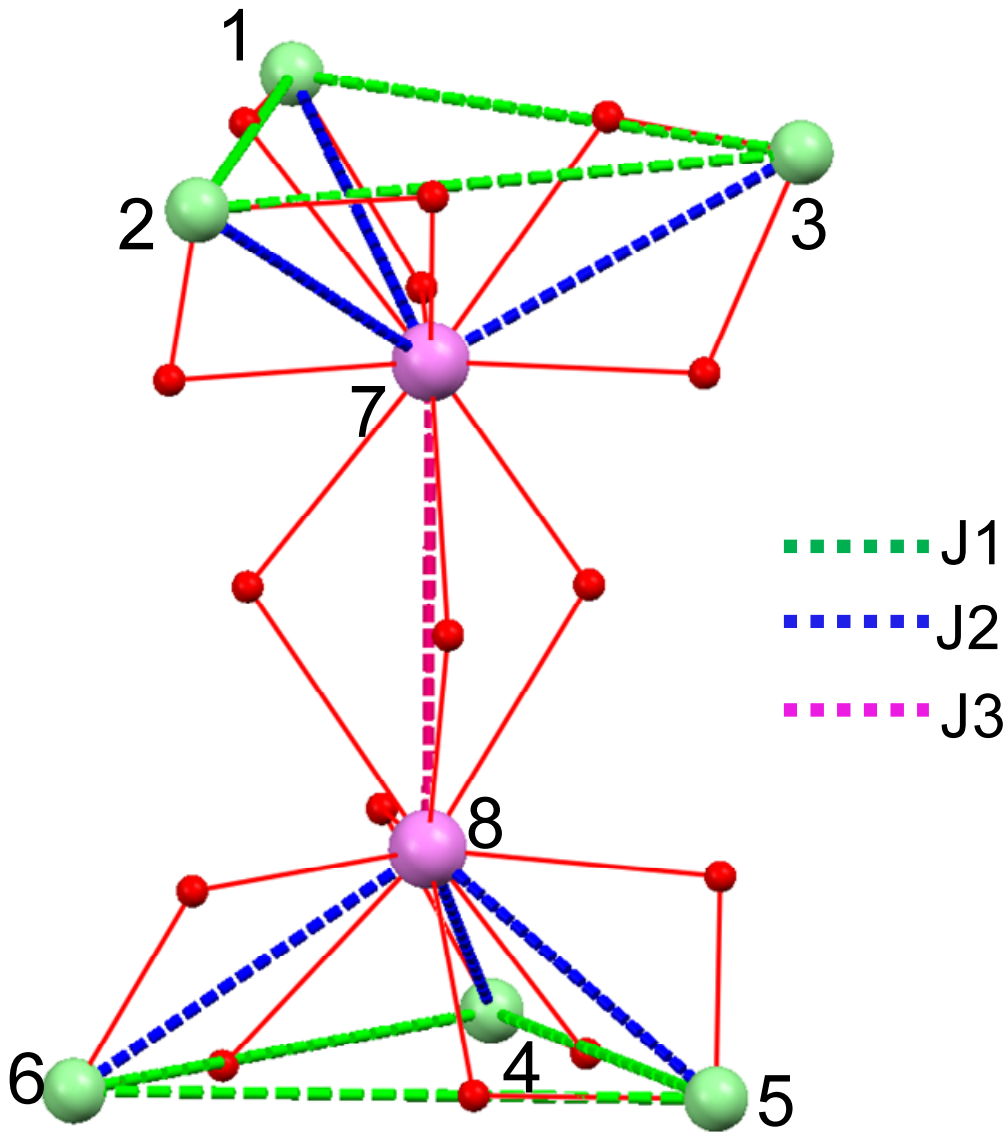


Figure 18. The spin coupling scheme and labels used in Equation (1).

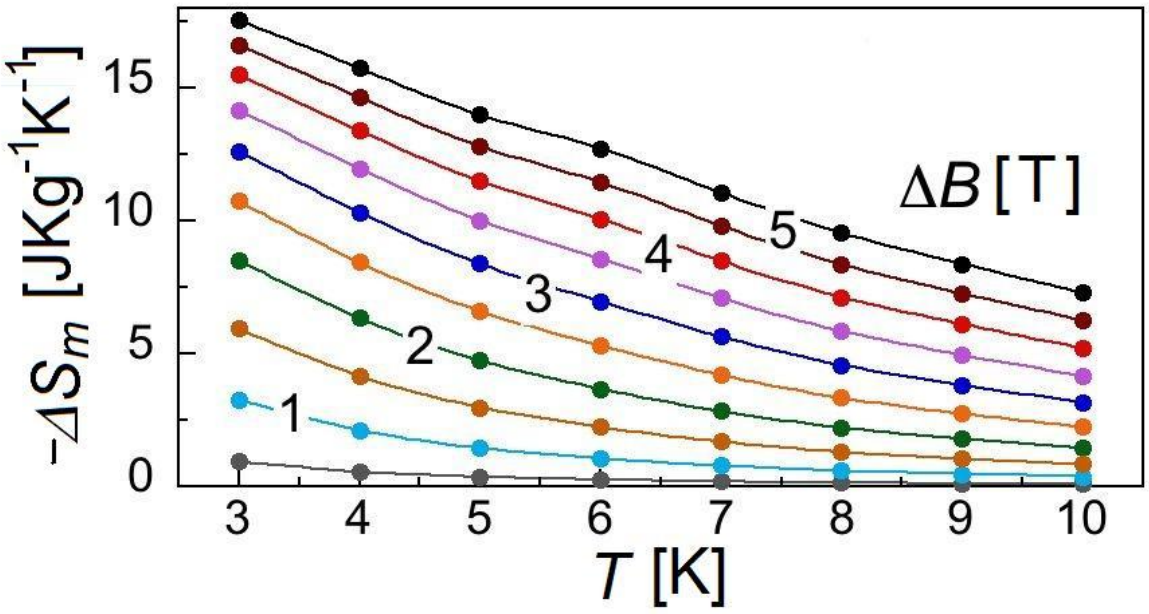


Figure 19. Plot of $-\Delta S_m$ versus T for compound $TEA[Gd_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6][Gd(NO_3)_5](ClO_4)_5$ (3) for various field increases, ΔB, ranging from 0.5 to 5 T.

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Appendix

Structure Factor Table for

$[Ce_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6][Ce(NO_3)_6]_2 \cdot n H_2O$ (**1**)

Table 1. Atomic coordinates and U_{eq}

atom	x	y	z	U_{eq}
Ce(1)	0.66185(5)	0.45021(4)	0.11884(3)	0.0608(3)
Ce(2)	0.82825(5)	0.51140(4)	0.11184(3)	0.0623(3)
Ce(3)	0.61667(6)	0.25311(5)	-0.16164(3)	0.0831(4)
Ce(4)	0.61152(7)	0.22663(5)	0.35854(4)	0.0946(4)
Ni(1)	0.5944(1)	0.38414(9)	0.02686(7)	0.0815(8)
Ni(2)	0.6348(1)	0.35244(9)	0.20005(7)	0.0707(7)
Ni(3)	0.5353(1)	0.53051(9)	0.14374(7)	0.0725(7)
Ni(4)	0.8853(1)	0.5628(1)	0.01016(8)	0.0997(9)
Ni(5)	0.8641(1)	0.61985(10)	0.17985(9)	0.0861(8)
Ni(6)	0.9577(1)	0.43400(9)	0.13877(7)	0.0719(7)
O(1)	0.6107(6)	0.3686(5)	0.0919(3)	0.080(3)
O(2)	0.5848(6)	0.3170(5)	0.1480(4)	0.091(4)
O(3)	0.6474(5)	0.4483(4)	0.0357(3)	0.068(3)
O(4)	0.6893(6)	0.5174(5)	0.0024(4)	0.092(4)
O(5)	0.5987(5)	0.4225(4)	0.1824(3)	0.066(3)
O(6)	0.5163(6)	0.4722(5)	0.1912(4)	0.085(4)
O(7)	0.7011(5)	0.3705(4)	0.1586(3)	0.070(3)
O(8)	0.7881(5)	0.3404(4)	0.1303(3)	0.070(3)
O(9)	0.5557(5)	0.4740(4)	0.1000(3)	0.067(3)
O(10)	0.5171(6)	0.4228(5)	0.0468(4)	0.090(4)
O(11)	0.6221(5)	0.5277(4)	0.1600(3)	0.069(3)
O(12)	0.6873(5)	0.5591(4)	0.2124(3)	0.073(3)
O(13)	0.8791(6)	0.5885(5)	0.0740(3)	0.082(3)
O(14)	0.9097(6)	0.6465(5)	0.1183(4)	0.094(4)
O(15)	0.8305(5)	0.5028(4)	0.0284(3)	0.070(3)
O(16)	0.7876(6)	0.4297(5)	0.0029(4)	0.096(4)
O(17)	0.8990(6)	0.5493(5)	0.1672(4)	0.092(4)
O(18)	0.9823(6)	0.5001(5)	0.1741(4)	0.090(4)
O(19)	0.7922(5)	0.5975(4)	0.1438(3)	0.070(3)
O(20)	0.7048(5)	0.6235(4)	0.1156(3)	0.072(3)

atom	x	y	z	U_{eq}
O(21)	0.9335(6)	0.4807(5)	0.0897(4)	0.088(4)
O(22)	0.9615(6)	0.5205(5)	0.0277(4)	0.103(4)
O(23)	0.8708(5)	0.4413(4)	0.1608(3)	0.072(3)
O(24)	0.8099(5)	0.4202(4)	0.2170(3)	0.071(3)
O(25)	0.7185(5)	0.5291(4)	0.0852(3)	0.059(3)
O(26)	0.7677(5)	0.4280(4)	0.0886(3)	0.064(3)
O(27)	0.7466(5)	0.4838(4)	0.1685(3)	0.069(3)
O(28)	0.7051(7)	0.2716(6)	-0.2195(5)	0.119(5)
O(29)	0.7277(7)	0.2891(6)	-0.1509(5)	0.127(5)
O(30)	0.790(1)	0.3112(9)	-0.2120(7)	0.190(8)
O(31)	0.6932(8)	0.1723(7)	-0.1602(5)	0.131(5)
O(32)	0.6018(7)	0.1567(6)	-0.1381(4)	0.106(4)
O(33)	0.670(1)	0.0954(10)	-0.1440(8)	0.209(9)
O(34)	0.6056(7)	0.1921(6)	-0.2320(5)	0.125(5)
O(35)	0.5782(6)	0.2725(6)	-0.2422(4)	0.098(4)
O(36)	0.5947(9)	0.2246(7)	-0.3015(6)	0.157(7)
O(37)	0.5145(7)	0.3042(6)	-0.1603(5)	0.118(5)
O(38)	0.5075(7)	0.2221(6)	-0.1686(5)	0.115(5)
O(39)	0.4263(10)	0.2706(8)	-0.1634(6)	0.171(7)
O(40)	0.6255(7)	0.3413(5)	-0.1154(4)	0.111(4)
O(41)	0.6339(6)	0.3512(5)	-0.1842(4)	0.101(4)
O(42)	0.6478(10)	0.4158(8)	-0.1424(6)	0.177(8)
O(43)	0.5596(8)	0.2443(7)	-0.0846(5)	0.138(6)
O(44)	0.6586(8)	0.2361(6)	-0.0806(5)	0.127(5)
O(45)	0.6076(8)	0.2246(7)	-0.0234(5)	0.138(5)
O(46)	0.6114(6)	0.3267(5)	0.3386(4)	0.083(3)
O(47)	0.6042(8)	0.3124(7)	0.4094(5)	0.134(5)
O(48)	0.6197(10)	0.3929(8)	0.3827(7)	0.181(7)
O(49)	0.5002(9)	0.2707(8)	0.3633(6)	0.151(6)
O(50)	0.5031(9)	0.1874(8)	0.3456(6)	0.155(7)
O(51)	0.422(1)	0.2273(8)	0.3516(6)	0.171(7)
O(52)	0.5742(7)	0.2449(6)	0.2768(4)	0.114(5)

atom	x	y	z	U_{eq}
O(53)	0.6065(8)	0.1683(7)	0.2845(5)	0.143(6)
O(54)	0.5831(8)	0.1988(7)	0.2188(5)	0.141(6)
O(55)	0.695(1)	0.1601(10)	0.3558(8)	0.203(9)
O(56)	0.6049(9)	0.1235(8)	0.3701(6)	0.158(7)
O(57)	0.667(2)	0.076(1)	0.355(1)	0.28(1)
O(58)	0.7169(7)	0.2682(6)	0.3671(5)	0.128(5)
O(59)	0.6951(6)	0.2477(5)	0.2989(4)	0.095(4)
O(60)	0.7779(9)	0.2919(8)	0.3132(6)	0.162(7)
O(61)	0.661(1)	0.202(1)	0.4382(8)	0.23(1)
O(62)	0.553(1)	0.1972(10)	0.4277(8)	0.209(9)
O(63)	0.589(3)	0.143(2)	0.476(2)	0.52(2)
O(71)	1.037(2)	0.356(2)	0.405(1)	0.39(2)
O(72)	0.778(3)	0.138(3)	0.486(2)	0.63(2)
O(73)	0.818(2)	0.042(2)	0.342(2)	0.44(2)
O(74)	0.270(2)	0.332(2)	-0.001(2)	0.49(2)
O(75)	0.413(2)	0.351(2)	0.423(2)	0.50(2)
O(76)	0.425(2)	0.384(2)	-0.093(1)	0.39(2)
O(77)	0.885(2)	0.213(2)	0.392(2)	0.52(2)
O(78)	0.376(2)	0.317(2)	0.160(1)	0.44(2)
O(79)	0.930(3)	0.077(2)	0.376(2)	0.57(2)
N(1)	0.5440(7)	0.3181(6)	0.0327(5)	0.082(4)
N(2)	0.5881(7)	0.4182(6)	-0.0352(5)	0.092(5)
N(3)	0.5609(8)	0.3480(7)	0.2403(5)	0.100(5)
N(4)	0.6831(6)	0.2856(5)	0.2063(4)	0.069(4)
N(5)	0.4491(7)	0.5203(6)	0.1203(5)	0.095(5)
N(6)	0.5339(6)	0.5854(5)	0.1925(4)	0.072(4)
N(7)	0.9406(8)	0.6268(8)	0.0060(6)	0.110(6)
N(8)	0.8796(9)	0.5229(7)	-0.0499(5)	0.110(5)
N(9)	0.9411(9)	0.6315(8)	0.2110(6)	0.126(6)
N(10)	0.8154(7)	0.6854(6)	0.1864(4)	0.080(4)
N(11)	1.0387(8)	0.4401(7)	0.1098(5)	0.108(5)
N(12)	0.9639(6)	0.3887(5)	0.1938(4)	0.063(4)

atom	x	y	z	U_{eq}
N(13)	0.6717(8)	0.3432(6)	0.0046(5)	0.087(4)
N(14)	0.6812(6)	0.3868(6)	0.2508(4)	0.074(4)
N(15)	0.5556(8)	0.5858(7)	0.0951(5)	0.095(5)
N(16)	0.8107(9)	0.6082(8)	-0.0050(6)	0.124(7)
N(17)	0.8239(9)	0.5914(8)	0.2330(6)	0.113(7)
N(18)	0.9377(7)	0.3679(6)	0.1020(5)	0.087(5)
N(19)	0.742(1)	0.2884(9)	-0.1936(7)	0.145(8)
N(20)	0.648(1)	0.1413(9)	-0.1493(7)	0.142(7)
N(21)	0.5917(9)	0.2295(8)	-0.2579(6)	0.123(6)
N(22)	0.4820(9)	0.2632(8)	-0.1653(6)	0.113(6)
N(23)	0.624(1)	0.3723(9)	-0.1472(7)	0.140(7)
N(24)	0.603(1)	0.2379(9)	-0.0624(7)	0.137(7)
N(25)	0.613(1)	0.3462(9)	0.3801(7)	0.136(7)
N(26)	0.478(1)	0.230(1)	0.3575(8)	0.170(9)
N(27)	0.5881(10)	0.2013(9)	0.2612(7)	0.133(7)
N(28)	0.661(2)	0.125(2)	0.349(1)	0.26(1)
N(29)	0.7313(10)	0.2702(8)	0.3237(6)	0.125(6)
N(30)	0.604(2)	0.180(1)	0.447(1)	0.24(1)
C(1)	0.5323(9)	0.3067(8)	0.0777(6)	0.092(6)
C(2)	0.5767(9)	0.3310(8)	0.1103(6)	0.090(6)
C(3)	0.525(2)	0.249(1)	0.0925(9)	0.1303
C(4)	0.471(2)	0.234(3)	0.063(2)	0.3076
C(5)	0.579(2)	0.213(2)	0.082(2)	0.2220
C(6)	0.6292(8)	0.4597(7)	-0.0416(5)	0.072(5)
C(7)	0.6559(9)	0.4783(7)	0.0009(5)	0.077(5)
C(8)	0.599(1)	0.503(1)	-0.0681(9)	0.1169
C(9)	0.559(2)	0.539(1)	-0.041(1)	0.1536
C(10)	0.648(2)	0.535(2)	-0.092(1)	0.2004
C(11)	0.520(1)	0.3812(10)	0.2234(7)	0.115(7)
C(12)	0.5454(9)	0.4298(7)	0.1975(5)	0.076(5)
C(13)	0.467(2)	0.402(2)	0.2587(10)	0.1872
C(14)	0.435(2)	0.355(2)	0.280(2)	0.2069

atom	x	y	z	U_{eq}
C(15)	0.504(2)	0.430(2)	0.294(1)	0.1956
C(16)	0.7463(7)	0.2923(6)	0.1883(5)	0.060(4)
C(17)	0.7486(8)	0.3386(7)	0.1552(5)	0.067(5)
C(18)	0.779(1)	0.249(1)	0.174(1)	0.1304
C(19)	0.746(2)	0.221(2)	0.135(1)	0.1520
C(20)	0.789(2)	0.211(2)	0.212(1)	0.2178
C(21)	0.450(1)	0.4713(9)	0.0925(7)	0.112(7)
C(22)	0.5128(8)	0.4553(7)	0.0774(5)	0.075(5)
C(23)	0.401(2)	0.479(1)	0.049(1)	0.1622
C(24)	0.409(2)	0.530(2)	0.023(2)	0.2120
C(25)	0.337(2)	0.475(3)	0.067(2)	0.3391
C(26)	0.5960(8)	0.6042(6)	0.2037(5)	0.067(5)
C(27)	0.6391(9)	0.5587(8)	0.1934(6)	0.086(6)
C(28)	0.605(1)	0.626(2)	0.249(1)	0.1735
C(29)	0.583(2)	0.594(2)	0.289(2)	0.2374
C(30)	0.578(2)	0.681(2)	0.252(2)	0.2056
C(31)	0.952(1)	0.6436(9)	0.0441(7)	0.110(7)
C(32)	0.9113(9)	0.6281(8)	0.0875(6)	0.086(6)
C(33)	0.945(3)	0.709(2)	0.055(1)	0.2453
C(34)	0.888(2)	0.726(3)	0.030(2)	0.3312
C(35)	1.001(2)	0.726(3)	0.028(2)	0.2523
C(36)	0.828(1)	0.4881(9)	-0.0514(7)	0.105(6)
C(37)	0.8160(10)	0.4713(9)	-0.0030(7)	0.099(6)
C(38)	0.828(2)	0.447(1)	-0.0860(10)	0.1351
C(39)	0.883(2)	0.411(2)	-0.082(2)	0.2267
C(40)	0.810(2)	0.451(2)	-0.135(1)	0.2523
C(41)	0.985(1)	0.5901(9)	0.1984(6)	0.100(6)
C(42)	0.955(1)	0.5436(9)	0.1812(6)	0.099(6)
C(43)	1.027(1)	0.574(1)	0.2398(8)	0.1238
C(44)	0.995(2)	0.555(1)	0.282(1)	0.1505
C(45)	1.069(2)	0.619(1)	0.251(1)	0.1499
C(46)	0.7539(8)	0.6810(7)	0.1681(5)	0.067(4)

atom	x	y	z	U_{eq}
C(47)	0.7489(8)	0.6311(6)	0.1378(5)	0.063(4)
C(48)	0.726(1)	0.7250(9)	0.1476(7)	0.0877
C(49)	0.763(2)	0.740(1)	0.1065(8)	0.1357
C(50)	0.721(2)	0.772(1)	0.1792(9)	0.1262
C(51)	1.036(1)	0.4732(9)	0.0681(7)	0.110(7)
C(52)	0.9747(9)	0.4932(8)	0.0614(6)	0.088(6)
C(53)	1.070(2)	0.451(2)	0.030(1)	0.1796
C(54)	1.045(3)	0.399(2)	0.012(2)	0.2663
C(55)	1.139(2)	0.450(3)	0.028(3)	0.3350
C(56)	0.9074(8)	0.3750(7)	0.2102(5)	0.067(4)
C(57)	0.8600(8)	0.4150(7)	0.1962(5)	0.076(5)
C(58)	0.899(1)	0.360(1)	0.2573(7)	0.1040
C(59)	0.918(2)	0.406(1)	0.288(1)	0.1232
C(60)	0.936(2)	0.312(1)	0.268(1)	0.1426
C(61)	0.712(1)	0.3272(9)	-0.0106(7)	0.100(6)
C(62)	0.758(1)	0.308(1)	-0.0356(8)	0.134(9)
C(63)	0.7059(9)	0.3993(8)	0.2823(6)	0.091(6)
C(64)	0.741(1)	0.416(1)	0.3201(9)	0.142(9)
C(65)	0.567(1)	0.617(1)	0.0739(7)	0.118(8)
C(66)	0.585(2)	0.664(1)	0.047(1)	0.19(1)
C(67)	0.778(1)	0.6335(9)	-0.0199(7)	0.108(7)
C(68)	0.737(1)	0.681(1)	-0.0337(9)	0.16(1)
C(69)	0.803(1)	0.584(1)	0.2502(8)	0.113(8)
C(70)	0.790(3)	0.554(2)	0.297(2)	0.38(2)
C(71)	0.9220(9)	0.3320(8)	0.0862(6)	0.091(6)
C(72)	0.908(1)	0.283(1)	0.0659(8)	0.148(9)
H(1)	0.7156	0.5300	0.0538	0.0686
H(2)	0.7035	0.5613	0.0971	0.0686
H(3)	0.7836	0.3971	0.1028	0.0762
H(4)	0.7676	0.4226	0.0575	0.0762
H(5)	0.7337	0.5136	0.1863	0.0815
H(6)	0.7611	0.4581	0.1886	0.0815

atom	x	y	z	U_{eq}
H(7)	0.5068	0.3219	0.0167	0.0967
H(8)	0.5651	0.2891	0.0195	0.0967
H(9)	0.5918	0.3915	-0.0578	0.1103
H(10)	0.5466	0.4318	-0.0388	0.1103
H(11)	0.5449	0.3125	0.2410	0.1143
H(12)	0.5697	0.3574	0.2703	0.1143
H(13)	0.6844	0.2758	0.2370	0.0813
H(14)	0.6630	0.2583	0.1901	0.0813
H(15)	0.4200	0.5176	0.1446	0.1157
H(16)	0.4358	0.5492	0.1022	0.1157
H(17)	0.5095	0.6154	0.1835	0.0843
H(18)	0.5158	0.5723	0.2194	0.0843
H(19)	0.9754	0.6188	-0.0106	0.1185
H(20)	0.9191	0.6545	-0.0098	0.1185
H(21)	0.8785	0.5472	-0.0738	0.1282
H(22)	0.9154	0.5018	-0.0534	0.1282
H(23)	0.9576	0.6663	0.2027	0.1433
H(24)	0.9361	0.6327	0.2425	0.1433
H(25)	0.8137	0.6945	0.2164	0.0910
H(26)	0.8358	0.7125	0.1700	0.0910
H(27)	1.0674	0.4548	0.1300	0.1264
H(28)	1.0532	0.4065	0.1009	0.1264
H(29)	0.9875	0.3575	0.1874	0.0783
H(30)	0.9860	0.4069	0.2172	0.0783
H(31)	0.4945	0.3236	0.0836	0.1068
H(32)	0.5097	0.2478	0.1243	0.1525
H(33)	0.4347	0.2553	0.0688	0.3698
H(34)	0.4797	0.2351	0.0333	0.3698
H(35)	0.4564	0.1979	0.0702	0.3698
H(36)	0.5646	0.1783	0.0897	0.2218
H(37)	0.5867	0.2173	0.0539	0.2218
H(38)	0.6076	0.2233	0.1029	0.2218

atom	x	y	z	U_{eq}
H(39)	0.6617	0.4456	-0.0597	0.0880
H(40)	0.5750	0.4897	-0.0897	0.1444
H(41)	0.5819	0.5580	-0.0174	0.1750
H(42)	0.5401	0.5654	-0.0583	0.1750
H(43)	0.5283	0.5203	-0.0250	0.1750
H(44)	0.6731	0.5150	-0.1074	0.2143
H(45)	0.6297	0.5622	-0.1090	0.2143
H(46)	0.6717	0.5545	-0.0683	0.2143
H(47)	0.4970	0.3601	0.2022	0.1435
H(48)	0.4384	0.4295	0.2481	0.2452
H(49)	0.4171	0.3632	0.3058	0.2291
H(50)	0.4142	0.3402	0.2581	0.2291
H(51)	0.4712	0.3320	0.2870	0.2291
H(52)	0.5401	0.4074	0.3029	0.2012
H(53)	0.5249	0.4623	0.2846	0.2012
H(54)	0.4862	0.4382	0.3223	0.2012
H(55)	0.7713	0.3025	0.2129	0.0668
H(56)	0.8154	0.2545	0.1585	0.1653
H(57)	0.7013	0.2109	0.1422	0.1670
H(58)	0.7350	0.2454	0.1079	0.1670
H(59)	0.7602	0.1909	0.1204	0.1670
H(60)	0.7442	0.1978	0.2190	0.2160
H(61)	0.8018	0.1754	0.1970	0.2160
H(62)	0.8067	0.2210	0.2307	0.2160
H(63)	0.4304	0.4428	0.1105	0.1204
H(64)	0.4070	0.4504	0.0287	0.1761
H(65)	0.4446	0.5330	0.0096	0.2425
H(66)	0.3765	0.5298	-0.0011	0.2425
H(67)	0.3983	0.5585	0.0415	0.2425
H(68)	0.3330	0.5000	0.0913	0.2726
H(69)	0.3086	0.4784	0.0466	0.2726
H(70)	0.3336	0.4405	0.0823	0.2726

atom	x	y	z	U_{eq}
H(71)	0.6061	0.6330	0.1836	0.0789
H(72)	0.6459	0.6302	0.2544	0.1815
H(73)	0.5868	0.6063	0.3148	0.2204
H(74)	0.5375	0.5855	0.2829	0.2204
H(75)	0.5990	0.5573	0.2860	0.2204
H(76)	0.5763	0.6926	0.2799	0.2159
H(77)	0.5914	0.7012	0.2300	0.2159
H(78)	0.5316	0.6744	0.2434	0.2159
H(79)	0.9950	0.6340	0.0516	0.1341
H(80)	0.9454	0.7240	0.0784	0.2628
H(81)	0.8909	0.7626	0.0163	0.3675
H(82)	0.8938	0.7089	-0.0073	0.3675
H(83)	0.8565	0.7154	0.0360	0.3675
H(84)	1.0389	0.7200	0.0413	0.2566
H(85)	1.0069	0.7115	-0.0040	0.2566
H(86)	1.0036	0.7653	0.0194	0.2566
H(87)	0.7945	0.5109	-0.0599	0.1244
H(88)	0.7981	0.4199	-0.0741	0.1565
H(89)	0.8972	0.4044	-0.0535	0.2412
H(90)	0.8805	0.3789	-0.0987	0.2412
H(91)	0.9177	0.4299	-0.0978	0.2412
H(92)	0.8408	0.4721	-0.1483	0.2614
H(93)	0.8045	0.4205	-0.1485	0.2614
H(94)	0.7736	0.4722	-0.1346	0.2614
H(95)	1.0097	0.6055	0.1755	0.1272
H(96)	1.0538	0.5450	0.2297	0.1451
H(97)	0.9681	0.5822	0.2910	0.1561
H(98)	0.9699	0.5251	0.2740	0.1561
H(99)	1.0210	0.5460	0.3043	0.1561
H(100)	1.0948	0.6114	0.2744	0.1565
H(101)	1.0888	0.6313	0.2258	0.1565
H(102)	1.0420	0.6477	0.2614	0.1565

atom	x	y	z	U_{eq}
H(103)	0.7291	0.6731	0.1933	0.0798
H(104)	0.6859	0.7166	0.1372	0.1014
H(105)	0.8038	0.7493	0.1174	0.1544
H(106)	0.7667	0.7125	0.0871	0.1544
H(107)	0.7476	0.7703	0.0927	0.1544
H(108)	0.7600	0.7816	0.1892	0.1407
H(109)	0.7024	0.8008	0.1651	0.1407
H(110)	0.6974	0.7624	0.2048	0.1407
H(111)	1.0625	0.5052	0.0745	0.1278
H(112)	1.0600	0.4796	0.0058	0.1951
H(113)	1.0034	0.4033	0.0058	0.2634
H(114)	1.0620	0.3997	-0.0220	0.2634
H(115)	1.0590	0.3746	0.0250	0.2634
H(116)	1.1495	0.4332	0.0555	0.2780
H(117)	1.1533	0.4395	0.0042	0.2780
H(118)	1.1516	0.4884	0.0345	0.2780
H(119)	0.8964	0.3424	0.1952	0.0790
H(120)	0.8572	0.3546	0.2642	0.1103
H(121)	0.9614	0.4132	0.2826	0.1360
H(122)	0.8976	0.4374	0.2811	0.1360
H(123)	0.9142	0.3981	0.3183	0.1360
H(124)	0.9327	0.3037	0.2983	0.1719
H(125)	0.9228	0.2850	0.2497	0.1719
H(126)	0.9774	0.3201	0.2611	0.1719
H(127)	0.7896	0.2906	-0.0200	0.1488
H(128)	0.7462	0.2843	-0.0601	0.1488
H(129)	0.7796	0.3366	-0.0527	0.1488
H(130)	0.7584	0.3845	0.3359	0.1482
H(131)	0.7757	0.4362	0.3124	0.1482
H(132)	0.7197	0.4340	0.3431	0.1482
H(133)	0.6179	0.6859	0.0592	0.1897
H(134)	0.5945	0.6596	0.0160	0.1897

atom	x	y	z	U_{eq}
H(135)	0.5510	0.6919	0.0456	0.1897
H(136)	0.7624	0.7107	-0.0420	0.1908
H(137)	0.7156	0.6716	-0.0606	0.1908
H(138)	0.7117	0.6897	-0.0114	0.1908
H(139)	0.7346	0.5603	0.3015	0.3216
H(140)	0.7825	0.5168	0.2966	0.3216
H(141)	0.7974	0.5670	0.3231	0.3216
H(142)	0.8647	0.2729	0.0671	0.1575
H(143)	0.9177	0.2809	0.0343	0.1575
H(144)	0.9283	0.2524	0.0792	0.1575

$$Ueq = \frac{1}{3}\left(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha\right)$$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ce(1)	0.0652(6)	0.0623(6)	0.0549(4)	-0.0042(5)	-0.0004(5)	-0.0024(5)
Ce(2)	0.0625(6)	0.0576(5)	0.0669(5)	0.0005(6)	0.0089(5)	0.0049(5)
Ce(3)	0.0899(8)	0.0782(7)	0.0811(6)	-0.0109(7)	0.0110(6)	0.0053(6)
Ce(4)	0.1019(10)	0.0922(8)	0.0898(7)	0.0032(8)	0.0245(7)	0.0195(6)
Ni(1)	0.108(2)	0.073(2)	0.064(1)	-0.002(2)	-0.017(1)	-0.007(1)
Ni(2)	0.067(2)	0.077(2)	0.068(1)	-0.003(1)	0.004(1)	0.010(1)
Ni(3)	0.074(2)	0.077(1)	0.067(1)	0.000(1)	-0.002(1)	-0.012(1)
Ni(4)	0.102(2)	0.091(2)	0.106(2)	0.016(2)	0.034(2)	0.037(1)
Ni(5)	0.071(2)	0.061(1)	0.126(2)	0.002(1)	-0.024(1)	-0.009(1)
Ni(6)	0.076(2)	0.066(1)	0.075(1)	0.013(1)	0.014(1)	0.010(1)

The general temperature factor expression:

$$\exp\left(-2\pi^2\left(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl\right)\right)$$

Table 3. Bond Lengths (Å)

atom	atom	distance	atom	atom	distance
Ce(1)	O(1)	2.52(1)	Ce(1)	O(3)	2.519(10)
Ce(1)	O(5)	2.47(1)	Ce(1)	O(7)	2.53(1)
Ce(1)	O(9)	2.51(1)	Ce(1)	O(11)	2.50(1)
Ce(1)	O(25)	2.59(1)	Ce(1)	O(26)	2.59(1)
Ce(1)	O(27)	2.55(1)	Ce(2)	O(13)	2.55(1)
Ce(2)	O(15)	2.516(10)	Ce(2)	O(17)	2.49(1)
Ce(2)	O(19)	2.54(1)	Ce(2)	O(21)	2.56(1)
Ce(2)	O(23)	2.51(1)	Ce(2)	O(25)	2.61(1)
Ce(2)	O(26)	2.62(1)	Ce(2)	O(27)	2.59(1)
Ce(3)	O(28)	2.67(2)	Ce(3)	O(29)	2.66(2)
Ce(3)	O(31)	2.68(2)	Ce(3)	O(32)	2.59(1)
Ce(3)	O(34)	2.64(1)	Ce(3)	O(35)	2.61(1)
Ce(3)	O(37)	2.63(2)	Ce(3)	O(38)	2.57(2)
Ce(3)	O(40)	2.66(1)	Ce(3)	O(41)	2.64(1)
Ce(3)	O(43)	2.65(2)	Ce(3)	O(44)	2.64(1)
Ce(4)	O(46)	2.64(1)	Ce(4)	O(47)	2.68(2)
Ce(4)	O(49)	2.73(2)	Ce(4)	O(50)	2.64(2)
Ce(4)	O(52)	2.63(1)	Ce(4)	O(53)	2.68(2)
Ce(4)	O(55)	2.53(3)	Ce(4)	O(56)	2.67(2)
Ce(4)	O(58)	2.59(2)	Ce(4)	O(59)	2.64(1)
Ce(4)	O(61)	2.71(2)	Ce(4)	O(62)	2.56(2)
Ni(1)	O(1)	2.02(1)	Ni(1)	O(3)	2.04(1)
Ni(1)	O(10)	2.07(1)	Ni(1)	N(1)	2.04(2)
Ni(1)	N(2)	2.06(1)	Ni(1)	N(13)	2.13(2)
Ni(2)	O(2)	2.12(1)	Ni(2)	O(5)	2.04(1)
Ni(2)	O(7)	1.98(1)	Ni(2)	N(3)	2.04(2)
Ni(2)	N(4)	2.03(1)	Ni(2)	N(14)	2.04(1)
Ni(3)	O(6)	2.11(1)	Ni(3)	O(9)	2.01(1)
Ni(3)	O(11)	1.99(1)	Ni(3)	N(5)	2.06(2)
Ni(3)	N(6)	2.03(1)	Ni(3)	N(15)	2.09(2)

atom	atom	distance	atom	atom	distance
Ni(4)	O(13)	2.03(1)	Ni(4)	O(15)	2.04(1)
Ni(4)	O(22)	2.08(1)	Ni(4)	N(7)	2.06(2)
Ni(4)	N(8)	2.08(2)	Ni(4)	N(16)	2.08(2)
Ni(5)	O(14)	2.21(1)	Ni(5)	O(17)	2.01(1)
Ni(5)	O(19)	2.01(1)	Ni(5)	N(9)	1.98(2)
Ni(5)	N(10)	2.01(2)	Ni(5)	N(17)	1.97(2)
Ni(6)	O(18)	2.07(1)	Ni(6)	O(21)	1.97(1)
Ni(6)	O(23)	2.05(1)	Ni(6)	N(11)	2.01(2)
Ni(6)	N(12)	2.02(1)	Ni(6)	N(18)	2.07(2)
O(1)	C(2)	1.35(2)	O(2)	C(2)	1.20(2)
O(3)	C(7)	1.31(2)	O(4)	C(7)	1.25(2)
O(5)	C(12)	1.28(2)	O(6)	C(12)	1.28(2)
O(7)	C(17)	1.34(2)	O(8)	C(17)	1.15(2)
O(9)	C(22)	1.27(2)	O(10)	C(22)	1.24(2)
O(11)	C(27)	1.34(2)	O(12)	C(27)	1.22(2)
O(13)	C(32)	1.31(2)	O(14)	C(32)	1.04(2)
O(15)	C(37)	1.28(2)	O(16)	C(37)	1.26(3)
O(17)	C(42)	1.32(3)	O(18)	C(42)	1.29(3)
O(19)	C(47)	1.31(2)	O(20)	C(47)	1.20(2)
O(21)	C(52)	1.29(2)	O(22)	C(52)	1.27(2)
O(23)	C(57)	1.28(2)	O(24)	C(57)	1.28(2)
O(25)	H(1)	0.946	O(25)	H(2)	0.960
O(26)	H(3)	0.968	O(26)	H(4)	0.945
O(27)	H(5)	0.976	O(27)	H(6)	0.951
O(28)	N(19)	1.22(3)	O(29)	N(19)	1.32(3)
O(30)	N(19)	1.33(3)	O(31)	N(20)	1.32(3)
O(32)	N(20)	1.16(3)	O(33)	N(20)	1.28(3)
O(34)	N(21)	1.27(3)	O(35)	N(21)	1.24(3)
O(36)	N(21)	1.32(3)	O(37)	N(22)	1.29(3)
O(38)	N(22)	1.20(3)	O(39)	N(22)	1.26(3)
O(40)	N(23)	1.24(3)	O(41)	N(23)	1.25(2)
O(42)	N(23)	1.24(3)	O(43)	N(24)	1.18(3)

atom	atom	distance	atom	atom	distance
O(44)	N(24)	1.36(3)	O(45)	N(24)	1.23(3)
O(46)	N(25)	1.34(2)	O(47)	N(25)	1.26(3)
O(48)	N(25)	1.21(3)	O(49)	N(26)	1.17(4)
O(50)	N(26)	1.28(4)	O(51)	N(26)	1.25(4)
O(52)	N(27)	1.25(3)	O(53)	N(27)	1.17(3)
O(54)	N(27)	1.28(3)	O(55)	N(28)	1.20(5)
O(56)	N(28)	1.39(5)	O(57)	N(28)	1.26(5)
O(58)	N(29)	1.34(2)	O(59)	N(29)	1.24(2)
O(60)	N(29)	1.22(3)	O(61)	N(30)	1.42(5)
O(62)	N(30)	1.35(5)	O(63)	N(30)	1.32(7)
N(1)	C(1)	1.41(2)	N(1)	H(7)	0.962
N(1)	H(8)	0.968	N(2)	C(6)	1.42(2)
N(2)	H(9)	0.967	N(2)	H(10)	0.994
N(3)	C(11)	1.35(3)	N(3)	H(11)	0.979
N(3)	H(12)	0.955	N(4)	C(16)	1.52(2)
N(4)	H(13)	0.954	N(4)	H(14)	0.964
N(5)	C(21)	1.51(3)	N(5)	H(15)	0.979
N(5)	H(16)	0.967	N(6)	C(26)	1.50(2)
N(6)	H(17)	0.980	N(6)	H(18)	0.963
N(7)	C(31)	1.25(3)	N(7)	H(19)	0.944
N(7)	H(20)	0.980	N(8)	C(36)	1.45(3)
N(8)	H(21)	0.952	N(8)	H(22)	0.968
N(9)	C(41)	1.49(3)	N(9)	H(23)	0.998
N(9)	H(24)	0.953	N(10)	C(46)	1.48(2)
N(10)	H(25)	0.934	N(10)	H(26)	0.966
N(11)	C(51)	1.51(3)	N(11)	H(27)	0.957
N(11)	H(28)	0.961	N(12)	C(56)	1.40(2)
N(12)	H(29)	0.977	N(12)	H(30)	0.978
N(13)	C(61)	1.09(3)	N(14)	C(63)	1.14(2)
N(15)	C(65)	1.06(3)	N(16)	C(67)	1.08(3)
N(17)	C(69)	0.72(3)	N(18)	C(71)	1.09(3)
C(1)	C(2)	1.52(3)	C(1)	H(31)	0.962

atom	atom	distance	atom	atom	distance
C(1)	C(3)	1.56(4)	C(6)	C(7)	1.49(2)
C(6)	H(39)	0.975	C(6)	C(8)	1.52(3)
C(11)	C(12)	1.58(3)	C(11)	H(47)	0.975
C(11)	C(13)	1.67(4)	C(16)	C(17)	1.55(2)
C(16)	H(55)	0.959	C(16)	C(18)	1.40(3)
C(21)	C(22)	1.52(3)	C(21)	H(63)	1.009
C(21)	C(23)	1.70(4)	C(26)	C(27)	1.54(3)
C(26)	H(71)	0.982	C(26)	C(28)	1.50(4)
C(31)	C(32)	1.64(3)	C(31)	H(79)	1.003
C(31)	C(33)	1.72(5)	C(36)	C(37)	1.54(3)
C(36)	H(87)	0.984	C(36)	C(38)	1.49(4)
C(41)	C(42)	1.46(3)	C(41)	H(95)	0.965
C(41)	C(43)	1.61(3)	C(46)	C(47)	1.58(2)
C(46)	H(103)	0.958	C(46)	C(48)	1.43(3)
C(51)	C(52)	1.48(3)	C(51)	H(111)	1.025
C(51)	C(53)	1.48(5)	C(56)	C(57)	1.53(2)
C(56)	H(119)	0.981	C(56)	C(58)	1.48(3)
C(61)	C(62)	1.37(3)	C(62)	H(127)	0.949
C(62)	H(128)	0.989	C(62)	H(129)	1.016
C(63)	C(64)	1.45(3)	C(64)	H(130)	1.014
C(64)	H(131)	0.951	C(64)	H(132)	0.960
C(65)	C(66)	1.49(4)	C(66)	H(133)	0.985
C(66)	H(134)	0.968	C(66)	H(135)	1.051
C(67)	C(68)	1.57(4)	C(68)	H(136)	0.975
C(68)	H(137)	0.972	C(68)	H(138)	0.909
C(69)	C(70)	1.64(6)	C(70)	H(139)	1.247
C(70)	H(140)	0.965	C(70)	H(141)	0.859
C(71)	C(72)	1.44(4)	C(72)	H(142)	0.992
C(72)	H(143)	0.975	C(72)	H(144)	0.984
C(3)	C(5)	1.54(6)	C(3)	C(4)	1.54(6)
C(8)	C(10)	1.54(5)	C(8)	C(9)	1.54(5)
C(13)	C(15)	1.54(6)	C(13)	C(14)	1.54(6)

atom	atom	distance	atom	atom	distance
C(18)	C(19)	1.54(5)	C(18)	C(20)	1.54(5)
C(23)	C(24)	1.54(6)	C(23)	C(25)	1.54(6)
C(28)	C(29)	1.54(6)	C(28)	C(30)	1.54(6)
C(38)	C(39)	1.54(6)	C(38)	C(40)	1.54(5)
C(43)	C(44)	1.54(4)	C(43)	C(45)	1.54(5)
C(48)	C(49)	1.54(4)	C(48)	C(50)	1.54(4)
C(53)	C(54)	1.54(7)	C(53)	C(55)	1.54(7)
C(58)	C(59)	1.54(4)	C(58)	C(60)	1.54(4)
C(33)	C(34)	1.54(8)	C(33)	C(35)	1.54(8)

Table 4. Bond Angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
O(1)	Ce(1)	O(3)	66.9(3)	O(1)	Ce(1)	O(5)	75.6(3)
O(1)	Ce(1)	O(7)	68.6(4)	O(1)	Ce(1)	O(9)	72.8(4)
O(1)	Ce(1)	O(11)	131.3(4)	O(1)	Ce(1)	O(25)	138.2(3)
O(1)	Ce(1)	O(26)	96.6(4)	O(1)	Ce(1)	O(27)	143.4(4)
O(3)	Ce(1)	O(5)	133.3(3)	O(3)	Ce(1)	O(7)	119.8(3)
O(3)	Ce(1)	O(9)	70.1(3)	O(3)	Ce(1)	O(11)	117.3(3)
O(3)	Ce(1)	O(25)	72.0(3)	O(3)	Ce(1)	O(26)	76.4(3)
O(3)	Ce(1)	O(27)	132.8(3)	O(5)	Ce(1)	O(7)	66.4(3)
O(5)	Ce(1)	O(9)	73.1(3)	O(5)	Ce(1)	O(11)	69.3(3)
O(5)	Ce(1)	O(25)	143.3(3)	O(5)	Ce(1)	O(26)	136.4(3)
O(5)	Ce(1)	O(27)	93.8(3)	O(7)	Ce(1)	O(9)	129.1(4)
O(7)	Ce(1)	O(11)	122.2(3)	O(7)	Ce(1)	O(25)	130.5(3)
O(7)	Ce(1)	O(26)	70.9(3)	O(7)	Ce(1)	O(27)	75.1(3)
O(9)	Ce(1)	O(11)	65.4(3)	O(9)	Ce(1)	O(25)	100.4(3)
O(9)	Ce(1)	O(26)	146.4(3)	O(9)	Ce(1)	O(27)	138.2(3)
O(11)	Ce(1)	O(25)	75.1(3)	O(11)	Ce(1)	O(26)	132.1(3)
O(11)	Ce(1)	O(27)	72.8(3)	O(25)	Ce(1)	O(26)	66.0(3)
O(25)	Ce(1)	O(27)	66.7(3)	O(26)	Ce(1)	O(27)	66.9(3)
O(13)	Ce(2)	O(15)	67.3(3)	O(13)	Ce(2)	O(17)	73.3(4)
O(13)	Ce(2)	O(19)	68.4(4)	O(13)	Ce(2)	O(21)	73.5(4)
O(13)	Ce(2)	O(23)	130.7(4)	O(13)	Ce(2)	O(25)	98.3(4)
O(13)	Ce(2)	O(26)	138.0(3)	O(13)	Ce(2)	O(27)	144.9(4)
O(15)	Ce(2)	O(17)	133.4(4)	O(15)	Ce(2)	O(19)	117.3(3)
O(15)	Ce(2)	O(21)	72.3(4)	O(15)	Ce(2)	O(23)	120.9(3)
O(15)	Ce(2)	O(25)	74.3(3)	O(15)	Ce(2)	O(26)	71.0(3)
O(15)	Ce(2)	O(27)	130.1(3)	O(17)	Ce(2)	O(19)	66.9(4)
O(17)	Ce(2)	O(21)	73.4(4)	O(17)	Ce(2)	O(23)	69.5(4)
O(17)	Ce(2)	O(25)	136.8(4)	O(17)	Ce(2)	O(26)	145.2(4)
O(17)	Ce(2)	O(27)	96.5(4)	O(19)	Ce(2)	O(21)	130.9(4)
O(19)	Ce(2)	O(23)	121.4(3)	O(19)	Ce(2)	O(25)	70.7(3)

atom	atom	atom	angle	atom	atom	atom	angle
O(19)	Ce(2)	O(26)	130.4(3)	O(19)	Ce(2)	O(27)	76.6(3)
O(21)	Ce(2)	O(23)	65.6(4)	O(21)	Ce(2)	O(25)	146.2(3)
O(21)	Ce(2)	O(26)	98.6(4)	O(21)	Ce(2)	O(27)	136.8(4)
O(23)	Ce(2)	O(25)	131.1(3)	O(23)	Ce(2)	O(26)	76.4(3)
O(23)	Ce(2)	O(27)	71.5(3)	O(25)	Ce(2)	O(26)	65.2(3)
O(25)	Ce(2)	O(27)	65.9(3)	O(26)	Ce(2)	O(27)	65.8(3)
O(28)	Ce(3)	O(29)	48.0(5)	O(28)	Ce(3)	O(31)	71.4(5)
O(28)	Ce(3)	O(32)	116.2(5)	O(28)	Ce(3)	O(34)	69.7(5)
O(28)	Ce(3)	O(35)	66.7(4)	O(28)	Ce(3)	O(37)	124.0(5)
O(28)	Ce(3)	O(38)	134.5(4)	O(28)	Ce(3)	O(40)	97.7(5)
O(28)	Ce(3)	O(41)	63.6(5)	O(28)	Ce(3)	O(43)	159.7(5)
O(28)	Ce(3)	O(44)	111.6(5)	O(29)	Ce(3)	O(31)	71.2(5)
O(29)	Ce(3)	O(32)	114.7(5)	O(29)	Ce(3)	O(34)	113.0(5)
O(29)	Ce(3)	O(35)	110.5(4)	O(29)	Ce(3)	O(37)	129.0(5)
O(29)	Ce(3)	O(38)	176.7(5)	O(29)	Ce(3)	O(40)	64.7(5)
O(29)	Ce(3)	O(41)	64.1(5)	O(29)	Ce(3)	O(43)	111.7(5)
O(29)	Ce(3)	O(44)	67.6(5)	O(31)	Ce(3)	O(32)	48.6(5)
O(31)	Ce(3)	O(34)	67.3(5)	O(31)	Ce(3)	O(35)	111.7(4)
O(31)	Ce(3)	O(37)	159.3(5)	O(31)	Ce(3)	O(38)	111.3(5)
O(31)	Ce(3)	O(40)	127.0(5)	O(31)	Ce(3)	O(41)	130.6(5)
O(31)	Ce(3)	O(43)	102.9(5)	O(31)	Ce(3)	O(44)	68.5(5)
O(32)	Ce(3)	O(34)	69.0(4)	O(32)	Ce(3)	O(35)	113.1(4)
O(32)	Ce(3)	O(37)	111.2(5)	O(32)	Ce(3)	O(38)	66.8(5)
O(32)	Ce(3)	O(40)	132.7(4)	O(32)	Ce(3)	O(41)	178.6(4)
O(32)	Ce(3)	O(43)	67.6(5)	O(32)	Ce(3)	O(44)	68.7(5)
O(34)	Ce(3)	O(35)	48.8(5)	O(34)	Ce(3)	O(37)	103.1(5)
O(34)	Ce(3)	O(38)	70.3(5)	O(34)	Ce(3)	O(40)	158.1(4)
O(34)	Ce(3)	O(41)	112.0(4)	O(34)	Ce(3)	O(43)	127.1(5)
O(34)	Ce(3)	O(44)	132.2(5)	O(35)	Ce(3)	O(37)	68.6(4)
O(35)	Ce(3)	O(38)	70.9(4)	O(35)	Ce(3)	O(40)	110.2(4)
O(35)	Ce(3)	O(41)	68.2(4)	O(35)	Ce(3)	O(43)	131.9(5)
O(35)	Ce(3)	O(44)	178.0(5)	O(37)	Ce(3)	O(38)	48.4(5)

atom	atom	atom	angle	atom	atom	atom	angle
O(37)	Ce(3)	O(40)	68.4(5)	O(37)	Ce(3)	O(41)	69.6(5)
O(37)	Ce(3)	O(43)	67.3(5)	O(37)	Ce(3)	O(44)	112.0(5)
O(38)	Ce(3)	O(40)	112.1(5)	O(38)	Ce(3)	O(41)	114.4(5)
O(38)	Ce(3)	O(43)	65.8(5)	O(38)	Ce(3)	O(44)	111.0(5)
O(40)	Ce(3)	O(41)	46.5(4)	O(40)	Ce(3)	O(43)	69.7(5)
O(40)	Ce(3)	O(44)	68.5(5)	O(41)	Ce(3)	O(43)	112.1(5)
O(41)	Ce(3)	O(44)	110.1(4)	O(43)	Ce(3)	O(44)	49.5(5)
O(46)	Ce(4)	O(47)	48.0(4)	O(46)	Ce(4)	O(49)	66.9(5)
O(46)	Ce(4)	O(50)	109.7(5)	O(46)	Ce(4)	O(52)	67.3(4)
O(46)	Ce(4)	O(53)	110.8(4)	O(46)	Ce(4)	O(55)	130.7(6)
O(46)	Ce(4)	O(56)	173.5(5)	O(46)	Ce(4)	O(58)	67.8(5)
O(46)	Ce(4)	O(59)	69.3(4)	O(46)	Ce(4)	O(61)	115.3(6)
O(46)	Ce(4)	O(62)	118.1(6)	O(47)	Ce(4)	O(49)	64.9(5)
O(47)	Ce(4)	O(50)	110.0(6)	O(47)	Ce(4)	O(52)	111.4(5)
O(47)	Ce(4)	O(53)	158.0(5)	O(47)	Ce(4)	O(55)	128.1(7)
O(47)	Ce(4)	O(56)	137.2(5)	O(47)	Ce(4)	O(58)	70.2(5)
O(47)	Ce(4)	O(59)	105.2(5)	O(47)	Ce(4)	O(61)	73.3(7)
O(47)	Ce(4)	O(62)	75.5(7)	O(49)	Ce(4)	O(50)	48.4(6)
O(49)	Ce(4)	O(52)	71.8(5)	O(49)	Ce(4)	O(53)	103.8(5)
O(49)	Ce(4)	O(55)	161.9(7)	O(49)	Ce(4)	O(56)	110.7(6)
O(49)	Ce(4)	O(58)	130.3(6)	O(49)	Ce(4)	O(59)	126.2(5)
O(49)	Ce(4)	O(61)	114.7(7)	O(49)	Ce(4)	O(62)	67.6(7)
O(50)	Ce(4)	O(52)	69.0(5)	O(50)	Ce(4)	O(53)	68.1(6)
O(50)	Ce(4)	O(55)	114.1(7)	O(50)	Ce(4)	O(56)	65.9(6)
O(50)	Ce(4)	O(58)	176.7(5)	O(50)	Ce(4)	O(59)	128.4(5)
O(50)	Ce(4)	O(61)	114.3(7)	O(50)	Ce(4)	O(62)	62.9(7)
O(52)	Ce(4)	O(53)	46.7(5)	O(52)	Ce(4)	O(55)	108.8(6)
O(52)	Ce(4)	O(56)	106.3(5)	O(52)	Ce(4)	O(58)	107.7(5)
O(52)	Ce(4)	O(59)	63.4(4)	O(52)	Ce(4)	O(61)	173.4(7)
O(52)	Ce(4)	O(62)	130.4(7)	O(53)	Ce(4)	O(55)	68.0(7)
O(53)	Ce(4)	O(56)	63.4(5)	O(53)	Ce(4)	O(58)	110.5(5)
O(53)	Ce(4)	O(59)	65.2(5)	O(53)	Ce(4)	O(61)	128.3(7)

atom	atom	atom	angle	atom	atom	atom	angle
O(53)	Ce(4)	O(62)	119.1(7)	O(55)	Ce(4)	O(56)	51.3(7)
O(55)	Ce(4)	O(58)	67.4(7)	O(55)	Ce(4)	O(59)	66.3(6)
O(55)	Ce(4)	O(61)	64.7(8)	O(55)	Ce(4)	O(62)	101.5(8)
O(56)	Ce(4)	O(58)	116.4(6)	O(56)	Ce(4)	O(59)	109.2(5)
O(56)	Ce(4)	O(61)	71.1(7)	O(56)	Ce(4)	O(62)	64.8(7)
O(58)	Ce(4)	O(59)	49.0(4)	O(58)	Ce(4)	O(61)	69.0(7)
O(58)	Ce(4)	O(62)	120.0(6)	O(59)	Ce(4)	O(61)	111.3(7)
O(59)	Ce(4)	O(62)	165.4(6)	O(61)	Ce(4)	O(62)	54.5(8)
O(1)	Ni(1)	O(3)	86.0(4)	O(1)	Ni(1)	O(10)	88.0(5)
O(1)	Ni(1)	N(1)	81.5(5)	O(1)	Ni(1)	N(2)	165.1(6)
O(1)	Ni(1)	N(13)	93.5(5)	O(3)	Ni(1)	O(10)	93.1(5)
O(3)	Ni(1)	N(1)	167.5(5)	O(3)	Ni(1)	N(2)	79.3(5)
O(3)	Ni(1)	N(13)	88.4(5)	O(10)	Ni(1)	N(1)	85.3(6)
O(10)	Ni(1)	N(2)	90.1(6)	O(10)	Ni(1)	N(13)	178.0(5)
N(1)	Ni(1)	N(2)	113.1(6)	N(1)	Ni(1)	N(13)	93.5(6)
N(2)	Ni(1)	N(13)	88.8(6)	O(2)	Ni(2)	O(5)	88.8(5)
O(2)	Ni(2)	O(7)	91.6(5)	O(2)	Ni(2)	N(3)	89.4(6)
O(2)	Ni(2)	N(4)	89.1(5)	O(2)	Ni(2)	N(14)	178.8(5)
O(5)	Ni(2)	O(7)	85.6(4)	O(5)	Ni(2)	N(3)	83.4(6)
O(5)	Ni(2)	N(4)	167.5(5)	O(5)	Ni(2)	N(14)	90.7(5)
O(7)	Ni(2)	N(3)	169.0(6)	O(7)	Ni(2)	N(4)	82.1(5)
O(7)	Ni(2)	N(14)	89.5(5)	N(3)	Ni(2)	N(4)	108.9(6)
N(3)	Ni(2)	N(14)	89.4(6)	N(4)	Ni(2)	N(14)	91.6(5)
O(6)	Ni(3)	O(9)	88.6(4)	O(6)	Ni(3)	O(11)	90.2(5)
O(6)	Ni(3)	N(5)	87.4(6)	O(6)	Ni(3)	N(6)	90.1(5)
O(6)	Ni(3)	N(15)	177.6(6)	O(9)	Ni(3)	O(11)	85.1(4)
O(9)	Ni(3)	N(5)	83.9(5)	O(9)	Ni(3)	N(6)	167.2(5)
O(9)	Ni(3)	N(15)	89.1(5)	O(11)	Ni(3)	N(5)	168.8(5)
O(11)	Ni(3)	N(6)	82.1(5)	O(11)	Ni(3)	N(15)	89.2(6)
N(5)	Ni(3)	N(6)	108.8(6)	N(5)	Ni(3)	N(15)	92.8(6)
N(6)	Ni(3)	N(15)	92.0(6)	O(13)	Ni(4)	O(15)	87.2(5)
O(13)	Ni(4)	O(22)	89.2(5)	O(13)	Ni(4)	N(7)	80.7(6)

atom	atom	atom	angle	atom	atom	atom	angle
O(13)	Ni(4)	N(8)	167.0(6)	O(13)	Ni(4)	N(16)	88.2(6)
O(15)	Ni(4)	O(22)	91.5(5)	O(15)	Ni(4)	N(7)	167.8(6)
O(15)	Ni(4)	N(8)	79.8(6)	O(15)	Ni(4)	N(16)	90.2(7)
O(22)	Ni(4)	N(7)	86.8(7)	O(22)	Ni(4)	N(8)	90.7(6)
O(22)	Ni(4)	N(16)	176.9(7)	N(7)	Ni(4)	N(8)	112.2(7)
N(7)	Ni(4)	N(16)	91.0(8)	N(8)	Ni(4)	N(16)	92.2(7)
O(14)	Ni(5)	O(17)	86.7(5)	O(14)	Ni(5)	O(19)	90.2(5)
O(14)	Ni(5)	N(9)	87.2(6)	O(14)	Ni(5)	N(10)	94.0(5)
O(14)	Ni(5)	N(17)	176.2(7)	O(17)	Ni(5)	O(19)	87.1(5)
O(17)	Ni(5)	N(9)	83.7(7)	O(17)	Ni(5)	N(10)	169.1(6)
O(17)	Ni(5)	N(17)	89.7(7)	O(19)	Ni(5)	N(9)	170.6(7)
O(19)	Ni(5)	N(10)	82.1(5)	O(19)	Ni(5)	N(17)	88.2(7)
N(9)	Ni(5)	N(10)	107.1(7)	N(9)	Ni(5)	N(17)	93.8(8)
N(10)	Ni(5)	N(17)	89.2(7)	O(18)	Ni(6)	O(21)	87.5(5)
O(18)	Ni(6)	O(23)	90.5(5)	O(18)	Ni(6)	N(11)	85.4(6)
O(18)	Ni(6)	N(12)	92.0(5)	O(18)	Ni(6)	N(18)	176.9(6)
O(21)	Ni(6)	O(23)	85.9(5)	O(21)	Ni(6)	N(11)	82.7(6)
O(21)	Ni(6)	N(12)	167.5(5)	O(21)	Ni(6)	N(18)	92.4(6)
O(23)	Ni(6)	N(11)	168.1(6)	O(23)	Ni(6)	N(12)	81.6(5)
O(23)	Ni(6)	N(18)	92.5(5)	N(11)	Ni(6)	N(12)	109.7(6)
N(11)	Ni(6)	N(18)	91.5(7)	N(12)	Ni(6)	N(18)	88.8(5)
Ce(1)	O(1)	Ni(1)	103.2(5)	Ce(1)	O(1)	C(2)	135(1)
Ni(1)	O(1)	C(2)	115(1)	Ni(2)	O(2)	C(2)	130(1)
Ce(1)	O(3)	Ni(1)	102.6(4)	Ce(1)	O(3)	C(7)	139(1)
Ni(1)	O(3)	C(7)	117.1(10)	Ce(1)	O(5)	Ni(2)	103.3(4)
Ce(1)	O(5)	C(12)	139(1)	Ni(2)	O(5)	C(12)	113(1)
Ni(3)	O(6)	C(12)	126(1)	Ce(1)	O(7)	Ni(2)	103.2(5)
Ce(1)	O(7)	C(17)	137.0(9)	Ni(2)	O(7)	C(17)	119.5(10)
Ce(1)	O(9)	Ni(3)	104.0(4)	Ce(1)	O(9)	C(22)	137(1)
Ni(3)	O(9)	C(22)	116(1)	Ni(1)	O(10)	C(22)	126(1)
Ce(1)	O(11)	Ni(3)	104.5(4)	Ce(1)	O(11)	C(27)	138(1)
Ni(3)	O(11)	C(27)	115(1)	Ce(2)	O(13)	Ni(4)	101.5(5)

atom	atom	atom	angle	atom	atom	atom	angle
Ce(2)	O(13)	C(32)	135(1)	Ni(4)	O(13)	C(32)	120(1)
Ni(5)	O(14)	C(32)	128(1)	Ce(2)	O(15)	Ni(4)	102.3(4)
Ce(2)	O(15)	C(37)	141(1)	Ni(4)	O(15)	C(37)	115(1)
Ce(2)	O(17)	Ni(5)	103.5(5)	Ce(2)	O(17)	C(42)	139(1)
Ni(5)	O(17)	C(42)	113(1)	Ni(6)	O(18)	C(42)	131(1)
Ce(2)	O(19)	Ni(5)	101.5(5)	Ce(2)	O(19)	C(47)	139.0(9)
Ni(5)	O(19)	C(47)	118.2(10)	Ce(2)	O(21)	Ni(6)	104.0(5)
Ce(2)	O(21)	C(52)	138(1)	Ni(6)	O(21)	C(52)	116(1)
Ni(4)	O(22)	C(52)	132(1)	Ce(2)	O(23)	Ni(6)	103.4(4)
Ce(2)	O(23)	C(57)	142(1)	Ni(6)	O(23)	C(57)	113(1)
Ce(1)	O(25)	Ce(2)	101.5(3)	Ce(1)	O(25)	H(1)	111.9
Ce(1)	O(25)	H(2)	111.2	Ce(2)	O(25)	H(1)	111.9
Ce(2)	O(25)	H(2)	111.2	H(1)	O(25)	H(2)	109.0
Ce(1)	O(26)	Ce(2)	101.2(3)	Ce(1)	O(26)	H(3)	111.1
Ce(1)	O(26)	H(4)	112.2	Ce(2)	O(26)	H(3)	111.4
Ce(2)	O(26)	H(4)	112.5	H(3)	O(26)	H(4)	108.4
Ce(1)	O(27)	Ce(2)	103.2(3)	Ce(1)	O(27)	H(5)	111.5
Ce(1)	O(27)	H(6)	112.7	Ce(2)	O(27)	H(5)	110.6
Ce(2)	O(27)	H(6)	111.7	H(5)	O(27)	H(6)	107.2
Ce(3)	O(28)	N(19)	98(1)	Ce(3)	O(29)	N(19)	96(1)
Ce(3)	O(31)	N(20)	89(1)	Ce(3)	O(32)	N(20)	97(1)
Ce(3)	O(34)	N(21)	93(1)	Ce(3)	O(35)	N(21)	95(1)
Ce(3)	O(37)	N(22)	94(1)	Ce(3)	O(38)	N(22)	99(1)
Ce(3)	O(40)	N(23)	98(1)	Ce(3)	O(41)	N(23)	99(1)
Ce(3)	O(43)	N(24)	96(1)	Ce(3)	O(44)	N(24)	92(1)
Ce(4)	O(46)	N(25)	98(1)	Ce(4)	O(47)	N(25)	99(1)
Ce(4)	O(49)	N(26)	90(1)	Ce(4)	O(50)	N(26)	92(1)
Ce(4)	O(52)	N(27)	96(1)	Ce(4)	O(53)	N(27)	96(1)
Ce(4)	O(55)	N(28)	92(2)	Ce(4)	O(56)	N(28)	82(1)
Ce(4)	O(58)	N(29)	97(1)	Ce(4)	O(59)	N(29)	98(1)
Ce(4)	O(61)	N(30)	84(1)	Ce(4)	O(62)	N(30)	91(1)
Ni(1)	N(1)	C(1)	110(1)	Ni(1)	N(1)	H(7)	110.2

atom	atom	atom	angle	atom	atom	atom	angle
Ni(1)	N(1)	H(8)	109.7	C(1)	N(1)	H(7)	110.0
C(1)	N(1)	H(8)	108.9	H(7)	N(1)	H(8)	107.0
Ni(1)	N(2)	C(6)	113(1)	Ni(1)	N(2)	H(9)	109.2
Ni(1)	N(2)	H(10)	108.1	C(6)	N(2)	H(9)	112.5
C(6)	N(2)	H(10)	108.6	H(9)	N(2)	H(10)	104.6
Ni(2)	N(3)	C(11)	106(1)	Ni(2)	N(3)	H(11)	111.0
Ni(2)	N(3)	H(12)	112.2	C(11)	N(3)	H(11)	110.4
C(11)	N(3)	H(12)	109.7	H(11)	N(3)	H(12)	106.7
Ni(2)	N(4)	C(16)	111.2(9)	Ni(2)	N(4)	H(13)	109.2
Ni(2)	N(4)	H(14)	108.8	C(16)	N(4)	H(13)	110.3
C(16)	N(4)	H(14)	109.5	H(13)	N(4)	H(14)	107.9
Ni(3)	N(5)	C(21)	106(1)	Ni(3)	N(5)	H(15)	111.7
Ni(3)	N(5)	H(16)	112.2	C(21)	N(5)	H(15)	111.3
C(21)	N(5)	H(16)	109.6	H(15)	N(5)	H(16)	105.7
Ni(3)	N(6)	C(26)	111.7(10)	Ni(3)	N(6)	H(17)	110.6
Ni(3)	N(6)	H(18)	111.5	C(26)	N(6)	H(17)	108.8
C(26)	N(6)	H(18)	108.1	H(17)	N(6)	H(18)	105.9
Ni(4)	N(7)	C(31)	110(1)	Ni(4)	N(7)	H(19)	110.4
Ni(4)	N(7)	H(20)	108.5	C(31)	N(7)	H(19)	112.8
C(31)	N(7)	H(20)	107.3	H(19)	N(7)	H(20)	107.5
Ni(4)	N(8)	C(36)	112(1)	Ni(4)	N(8)	H(21)	109.5
Ni(4)	N(8)	H(22)	108.7	C(36)	N(8)	H(21)	111.0
C(36)	N(8)	H(22)	107.5	H(21)	N(8)	H(22)	107.8
Ni(5)	N(9)	C(41)	109(1)	Ni(5)	N(9)	H(23)	109.6
Ni(5)	N(9)	H(24)	111.9	C(41)	N(9)	H(23)	109.5
C(41)	N(9)	H(24)	110.6	H(23)	N(9)	H(24)	105.4
Ni(5)	N(10)	C(46)	113(1)	Ni(5)	N(10)	H(25)	109.0
Ni(5)	N(10)	H(26)	107.5	C(46)	N(10)	H(25)	109.8
C(46)	N(10)	H(26)	107.5	H(25)	N(10)	H(26)	109.4
Ni(6)	N(11)	C(51)	111(1)	Ni(6)	N(11)	H(27)	110.9
Ni(6)	N(11)	H(28)	110.6	C(51)	N(11)	H(27)	108.9
C(51)	N(11)	H(28)	106.5	H(27)	N(11)	H(28)	107.9

atom	atom	atom	angle	atom	atom	atom	angle
Ni(6)	N(12)	C(56)	111.8(10)	Ni(6)	N(12)	H(29)	110.4
Ni(6)	N(12)	H(30)	110.3	C(56)	N(12)	H(29)	110.3
C(56)	N(12)	H(30)	108.7	H(29)	N(12)	H(30)	105.1
Ni(1)	N(13)	C(61)	170(1)	Ni(2)	N(14)	C(63)	170(1)
Ni(3)	N(15)	C(65)	172(1)	Ni(4)	N(16)	C(67)	166(1)
Ni(5)	N(17)	C(69)	166(2)	Ni(6)	N(18)	C(71)	171(1)
O(28)	N(19)	O(29)	116(2)	O(28)	N(19)	O(30)	115(2)
O(29)	N(19)	O(30)	126(2)	O(31)	N(20)	O(32)	122(2)
O(31)	N(20)	O(33)	107(2)	O(32)	N(20)	O(33)	127(2)
O(34)	N(21)	O(35)	120(1)	O(34)	N(21)	O(36)	121(1)
O(35)	N(21)	O(36)	118(1)	O(37)	N(22)	O(38)	117(1)
O(37)	N(22)	O(39)	115(1)	O(38)	N(22)	O(39)	127(2)
O(40)	N(23)	O(41)	113(1)	O(40)	N(23)	O(42)	118(2)
O(41)	N(23)	O(42)	114(2)	O(43)	N(24)	O(44)	121(1)
O(43)	N(24)	O(45)	130(2)	O(44)	N(24)	O(45)	107(1)
O(46)	N(25)	O(47)	112(1)	O(46)	N(25)	O(48)	115(1)
O(47)	N(25)	O(48)	131(2)	O(49)	N(26)	O(50)	128(2)
O(49)	N(26)	O(51)	119(2)	O(50)	N(26)	O(51)	110(2)
O(52)	N(27)	O(53)	120(1)	O(52)	N(27)	O(54)	113(1)
O(53)	N(27)	O(54)	126(2)	O(55)	N(28)	O(56)	121(3)
O(55)	N(28)	O(57)	130(4)	O(56)	N(28)	O(57)	90(3)
O(58)	N(29)	O(59)	114(1)	O(58)	N(29)	O(60)	118(1)
O(59)	N(29)	O(60)	127(1)	O(61)	N(30)	O(62)	121(2)
O(61)	N(30)	O(63)	129(3)	O(62)	N(30)	O(63)	108(3)
N(1)	C(1)	C(2)	114(1)	N(1)	C(1)	H(31)	104.2
N(1)	C(1)	C(3)	119(1)	C(2)	C(1)	H(31)	105.3
C(2)	C(1)	C(3)	105(1)	H(31)	C(1)	C(3)	106.5
O(1)	C(2)	O(2)	121(1)	O(1)	C(2)	C(1)	113(1)
O(2)	C(2)	C(1)	125(1)	N(2)	C(6)	C(7)	112(1)
N(2)	C(6)	H(39)	105.9	N(2)	C(6)	C(8)	109(1)
C(7)	C(6)	H(39)	107.5	C(7)	C(6)	C(8)	112(1)
H(39)	C(6)	C(8)	107.6	O(3)	C(7)	O(4)	122(1)

atom	atom	atom	angle	atom	atom	atom	angle
O(3)	C(7)	C(6)	115(1)	O(4)	C(7)	C(6)	121(1)
N(3)	C(11)	C(12)	115(1)	N(3)	C(11)	H(47)	104.3
N(3)	C(11)	C(13)	116(1)	C(12)	C(11)	H(47)	107.8
C(12)	C(11)	C(13)	108(2)	H(47)	C(11)	C(13)	103.1
O(5)	C(12)	O(6)	122(1)	O(5)	C(12)	C(11)	113(1)
O(6)	C(12)	C(11)	124(1)	N(4)	C(16)	C(17)	110(1)
N(4)	C(16)	H(55)	107.1	N(4)	C(16)	C(18)	119(1)
C(17)	C(16)	H(55)	105.4	C(17)	C(16)	C(18)	112(1)
H(55)	C(16)	C(18)	99.4	O(7)	C(17)	O(8)	128(1)
O(7)	C(17)	C(16)	113(1)	O(8)	C(17)	C(16)	118(1)
N(5)	C(21)	C(22)	113(1)	N(5)	C(21)	H(63)	107.7
N(5)	C(21)	C(23)	108(1)	C(22)	C(21)	H(63)	111.2
C(22)	C(21)	C(23)	112(1)	H(63)	C(21)	C(23)	102.0
O(9)	C(22)	O(10)	126(1)	O(9)	C(22)	C(21)	115(1)
O(10)	C(22)	C(21)	118(1)	N(6)	C(26)	C(27)	106(1)
N(6)	C(26)	H(71)	108.4	N(6)	C(26)	C(28)	117(1)
C(27)	C(26)	H(71)	107.8	C(27)	C(26)	C(28)	112(1)
H(71)	C(26)	C(28)	104.0	O(11)	C(27)	O(12)	127(1)
O(11)	C(27)	C(26)	115(1)	O(12)	C(27)	C(26)	116(1)
N(7)	C(31)	C(32)	121(1)	N(7)	C(31)	H(79)	108.6
N(7)	C(31)	C(33)	119(2)	C(32)	C(31)	H(79)	106.8
C(32)	C(31)	C(33)	92(1)	H(79)	C(31)	C(33)	106.5
O(13)	C(32)	O(14)	127(1)	O(13)	C(32)	C(31)	104(1)
O(14)	C(32)	C(31)	128(1)	N(8)	C(36)	C(37)	106(1)
N(8)	C(36)	H(87)	104.1	N(8)	C(36)	C(38)	117(2)
C(37)	C(36)	H(87)	106.2	C(37)	C(36)	C(38)	117(2)
H(87)	C(36)	C(38)	103.9	O(15)	C(37)	O(16)	124(1)
O(15)	C(37)	C(36)	118(1)	O(16)	C(37)	C(36)	117(1)
N(9)	C(41)	C(42)	111(1)	N(9)	C(41)	H(95)	105.2
N(9)	C(41)	C(43)	111(1)	C(42)	C(41)	H(95)	110.1
C(42)	C(41)	C(43)	108(1)	H(95)	C(41)	C(43)	109.0
O(17)	C(42)	O(18)	119(1)	O(17)	C(42)	C(41)	116(1)

atom	atom	atom	angle	atom	atom	atom	angle
O(18)	C(42)	C(41)	123(1)	N(10)	C(46)	C(47)	109(1)
N(10)	C(46)	H(103)	104.8	N(10)	C(46)	C(48)	120(1)
C(47)	C(46)	H(103)	104.0	C(47)	C(46)	C(48)	111(1)
H(103)	C(46)	C(48)	104.9	O(19)	C(47)	O(20)	124(1)
O(19)	C(47)	C(46)	113(1)	O(20)	C(47)	C(46)	120(1)
N(11)	C(51)	C(52)	109(1)	N(11)	C(51)	H(111)	106.1
N(11)	C(51)	C(53)	113(2)	C(52)	C(51)	H(111)	105.7
C(52)	C(51)	C(53)	120(2)	H(111)	C(51)	C(53)	99.7
O(21)	C(52)	O(22)	119(1)	O(21)	C(52)	C(51)	118(1)
O(22)	C(52)	C(51)	121(1)	N(12)	C(56)	C(57)	110(1)
N(12)	C(56)	H(119)	106.2	N(12)	C(56)	C(58)	121(1)
C(57)	C(56)	H(119)	105.9	C(57)	C(56)	C(58)	109(1)
H(119)	C(56)	C(58)	100.9	O(23)	C(57)	O(24)	120(1)
O(23)	C(57)	C(56)	116(1)	O(24)	C(57)	C(56)	122(1)
N(13)	C(61)	C(62)	171(2)	C(61)	C(62)	H(127)	116.7
C(61)	C(62)	H(128)	115.2	C(61)	C(62)	H(129)	111.3
H(127)	C(62)	H(128)	106.4	H(127)	C(62)	H(129)	104.3
H(128)	C(62)	H(129)	101.4	N(14)	C(63)	C(64)	175(2)
C(63)	C(64)	H(130)	109.5	C(63)	C(64)	H(131)	114.1
C(63)	C(64)	H(132)	115.8	H(130)	C(64)	H(131)	104.2
H(130)	C(64)	H(132)	103.6	H(131)	C(64)	H(132)	108.5
N(15)	C(65)	C(66)	175(2)	C(65)	C(66)	H(133)	117.8
C(65)	C(66)	H(134)	119.2	C(65)	C(66)	H(135)	112.1
H(133)	C(66)	H(134)	105.2	H(133)	C(66)	H(135)	99.2
H(134)	C(66)	H(135)	100.3	N(16)	C(67)	C(68)	165(2)
C(67)	C(68)	H(136)	110.1	C(67)	C(68)	H(137)	108.1
C(67)	C(68)	H(138)	110.9	H(136)	C(68)	H(137)	105.6
H(136)	C(68)	H(138)	110.8	H(137)	C(68)	H(138)	111.1
N(17)	C(69)	C(70)	149(3)	C(69)	C(70)	H(139)	101.4
C(69)	C(70)	H(140)	117.9	C(69)	C(70)	H(141)	123.9
H(139)	C(70)	H(140)	88.1	H(139)	C(70)	H(141)	93.0
H(140)	C(70)	H(141)	116.4	N(18)	C(71)	C(72)	173(2)

atom	atom	atom	angle	atom	atom	atom	angle
C(71)	C(72)	H(142)	114.6	C(71)	C(72)	H(143)	113.8
C(71)	C(72)	H(144)	114.9	H(142)	C(72)	H(143)	104.1
H(142)	C(72)	H(144)	103.5	H(143)	C(72)	H(144)	104.8
C(1)	C(3)	H(32)	109.1	C(1)	C(3)	C(5)	115(2)
C(1)	C(3)	C(4)	98(3)	H(32)	C(3)	C(5)	116.0
H(32)	C(3)	C(4)	106.4	C(5)	C(3)	C(4)	109(3)
H(36)	C(5)	H(37)	114.5	H(36)	C(5)	H(38)	108.5
H(36)	C(5)	C(3)	104.4	H(37)	C(5)	H(38)	118.2
H(37)	C(5)	C(3)	106.5	H(38)	C(5)	C(3)	103.2
H(33)	C(4)	H(34)	109.1	H(33)	C(4)	H(35)	101.3
H(33)	C(4)	C(3)	113.0	H(34)	C(4)	H(35)	108.4
H(34)	C(4)	C(3)	113.6	H(35)	C(4)	C(3)	110.7
C(6)	C(8)	H(40)	111.3	C(6)	C(8)	C(10)	109(2)
C(6)	C(8)	C(9)	114(2)	H(40)	C(8)	C(10)	106.1
H(40)	C(8)	C(9)	105.1	C(10)	C(8)	C(9)	109(2)
H(44)	C(10)	H(45)	115.6	H(44)	C(10)	H(46)	107.6
H(44)	C(10)	C(8)	111.8	H(45)	C(10)	H(46)	103.6
H(45)	C(10)	C(8)	110.7	H(46)	C(10)	C(8)	106.9
H(41)	C(9)	H(42)	106.3	H(41)	C(9)	H(43)	105.6
H(41)	C(9)	C(8)	111.9	H(42)	C(9)	H(43)	108.4
H(42)	C(9)	C(8)	112.7	H(43)	C(9)	C(8)	111.6
C(11)	C(13)	H(48)	117.9	C(11)	C(13)	C(15)	102(2)
C(11)	C(13)	C(14)	109(2)	H(48)	C(13)	C(15)	103.1
H(48)	C(13)	C(14)	113.7	C(15)	C(13)	C(14)	109(3)
H(52)	C(15)	H(53)	100.9	H(52)	C(15)	H(54)	103.3
H(52)	C(15)	C(13)	109.2	H(53)	C(15)	H(54)	105.8
H(53)	C(15)	C(13)	116.2	H(54)	C(15)	C(13)	119.1
H(49)	C(14)	H(50)	120.4	H(49)	C(14)	H(51)	107.8
H(49)	C(14)	C(13)	111.4	H(50)	C(14)	H(51)	109.9
H(50)	C(14)	C(13)	105.4	H(51)	C(14)	C(13)	100.1
C(16)	C(18)	H(56)	118.4	C(16)	C(18)	C(19)	111(2)
C(16)	C(18)	C(20)	110(2)	H(56)	C(18)	C(19)	97.5

atom	atom	atom	angle	atom	atom	atom	angle
H(56)	C(18)	C(20)	108.8	C(19)	C(18)	C(20)	109(2)
H(57)	C(19)	H(58)	95.2	H(57)	C(19)	H(59)	102.8
H(57)	C(19)	C(18)	115.0	H(58)	C(19)	H(59)	100.6
H(58)	C(19)	C(18)	113.8	H(59)	C(19)	C(18)	124.6
H(60)	C(20)	H(61)	93.8	H(60)	C(20)	H(62)	117.2
H(60)	C(20)	C(18)	101.3	H(61)	C(20)	H(62)	120.5
H(61)	C(20)	C(18)	105.5	H(62)	C(20)	C(18)	115.1
C(21)	C(23)	H(64)	108.9	C(21)	C(23)	C(24)	114(3)
C(21)	C(23)	C(25)	109(3)	H(64)	C(23)	C(24)	107.2
H(64)	C(23)	C(25)	107.8	C(24)	C(23)	C(25)	109(3)
H(65)	C(24)	H(66)	107.2	H(65)	C(24)	H(67)	114.3
H(65)	C(24)	C(23)	114.2	H(66)	C(24)	H(67)	103.5
H(66)	C(24)	C(23)	106.7	H(67)	C(24)	C(23)	110.1
H(68)	C(25)	H(69)	113.5	H(68)	C(25)	H(70)	104.3
H(68)	C(25)	C(23)	107.2	H(69)	C(25)	H(70)	111.3
H(69)	C(25)	C(23)	114.0	H(70)	C(25)	C(23)	105.9
C(26)	C(28)	H(72)	109.1	C(26)	C(28)	C(29)	117(3)
C(26)	C(28)	C(30)	109(2)	H(72)	C(28)	C(29)	104.0
H(72)	C(28)	C(30)	106.7	C(29)	C(28)	C(30)	109(3)
H(73)	C(29)	H(74)	108.7	H(73)	C(29)	H(75)	114.7
H(73)	C(29)	C(28)	118.0	H(74)	C(29)	H(75)	97.8
H(74)	C(29)	C(28)	106.1	H(75)	C(29)	C(28)	109.3
H(76)	C(30)	H(77)	121.9	H(76)	C(30)	H(78)	104.3
H(76)	C(30)	C(28)	111.4	H(77)	C(30)	H(78)	103.9
H(77)	C(30)	C(28)	110.4	H(78)	C(30)	C(28)	102.6
C(36)	C(38)	H(88)	103.7	C(36)	C(38)	C(39)	111(2)
C(36)	C(38)	C(40)	128(3)	H(88)	C(38)	C(39)	95.2
H(88)	C(38)	C(40)	102.8	C(39)	C(38)	C(40)	109(3)
H(89)	C(39)	H(90)	110.6	H(89)	C(39)	H(91)	105.5
H(89)	C(39)	C(38)	117.3	H(90)	C(39)	H(91)	101.6
H(90)	C(39)	C(38)	114.2	H(91)	C(39)	C(38)	105.9
H(92)	C(40)	H(93)	114.7	H(92)	C(40)	H(94)	107.2

atom	atom	atom	angle	atom	atom	atom	angle
H(92)	C(40)	C(38)	104.4	H(93)	C(40)	H(94)	112.7
H(93)	C(40)	C(38)	113.3	H(94)	C(40)	C(38)	103.6
C(41)	C(43)	H(96)	107.9	C(41)	C(43)	C(44)	116(2)
C(41)	C(43)	C(45)	109(2)	H(96)	C(43)	C(44)	107.4
H(96)	C(43)	C(45)	105.7	C(44)	C(43)	C(45)	109(2)
H(97)	C(44)	H(98)	106.6	H(97)	C(44)	H(99)	111.9
H(97)	C(44)	C(43)	106.6	H(98)	C(44)	H(99)	111.1
H(98)	C(44)	C(43)	107.7	H(99)	C(44)	C(43)	112.6
H(100)	C(45)	H(101)	113.5	H(100)	C(45)	H(102)	108.2
H(100)	C(45)	C(43)	112.5	H(101)	C(45)	H(102)	106.5
H(101)	C(45)	C(43)	110.4	H(102)	C(45)	C(43)	105.1
C(46)	C(48)	H(104)	111.4	C(46)	C(48)	C(49)	108(2)
C(46)	C(48)	C(50)	112(1)	H(104)	C(48)	C(49)	107.1
H(104)	C(48)	C(50)	107.7	C(49)	C(48)	C(50)	109(2)
H(105)	C(49)	H(106)	108.0	H(105)	C(49)	H(107)	107.3
H(105)	C(49)	C(48)	106.6	H(106)	C(49)	H(107)	112.7
H(106)	C(49)	C(48)	110.5	H(107)	C(49)	C(48)	111.5
H(108)	C(50)	H(109)	109.2	H(108)	C(50)	H(110)	108.0
H(108)	C(50)	C(48)	109.1	H(109)	C(50)	H(110)	109.2
H(109)	C(50)	C(48)	111.7	H(110)	C(50)	C(48)	109.6
C(51)	C(53)	H(112)	98.8	C(51)	C(53)	C(54)	115(3)
C(51)	C(53)	C(55)	123(3)	H(112)	C(53)	C(54)	105.3
H(112)	C(53)	C(55)	100.4	C(54)	C(53)	C(55)	109(4)
H(113)	C(54)	H(114)	99.8	H(113)	C(54)	H(115)	122.8
H(113)	C(54)	C(53)	109.2	H(114)	C(54)	H(115)	109.8
H(114)	C(54)	C(53)	102.2	H(115)	C(54)	C(53)	110.7
H(116)	C(55)	H(117)	119.9	H(116)	C(55)	H(118)	101.1
H(116)	C(55)	C(53)	101.2	H(117)	C(55)	H(118)	112.8
H(117)	C(55)	C(53)	115.4	H(118)	C(55)	C(53)	104.3
C(56)	C(58)	H(120)	111.9	C(56)	C(58)	C(59)	109(2)
C(56)	C(58)	C(60)	109(2)	H(120)	C(58)	C(59)	105.3
H(120)	C(58)	C(60)	110.3	C(59)	C(58)	C(60)	109(2)

atom	atom	atom	angle	atom	atom	atom	angle
H(121)	C(59)	H(122)	105.3	H(121)	C(59)	H(123)	106.6
H(121)	C(59)	C(58)	109.2	H(122)	C(59)	H(123)	109.3
H(122)	C(59)	C(58)	112.5	H(123)	C(59)	C(58)	113.4
H(124)	C(60)	H(125)	113.4	H(124)	C(60)	H(126)	109.6
H(124)	C(60)	C(58)	110.1	H(125)	C(60)	H(126)	109.5
H(125)	C(60)	C(58)	107.5	H(126)	C(60)	C(58)	106.4
C(31)	C(33)	H(80)	129.3	C(31)	C(33)	C(34)	104(3)
C(31)	C(33)	C(35)	96(3)	H(80)	C(33)	C(34)	107.5
H(80)	C(33)	C(35)	108.5	C(34)	C(33)	C(35)	109(3)
H(81)	C(34)	H(82)	87.1	H(81)	C(34)	H(83)	117.6
H(81)	C(34)	C(33)	113.0	H(82)	C(34)	H(83)	101.2
H(82)	C(34)	C(33)	105.4	H(83)	C(34)	C(33)	123.3
H(84)	C(35)	H(85)	101.8	H(84)	C(35)	H(86)	102.8
H(84)	C(35)	C(33)	116.9	H(85)	C(35)	H(86)	96.1
H(85)	C(35)	C(33)	118.6	H(86)	C(35)	C(33)	117.3

Table 5. Special Distances (Å)

atom	atom	distance	atom	atom	distance
Ce(1)	Ce(2)	4.028(1)	Ce(1)	Ni(1)	3.572(2)
Ce(1)	Ni(2)	3.551(2)	Ce(1)	Ni(3)	3.570(3)
Ce(2)	Ni(4)	3.560(3)	Ce(2)	Ni(5)	3.544(3)
Ce(2)	Ni(6)	3.591(3)	Ni(1)	Ni(2)	5.340(3)
Ni(2)	Ni(3)	5.354(3)	Ni(3)	Ni(1)	5.307(3)
Ni(4)	Ni(5)	5.322(4)	Ni(5)	Ni(6)	5.350(3)
Ni(6)	Ni(4)	5.333(3)			

Table 6. Special Angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Ni(1)	Ce(1)	Ni(2)	97.12(5)	Ni(2)	Ce(1)	Ni(3)	97.52(5)
Ni(3)	Ce(1)	Ni(1)	95.99(6)	Ni(4)	Ce(2)	Ni(5)	97.03(6)
Ni(5)	Ce(2)	Ni(6)	97.14(6)	Ni(6)	Ce(2)	Ni(4)	96.43(6)
Ni(1)	Ce(1)	Ce(2)	122.10(5)	Ni(2)	Ce(1)	Ce(2)	117.86(4)
Ni(3)	Ce(1)	Ce(2)	120.74(5)	Ni(4)	Ce(2)	Ce(1)	121.16(5)
Ni(5)	Ce(2)	Ce(1)	118.91(5)	Ni(6)	Ce(2)	Ce(1)	120.65(5)

Structure Factor Table for

$[Pr_2\{Ni(val)_2\}_6(H_2O)_3(CH_3CN)_6][Pr(NO_3)_6]_2 \cdot n H_2O$ (2)

Table 1. Atomic coordinates, U_{eq} and occupancy

atom	x	y	z	U_{eq}	occ
Pr(1)	0.66194(3)	0.44990(3)	0.11923(2)	0.0565(2)	1.0000
Pr(2)	0.82752(3)	0.51090(3)	0.11223(2)	0.0588(2)	1.0000
Pr(3)	0.61742(4)	0.25350(4)	-0.16128(3)	0.0782(3)	1.0000
Pr(4)	0.61185(5)	0.22682(4)	0.35897(3)	0.0921(3)	1.0000
Ni(1)	0.59532(9)	0.38367(7)	0.02713(5)	0.0755(6)	1.0000
Ni(2)	0.63512(8)	0.35272(7)	0.20078(5)	0.0662(5)	1.0000
Ni(3)	0.53536(8)	0.53048(7)	0.14380(5)	0.0676(5)	1.0000
Ni(4)	0.8841(1)	0.56299(9)	0.01069(6)	0.0988(7)	1.0000
Ni(5)	0.86292(9)	0.61886(8)	0.18078(7)	0.0817(6)	1.0000
Ni(6)	0.95712(8)	0.43335(7)	0.13856(5)	0.0696(5)	1.0000
O(1)	0.6121(4)	0.3682(4)	0.0919(3)	0.073(2)	1.0000
O(2)	0.5850(5)	0.3176(4)	0.1479(3)	0.083(3)	1.0000
O(3)	0.6476(4)	0.4484(3)	0.0365(2)	0.065(2)	1.0000
O(4)	0.6884(4)	0.5165(4)	0.0034(3)	0.084(3)	1.0000
O(5)	0.5986(4)	0.4230(3)	0.1829(2)	0.059(2)	1.0000
O(6)	0.5172(4)	0.4732(4)	0.1919(3)	0.083(3)	1.0000
O(7)	0.7024(4)	0.3716(3)	0.1587(2)	0.059(2)	1.0000
O(8)	0.7900(4)	0.3403(4)	0.1298(3)	0.073(2)	1.0000
O(9)	0.5561(4)	0.4737(4)	0.0997(3)	0.070(2)	1.0000
O(10)	0.5172(4)	0.4230(4)	0.0472(3)	0.080(3)	1.0000
O(11)	0.6238(4)	0.5276(3)	0.1608(2)	0.063(2)	1.0000
O(12)	0.6885(4)	0.5583(4)	0.2115(3)	0.077(3)	1.0000
O(13)	0.8795(5)	0.5874(4)	0.0749(3)	0.090(3)	1.0000
O(14)	0.9094(5)	0.6456(4)	0.1199(4)	0.103(3)	1.0000
O(15)	0.8299(4)	0.5024(3)	0.0289(3)	0.074(2)	1.0000
O(16)	0.7875(5)	0.4282(4)	0.0038(3)	0.093(3)	1.0000
O(17)	0.8982(5)	0.5481(4)	0.1684(3)	0.088(3)	1.0000
O(18)	0.9798(5)	0.4980(4)	0.1758(3)	0.088(3)	1.0000
O(19)	0.7911(4)	0.5965(3)	0.1450(2)	0.061(2)	1.0000
O(20)	0.7047(4)	0.6239(4)	0.1151(3)	0.079(3)	1.0000

atom	x	y	z	U_{eq}	occ
O(21)	0.9302(4)	0.4807(4)	0.0888(3)	0.083(3)	1.0000
O(22)	0.9600(5)	0.5199(4)	0.0263(3)	0.096(3)	1.0000
O(23)	0.8702(4)	0.4405(3)	0.1602(2)	0.058(2)	1.0000
O(24)	0.8106(4)	0.4200(3)	0.2172(3)	0.068(2)	1.0000
O(25)	0.7181(4)	0.5280(3)	0.0857(2)	0.055(2)	1.0000
O(26)	0.7682(4)	0.4275(3)	0.0893(2)	0.053(2)	1.0000
O(27)	0.7478(4)	0.4833(3)	0.1695(2)	0.065(2)	1.0000
O(28)	0.7036(6)	0.2677(5)	-0.2198(4)	0.117(4)	1.0000
O(29)	0.7304(6)	0.2885(5)	-0.1521(4)	0.120(4)	1.0000
O(30)	0.7888(9)	0.3125(8)	-0.2103(6)	0.198(7)	1.0000
O(31)	0.6918(6)	0.1741(5)	-0.1615(4)	0.127(4)	1.0000
O(32)	0.6019(5)	0.1574(5)	-0.1389(3)	0.103(3)	1.0000
O(33)	0.6693(9)	0.0971(8)	-0.1430(6)	0.204(7)	1.0000
O(34)	0.6049(6)	0.1928(5)	-0.2310(4)	0.115(4)	1.0000
O(35)	0.5806(5)	0.2728(4)	-0.2421(3)	0.094(3)	1.0000
O(36)	0.5945(7)	0.2245(6)	-0.3003(4)	0.145(5)	1.0000
O(37)	0.5152(6)	0.3056(5)	-0.1605(4)	0.118(4)	1.0000
O(38)	0.5088(5)	0.2208(5)	-0.1674(3)	0.109(4)	1.0000
O(39)	0.4258(7)	0.2711(6)	-0.1650(5)	0.158(5)	1.0000
O(40)	0.6265(5)	0.3409(5)	-0.1143(4)	0.109(3)	1.0000
O(41)	0.6335(5)	0.3508(4)	-0.1858(3)	0.099(3)	1.0000
O(42)	0.6483(8)	0.4157(7)	-0.1436(5)	0.165(6)	1.0000
O(43)	0.5597(6)	0.2458(5)	-0.0842(4)	0.121(4)	1.0000
O(44)	0.6599(6)	0.2351(5)	-0.0816(4)	0.122(4)	1.0000
O(45)	0.6080(6)	0.2248(5)	-0.0229(4)	0.135(4)	1.0000
O(46)	0.6122(5)	0.3263(4)	0.3384(3)	0.085(3)	1.0000
O(47)	0.6091(6)	0.3103(5)	0.4103(4)	0.135(4)	1.0000
O(48)	0.6216(8)	0.3901(7)	0.3853(5)	0.172(6)	1.0000
O(49)	0.5055(7)	0.2727(6)	0.3642(4)	0.146(5)	1.0000
O(50)	0.5060(7)	0.1877(6)	0.3455(4)	0.138(5)	1.0000
O(51)	0.4218(10)	0.2292(8)	0.3563(6)	0.206(7)	1.0000
O(52)	0.5754(5)	0.2453(5)	0.2771(4)	0.111(4)	1.0000

atom	x	y	z	U_{eq}	occ
O(53)	0.6065(7)	0.1663(6)	0.2876(4)	0.140(5)	1.0000
O(54)	0.5820(6)	0.1982(6)	0.2212(4)	0.137(5)	1.0000
O(55)	0.6947(8)	0.1578(7)	0.3562(5)	0.161(6)	1.0000
O(56)	0.6078(7)	0.1245(6)	0.3725(5)	0.154(5)	1.0000
O(57)	0.675(1)	0.0730(10)	0.3572(8)	0.259(10)	1.0000
O(58)	0.7196(6)	0.2662(5)	0.3668(4)	0.115(4)	1.0000
O(59)	0.6942(5)	0.2483(4)	0.2998(3)	0.093(3)	1.0000
O(60)	0.7783(7)	0.2910(6)	0.3130(5)	0.151(5)	1.0000
O(61)	0.6533(9)	0.2029(8)	0.4384(6)	0.204(7)	1.0000
O(62)	0.5543(9)	0.1984(8)	0.4264(6)	0.200(8)	1.0000
O(63)	0.586(2)	0.143(2)	0.484(1)	0.44(1)	1.0000
O(71)	1.033(1)	0.354(1)	0.4059(9)	0.36(1)	1.0000
O(72)	0.778(2)	0.143(2)	0.488(2)	0.64(2)	1.0000
O(73)	0.818(2)	0.038(2)	0.341(1)	0.48(2)	1.0000
O(74)	0.268(2)	0.340(2)	-0.010(1)	0.50(2)	1.0000
O(75)	0.426(2)	0.363(2)	0.420(1)	0.47(1)	0.76(4)
O(76)	0.711(4)	0.260(4)	0.514(3)	0.82(3)	1.0000
O(77)	0.423(2)	0.387(1)	-0.091(1)	0.38(1)	1.0000
O(78)	0.889(2)	0.209(2)	0.379(1)	0.49(2)	1.0000
O(79)	0.410(2)	0.559(2)	0.377(2)	0.47(2)	0.81(3)
O(80)	0.466(5)	0.113(4)	0.433(3)	0.30(3)	0.31(3)
O(81)	0.385(1)	0.330(1)	0.1491(9)	0.34(1)	1.0000
O(82)	0.909(2)	0.095(2)	0.373(2)	0.58(2)	1.06(4)
N(1)	0.5477(5)	0.3166(5)	0.0342(3)	0.078(3)	1.0000
N(2)	0.5893(6)	0.4168(5)	-0.0350(4)	0.085(3)	1.0000
N(3)	0.5597(6)	0.3464(5)	0.2388(4)	0.082(3)	1.0000
N(4)	0.6841(5)	0.2842(4)	0.2061(3)	0.069(3)	1.0000
N(5)	0.4497(6)	0.5207(5)	0.1194(4)	0.097(4)	1.0000
N(6)	0.5329(5)	0.5851(5)	0.1934(3)	0.075(3)	1.0000
N(7)	0.9409(7)	0.6252(6)	0.0061(5)	0.115(5)	1.0000
N(8)	0.8774(6)	0.5233(5)	-0.0508(4)	0.094(4)	1.0000
N(9)	0.9401(8)	0.6316(7)	0.2113(5)	0.136(6)	1.0000

atom	x	y	z	U_{eq}	occ
N(10)	0.8170(6)	0.6858(5)	0.1850(4)	0.086(4)	1.0000
N(11)	1.0390(6)	0.4399(5)	0.1082(4)	0.097(4)	1.0000
N(12)	0.9654(5)	0.3868(4)	0.1928(3)	0.067(3)	1.0000
N(13)	0.6725(6)	0.3416(5)	0.0051(4)	0.091(4)	1.0000
N(14)	0.6830(5)	0.3877(4)	0.2525(3)	0.071(3)	1.0000
N(15)	0.5546(7)	0.5862(6)	0.0953(4)	0.096(4)	1.0000
N(16)	0.8067(7)	0.6079(6)	-0.0069(5)	0.111(5)	1.0000
N(17)	0.8239(7)	0.5915(6)	0.2329(5)	0.107(5)	1.0000
N(18)	0.9368(5)	0.3669(5)	0.1018(4)	0.081(3)	1.0000
N(19)	0.7406(8)	0.2856(7)	-0.1943(5)	0.130(5)	1.0000
N(20)	0.6499(9)	0.1415(8)	-0.1499(5)	0.138(6)	1.0000
N(21)	0.5946(6)	0.2289(6)	-0.2572(4)	0.099(4)	1.0000
N(22)	0.4819(8)	0.2646(7)	-0.1651(5)	0.116(5)	1.0000
N(23)	0.6330(9)	0.3685(8)	-0.1475(6)	0.145(6)	1.0000
N(24)	0.6034(7)	0.2386(6)	-0.0645(5)	0.113(5)	1.0000
N(25)	0.6117(8)	0.3430(7)	0.3814(5)	0.130(5)	1.0000
N(26)	0.479(1)	0.2298(9)	0.3576(6)	0.164(7)	1.0000
N(27)	0.5892(7)	0.1985(7)	0.2621(5)	0.120(5)	1.0000
N(28)	0.659(2)	0.119(1)	0.354(1)	0.28(1)	1.0000
N(29)	0.7328(7)	0.2676(6)	0.3259(5)	0.119(5)	1.0000
N(30)	0.595(1)	0.177(1)	0.4417(9)	0.23(1)	1.0000
C(1)	0.5312(7)	0.3076(6)	0.0785(4)	0.081(4)	1.0000
C(2)	0.5801(6)	0.3306(5)	0.1098(4)	0.070(4)	1.0000
C(3)	0.522(1)	0.2492(9)	0.0945(7)	0.1333	1.0000
C(4)	0.470(1)	0.240(2)	0.062(1)	0.3356	1.0000
C(5)	0.575(1)	0.214(1)	0.082(1)	0.1895	1.0000
C(6)	0.6308(6)	0.4589(5)	-0.0405(4)	0.071(4)	1.0000
C(7)	0.6563(6)	0.4777(5)	0.0027(4)	0.063(3)	1.0000
C(8)	0.600(1)	0.5032(7)	-0.0659(7)	0.1173	1.0000
C(9)	0.557(1)	0.539(1)	-0.0397(10)	0.1706	1.0000
C(10)	0.646(1)	0.537(1)	-0.0911(10)	0.1797	1.0000
C(11)	0.5172(8)	0.3845(7)	0.2237(5)	0.099(5)	1.0000

atom	x	y	z	U_{eq}	occ
C(12)	0.5443(6)	0.4317(5)	0.1978(4)	0.066(3)	1.0000
C(13)	0.468(1)	0.405(1)	0.2601(7)	0.1931	1.0000
C(14)	0.436(2)	0.356(1)	0.279(1)	0.2258	1.0000
C(15)	0.507(2)	0.430(1)	0.297(1)	0.1992	1.0000
C(16)	0.7463(6)	0.2923(5)	0.1900(4)	0.062(3)	1.0000
C(17)	0.7468(6)	0.3381(5)	0.1563(4)	0.062(3)	1.0000
C(18)	0.7789(10)	0.2460(8)	0.1718(7)	0.1188	1.0000
C(19)	0.746(1)	0.219(1)	0.1330(7)	0.1490	1.0000
C(20)	0.789(2)	0.207(1)	0.2098(8)	0.1847	1.0000
C(21)	0.4485(8)	0.4730(7)	0.0932(5)	0.106(5)	1.0000
C(22)	0.5110(6)	0.4550(5)	0.0773(4)	0.067(3)	1.0000
C(23)	0.400(1)	0.4755(10)	0.0519(8)	0.1434	1.0000
C(24)	0.406(2)	0.526(1)	0.024(1)	0.2136	1.0000
C(25)	0.335(1)	0.472(2)	0.071(2)	0.3047	1.0000
C(26)	0.5952(7)	0.6045(6)	0.2049(4)	0.075(4)	1.0000
C(27)	0.6398(7)	0.5591(6)	0.1939(4)	0.082(4)	1.0000
C(28)	0.610(1)	0.629(1)	0.2490(7)	0.1610	1.0000
C(29)	0.582(2)	0.591(1)	0.283(1)	0.1841	1.0000
C(30)	0.577(2)	0.681(1)	0.251(1)	0.2022	1.0000
C(31)	0.9513(9)	0.6426(8)	0.0440(6)	0.109(6)	1.0000
C(32)	0.9122(8)	0.6288(7)	0.0889(5)	0.090(5)	1.0000
C(33)	0.958(2)	0.704(1)	0.0565(10)	0.2580	1.0000
C(34)	0.900(2)	0.727(2)	0.037(2)	0.3721	1.0000
C(35)	1.012(2)	0.724(2)	0.029(2)	0.3058	1.0000
C(36)	0.8291(8)	0.4890(7)	-0.0512(5)	0.104(5)	1.0000
C(37)	0.8147(8)	0.4701(7)	-0.0012(5)	0.091(5)	1.0000
C(38)	0.829(1)	0.4485(9)	-0.0841(7)	0.1353	1.0000
C(39)	0.885(2)	0.413(1)	-0.080(1)	0.2165	1.0000
C(40)	0.814(2)	0.456(1)	-0.1335(8)	0.2033	1.0000
C(41)	0.9875(8)	0.5864(7)	0.1995(5)	0.100(5)	1.0000
C(42)	0.9525(8)	0.5413(7)	0.1840(5)	0.097(5)	1.0000
C(43)	1.0264(9)	0.5709(8)	0.2388(5)	0.1150	1.0000

atom	x	y	z	U_{eq}	occ
C(44)	0.990(1)	0.554(1)	0.2798(8)	0.1469	1.0000
C(45)	1.068(1)	0.617(1)	0.2516(9)	0.1519	1.0000
C(46)	0.7549(6)	0.6803(6)	0.1680(4)	0.070(4)	1.0000
C(47)	0.7491(6)	0.6293(5)	0.1415(4)	0.069(4)	1.0000
C(48)	0.7258(8)	0.7242(6)	0.1483(5)	0.0930	1.0000
C(49)	0.764(1)	0.7392(9)	0.1072(6)	0.1336	1.0000
C(50)	0.721(1)	0.7714(8)	0.1797(6)	0.1170	1.0000
C(51)	1.0347(8)	0.4744(7)	0.0696(5)	0.092(5)	1.0000
C(52)	0.9735(8)	0.4930(7)	0.0596(5)	0.099(5)	1.0000
C(53)	1.068(1)	0.450(1)	0.0299(9)	0.1699	1.0000
C(54)	1.041(2)	0.399(2)	0.011(2)	0.2880	1.0000
C(55)	1.137(1)	0.446(2)	0.029(2)	0.3001	1.0000
C(56)	0.9046(6)	0.3724(5)	0.2094(4)	0.068(4)	1.0000
C(57)	0.8590(6)	0.4148(5)	0.1958(4)	0.061(3)	1.0000
C(58)	0.8987(7)	0.3583(7)	0.2586(5)	0.0920	1.0000
C(59)	0.919(1)	0.4046(7)	0.2876(7)	0.1087	1.0000
C(60)	0.937(1)	0.3102(7)	0.2697(8)	0.1224	1.0000
C(61)	0.7122(9)	0.3260(8)	-0.0104(6)	0.112(6)	1.0000
C(62)	0.761(1)	0.3078(9)	-0.0352(7)	0.139(7)	1.0000
C(63)	0.7074(7)	0.3997(6)	0.2823(5)	0.085(4)	1.0000
C(64)	0.746(1)	0.4173(10)	0.3205(8)	0.156(8)	1.0000
C(65)	0.5698(9)	0.6188(8)	0.0749(6)	0.103(6)	1.0000
C(66)	0.590(1)	0.6613(10)	0.0464(7)	0.153(8)	1.0000
C(67)	0.7780(9)	0.6356(8)	-0.0205(6)	0.111(6)	1.0000
C(68)	0.735(1)	0.684(1)	-0.0377(8)	0.174(9)	1.0000
C(69)	0.8056(9)	0.5805(8)	0.2509(6)	0.104(6)	1.0000
C(70)	0.767(2)	0.549(2)	0.293(2)	0.39(2)	1.0000
C(71)	0.9215(7)	0.3308(7)	0.0868(5)	0.087(4)	1.0000
C(72)	0.904(1)	0.284(1)	0.0687(8)	0.177(9)	1.0000
H(1)	0.5117	0.3192	0.0176	0.0945	1.0000
H(2)	0.5713	0.2884	0.0237	0.0945	1.0000
H(3)	0.5960	0.3915	-0.0565	0.1001	1.0000

atom	x	y	z	U_{eq}	occ
H(4)	0.5487	0.4305	-0.0382	0.1001	1.0000
H(5)	0.5425	0.3128	0.2354	0.0981	1.0000
H(6)	0.5691	0.3524	0.2692	0.0981	1.0000
H(7)	0.6845	0.2734	0.2361	0.0837	1.0000
H(8)	0.6653	0.2582	0.1882	0.0837	1.0000
H(9)	0.4218	0.5186	0.1432	0.1173	1.0000
H(10)	0.4393	0.5500	0.1009	0.1173	1.0000
H(11)	0.5082	0.6136	0.1835	0.0883	1.0000
H(12)	0.5142	0.5699	0.2189	0.0883	1.0000
H(13)	0.9771	0.6132	-0.0079	0.1406	1.0000
H(14)	0.9223	0.6502	-0.0131	0.1406	1.0000
H(15)	0.8720	0.5481	-0.0739	0.1125	1.0000
H(16)	0.9133	0.5042	-0.0557	0.1125	1.0000
H(17)	0.9557	0.6631	0.2048	0.1619	1.0000
H(18)	0.9331	0.6285	0.2437	0.1619	1.0000
H(19)	0.8144	0.6962	0.2152	0.1008	1.0000
H(20)	0.8367	0.7118	0.1681	0.1008	1.0000
H(21)	1.0678	0.4538	0.1288	0.1160	1.0000
H(22)	1.0526	0.4067	0.0984	0.1160	1.0000
H(23)	0.9875	0.3564	0.1860	0.0805	1.0000
H(24)	0.9865	0.4054	0.2162	0.0805	1.0000
H(25)	0.4953	0.3236	0.0848	0.0990	1.0000
H(26)	0.5141	0.2440	0.1249	0.1565	1.0000
H(27)	0.4416	0.2554	0.0670	0.4178	1.0000
H(28)	0.4893	0.2386	0.0321	0.4178	1.0000
H(29)	0.4640	0.1981	0.0656	0.4178	1.0000
H(30)	0.5738	0.1793	0.0856	0.2252	1.0000
H(31)	0.5953	0.2233	0.0539	0.2252	1.0000
H(32)	0.6140	0.2240	0.1036	0.2252	1.0000
H(33)	0.6623	0.4466	-0.0583	0.0864	1.0000
H(34)	0.5741	0.4858	-0.0868	0.1396	1.0000
H(35)	0.5794	0.5591	-0.0186	0.2166	1.0000

atom	x	y	z	U_{eq}	occ
H(36)	0.5346	0.5599	-0.0583	0.2166	1.0000
H(37)	0.5288	0.5175	-0.0217	0.2166	1.0000
H(38)	0.6717	0.5135	-0.1062	0.2415	1.0000
H(39)	0.6232	0.5564	-0.1124	0.2415	1.0000
H(40)	0.6653	0.5577	-0.0712	0.2415	1.0000
H(41)	0.4947	0.3674	0.2016	0.1152	1.0000
H(42)	0.4375	0.4278	0.2450	0.2405	1.0000
H(43)	0.4059	0.3666	0.3006	0.2569	1.0000
H(44)	0.4111	0.3389	0.2548	0.2569	1.0000
H(45)	0.4620	0.3327	0.2898	0.2569	1.0000
H(46)	0.5306	0.4059	0.3070	0.2389	1.0000
H(47)	0.5242	0.4590	0.2829	0.2389	1.0000
H(48)	0.4769	0.4424	0.3182	0.2389	1.0000
H(49)	0.7694	0.3036	0.2152	0.0715	1.0000
H(50)	0.8153	0.2580	0.1603	0.1464	1.0000
H(51)	0.7056	0.2077	0.1426	0.1742	1.0000
H(52)	0.7380	0.2434	0.1085	0.1742	1.0000
H(53)	0.7669	0.1908	0.1224	0.1742	1.0000
H(54)	0.7480	0.1993	0.2215	0.2436	1.0000
H(55)	0.8060	0.1785	0.1989	0.2436	1.0000
H(56)	0.8098	0.2248	0.2320	0.2436	1.0000
H(57)	0.4345	0.4469	0.1126	0.1302	1.0000
H(58)	0.4054	0.4476	0.0322	0.1781	1.0000
H(59)	0.4435	0.5286	0.0106	0.2691	1.0000
H(60)	0.3746	0.5283	0.0022	0.2691	1.0000
H(61)	0.4006	0.5564	0.0438	0.2691	1.0000
H(62)	0.3299	0.5018	0.0915	0.3420	1.0000
H(63)	0.3068	0.4739	0.0489	0.3420	1.0000
H(64)	0.3323	0.4414	0.0882	0.3420	1.0000
H(65)	0.6033	0.6317	0.1844	0.0915	1.0000
H(66)	0.6490	0.6308	0.2559	0.1921	1.0000
H(67)	0.5880	0.6055	0.3160	0.2572	1.0000

atom	x	y	z	U_{eq}	occ
H(68)	0.5375	0.5889	0.2832	0.2572	1.0000
H(69)	0.5973	0.5576	0.2852	0.2572	1.0000
H(70)	0.5826	0.6961	0.2816	0.2592	1.0000
H(71)	0.5924	0.7026	0.2307	0.2592	1.0000
H(72)	0.5340	0.6766	0.2484	0.2592	1.0000
H(73)	0.9899	0.6301	0.0490	0.1286	1.0000
H(74)	0.9601	0.7142	0.0859	0.2739	1.0000
H(75)	0.9008	0.7677	0.0364	0.4485	1.0000
H(76)	0.8991	0.7220	0.0027	0.4485	1.0000
H(77)	0.8655	0.7173	0.0478	0.4485	1.0000
H(78)	1.0481	0.7110	0.0419	0.3851	1.0000
H(79)	1.0100	0.7125	-0.0014	0.3851	1.0000
H(80)	1.0152	0.7619	0.0282	0.3851	1.0000
H(81)	0.7948	0.5087	-0.0603	0.1203	1.0000
H(82)	0.8025	0.4253	-0.0730	0.1675	1.0000
H(83)	0.8745	0.3763	-0.0924	0.2469	1.0000
H(84)	0.9189	0.4222	-0.0996	0.2469	1.0000
H(85)	0.9005	0.4060	-0.0517	0.2469	1.0000
H(86)	0.7819	0.4797	-0.1333	0.2552	1.0000
H(87)	0.8461	0.4655	-0.1497	0.2552	1.0000
H(88)	0.7984	0.4220	-0.1430	0.2552	1.0000
H(89)	1.0133	0.5983	0.1760	0.1186	1.0000
H(90)	1.0494	0.5406	0.2305	0.1347	1.0000
H(91)	0.9639	0.5831	0.2891	0.1807	1.0000
H(92)	0.9615	0.5261	0.2720	0.1807	1.0000
H(93)	1.0132	0.5436	0.3033	0.1807	1.0000
H(94)	1.0912	0.6053	0.2766	0.1873	1.0000
H(95)	1.0932	0.6227	0.2271	0.1873	1.0000
H(96)	1.0442	0.6448	0.2587	0.1873	1.0000
H(97)	0.7313	0.6746	0.1937	0.0853	1.0000
H(98)	0.6860	0.7146	0.1386	0.1098	1.0000
H(99)	0.8034	0.7470	0.1165	0.1673	1.0000

atom	x	y	z	U_{eq}	occ
H(100)	0.7643	0.7107	0.0870	0.1673	1.0000
H(101)	0.7465	0.7687	0.0930	0.1673	1.0000
H(102)	0.7596	0.7824	0.1883	0.1335	1.0000
H(103)	0.7011	0.7998	0.1643	0.1335	1.0000
H(104)	0.6975	0.7626	0.2050	0.1335	1.0000
H(105)	1.0574	0.5053	0.0777	0.1097	1.0000
H(106)	1.0591	0.4755	0.0086	0.2245	1.0000
H(107)	1.0031	0.4000	0.0103	0.3467	1.0000
H(108)	1.0603	0.3979	-0.0193	0.3467	1.0000
H(109)	1.0603	0.3715	0.0272	0.3467	1.0000
H(110)	1.1534	0.4238	0.0461	0.3697	1.0000
H(111)	1.1509	0.4512	0.0000	0.3697	1.0000
H(112)	1.1516	0.4842	0.0434	0.3697	1.0000
H(113)	0.8930	0.3421	0.1935	0.0821	1.0000
H(114)	0.8569	0.3516	0.2647	0.1083	1.0000
H(115)	0.9153	0.3968	0.3176	0.1325	1.0000
H(116)	0.9590	0.4139	0.2801	0.1325	1.0000
H(117)	0.8934	0.4348	0.2808	0.1325	1.0000
H(118)	0.9320	0.3033	0.3011	0.1424	1.0000
H(119)	0.9228	0.2818	0.2532	0.1424	1.0000
H(120)	0.9772	0.3177	0.2637	0.1424	1.0000
H(121)	0.7146	0.5295	0.0540	0.0670	1.0000
H(122)	0.7025	0.5610	0.0972	0.0670	1.0000
H(123)	0.7837	0.3965	0.1031	0.0665	1.0000
H(124)	0.7676	0.4221	0.0578	0.0665	1.0000
H(125)	0.7357	0.5119	0.1879	0.0803	1.0000
H(126)	0.7631	0.4563	0.1890	0.0803	1.0000
H(127)	0.7478	0.2793	-0.0544	0.1518	1.0000
H(128)	0.7758	0.3347	-0.0551	0.1518	1.0000
H(129)	0.7923	0.2962	-0.0172	0.1518	1.0000
H(130)	0.7793	0.3900	0.3243	0.1659	1.0000
H(131)	0.7664	0.4481	0.3138	0.1659	1.0000

atom	x	y	z	U_{eq}	occ
H(132)	0.7257	0.4182	0.3471	0.1659	1.0000
H(133)	0.6202	0.6855	0.0646	0.1837	1.0000
H(134)	0.6140	0.6521	0.0217	0.1837	1.0000
H(135)	0.5609	0.6870	0.0373	0.1837	1.0000
H(136)	0.7572	0.7093	-0.0539	0.1933	1.0000
H(137)	0.7047	0.6699	-0.0589	0.1933	1.0000
H(138)	0.7131	0.7001	-0.0146	0.1933	1.0000
H(139)	0.7393	0.5671	0.3101	0.4253	1.0000
H(140)	0.7428	0.5173	0.2809	0.4253	1.0000
H(141)	0.7938	0.5296	0.3145	0.4253	1.0000
H(142)	0.8809	0.2590	0.0891	0.1951	1.0000
H(143)	0.8794	0.2834	0.0419	0.1951	1.0000
H(144)	0.9383	0.2586	0.0598	0.1951	1.0000

$$Ueq = \frac{1}{3}\left(U_{11}\left(aa^*\right)^2 + U_{22}\left(bb^*\right)^2 + U_{33}\left(cc^*\right)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha\right)$$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pr(1)	0.0622(4)	0.0573(4)	0.0499(3)	-0.0036(4)	-0.0014(3)	-0.0020(3)
Pr(2)	0.0599(4)	0.0529(4)	0.0637(3)	0.0000(4)	0.0093(4)	0.0058(3)
Pr(3)	0.0835(6)	0.0730(5)	0.0779(4)	-0.0123(5)	0.0112(4)	0.0041(4)
Pr(4)	0.0977(7)	0.0911(7)	0.0876(5)	0.0052(6)	0.0238(5)	0.0189(5)
Ni(1)	0.100(1)	0.068(1)	0.0586(8)	-0.001(1)	-0.0155(9)	-0.0082(8)
Ni(2)	0.062(1)	0.073(1)	0.0639(8)	-0.0068(10)	-0.0002(8)	0.0095(8)
Ni(3)	0.068(1)	0.072(1)	0.0627(8)	0.002(1)	-0.0032(8)	-0.0109(9)
Ni(4)	0.099(2)	0.092(1)	0.105(1)	0.020(1)	0.037(1)	0.048(1)
Ni(5)	0.065(1)	0.056(1)	0.124(1)	0.001(1)	-0.025(1)	-0.011(1)
Ni(6)	0.070(1)	0.065(1)	0.0738(9)	0.013(1)	0.0154(9)	0.0119(9)

The general temperature factor expression:

$$\exp\left(-2\pi^2\left(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl\right)\right)$$

Table 3. Bond Lengths (Å)

atom	atom	distance	atom	atom	distance
Pr(1)	O(1)	2.507(9)	Pr(1)	O(3)	2.504(7)
Pr(1)	O(5)	2.472(8)	Pr(1)	O(7)	2.499(8)
Pr(1)	O(9)	2.498(9)	Pr(1)	O(11)	2.500(8)
Pr(1)	O(25)	2.567(8)	Pr(1)	O(26)	2.588(8)
Pr(1)	O(27)	2.578(8)	Pr(2)	O(13)	2.54(1)
Pr(2)	O(15)	2.512(8)	Pr(2)	O(17)	2.493(10)
Pr(2)	O(19)	2.537(8)	Pr(2)	O(21)	2.510(10)
Pr(2)	O(23)	2.498(8)	Pr(2)	O(25)	2.594(8)
Pr(2)	O(26)	2.605(8)	Pr(2)	O(27)	2.567(8)
Pr(3)	O(28)	2.62(1)	Pr(3)	O(29)	2.68(1)
Pr(3)	O(31)	2.62(1)	Pr(3)	O(32)	2.58(1)
Pr(3)	O(34)	2.62(1)	Pr(3)	O(35)	2.609(10)
Pr(3)	O(37)	2.63(1)	Pr(3)	O(38)	2.56(1)
Pr(3)	O(40)	2.66(1)	Pr(3)	O(41)	2.63(1)
Pr(3)	O(43)	2.65(1)	Pr(3)	O(44)	2.61(1)
Pr(4)	O(46)	2.626(10)	Pr(4)	O(47)	2.64(1)
Pr(4)	O(49)	2.64(2)	Pr(4)	O(50)	2.59(1)
Pr(4)	O(52)	2.63(1)	Pr(4)	O(53)	2.65(1)
Pr(4)	O(55)	2.56(2)	Pr(4)	O(56)	2.66(2)
Pr(4)	O(58)	2.61(1)	Pr(4)	O(59)	2.607(10)
Pr(4)	O(61)	2.63(2)	Pr(4)	O(62)	2.50(2)
Ni(1)	O(1)	2.020(8)	Ni(1)	O(3)	2.045(9)
Ni(1)	O(10)	2.096(10)	Ni(1)	N(1)	2.03(1)
Ni(1)	N(2)	2.05(1)	Ni(1)	N(13)	2.13(1)
Ni(2)	O(2)	2.136(10)	Ni(2)	O(5)	2.049(8)
Ni(2)	O(7)	2.015(8)	Ni(2)	N(3)	2.03(1)
Ni(2)	N(4)	2.07(1)	Ni(2)	N(14)	2.08(1)
Ni(3)	O(6)	2.099(10)	Ni(3)	O(9)	2.023(9)
Ni(3)	O(11)	2.031(9)	Ni(3)	N(5)	2.05(1)
Ni(3)	N(6)	2.05(1)	Ni(3)	N(15)	2.08(1)

atom	atom	distance	atom	atom	distance
Ni(4)	O(13)	2.028(9)	Ni(4)	O(15)	2.040(9)
Ni(4)	O(22)	2.07(1)	Ni(4)	N(7)	2.04(2)
Ni(4)	N(8)	2.11(1)	Ni(4)	N(16)	2.13(2)
Ni(5)	O(14)	2.21(1)	Ni(5)	O(17)	2.01(1)
Ni(5)	O(19)	2.007(8)	Ni(5)	N(9)	1.97(2)
Ni(5)	N(10)	2.00(1)	Ni(5)	N(17)	1.92(1)
Ni(6)	O(18)	2.06(1)	Ni(6)	O(21)	2.015(10)
Ni(6)	O(23)	2.045(8)	Ni(6)	N(11)	2.04(1)
Ni(6)	N(12)	2.03(1)	Ni(6)	N(18)	2.08(1)
O(1)	C(2)	1.31(2)	O(2)	C(2)	1.20(2)
O(3)	C(7)	1.28(1)	O(4)	C(7)	1.23(2)
O(5)	C(12)	1.31(2)	O(6)	C(12)	1.23(2)
O(7)	C(17)	1.31(2)	O(8)	C(17)	1.25(2)
O(9)	C(22)	1.30(2)	O(10)	C(22)	1.23(2)
O(11)	C(27)	1.33(2)	O(12)	C(27)	1.20(2)
O(13)	C(32)	1.35(2)	O(14)	C(32)	1.03(2)
O(15)	C(37)	1.27(2)	O(16)	C(37)	1.24(2)
O(17)	C(42)	1.31(2)	O(18)	C(42)	1.29(2)
O(19)	C(47)	1.26(2)	O(20)	C(47)	1.27(2)
O(21)	C(52)	1.34(2)	O(22)	C(52)	1.25(2)
O(23)	C(57)	1.28(1)	O(24)	C(57)	1.26(2)
O(25)	H(121)	0.953	O(25)	H(122)	0.979
O(26)	H(123)	0.960	O(26)	H(124)	0.958
O(27)	H(125)	0.957	O(27)	H(126)	0.970
O(28)	N(19)	1.21(2)	O(29)	N(19)	1.29(2)
O(30)	N(19)	1.36(3)	O(31)	N(20)	1.30(2)
O(32)	N(20)	1.19(2)	O(33)	N(20)	1.24(3)
O(34)	N(21)	1.24(2)	O(35)	N(21)	1.25(2)
O(36)	N(21)	1.30(2)	O(37)	N(22)	1.29(2)
O(38)	N(22)	1.27(2)	O(39)	N(22)	1.26(2)
O(40)	N(23)	1.23(2)	O(41)	N(23)	1.24(2)
O(42)	N(23)	1.26(3)	O(43)	N(24)	1.15(2)

atom	atom	distance	atom	atom	distance
O(44)	N(24)	1.36(2)	O(45)	N(24)	1.30(2)
O(46)	N(25)	1.36(2)	O(47)	N(25)	1.21(2)
O(48)	N(25)	1.23(2)	O(49)	N(26)	1.26(3)
O(50)	N(26)	1.28(3)	O(51)	N(26)	1.28(3)
O(52)	N(27)	1.32(2)	O(53)	N(27)	1.19(2)
O(54)	N(27)	1.24(2)	O(55)	N(28)	1.29(4)
O(56)	N(28)	1.27(4)	O(57)	N(28)	1.23(4)
O(58)	N(29)	1.26(2)	O(59)	N(29)	1.26(2)
O(60)	N(29)	1.24(2)	O(61)	N(30)	1.45(4)
O(62)	N(30)	1.16(4)	O(63)	N(30)	1.56(5)
N(1)	C(1)	1.40(2)	N(1)	H(1)	0.945
N(1)	H(2)	0.946	N(2)	C(6)	1.43(2)
N(2)	H(3)	0.929	N(2)	H(4)	0.971
N(3)	C(11)	1.43(2)	N(3)	H(5)	0.948
N(3)	H(6)	0.948	N(4)	C(16)	1.48(2)
N(4)	H(7)	0.944	N(4)	H(8)	0.952
N(5)	C(21)	1.46(2)	N(5)	H(9)	0.947
N(5)	H(10)	0.961	N(6)	C(26)	1.51(2)
N(6)	H(11)	0.963	N(6)	H(12)	0.953
N(7)	C(31)	1.24(2)	N(7)	H(13)	0.957
N(7)	H(14)	0.957	N(8)	C(36)	1.39(2)
N(8)	H(15)	0.950	N(8)	H(16)	0.948
N(9)	C(41)	1.61(3)	N(9)	H(17)	0.903
N(9)	H(18)	0.988	N(10)	C(46)	1.48(2)
N(10)	H(19)	0.945	N(10)	H(20)	0.946
N(11)	C(51)	1.46(2)	N(11)	H(21)	0.960
N(11)	H(22)	0.950	N(12)	C(56)	1.49(2)
N(12)	H(23)	0.943	N(12)	H(24)	0.970
N(13)	C(61)	1.08(2)	N(14)	C(63)	1.09(2)
N(15)	C(65)	1.09(2)	N(16)	C(67)	1.04(3)
N(17)	C(69)	0.73(2)	N(18)	C(71)	1.09(2)
C(1)	C(2)	1.55(2)	C(1)	H(25)	0.919

atom	atom	distance	atom	atom	distance
C(1)	C(3)	1.58(3)	C(6)	C(7)	1.49(2)
C(6)	H(33)	0.935	C(6)	C(8)	1.53(2)
C(11)	C(12)	1.56(2)	C(11)	H(41)	0.940
C(11)	C(13)	1.63(3)	C(16)	C(17)	1.55(2)
C(16)	H(49)	0.960	C(16)	C(18)	1.49(2)
C(21)	C(22)	1.54(2)	C(21)	H(57)	0.940
C(21)	C(23)	1.65(3)	C(26)	C(27)	1.56(2)
C(26)	H(65)	0.947	C(26)	C(28)	1.50(3)
C(31)	C(32)	1.64(2)	C(31)	H(73)	0.927
C(31)	C(33)	1.63(4)	C(36)	C(37)	1.61(2)
C(36)	H(81)	0.954	C(36)	C(38)	1.43(3)
C(41)	C(42)	1.47(3)	C(41)	H(89)	0.958
C(41)	C(43)	1.51(2)	C(46)	C(47)	1.54(2)
C(46)	H(97)	0.943	C(46)	C(48)	1.43(2)
C(51)	C(52)	1.47(2)	C(51)	H(105)	0.969
C(51)	C(53)	1.54(3)	C(56)	C(57)	1.54(2)
C(56)	H(113)	0.947	C(56)	C(58)	1.53(2)
C(61)	C(62)	1.39(3)	C(62)	H(127)	0.972
C(62)	H(128)	0.973	C(62)	H(129)	0.935
C(63)	C(64)	1.50(3)	C(64)	H(130)	1.020
C(64)	H(131)	0.931	C(64)	H(132)	0.919
C(65)	C(66)	1.46(3)	C(66)	H(133)	1.059
C(66)	H(134)	0.938	C(66)	H(135)	0.969
C(67)	C(68)	1.65(3)	C(68)	H(136)	0.936
C(68)	H(137)	1.005	C(68)	H(138)	0.942
C(69)	C(70)	1.73(5)	C(70)	H(139)	0.929
C(70)	H(140)	1.049	C(70)	H(141)	1.002
C(71)	C(72)	1.39(3)	C(72)	H(142)	1.018
C(72)	H(143)	0.971	C(72)	H(144)	1.031
C(3)	C(5)	1.54(4)	C(3)	C(4)	1.54(4)
C(8)	C(10)	1.54(4)	C(8)	C(9)	1.54(4)
C(13)	C(15)	1.54(4)	C(13)	C(14)	1.54(5)

atom	atom	distance	atom	atom	distance
C(18)	C(19)	1.54(3)	C(18)	C(20)	1.54(3)
C(23)	C(24)	1.54(4)	C(23)	C(25)	1.54(4)
C(28)	C(29)	1.54(4)	C(28)	C(30)	1.54(4)
C(38)	C(39)	1.54(4)	C(38)	C(40)	1.54(3)
C(43)	C(44)	1.54(3)	C(43)	C(45)	1.54(3)
C(48)	C(49)	1.54(3)	C(48)	C(50)	1.54(3)
C(53)	C(54)	1.54(5)	C(53)	C(55)	1.54(4)
C(58)	C(59)	1.54(2)	C(58)	C(60)	1.54(3)
C(33)	C(34)	1.54(6)	C(33)	C(35)	1.54(6)

Table 4. Bond Angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
O(1)	Pr(1)	O(3)	66.8(3)	O(1)	Pr(1)	O(5)	76.6(3)
O(1)	Pr(1)	O(7)	69.0(3)	O(1)	Pr(1)	O(9)	73.3(3)
O(1)	Pr(1)	O(11)	132.9(3)	O(1)	Pr(1)	O(25)	137.6(2)
O(1)	Pr(1)	O(26)	95.9(3)	O(1)	Pr(1)	O(27)	142.7(3)
O(3)	Pr(1)	O(5)	133.7(3)	O(3)	Pr(1)	O(7)	120.2(3)
O(3)	Pr(1)	O(9)	69.6(3)	O(3)	Pr(1)	O(11)	117.7(3)
O(3)	Pr(1)	O(25)	71.6(2)	O(3)	Pr(1)	O(26)	76.6(2)
O(3)	Pr(1)	O(27)	132.8(3)	O(5)	Pr(1)	O(7)	67.3(3)
O(5)	Pr(1)	O(9)	73.4(3)	O(5)	Pr(1)	O(11)	69.1(3)
O(5)	Pr(1)	O(25)	142.9(2)	O(5)	Pr(1)	O(26)	136.5(2)
O(5)	Pr(1)	O(27)	93.5(2)	O(7)	Pr(1)	O(9)	130.2(3)
O(7)	Pr(1)	O(11)	121.8(2)	O(7)	Pr(1)	O(25)	129.7(3)
O(7)	Pr(1)	O(26)	70.0(2)	O(7)	Pr(1)	O(27)	74.0(3)
O(9)	Pr(1)	O(11)	66.7(3)	O(9)	Pr(1)	O(25)	100.1(3)
O(9)	Pr(1)	O(26)	146.1(2)	O(9)	Pr(1)	O(27)	138.8(3)
O(11)	Pr(1)	O(25)	74.8(2)	O(11)	Pr(1)	O(26)	131.2(3)
O(11)	Pr(1)	O(27)	72.1(3)	O(25)	Pr(1)	O(26)	66.0(2)
O(25)	Pr(1)	O(27)	67.1(2)	O(26)	Pr(1)	O(27)	66.6(2)
O(13)	Pr(2)	O(15)	67.5(3)	O(13)	Pr(2)	O(17)	73.6(3)
O(13)	Pr(2)	O(19)	69.4(3)	O(13)	Pr(2)	O(21)	72.6(3)
O(13)	Pr(2)	O(23)	129.9(3)	O(13)	Pr(2)	O(25)	99.2(3)
O(13)	Pr(2)	O(26)	138.5(3)	O(13)	Pr(2)	O(27)	145.4(3)
O(15)	Pr(2)	O(17)	133.9(3)	O(15)	Pr(2)	O(19)	117.9(3)
O(15)	Pr(2)	O(21)	71.0(3)	O(15)	Pr(2)	O(23)	120.3(3)
O(15)	Pr(2)	O(25)	74.2(3)	O(15)	Pr(2)	O(26)	71.1(3)
O(15)	Pr(2)	O(27)	131.1(3)	O(17)	Pr(2)	O(19)	66.9(3)
O(17)	Pr(2)	O(21)	74.7(3)	O(17)	Pr(2)	O(23)	69.3(3)
O(17)	Pr(2)	O(25)	137.1(3)	O(17)	Pr(2)	O(26)	144.2(3)
O(17)	Pr(2)	O(27)	95.0(3)	O(19)	Pr(2)	O(21)	131.7(3)
O(19)	Pr(2)	O(23)	121.5(2)	O(19)	Pr(2)	O(25)	71.0(2)

atom	atom	atom	angle	atom	atom	atom	angle
O(19)	Pr(2)	O(26)	130.6(3)	O(19)	Pr(2)	O(27)	76.0(3)
O(21)	Pr(2)	O(23)	66.0(3)	O(21)	Pr(2)	O(25)	144.8(3)
O(21)	Pr(2)	O(26)	97.6(3)	O(21)	Pr(2)	O(27)	136.8(3)
O(23)	Pr(2)	O(25)	130.9(2)	O(23)	Pr(2)	O(26)	75.5(2)
O(23)	Pr(2)	O(27)	71.1(3)	O(25)	Pr(2)	O(26)	65.4(2)
O(25)	Pr(2)	O(27)	66.8(2)	O(26)	Pr(2)	O(27)	66.5(2)
O(28)	Pr(3)	O(29)	48.6(4)	O(28)	Pr(3)	O(31)	69.3(4)
O(28)	Pr(3)	O(32)	113.9(4)	O(28)	Pr(3)	O(34)	68.0(4)
O(28)	Pr(3)	O(35)	65.1(4)	O(28)	Pr(3)	O(37)	124.3(4)
O(28)	Pr(3)	O(38)	133.2(4)	O(28)	Pr(3)	O(40)	100.5(4)
O(28)	Pr(3)	O(41)	65.2(4)	O(28)	Pr(3)	O(43)	161.3(4)
O(28)	Pr(3)	O(44)	112.0(4)	O(29)	Pr(3)	O(31)	70.7(4)
O(29)	Pr(3)	O(32)	114.7(4)	O(29)	Pr(3)	O(34)	112.3(4)
O(29)	Pr(3)	O(35)	109.0(3)	O(29)	Pr(3)	O(37)	129.5(4)
O(29)	Pr(3)	O(38)	178.1(3)	O(29)	Pr(3)	O(40)	65.9(4)
O(29)	Pr(3)	O(41)	65.4(4)	O(29)	Pr(3)	O(43)	112.8(4)
O(29)	Pr(3)	O(44)	68.2(4)	O(31)	Pr(3)	O(32)	48.9(4)
O(31)	Pr(3)	O(34)	66.7(4)	O(31)	Pr(3)	O(35)	110.0(4)
O(31)	Pr(3)	O(37)	159.6(4)	O(31)	Pr(3)	O(38)	109.8(4)
O(31)	Pr(3)	O(40)	127.5(4)	O(31)	Pr(3)	O(41)	130.7(4)
O(31)	Pr(3)	O(43)	104.4(4)	O(31)	Pr(3)	O(44)	68.6(4)
O(32)	Pr(3)	O(34)	68.1(3)	O(32)	Pr(3)	O(35)	112.5(3)
O(32)	Pr(3)	O(37)	111.6(4)	O(32)	Pr(3)	O(38)	65.1(4)
O(32)	Pr(3)	O(40)	132.7(3)	O(32)	Pr(3)	O(41)	178.8(3)
O(32)	Pr(3)	O(43)	68.7(4)	O(32)	Pr(3)	O(44)	68.7(4)
O(34)	Pr(3)	O(35)	48.5(4)	O(34)	Pr(3)	O(37)	102.5(4)
O(34)	Pr(3)	O(38)	69.4(4)	O(34)	Pr(3)	O(40)	158.8(4)
O(34)	Pr(3)	O(41)	110.8(3)	O(34)	Pr(3)	O(43)	126.9(4)
O(34)	Pr(3)	O(44)	131.4(4)	O(35)	Pr(3)	O(37)	69.0(3)
O(35)	Pr(3)	O(38)	72.5(3)	O(35)	Pr(3)	O(40)	110.9(3)
O(35)	Pr(3)	O(41)	66.5(3)	O(35)	Pr(3)	O(43)	132.4(4)
O(35)	Pr(3)	O(44)	177.1(4)	O(37)	Pr(3)	O(38)	49.8(4)

atom	atom	atom	angle	atom	atom	atom	angle
O(37)	Pr(3)	O(40)	68.4(4)	O(37)	Pr(3)	O(41)	68.7(4)
O(37)	Pr(3)	O(43)	67.3(4)	O(37)	Pr(3)	O(44)	113.2(4)
O(38)	Pr(3)	O(40)	112.7(4)	O(38)	Pr(3)	O(41)	114.8(4)
O(38)	Pr(3)	O(43)	65.3(4)	O(38)	Pr(3)	O(44)	110.3(4)
O(40)	Pr(3)	O(41)	48.4(3)	O(40)	Pr(3)	O(43)	68.7(4)
O(40)	Pr(3)	O(44)	68.8(4)	O(41)	Pr(3)	O(43)	112.4(4)
O(41)	Pr(3)	O(44)	112.3(4)	O(43)	Pr(3)	O(44)	50.4(4)
O(46)	Pr(4)	O(47)	49.3(3)	O(46)	Pr(4)	O(49)	65.4(4)
O(46)	Pr(4)	O(50)	110.1(4)	O(46)	Pr(4)	O(52)	66.8(3)
O(46)	Pr(4)	O(53)	112.3(4)	O(46)	Pr(4)	O(55)	131.6(4)
O(46)	Pr(4)	O(56)	174.9(4)	O(46)	Pr(4)	O(58)	69.0(4)
O(46)	Pr(4)	O(59)	68.4(3)	O(46)	Pr(4)	O(61)	116.0(5)
O(46)	Pr(4)	O(62)	118.4(5)	O(47)	Pr(4)	O(49)	65.4(4)
O(47)	Pr(4)	O(50)	112.6(4)	O(47)	Pr(4)	O(52)	113.1(4)
O(47)	Pr(4)	O(53)	161.2(4)	O(47)	Pr(4)	O(55)	126.7(5)
O(47)	Pr(4)	O(56)	135.4(4)	O(47)	Pr(4)	O(58)	69.7(4)
O(47)	Pr(4)	O(59)	104.0(4)	O(47)	Pr(4)	O(61)	70.6(5)
O(47)	Pr(4)	O(62)	75.7(6)	O(49)	Pr(4)	O(50)	51.0(5)
O(49)	Pr(4)	O(52)	72.6(4)	O(49)	Pr(4)	O(53)	105.7(4)
O(49)	Pr(4)	O(55)	162.6(5)	O(49)	Pr(4)	O(56)	113.6(5)
O(49)	Pr(4)	O(58)	129.9(4)	O(49)	Pr(4)	O(59)	125.0(4)
O(49)	Pr(4)	O(61)	111.3(5)	O(49)	Pr(4)	O(62)	68.0(6)
O(50)	Pr(4)	O(52)	69.2(4)	O(50)	Pr(4)	O(53)	66.8(4)
O(50)	Pr(4)	O(55)	112.4(5)	O(50)	Pr(4)	O(56)	67.1(5)
O(50)	Pr(4)	O(58)	176.2(4)	O(50)	Pr(4)	O(59)	127.8(4)
O(50)	Pr(4)	O(61)	111.7(5)	O(50)	Pr(4)	O(62)	63.2(5)
O(52)	Pr(4)	O(53)	48.4(4)	O(52)	Pr(4)	O(55)	108.4(4)
O(52)	Pr(4)	O(56)	108.0(4)	O(52)	Pr(4)	O(58)	107.3(4)
O(52)	Pr(4)	O(59)	62.7(3)	O(52)	Pr(4)	O(61)	175.8(5)
O(52)	Pr(4)	O(62)	130.6(5)	O(53)	Pr(4)	O(55)	66.4(5)
O(53)	Pr(4)	O(56)	62.8(4)	O(53)	Pr(4)	O(58)	110.0(4)
O(53)	Pr(4)	O(59)	66.7(4)	O(53)	Pr(4)	O(61)	127.8(5)

atom	atom	atom	angle	atom	atom	atom	angle
O(53)	Pr(4)	O(62)	117.4(6)	O(55)	Pr(4)	O(56)	49.1(5)
O(55)	Pr(4)	O(58)	67.1(5)	O(55)	Pr(4)	O(59)	67.6(4)
O(55)	Pr(4)	O(61)	67.4(5)	O(55)	Pr(4)	O(62)	101.1(6)
O(56)	Pr(4)	O(58)	113.6(5)	O(56)	Pr(4)	O(59)	109.6(4)
O(56)	Pr(4)	O(61)	69.1(5)	O(56)	Pr(4)	O(62)	64.6(6)
O(58)	Pr(4)	O(59)	48.4(3)	O(58)	Pr(4)	O(61)	71.7(5)
O(58)	Pr(4)	O(62)	120.6(5)	O(59)	Pr(4)	O(61)	114.9(5)
O(59)	Pr(4)	O(62)	166.1(5)	O(61)	Pr(4)	O(62)	51.5(6)
O(1)	Ni(1)	O(3)	85.5(3)	O(1)	Ni(1)	O(10)	88.3(4)
O(1)	Ni(1)	N(1)	80.2(4)	O(1)	Ni(1)	N(2)	165.4(4)
O(1)	Ni(1)	N(13)	92.9(4)	O(3)	Ni(1)	O(10)	92.3(4)
O(3)	Ni(1)	N(1)	165.7(4)	O(3)	Ni(1)	N(2)	79.9(4)
O(3)	Ni(1)	N(13)	89.8(4)	O(10)	Ni(1)	N(1)	86.9(4)
O(10)	Ni(1)	N(2)	90.5(4)	O(10)	Ni(1)	N(13)	177.6(4)
N(1)	Ni(1)	N(2)	114.3(5)	N(1)	Ni(1)	N(13)	91.2(5)
N(2)	Ni(1)	N(13)	88.9(5)	O(2)	Ni(2)	O(5)	88.3(3)
O(2)	Ni(2)	O(7)	91.2(3)	O(2)	Ni(2)	N(3)	87.4(4)
O(2)	Ni(2)	N(4)	88.4(4)	O(2)	Ni(2)	N(14)	179.2(4)
O(5)	Ni(2)	O(7)	85.3(3)	O(5)	Ni(2)	N(3)	83.7(4)
O(5)	Ni(2)	N(4)	166.9(4)	O(5)	Ni(2)	N(14)	91.0(4)
O(7)	Ni(2)	N(3)	169.0(4)	O(7)	Ni(2)	N(4)	82.1(4)
O(7)	Ni(2)	N(14)	89.2(4)	N(3)	Ni(2)	N(4)	108.8(5)
N(3)	Ni(2)	N(14)	92.1(4)	N(4)	Ni(2)	N(14)	92.3(4)
O(6)	Ni(3)	O(9)	89.4(4)	O(6)	Ni(3)	O(11)	89.3(4)
O(6)	Ni(3)	N(5)	89.0(5)	O(6)	Ni(3)	N(6)	88.5(4)
O(6)	Ni(3)	N(15)	178.7(5)	O(9)	Ni(3)	O(11)	85.3(3)
O(9)	Ni(3)	N(5)	83.6(4)	O(9)	Ni(3)	N(6)	167.5(4)
O(9)	Ni(3)	N(15)	89.4(5)	O(11)	Ni(3)	N(5)	168.8(4)
O(11)	Ni(3)	N(6)	82.4(4)	O(11)	Ni(3)	N(15)	90.1(5)
N(5)	Ni(3)	N(6)	108.6(5)	N(5)	Ni(3)	N(15)	91.4(5)
N(6)	Ni(3)	N(15)	92.6(5)	O(13)	Ni(4)	O(15)	87.2(4)
O(13)	Ni(4)	O(22)	89.5(4)	O(13)	Ni(4)	N(7)	81.6(5)

atom	atom	atom	angle	atom	atom	atom	angle
O(13)	Ni(4)	N(8)	167.1(5)	O(13)	Ni(4)	N(16)	91.6(5)
O(15)	Ni(4)	O(22)	90.7(4)	O(15)	Ni(4)	N(7)	168.4(5)
O(15)	Ni(4)	N(8)	79.9(4)	O(15)	Ni(4)	N(16)	90.2(5)
O(22)	Ni(4)	N(7)	86.0(5)	O(22)	Ni(4)	N(8)	89.8(5)
O(22)	Ni(4)	N(16)	178.6(5)	N(7)	Ni(4)	N(8)	111.2(5)
N(7)	Ni(4)	N(16)	93.4(6)	N(8)	Ni(4)	N(16)	89.3(5)
O(14)	Ni(5)	O(17)	86.9(4)	O(14)	Ni(5)	O(19)	91.0(4)
O(14)	Ni(5)	N(9)	85.8(6)	O(14)	Ni(5)	N(10)	91.4(4)
O(14)	Ni(5)	N(17)	176.6(6)	O(17)	Ni(5)	O(19)	87.3(4)
O(17)	Ni(5)	N(9)	84.1(6)	O(17)	Ni(5)	N(10)	169.9(4)
O(17)	Ni(5)	N(17)	89.8(5)	O(19)	Ni(5)	N(9)	170.9(6)
O(19)	Ni(5)	N(10)	82.8(4)	O(19)	Ni(5)	N(17)	88.5(5)
N(9)	Ni(5)	N(10)	105.7(6)	N(9)	Ni(5)	N(17)	94.2(7)
N(10)	Ni(5)	N(17)	91.8(6)	O(18)	Ni(6)	O(21)	89.4(4)
O(18)	Ni(6)	O(23)	89.2(4)	O(18)	Ni(6)	N(11)	87.6(5)
O(18)	Ni(6)	N(12)	90.9(4)	O(18)	Ni(6)	N(18)	178.1(4)
O(21)	Ni(6)	O(23)	84.4(4)	O(21)	Ni(6)	N(11)	83.3(5)
O(21)	Ni(6)	N(12)	167.7(4)	O(21)	Ni(6)	N(18)	92.1(4)
O(23)	Ni(6)	N(11)	167.3(4)	O(23)	Ni(6)	N(12)	83.3(4)
O(23)	Ni(6)	N(18)	92.1(4)	N(11)	Ni(6)	N(12)	109.1(5)
N(11)	Ni(6)	N(18)	91.4(5)	N(12)	Ni(6)	N(18)	87.9(4)
Pr(1)	O(1)	Ni(1)	103.4(4)	Pr(1)	O(1)	C(2)	136.0(7)
Ni(1)	O(1)	C(2)	116.0(8)	Ni(2)	O(2)	C(2)	129.8(10)
Pr(1)	O(3)	Ni(1)	102.8(3)	Pr(1)	O(3)	C(7)	139.4(8)
Ni(1)	O(3)	C(7)	117.0(7)	Pr(1)	O(5)	Ni(2)	102.9(3)
Pr(1)	O(5)	C(12)	138.0(7)	Ni(2)	O(5)	C(12)	115.3(8)
Ni(3)	O(6)	C(12)	127.5(9)	Pr(1)	O(7)	Ni(2)	102.9(3)
Pr(1)	O(7)	C(17)	140.5(7)	Ni(2)	O(7)	C(17)	115.8(7)
Pr(1)	O(9)	Ni(3)	103.7(3)	Pr(1)	O(9)	C(22)	139.3(8)
Ni(3)	O(9)	C(22)	115.4(8)	Ni(1)	O(10)	C(22)	128.8(9)
Pr(1)	O(11)	Ni(3)	103.4(3)	Pr(1)	O(11)	C(27)	140.1(9)
Ni(3)	O(11)	C(27)	115.1(8)	Pr(2)	O(13)	Ni(4)	101.8(4)

atom	atom	atom	angle	atom	atom	atom	angle
Pr(2)	O(13)	C(32)	135.4(8)	Ni(4)	O(13)	C(32)	120.8(9)
Ni(5)	O(14)	C(32)	130(1)	Pr(2)	O(15)	Ni(4)	102.3(3)
Pr(2)	O(15)	C(37)	139.3(9)	Ni(4)	O(15)	C(37)	117.6(9)
Pr(2)	O(17)	Ni(5)	103.0(4)	Pr(2)	O(17)	C(42)	140.7(10)
Ni(5)	O(17)	C(42)	114.4(10)	Ni(6)	O(18)	C(42)	132(1)
Pr(2)	O(19)	Ni(5)	101.6(3)	Pr(2)	O(19)	C(47)	141.4(8)
Ni(5)	O(19)	C(47)	116.1(8)	Pr(2)	O(21)	Ni(6)	104.4(4)
Pr(2)	O(21)	C(52)	139.7(10)	Ni(6)	O(21)	C(52)	114.5(10)
Ni(4)	O(22)	C(52)	132(1)	Pr(2)	O(23)	Ni(6)	103.8(3)
Pr(2)	O(23)	C(57)	141.4(8)	Ni(6)	O(23)	C(57)	113.7(8)
Pr(1)	O(25)	Pr(2)	101.7(3)	Pr(1)	O(25)	H(121)	112.5
Pr(1)	O(25)	H(122)	111.3	Pr(2)	O(25)	H(121)	112.9
Pr(2)	O(25)	H(122)	111.7	H(121)	O(25)	H(122)	106.8
Pr(1)	O(26)	Pr(2)	100.8(3)	Pr(1)	O(26)	H(123)	111.3
Pr(1)	O(26)	H(124)	111.4	Pr(2)	O(26)	H(123)	112.6
Pr(2)	O(26)	H(124)	112.7	H(123)	O(26)	H(124)	108.0
Pr(1)	O(27)	Pr(2)	102.1(3)	Pr(1)	O(27)	H(125)	112.7
Pr(1)	O(27)	H(126)	112.0	Pr(2)	O(27)	H(125)	111.7
Pr(2)	O(27)	H(126)	111.1	H(125)	O(27)	H(126)	107.2
Pr(3)	O(28)	N(19)	97(1)	Pr(3)	O(29)	N(19)	92(1)
Pr(3)	O(31)	N(20)	92(1)	Pr(3)	O(32)	N(20)	97(1)
Pr(3)	O(34)	N(21)	94.7(9)	Pr(3)	O(35)	N(21)	95.0(8)
Pr(3)	O(37)	N(22)	94.5(10)	Pr(3)	O(38)	N(22)	98.5(10)
Pr(3)	O(40)	N(23)	93(1)	Pr(3)	O(41)	N(23)	95(1)
Pr(3)	O(43)	N(24)	93.1(10)	Pr(3)	O(44)	N(24)	90.1(8)
Pr(4)	O(46)	N(25)	94.7(9)	Pr(4)	O(47)	N(25)	98(1)
Pr(4)	O(49)	N(26)	90(1)	Pr(4)	O(50)	N(26)	92(1)
Pr(4)	O(52)	N(27)	94.8(9)	Pr(4)	O(53)	N(27)	97(1)
Pr(4)	O(55)	N(28)	95(1)	Pr(4)	O(56)	N(28)	91(1)
Pr(4)	O(58)	N(29)	97.8(10)	Pr(4)	O(59)	N(29)	97.8(9)
Pr(4)	O(61)	N(30)	81(1)	Pr(4)	O(62)	N(30)	93(1)
Ni(1)	N(1)	C(1)	112.1(9)	Ni(1)	N(1)	H(1)	109.0

atom	atom	atom	angle	atom	atom	atom	angle
Ni(1)	N(1)	H(2)	108.9	C(1)	N(1)	H(1)	107.0
C(1)	N(1)	H(2)	109.6	H(1)	N(1)	H(2)	110.3
Ni(1)	N(2)	C(6)	112.1(8)	Ni(1)	N(2)	H(3)	109.3
Ni(1)	N(2)	H(4)	107.3	C(6)	N(2)	H(3)	110.3
C(6)	N(2)	H(4)	108.4	H(3)	N(2)	H(4)	109.4
Ni(2)	N(3)	C(11)	108.1(9)	Ni(2)	N(3)	H(5)	110.2
Ni(2)	N(3)	H(6)	110.1	C(11)	N(3)	H(5)	108.8
C(11)	N(3)	H(6)	109.8	H(5)	N(3)	H(6)	109.8
Ni(2)	N(4)	C(16)	110.3(8)	Ni(2)	N(4)	H(7)	109.1
Ni(2)	N(4)	H(8)	108.7	C(16)	N(4)	H(7)	110.1
C(16)	N(4)	H(8)	108.9	H(7)	N(4)	H(8)	109.8
Ni(3)	N(5)	C(21)	108(1)	Ni(3)	N(5)	H(9)	110.0
Ni(3)	N(5)	H(10)	109.4	C(21)	N(5)	H(9)	110.4
C(21)	N(5)	H(10)	110.0	H(9)	N(5)	H(10)	108.8
Ni(3)	N(6)	C(26)	111.6(8)	Ni(3)	N(6)	H(11)	108.1
Ni(3)	N(6)	H(12)	108.5	C(26)	N(6)	H(11)	110.0
C(26)	N(6)	H(12)	110.6	H(11)	N(6)	H(12)	108.1
Ni(4)	N(7)	C(31)	109(1)	Ni(4)	N(7)	H(13)	107.4
Ni(4)	N(7)	H(14)	107.5	C(31)	N(7)	H(13)	111.1
C(31)	N(7)	H(14)	112.9	H(13)	N(7)	H(14)	108.3
Ni(4)	N(8)	C(36)	111.6(9)	Ni(4)	N(8)	H(15)	109.1
Ni(4)	N(8)	H(16)	109.1	C(36)	N(8)	H(15)	108.7
C(36)	N(8)	H(16)	108.8	H(15)	N(8)	H(16)	109.6
Ni(5)	N(9)	C(41)	110(1)	Ni(5)	N(9)	H(17)	112.5
Ni(5)	N(9)	H(18)	108.0	C(41)	N(9)	H(17)	110.3
C(41)	N(9)	H(18)	105.3	H(17)	N(9)	H(18)	110.2
Ni(5)	N(10)	C(46)	111.8(9)	Ni(5)	N(10)	H(19)	109.5
Ni(5)	N(10)	H(20)	109.4	C(46)	N(10)	H(19)	107.5
C(46)	N(10)	H(20)	108.3	H(19)	N(10)	H(20)	110.3
Ni(6)	N(11)	C(51)	110.3(10)	Ni(6)	N(11)	H(21)	109.7
Ni(6)	N(11)	H(22)	110.3	C(51)	N(11)	H(21)	109.2
C(51)	N(11)	H(22)	108.7	H(21)	N(11)	H(22)	108.6

atom	atom	atom	angle	atom	atom	atom	angle
Ni(6)	N(12)	C(56)	109.4(8)	Ni(6)	N(12)	H(23)	111.0
Ni(6)	N(12)	H(24)	109.6	C(56)	N(12)	H(23)	109.8
C(56)	N(12)	H(24)	108.5	H(23)	N(12)	H(24)	108.4
Ni(1)	N(13)	C(61)	169(1)	Ni(2)	N(14)	C(63)	170(1)
Ni(3)	N(15)	C(65)	169(1)	Ni(4)	N(16)	C(67)	163(1)
Ni(5)	N(17)	C(69)	172(2)	Ni(6)	N(18)	C(71)	171(1)
O(28)	N(19)	O(29)	121(1)	O(28)	N(19)	O(30)	120(1)
O(29)	N(19)	O(30)	117(1)	O(31)	N(20)	O(32)	119(1)
O(31)	N(20)	O(33)	112(1)	O(32)	N(20)	O(33)	125(1)
O(34)	N(21)	O(35)	119(1)	O(34)	N(21)	O(36)	124(1)
O(35)	N(21)	O(36)	115(1)	O(37)	N(22)	O(38)	117(1)
O(37)	N(22)	O(39)	117(1)	O(38)	N(22)	O(39)	125(1)
O(40)	N(23)	O(41)	122(1)	O(40)	N(23)	O(42)	120(1)
O(41)	N(23)	O(42)	115(1)	O(43)	N(24)	O(44)	126(1)
O(43)	N(24)	O(45)	127(1)	O(44)	N(24)	O(45)	105(1)
O(46)	N(25)	O(47)	117(1)	O(46)	N(25)	O(48)	113(1)
O(47)	N(25)	O(48)	128(1)	O(49)	N(26)	O(50)	124(2)
O(49)	N(26)	O(51)	118(2)	O(50)	N(26)	O(51)	116(2)
O(52)	N(27)	O(53)	119(1)	O(52)	N(27)	O(54)	108(1)
O(53)	N(27)	O(54)	132(1)	O(55)	N(28)	O(56)	115(2)
O(55)	N(28)	O(57)	123(3)	O(56)	N(28)	O(57)	110(3)
O(58)	N(29)	O(59)	115(1)	O(58)	N(29)	O(60)	120(1)
O(59)	N(29)	O(60)	123(1)	O(61)	N(30)	O(62)	117(2)
O(61)	N(30)	O(63)	115(2)	O(62)	N(30)	O(63)	119(2)
N(1)	C(1)	C(2)	109(1)	N(1)	C(1)	H(25)	110.4
N(1)	C(1)	C(3)	118(1)	C(2)	C(1)	H(25)	108.2
C(2)	C(1)	C(3)	105(1)	H(25)	C(1)	C(3)	104.4
O(1)	C(2)	O(2)	123(1)	O(1)	C(2)	C(1)	114(1)
O(2)	C(2)	C(1)	122(1)	N(2)	C(6)	C(7)	112(1)
N(2)	C(6)	H(33)	107.1	N(2)	C(6)	C(8)	109(1)
C(7)	C(6)	H(33)	108.8	C(7)	C(6)	C(8)	111(1)
H(33)	C(6)	C(8)	107.4	O(3)	C(7)	O(4)	123(1)

atom	atom	atom	angle	atom	atom	atom	angle
O(3)	C(7)	C(6)	116(1)	O(4)	C(7)	C(6)	119(1)
N(3)	C(11)	C(12)	115(1)	N(3)	C(11)	H(41)	104.7
N(3)	C(11)	C(13)	116(1)	C(12)	C(11)	H(41)	102.5
C(12)	C(11)	C(13)	110(1)	H(41)	C(11)	C(13)	105.5
O(5)	C(12)	O(6)	123(1)	O(5)	C(12)	C(11)	113(1)
O(6)	C(12)	C(11)	123(1)	N(4)	C(16)	C(17)	109(1)
N(4)	C(16)	H(49)	106.4	N(4)	C(16)	C(18)	117(1)
C(17)	C(16)	H(49)	106.3	C(17)	C(16)	C(18)	111(1)
H(49)	C(16)	C(18)	105.6	O(7)	C(17)	O(8)	125(1)
O(7)	C(17)	C(16)	117(1)	O(8)	C(17)	C(16)	117(1)
N(5)	C(21)	C(22)	113(1)	N(5)	C(21)	H(57)	105.7
N(5)	C(21)	C(23)	112(1)	C(22)	C(21)	H(57)	106.2
C(22)	C(21)	C(23)	111(1)	H(57)	C(21)	C(23)	106.0
O(9)	C(22)	O(10)	122(1)	O(9)	C(22)	C(21)	115(1)
O(10)	C(22)	C(21)	121(1)	N(6)	C(26)	C(27)	106(1)
N(6)	C(26)	H(65)	105.6	N(6)	C(26)	C(28)	122(1)
C(27)	C(26)	H(65)	107.0	C(27)	C(26)	C(28)	111(1)
H(65)	C(26)	C(28)	103.0	O(11)	C(27)	O(12)	123(1)
O(11)	C(27)	C(26)	116(1)	O(12)	C(27)	C(26)	119(1)
N(7)	C(31)	C(32)	125(1)	N(7)	C(31)	H(73)	101.2
N(7)	C(31)	C(33)	125(1)	C(32)	C(31)	H(73)	106.4
C(32)	C(31)	C(33)	94(1)	H(73)	C(31)	C(33)	102.1
O(13)	C(32)	O(14)	125(1)	O(13)	C(32)	C(31)	101(1)
O(14)	C(32)	C(31)	133(1)	N(8)	C(36)	C(37)	109(1)
N(8)	C(36)	H(81)	106.5	N(8)	C(36)	C(38)	117(1)
C(37)	C(36)	H(81)	105.7	C(37)	C(36)	C(38)	115(1)
H(81)	C(36)	C(38)	100.8	O(15)	C(37)	O(16)	127(1)
O(15)	C(37)	C(36)	114(1)	O(16)	C(37)	C(36)	118(1)
N(9)	C(41)	C(42)	106(1)	N(9)	C(41)	H(89)	109.0
N(9)	C(41)	C(43)	113(1)	C(42)	C(41)	H(89)	109.5
C(42)	C(41)	C(43)	109(1)	H(89)	C(41)	C(43)	108.4
O(17)	C(42)	O(18)	118(1)	O(17)	C(42)	C(41)	119(1)

atom	atom	atom	angle	atom	atom	atom	angle
O(18)	C(42)	C(41)	119(1)	N(10)	C(46)	C(47)	109(1)
N(10)	C(46)	H(97)	104.6	N(10)	C(46)	C(48)	119(1)
C(47)	C(46)	H(97)	104.1	C(47)	C(46)	C(48)	114(1)
H(97)	C(46)	C(48)	102.1	O(19)	C(47)	O(20)	123(1)
O(19)	C(47)	C(46)	117(1)	O(20)	C(47)	C(46)	118(1)
N(11)	C(51)	C(52)	114(1)	N(11)	C(51)	H(105)	105.2
N(11)	C(51)	C(53)	109(1)	C(52)	C(51)	H(105)	105.5
C(52)	C(51)	C(53)	114(1)	H(105)	C(51)	C(53)	106.0
O(21)	C(52)	O(22)	118(1)	O(21)	C(52)	C(51)	116(1)
O(22)	C(52)	C(51)	124(1)	N(12)	C(56)	C(57)	109(1)
N(12)	C(56)	H(113)	106.4	N(12)	C(56)	C(58)	117(1)
C(57)	C(56)	H(113)	105.6	C(57)	C(56)	C(58)	111(1)
H(113)	C(56)	C(58)	105.6	O(23)	C(57)	O(24)	122(1)
O(23)	C(57)	C(56)	117(1)	O(24)	C(57)	C(56)	120(1)
N(13)	C(61)	C(62)	173(2)	C(61)	C(62)	H(127)	109.9
C(61)	C(62)	H(128)	111.0	C(61)	C(62)	H(129)	112.2
H(127)	C(62)	H(128)	105.8	H(127)	C(62)	H(129)	108.9
H(128)	C(62)	H(129)	108.8	N(14)	C(63)	C(64)	174(1)
C(63)	C(64)	H(130)	106.9	C(63)	C(64)	H(131)	111.3
C(63)	C(64)	H(132)	112.7	H(130)	C(64)	H(131)	105.2
H(130)	C(64)	H(132)	106.1	H(131)	C(64)	H(132)	113.9
N(15)	C(65)	C(66)	178(2)	C(65)	C(66)	H(133)	109.4
C(65)	C(66)	H(134)	116.8	C(65)	C(66)	H(135)	117.6
H(133)	C(66)	H(134)	101.8	H(133)	C(66)	H(135)	99.8
H(134)	C(66)	H(135)	108.9	N(16)	C(67)	C(68)	173(2)
C(67)	C(68)	H(136)	112.5	C(67)	C(68)	H(137)	107.7
C(67)	C(68)	H(138)	113.1	H(136)	C(68)	H(137)	106.0
H(136)	C(68)	H(138)	111.4	H(137)	C(68)	H(138)	105.6
N(17)	C(69)	C(70)	174(3)	C(69)	C(70)	H(139)	120.0
C(69)	C(70)	H(140)	111.1	C(69)	C(70)	H(141)	114.6
H(139)	C(70)	H(140)	103.2	H(139)	C(70)	H(141)	106.9
H(140)	C(70)	H(141)	98.3	N(18)	C(71)	C(72)	177(1)

atom	atom	atom	angle	atom	atom	atom	angle
C(71)	C(72)	H(142)	116.5	C(71)	C(72)	H(143)	118.9
C(71)	C(72)	H(144)	115.9	H(142)	C(72)	H(143)	102.4
H(142)	C(72)	H(144)	98.4	H(143)	C(72)	H(144)	101.5
C(1)	C(3)	H(26)	116.9	C(1)	C(3)	C(5)	112(2)
C(1)	C(3)	C(4)	92(2)	H(26)	C(3)	C(5)	107.4
H(26)	C(3)	C(4)	117.3	C(5)	C(3)	C(4)	109(2)
H(30)	C(5)	H(31)	111.5	H(30)	C(5)	H(32)	100.7
H(30)	C(5)	C(3)	121.4	H(31)	C(5)	H(32)	95.9
H(31)	C(5)	C(3)	114.6	H(32)	C(5)	C(3)	108.3
H(27)	C(4)	H(28)	124.7	H(27)	C(4)	H(29)	113.4
H(27)	C(4)	C(3)	114.2	H(28)	C(4)	H(29)	96.4
H(28)	C(4)	C(3)	104.4	H(29)	C(4)	C(3)	99.8
C(6)	C(8)	H(34)	104.4	C(6)	C(8)	C(10)	111(1)
C(6)	C(8)	C(9)	117(1)	H(34)	C(8)	C(10)	109.8
H(34)	C(8)	C(9)	103.5	C(10)	C(8)	C(9)	109(1)
H(38)	C(10)	H(39)	109.3	H(38)	C(10)	H(40)	113.9
H(38)	C(10)	C(8)	106.2	H(39)	C(10)	H(40)	112.6
H(39)	C(10)	C(8)	105.6	H(40)	C(10)	C(8)	108.7
H(35)	C(9)	H(36)	110.5	H(35)	C(9)	H(37)	105.5
H(35)	C(9)	C(8)	109.3	H(36)	C(9)	H(37)	109.0
H(36)	C(9)	C(8)	111.9	H(37)	C(9)	C(8)	110.4
C(11)	C(13)	H(42)	109.7	C(11)	C(13)	C(15)	104(2)
C(11)	C(13)	C(14)	107(2)	H(42)	C(13)	C(15)	116.4
H(42)	C(13)	C(14)	108.9	C(15)	C(13)	C(14)	109(2)
H(46)	C(15)	H(47)	117.9	H(46)	C(15)	H(48)	114.1
H(46)	C(15)	C(13)	106.2	H(47)	C(15)	H(48)	109.3
H(47)	C(15)	C(13)	104.3	H(48)	C(15)	C(13)	103.5
H(43)	C(14)	H(44)	102.5	H(43)	C(14)	H(45)	113.1
H(43)	C(14)	C(13)	110.7	H(44)	C(14)	H(45)	107.7
H(44)	C(14)	C(13)	109.9	H(45)	C(14)	C(13)	112.5
C(16)	C(18)	H(50)	107.1	C(16)	C(18)	C(19)	113(1)
C(16)	C(18)	C(20)	108(1)	H(50)	C(18)	C(19)	106.3

atom	atom	atom	angle	atom	atom	atom	angle
H(50)	C(18)	C(20)	111.7	C(19)	C(18)	C(20)	109(1)
H(51)	C(19)	H(52)	104.5	H(51)	C(19)	H(53)	108.9
H(51)	C(19)	C(18)	110.2	H(52)	C(19)	H(53)	109.4
H(52)	C(19)	C(18)	111.8	H(53)	C(19)	C(18)	111.8
H(54)	C(20)	H(55)	112.3	H(54)	C(20)	H(56)	107.2
H(54)	C(20)	C(18)	105.1	H(55)	C(20)	H(56)	116.9
H(55)	C(20)	C(18)	109.0	H(56)	C(20)	C(18)	105.6
C(21)	C(23)	H(58)	110.8	C(21)	C(23)	C(24)	112(2)
C(21)	C(23)	C(25)	109(2)	H(58)	C(23)	C(24)	106.7
H(58)	C(23)	C(25)	108.2	C(24)	C(23)	C(25)	109(2)
H(59)	C(24)	H(60)	110.0	H(59)	C(24)	H(61)	107.9
H(59)	C(24)	C(23)	112.5	H(60)	C(24)	H(61)	105.5
H(60)	C(24)	C(23)	111.1	H(61)	C(24)	C(23)	109.5
H(62)	C(25)	H(63)	108.5	H(62)	C(25)	H(64)	106.7
H(62)	C(25)	C(23)	107.5	H(63)	C(25)	H(64)	113.0
H(63)	C(25)	C(23)	112.0	H(64)	C(25)	C(23)	108.9
C(26)	C(28)	H(66)	116.0	C(26)	C(28)	C(29)	103(2)
C(26)	C(28)	C(30)	107(2)	H(66)	C(28)	C(29)	105.6
H(66)	C(28)	C(30)	113.5	C(29)	C(28)	C(30)	109(2)
H(67)	C(29)	H(68)	97.8	H(67)	C(29)	H(69)	102.4
H(67)	C(29)	C(28)	110.1	H(68)	C(29)	H(69)	108.7
H(68)	C(29)	C(28)	115.8	H(69)	C(29)	C(28)	119.1
H(70)	C(30)	H(71)	110.9	H(70)	C(30)	H(72)	105.5
H(70)	C(30)	C(28)	108.4	H(71)	C(30)	H(72)	113.1
H(71)	C(30)	C(28)	108.3	H(72)	C(30)	C(28)	110.5
C(36)	C(38)	H(82)	102.9	C(36)	C(38)	C(39)	112(2)
C(36)	C(38)	C(40)	124(2)	H(82)	C(38)	C(39)	95.8
H(82)	C(38)	C(40)	107.0	C(39)	C(38)	C(40)	109(2)
H(83)	C(39)	H(84)	100.3	H(83)	C(39)	H(85)	104.0
H(83)	C(39)	C(38)	109.9	H(84)	C(39)	H(85)	107.0
H(84)	C(39)	C(38)	114.9	H(85)	C(39)	C(38)	118.7
H(86)	C(40)	H(87)	116.5	H(86)	C(40)	H(88)	108.8

atom	atom	atom	angle	atom	atom	atom	angle
H(86)	C(40)	C(38)	104.5	H(87)	C(40)	H(88)	110.7
H(87)	C(40)	C(38)	111.8	H(88)	C(40)	C(38)	103.8
C(41)	C(43)	H(90)	108.2	C(41)	C(43)	C(44)	113(1)
C(41)	C(43)	C(45)	109(1)	H(90)	C(43)	C(44)	104.9
H(90)	C(43)	C(45)	111.2	C(44)	C(43)	C(45)	109(1)
H(91)	C(44)	H(92)	104.7	H(91)	C(44)	H(93)	109.2
H(91)	C(44)	C(43)	108.5	H(92)	C(44)	H(93)	110.0
H(92)	C(44)	C(43)	110.9	H(93)	C(44)	C(43)	113.2
H(94)	C(45)	H(95)	109.8	H(94)	C(45)	H(96)	111.5
H(94)	C(45)	C(43)	107.0	H(95)	C(45)	H(96)	113.0
H(95)	C(45)	C(43)	106.9	H(96)	C(45)	C(43)	108.4
C(46)	C(48)	H(98)	109.9	C(46)	C(48)	C(49)	106(1)
C(46)	C(48)	C(50)	113(1)	H(98)	C(48)	C(49)	108.9
H(98)	C(48)	C(50)	108.6	C(49)	C(48)	C(50)	109(1)
H(99)	C(49)	H(100)	109.6	H(99)	C(49)	H(101)	109.8
H(99)	C(49)	C(48)	108.9	H(100)	C(49)	H(101)	109.4
H(100)	C(49)	C(48)	109.1	H(101)	C(49)	C(48)	110.0
H(102)	C(50)	H(103)	108.6	H(102)	C(50)	H(104)	110.5
H(102)	C(50)	C(48)	109.9	H(103)	C(50)	H(104)	108.3
H(103)	C(50)	C(48)	109.4	H(104)	C(50)	C(48)	110.2
C(51)	C(53)	H(106)	98.0	C(51)	C(53)	C(54)	115(2)
C(51)	C(53)	C(55)	121(2)	H(106)	C(53)	C(54)	104.9
H(106)	C(53)	C(55)	104.5	C(54)	C(53)	C(55)	109(2)
H(107)	C(54)	H(108)	113.1	H(107)	C(54)	H(109)	118.4
H(107)	C(54)	C(53)	112.4	H(108)	C(54)	H(109)	104.0
H(108)	C(54)	C(53)	101.3	H(109)	C(54)	C(53)	105.9
H(110)	C(55)	H(111)	121.0	H(110)	C(55)	H(112)	104.7
H(110)	C(55)	C(53)	116.9	H(111)	C(55)	H(112)	98.7
H(111)	C(55)	C(53)	108.8	H(112)	C(55)	C(53)	103.2
C(56)	C(58)	H(114)	107.9	C(56)	C(58)	C(59)	109(1)
C(56)	C(58)	C(60)	110(1)	H(114)	C(58)	C(59)	108.2
H(114)	C(58)	C(60)	110.7	C(59)	C(58)	C(60)	109(1)

atom	atom	atom	angle	atom	atom	atom	angle
H(115)	C(59)	H(116)	111.8	H(115)	C(59)	H(117)	108.6
H(115)	C(59)	C(58)	110.8	H(116)	C(59)	H(117)	107.2
H(116)	C(59)	C(58)	109.6	H(117)	C(59)	C(58)	108.7
H(118)	C(60)	H(119)	109.2	H(118)	C(60)	H(120)	110.3
H(118)	C(60)	C(58)	106.9	H(119)	C(60)	H(120)	112.8
H(119)	C(60)	C(58)	108.5	H(120)	C(60)	C(58)	109.0
C(31)	C(33)	H(74)	119.9	C(31)	C(33)	C(34)	101(3)
C(31)	C(33)	C(35)	106(3)	H(74)	C(33)	C(34)	106.5
H(74)	C(33)	C(35)	112.4	C(34)	C(33)	C(35)	109(3)
H(75)	C(34)	H(76)	95.2	H(75)	C(34)	H(77)	108.3
H(75)	C(34)	C(33)	111.5	H(76)	C(34)	H(77)	108.6
H(76)	C(34)	C(33)	109.6	H(77)	C(34)	C(33)	120.6
H(78)	C(35)	H(79)	108.0	H(78)	C(35)	H(80)	108.7
H(78)	C(35)	C(33)	108.6	H(79)	C(35)	H(80)	106.4
H(79)	C(35)	C(33)	110.8	H(80)	C(35)	C(33)	114.1

Table 5. Special Distances (Å)

atom	atom	distance	atom	atom	distance
Pr(1)	Pr(2)	4.0016(8)	Pr(1)	Ni(1)	3.566(2)
Pr(1)	Ni(2)	3.544(2)	Pr(1)	Ni(3)	3.566(2)
Pr(2)	Ni(4)	3.557(2)	Pr(2)	Ni(5)	3.539(2)
Pr(2)	Ni(6)	3.587(2)	Ni(1)	Ni(2)	5.346(2)
Ni(2)	Ni(3)	5.351(3)	Ni(3)	Pr(1)	3.566(2)
Ni(4)	Ni(5)	5.324(3)	Ni(5)	Ni(6)	5.351(3)
Ni(6)	Ni(4)	5.331(3)			

Table 6. Special Angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Ni(1)	Pr(1)	Ni(2)	97.50(4)	Ni(2)	Pr(1)	Ni(3)	97.61(4)
Ni(3)	Pr(1)	Ni(1)	96.29(4)	Ni(1)	Pr(1)	Pr(2)	121.79(3)
Ni(2)	Pr(1)	Pr(2)	117.76(3)	Ni(3)	Pr(1)	Pr(2)	120.56(4)
Ni(4)	Pr(2)	Ni(5)	97.23(5)	Ni(5)	Pr(2)	Ni(6)	97.34(5)
Ni(6)	Pr(2)	Ni(4)	96.54(5)	Ni(4)	Pr(2)	Pr(1)	121.09(4)
Ni(5)	Pr(2)	Pr(1)	118.66(4)	Ni(6)	Pr(2)	Pr(1)	120.58(4)

Structure Factor Table for

TEA[Gd_2{$Ni(val)_2$}$_6(H_2O)_3(CH_3CN)_6$][$Gd(NO_3)_5$]$(ClO_4)_5 \cdot 7CH_3CN \cdot 2H_2O$ (3)

Table 1. Atomic coordinates and U_{eq}

atom	x	y	z	U_{eq}
Gd1	0.28632(4)	0.50180(4)	0.51929(2)	0.0313(2)
Gd2	0.40799(4)	0.48406(4)	0.60659(3)	0.0292(2)
Ni1	0.32993(10)	0.49570(10)	0.41286(6)	0.0360(6)
Ni2	0.16924(11)	0.39799(10)	0.51577(7)	0.0383(6)
Ni3	0.19752(11)	0.62975(10)	0.51320(7)	0.0362(6)
Ni4	0.55536(11)	0.54128(10)	0.59210(7)	0.0354(6)
Ni5	0.45192(11)	0.34088(9)	0.63759(7)	0.0326(6)
Ni6	0.38164(11)	0.54188(10)	0.70823(7)	0.0332(6)
O1	0.3775(5)	0.4432(5)	0.5375(3)	0.030(3)
H1A	0.3678	0.4009	0.5398	0.035
H1B	0.4097	0.4485	0.5162	0.035
O2	0.3675(5)	0.5586(5)	0.5559(4)	0.045(4)
H2B	0.3508	0.5932	0.5708	0.055
H2C	0.3989	0.5718	0.5358	0.055
O3	0.2975(5)	0.4789(4)	0.5969(3)	0.028(3)
H3B	0.2765	0.5084	0.6145	0.034
H3C	0.2818	0.4393	0.6037	0.034
O4	0.3630(5)	0.5314(5)	0.4680(3)	0.032(3)
O5	0.4331(6)	0.5905(5)	0.4927(3)	0.042(3)
O6	0.2694(5)	0.4558(5)	0.4507(3)	0.028(3)
O7	0.1884(5)	0.3995(5)	0.4504(3)	0.033(3)
O8	0.2480(5)	0.5799(5)	0.4740(4)	0.038(3)
O9	0.2683(5)	0.5655(5)	0.4058(4)	0.035(3)
O10	0.2592(5)	0.3990(5)	0.5279(3)	0.032(3)
O11	0.3381(6)	0.3368(5)	0.5320(4)	0.041(3)
O12	0.1785(5)	0.4870(5)	0.5166(3)	0.034(3)
O13	0.1269(6)	0.5696(6)	0.5056(3)	0.043(3)
O14	0.2334(6)	0.5770(5)	0.5591(4)	0.037(3)
O15	0.2267(6)	0.5601(5)	0.6297(4)	0.039(3)
O16	0.4899(5)	0.5022(5)	0.5564(3)	0.035(3)

atom	x	y	z	U_{eq}
O17	0.4746(5)	0.4587(5)	0.4952(4)	0.038(3)
O18	0.4904(5)	0.5433(4)	0.6370(3)	0.030(3)
O19	0.4726(5)	0.5682(5)	0.7035(4)	0.033(3)
O20	0.4938(6)	0.4168(5)	0.6189(3)	0.037(3)
O21	0.5811(6)	0.4594(5)	0.6178(3)	0.041(3)
O22	0.3752(5)	0.3815(5)	0.6198(4)	0.033(3)
O23	0.2760(6)	0.3751(5)	0.6239(3)	0.036(3)
O24	0.4053(6)	0.4628(4)	0.6834(3)	0.038(3)
O25	0.4452(5)	0.3758(5)	0.6982(3)	0.032(3)
O26	0.3672(5)	0.5652(5)	0.6470(3)	0.032(3)
O27	0.3393(6)	0.6424(5)	0.6073(4)	0.039(3)
N1	0.3966(6)	0.5478(6)	0.3863(4)	0.038(4)
N2	0.2861(6)	0.4514(6)	0.3652(4)	0.036(4)
N3	0.1707(7)	0.6716(6)	0.4595(4)	0.044(4)
N4	0.1810(8)	0.3079(7)	0.5133(5)	0.062(5)
N5	0.0795(7)	0.4157(7)	0.5071(5)	0.045(4)
N6	0.1507(6)	0.6673(6)	0.5620(4)	0.037(4)
N7	0.3896(9)	0.4277(8)	0.4174(6)	0.050(6)
N8	0.1543(7)	0.3945(7)	0.5799(5)	0.052(5)
N9	0.2689(7)	0.6885(6)	0.5227(4)	0.030(4)
N10	0.6102(7)	0.5237(7)	0.5398(4)	0.049(5)
N11	0.6080(6)	0.5780(6)	0.6391(4)	0.034(4)
N12	0.5373(7)	0.3179(6)	0.6552(4)	0.041(4)
N13	0.3921(6)	0.2775(6)	0.6573(4)	0.033(4)
N14	0.4014(6)	0.4980(6)	0.7632(4)	0.034(4)
N15	0.3595(6)	0.6304(6)	0.7198(4)	0.032(4)
N16	0.5315(7)	0.6231(6)	0.5656(5)	0.038(4)
N17	0.4626(8)	0.3013(7)	0.5792(5)	0.049(5)
N18	0.2917(9)	0.5178(7)	0.7147(4)	0.047(4)
C1	0.4127(9)	0.5619(8)	0.4634(6)	0.035(4)
C2	0.4432(8)	0.5571(8)	0.4204(5)	0.040(4)
H2A	0.4691	0.5213	0.4211	0.048

atom	x	y	z	U_{eq}
C3	0.4852(9)	0.6101(8)	0.4126(6)	0.056(6)
H3A	0.5112	0.6144	0.4382	0.067
C4	0.5278(10)	0.5960(11)	0.3749(7)	0.078(7)
H4A	0.5487	0.5589	0.3802	0.118
H4B	0.5574	0.6276	0.3717	0.118
H4C	0.5039	0.5926	0.3490	0.118
C5	0.4476(12)	0.6686(9)	0.4081(7)	0.079(8)
H5A	0.4751	0.7016	0.4032	0.119
H5B	0.4245	0.6754	0.4339	0.119
H5C	0.4198	0.6650	0.3841	0.119
C6	0.2303(9)	0.4257(8)	0.4324(5)	0.030(5)
C7	0.2334(8)	0.4195(8)	0.3836(5)	0.038(5)
H7A	0.1970	0.4406	0.3727	0.046
C8	0.2266(11)	0.3561(9)	0.3680(6)	0.059(6)
H8A	0.1918	0.3386	0.3835	0.071
C9	0.2096(11)	0.3563(10)	0.3205(7)	0.081(8)
H9A	0.1724	0.3789	0.3165	0.121
H9B	0.2033	0.3158	0.3109	0.121
H9C	0.2423	0.3742	0.3042	0.121
C10	0.2823(11)	0.3194(9)	0.3791(6)	0.073(7)
H10A	0.2887	0.3204	0.4097	0.110
H10B	0.3177	0.3357	0.3648	0.110
H10C	0.2760	0.2787	0.3700	0.110
C11	0.2439(7)	0.5915(7)	0.4339(7)	0.030(5)
C12	0.2011(8)	0.6423(7)	0.4224(5)	0.035(5)
H12A	0.1682	0.6248	0.4048	0.042
C13	0.2345(8)	0.6853(8)	0.3942(5)	0.041(5)
H13A	0.2506	0.6622	0.3699	0.049
C14	0.2880(10)	0.7124(9)	0.4160(6)	0.057(6)
H14A	0.3140	0.6814	0.4272	0.086
H14B	0.2740	0.7374	0.4392	0.086
H14C	0.3107	0.7363	0.3957	0.086

atom	x	y	z	U_{eq}
C15	0.1937(11)	0.7327(9)	0.3758(5)	0.072(8)
H15A	0.1595	0.7142	0.3614	0.108
H15B	0.2166	0.7565	0.3557	0.108
H15C	0.1787	0.7579	0.3986	0.108
C16	0.2823(12)	0.3483(9)	0.5318(5)	0.047(6)
C17	0.2396(10)	0.2957(8)	0.5341(7)	0.056(6)
H17A	0.2300	0.2906	0.5647	0.067
C18	0.2690(12)	0.2342(9)	0.5193(8)	0.080(5)
H18A	0.3066	0.2298	0.5364	0.096
C19	0.2886(12)	0.2339(9)	0.4756(7)	0.083(6)
H19A	0.3074	0.1960	0.4690	0.124
H19B	0.3179	0.2655	0.4711	0.124
H19C	0.2537	0.2400	0.4571	0.124
C20	0.2295(11)	0.1853(10)	0.5325(8)	0.082(6)
H20A	0.2472	0.1479	0.5234	0.124
H20B	0.1897	0.1900	0.5195	0.124
H20C	0.2253	0.1855	0.5632	0.124
C21	0.1301(8)	0.5168(9)	0.5090(5)	0.028(4)
C22	0.0702(9)	0.4819(9)	0.4997(6)	0.055(6)
H22A	0.0600	0.4877	0.4692	0.066
C23	0.0206(8)	0.5044(9)	0.5244(6)	0.044(5)
H23A	0.0196	0.5476	0.5188	0.052
C24	0.0287(9)	0.4985(10)	0.5721(6)	0.064(6)
H24A	0.0679	0.5147	0.5803	0.096
H24B	0.0269	0.4569	0.5800	0.096
H24C	-0.0035	0.5200	0.5866	0.096
C25	-0.0422(9)	0.4807(9)	0.5099(6)	0.058(6)
H25A	-0.0462	0.4856	0.4793	0.088
H25B	-0.0743	0.5026	0.5241	0.088
H25C	-0.0455	0.4389	0.5170	0.088
C26	0.2158(9)	0.5924(10)	0.5985(8)	0.058(6)
C27	0.1822(8)	0.6530(7)	0.6011(5)	0.031(5)

atom	x	y	z	U_{eq}
H27A	0.2149	0.6831	0.6037	0.038
C28	0.1465(10)	0.6570(9)	0.6424(6)	0.061(7)
H28A	0.1743	0.6453	0.6658	0.074
C29	0.1277(10)	0.7163(9)	0.6504(7)	0.062(6)
H29A	0.1629	0.7422	0.6502	0.093
H29B	0.1078	0.7184	0.6779	0.093
H29C	0.0993	0.7287	0.6284	0.093
C30	0.0921(9)	0.6128(9)	0.6426(6)	0.053(5)
H30A	0.0710	0.6151	0.6697	0.079
H30B	0.1071	0.5727	0.6383	0.079
H30C	0.0641	0.6229	0.6198	0.079
C31	0.4223(12)	0.3953(13)	0.4151(7)	0.067(7)
C32	0.4721(10)	0.3430(12)	0.4148(8)	0.090(9)
H32A	0.4994	0.3485	0.3908	0.134
H32B	0.4516	0.3050	0.4122	0.134
H32C	0.4952	0.3440	0.4411	0.134
C33	0.1440(11)	0.3816(11)	0.6135(9)	0.081(8)
C34	0.1227(16)	0.3684(16)	0.6602(11)	0.156(14)
H34A	0.1464	0.3357	0.6717	0.234
H34B	0.0799	0.3578	0.6601	0.234
H34C	0.1287	0.4034	0.6777	0.234
C35	0.3020(9)	0.7215(9)	0.5330(6)	0.036(5)
C36	0.3489(10)	0.7655(10)	0.5489(6)	0.072(7)
H36A	0.3287	0.7963	0.5653	0.108
H36B	0.3697	0.7833	0.5249	0.108
H36C	0.3782	0.7452	0.5669	0.108
C37	0.5052(9)	0.4860(8)	0.5196(6)	0.036(5)
C38	0.5699(8)	0.5057(8)	0.5041(5)	0.044(5)
H38A	0.5644	0.5408	0.4856	0.053
C39	0.5979(9)	0.4550(10)	0.4759(7)	0.068(5)
H39A	0.5699	0.4481	0.4516	0.081
C40	0.6561(9)	0.4763(11)	0.4584(7)	0.083(6)

atom	x	y	z	U_{eq}
H40A	0.6741	0.4456	0.4408	0.125
H40B	0.6836	0.4859	0.4817	0.125
H40C	0.6490	0.5115	0.4413	0.125
C41	0.6028(10)	0.3979(11)	0.5006(7)	0.081(6)
H41A	0.6196	0.3672	0.4824	0.122
H41B	0.5627	0.3860	0.5103	0.122
H41C	0.6293	0.4037	0.5249	0.122
C42	0.5052(9)	0.5644(7)	0.6719(6)	0.034(5)
C43	0.5712(9)	0.5819(8)	0.6782(6)	0.042(5)
H43A	0.5888	0.5530	0.6985	0.050
C44	0.5746(8)	0.6429(8)	0.7000(6)	0.038(5)
H44A	0.5482	0.6411	0.7255	0.046
C45	0.6360(11)	0.6573(10)	0.7148(6)	0.071(7)
H45A	0.6358	0.6960	0.7283	0.106
H45B	0.6638	0.6577	0.6908	0.106
H45C	0.6492	0.6276	0.7352	0.106
C46	0.5494(10)	0.6907(9)	0.6717(7)	0.067(7)
H46A	0.5514	0.7285	0.6863	0.100
H46B	0.5073	0.6817	0.6648	0.100
H46C	0.5731	0.6927	0.6457	0.100
C47	0.5499(10)	0.4197(9)	0.6278(6)	0.039(4)
C48	0.5727(8)	0.3714(8)	0.6574(6)	0.048(3)
H48A	0.5683	0.3868	0.6868	0.057
C49	0.6411(9)	0.3585(9)	0.6510(6)	0.053(3)
H49A	0.6616	0.3976	0.6514	0.064
C50	0.6661(10)	0.3239(10)	0.6899(7)	0.079(5)
H50A	0.7092	0.3160	0.6857	0.118
H50B	0.6444	0.2867	0.6928	0.118
H50C	0.6606	0.3475	0.7155	0.118
C51	0.6569(10)	0.3317(9)	0.6103(7)	0.067(5)
H51A	0.7006	0.3257	0.6090	0.100
H51B	0.6443	0.3578	0.5874	0.100

atom	x	y	z	U_{eq}
H51C	0.6363	0.2938	0.6076	0.100
C52	0.3271(10)	0.3540(8)	0.6263(5)	0.033(5)
C53	0.3343(9)	0.2861(7)	0.6361(5)	0.034(5)
H53A	0.3358	0.2647	0.6086	0.041
C54	0.2828(10)	0.2633(8)	0.6603(6)	0.049(6)
H54A	0.2454	0.2738	0.6443	0.058
C55	0.2831(9)	0.1965(8)	0.6655(6)	0.052(6)
H55A	0.2865	0.1779	0.6377	0.078
H55B	0.2455	0.1839	0.6790	0.078
H55C	0.3174	0.1848	0.6831	0.078
C56	0.2755(9)	0.2881(9)	0.7060(6)	0.052(6)
H56A	0.2739	0.3311	0.7049	0.078
H56B	0.3099	0.2758	0.7233	0.078
H56C	0.2381	0.2731	0.7184	0.078
C57	0.4295(8)	0.4249(8)	0.7068(5)	0.028(4)
C58	0.4436(9)	0.4480(8)	0.7525(5)	0.041(5)
H58A	0.4848	0.4656	0.7511	0.049
C59	0.4464(9)	0.4011(8)	0.7866(5)	0.042(5)
H59A	0.4443	0.4234	0.8138	0.051
C60	0.3924(10)	0.3591(8)	0.7882(6)	0.052(6)
H60A	0.3549	0.3819	0.7883	0.078
H60B	0.3946	0.3353	0.8139	0.078
H60C	0.3931	0.3334	0.7635	0.078
C61	0.5079(10)	0.3678(9)	0.7886(7)	0.063(6)
H61A	0.5411	0.3963	0.7880	0.095
H61B	0.5113	0.3414	0.7643	0.095
H61C	0.5101	0.3449	0.8147	0.095
C62	0.3473(8)	0.6198(8)	0.6429(6)	0.037(5)
C63	0.3252(9)	0.6511(7)	0.6816(5)	0.037(5)
H63A	0.2829	0.6370	0.6859	0.044
C64	0.3206(9)	0.7143(8)	0.6764(5)	0.036(5)
H64A	0.2939	0.7226	0.6516	0.043

atom	x	y	z	U_{eq}
C65	0.2925(12)	0.7438(9)	0.7167(6)	0.071(7)
H65A	0.2530	0.7263	0.7226	0.107
H65B	0.2878	0.7861	0.7119	0.107
H65C	0.3192	0.7375	0.7409	0.107
C66	0.3800(10)	0.7427(8)	0.6691(6)	0.061(7)
H66A	0.3992	0.7254	0.6442	0.091
H66B	0.4059	0.7365	0.6938	0.091
H66C	0.3742	0.7849	0.6646	0.091
C67	0.5249(8)	0.6598(10)	0.5458(6)	0.041(5)
C68	0.5122(10)	0.7130(8)	0.5193(6)	0.057(6)
H68A	0.4709	0.7109	0.5083	0.085
H68B	0.5407	0.7146	0.4958	0.085
H68C	0.5165	0.7485	0.5366	0.085
C69	0.4581(10)	0.2772(10)	0.5489(8)	0.063(7)
C70	0.4507(11)	0.2409(10)	0.5102(7)	0.076(7)
H70A	0.4433	0.2667	0.4859	0.114
H70B	0.4164	0.2142	0.5138	0.114
H70C	0.4875	0.2181	0.5053	0.114
C71	0.2426(13)	0.5131(11)	0.7172(7)	0.066(6)
C72	0.1731(10)	0.5065(12)	0.7176(8)	0.089(6)
H72A	0.1564	0.5282	0.7416	0.134
H72B	0.1625	0.4649	0.7201	0.134
H72C	0.1564	0.5223	0.6913	0.134
Gd3	0.50256(4)	0.60619(4)	0.85847(3)	0.0357(2)
O30	0.4658(6)	0.6347(5)	0.9298(3)	0.039(3)
N30	0.4372(8)	0.6789(8)	0.9198(5)	0.044(4)
O31	0.4333(6)	0.6899(5)	0.8774(3)	0.045(3)
O32	0.4085(6)	0.7116(5)	0.9437(4)	0.051(4)
O40	0.4698(6)	0.5158(5)	0.8972(3)	0.042(3)
N40	0.4168(8)	0.5124(8)	0.8820(4)	0.037(4)
O41	0.4069(6)	0.5538(5)	0.8547(4)	0.042(3)
O42	0.3826(6)	0.4761(6)	0.8916(4)	0.056(4)

atom	x	y	z	U_{eq}
O50	0.4492(5)	0.6345(5)	0.7946(3)	0.038(3)
N50	0.4712(7)	0.6839(7)	0.7904(5)	0.036(4)
O51	0.5164(7)	0.6957(5)	0.8133(4)	0.055(4)
O52	0.4526(6)	0.7205(5)	0.7644(4)	0.050(4)
O60	0.5869(6)	0.5922(5)	0.8088(4)	0.047(3)
N60	0.5704(8)	0.5413(7)	0.7972(5)	0.045(4)
O61	0.5229(5)	0.5209(5)	0.8158(3)	0.037(3)
O62	0.5964(7)	0.5119(6)	0.7709(5)	0.067(4)
O70	0.5803(5)	0.6658(5)	0.8911(3)	0.040(3)
N70	0.6053(8)	0.6240(7)	0.9123(5)	0.045(4)
O71	0.5839(6)	0.5720(5)	0.9033(4)	0.048(3)
O72	0.6480(7)	0.6339(6)	0.9350(5)	0.080(5)
Cl1	0.9495(3)	0.6625(2)	0.54559(18)	0.0720(16)
O33	1.0092(6)	0.6797(6)	0.5528(5)	0.099(5)
O34	0.9450(7)	0.6406(7)	0.5034(4)	0.106(5)
O35	0.9324(7)	0.6168(6)	0.5736(4)	0.107(5)
O36	0.9100(6)	0.7102(6)	0.5496(4)	0.095(5)
Cl2	0.8305(3)	0.3303(3)	0.9729(2)	0.0838(18)
O43	0.7712(6)	0.3413(8)	0.9576(6)	0.152(6)
O44	0.8286(7)	0.2964(6)	1.0103(4)	0.113(5)
O45	0.8606(8)	0.2958(6)	0.9403(5)	0.122(5)
O46	0.8633(7)	0.3823(6)	0.9787(5)	0.109(5)
Cl3	0.1586(4)	0.3656(4)	0.7879(2)	0.123(3)
O53	0.1479(10)	0.3311(9)	0.8191(5)	0.186(7)
O54	0.1328(8)	0.3497(9)	0.7523(5)	0.156(6)
O55	0.1380(10)	0.4193(8)	0.7985(6)	0.196(8)
O56	0.2171(7)	0.3723(10)	0.7797(6)	0.190(7)
Cl4	0.0580(5)	0.5802(4)	0.7974(3)	0.159(4)
O63	0.0151(10)	0.6295(10)	0.8151(7)	0.220(8)
O64	0.0426(10)	0.5224(8)	0.8199(6)	0.181(7)
O65	0.1239(9)	0.6011(10)	0.8082(6)	0.183(7)
O66	0.0506(10)	0.5763(9)	0.7498(5)	0.177(7)

atom	x	y	z	U_{eq}
Cl5	0.4698(5)	0.1721(4)	0.3934(3)	0.172(4)
O73	0.5092(10)	0.1591(10)	0.4319(6)	0.190(7)
O74	0.5067(11)	0.2148(10)	0.3636(8)	0.238(9)
O75	0.4563(10)	0.1150(9)	0.3682(7)	0.211(8)
O76	0.4103(9)	0.2027(10)	0.4056(7)	0.198(8)
O1W	0.2902(7)	0.4645(6)	0.8165(4)	0.067(4)
O2W	0.5823(11)	0.2517(10)	0.4356(7)	0.156(9)
N2S	-0.0477(10)	0.1712(10)	0.0873(7)	0.106(6)
C9S	-0.0082(11)	0.1427(12)	0.0930(9)	0.098(6)
C10S	0.0530(10)	0.1068(11)	0.0932(8)	0.101(7)
H10D	0.0505	0.0751	0.1141	0.151
H10E	0.0864	0.1331	0.1005	0.151
H10F	0.0600	0.0899	0.0652	0.151
N3S	0.2867(14)	0.9942(14)	0.8106(9)	0.159(9)
C11S	0.2732(18)	0.9789(18)	0.7793(11)	0.169(9)
C12S	0.2701(17)	0.9514(17)	0.7335(10)	0.177(10)
H12B	0.2296	0.9571	0.7219	0.265
H12C	0.2791	0.9093	0.7350	0.265
H12D	0.2997	0.9708	0.7153	0.265
N4S	0.8033(13)	0.6320(17)	0.3684(13)	0.199(11)
C13S	0.7547(15)	0.627(2)	0.3633(15)	0.195(11)
C14S	0.6888(13)	0.6124(18)	0.3476(13)	0.197(12)
H14D	0.6835	0.5698	0.3456	0.295
H14E	0.6823	0.6302	0.3198	0.295
H14F	0.6595	0.6285	0.3677	0.295
N5S	0.2379(16)	0.9691(16)	0.1372(11)	0.197(12)
C15S	0.2182(19)	0.9871(19)	0.1082(12)	0.185(12)
C16S	0.1916(16)	1.0164(16)	0.0669(10)	0.174(13)
H16A	0.1744	0.9859	0.0487	0.261
H16B	0.2239	1.0368	0.0518	0.261
H16C	0.1601	1.0445	0.0747	0.261
N6S	0.741(2)	0.6160(19)	0.6121(13)	0.247(15)

atom	x	y	z	U_{eq}
C17S	0.766(2)	0.597(2)	0.5853(15)	0.232(14)
C18S	0.8077(19)	0.6001(19)	0.5450(13)	0.217(16)
H18B	0.8028	0.5641	0.5284	0.326
H18C	0.8498	0.6040	0.5538	0.326
H18D	0.7963	0.6341	0.5277	0.326
N1S	0.8981(13)	0.6524(12)	0.7070(9)	0.386(16)
C1S	0.9557(17)	0.668(2)	0.6894(16)	0.386(16)
C2S	0.925(3)	0.716(2)	0.6670(17)	0.386(16)
C3S	0.885(2)	0.694(2)	0.7410(14)	0.386(16)
C4S	0.934(2)	0.666(3)	0.7647(15)	0.386(16)
C5S	0.852(2)	0.657(2)	0.6757(14)	0.386(16)
C6S	0.807(2)	0.652(2)	0.711(2)	0.386(16)
C7S	0.900(2)	0.5949(15)	0.7243(16)	0.386(16)
C8S	0.926(2)	0.574(2)	0.6846(18)	0.386(16)

$$Ueq = \frac{1}{3}\left(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha\right)$$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Gd1	0.0459(6)	0.0276(5)	0.0203(4)	-0.0021(4)	-0.0040(4)	0.0022(5)
Gd2	0.0427(6)	0.0243(5)	0.0205(5)	-0.0001(4)	-0.0049(4)	0.0001(4)
Ni1	0.0479(15)	0.0389(15)	0.0212(12)	-0.0014(11)	-0.0025(11)	0.0050(13)
Ni2	0.0505(16)	0.0409(14)	0.0234(13)	0.0021(12)	-0.0082(12)	-0.0048(13)
Ni3	0.0470(16)	0.0361(14)	0.0256(14)	0.0001(11)	-0.0018(12)	0.0066(12)
Ni4	0.0468(16)	0.0345(14)	0.0247(13)	0.0025(11)	0.0002(12)	-0.0031(12)
Ni5	0.0436(15)	0.0285(13)	0.0258(13)	0.0031(11)	-0.0030(12)	-0.0023(12)
Ni6	0.0504(16)	0.0288(14)	0.0204(13)	-0.0017(11)	-0.0031(12)	-0.0024(12)
O1	0.033(7)	0.035(7)	0.021(7)	-0.001(5)	-0.006(6)	0.000(6)
O2	0.044(9)	0.052(9)	0.041(8)	0.015(7)	-0.001(7)	0.009(7)
O3	0.040(7)	0.018(6)	0.027(6)	0.003(5)	0.003(6)	-0.007(6)
O4	0.045(7)	0.042(6)	0.010(5)	-0.009(5)	-0.004(5)	0.013(6)
O5	0.067(10)	0.041(8)	0.018(7)	-0.014(6)	-0.004(6)	-0.006(7)
O6	0.021(7)	0.032(7)	0.032(7)	0.010(6)	-0.002(6)	-0.004(6)
O7	0.044(7)	0.029(6)	0.026(6)	-0.018(5)	-0.004(5)	0.008(6)
O8	0.041(8)	0.051(8)	0.023(8)	-0.011(6)	-0.002(6)	0.007(6)
O9	0.044(8)	0.048(8)	0.013(7)	0.001(6)	-0.010(6)	0.005(7)
O10	0.054(8)	0.011(7)	0.030(7)	-0.006(6)	-0.004(6)	0.001(6)
O11	0.045(9)	0.024(7)	0.055(9)	0.007(6)	-0.014(7)	0.011(7)
O12	0.041(7)	0.046(7)	0.014(6)	-0.015(6)	-0.011(6)	0.015(7)
O13	0.052(9)	0.054(9)	0.024(7)	-0.011(6)	-0.010(6)	-0.005(7)
O14	0.056(9)	0.033(7)	0.023(7)	0.008(6)	-0.010(7)	-0.001(6)
O15	0.051(9)	0.037(8)	0.030(8)	0.002(6)	0.007(7)	0.002(7)
O16	0.045(7)	0.033(7)	0.026(7)	-0.010(6)	0.001(6)	-0.005(7)
O17	0.040(8)	0.040(8)	0.034(8)	-0.009(6)	-0.008(6)	0.007(6)
O18	0.047(8)	0.027(6)	0.016(7)	-0.006(5)	0.009(6)	-0.008(6)
O19	0.045(8)	0.032(7)	0.022(7)	0.000(6)	-0.003(7)	-0.021(6)
O20	0.058(9)	0.031(7)	0.022(6)	-0.009(5)	0.017(6)	-0.013(7)
O21	0.062(9)	0.041(8)	0.020(7)	0.000(6)	-0.003(6)	-0.009(7)
O22	0.025(7)	0.023(7)	0.052(8)	0.002(6)	-0.021(6)	-0.007(6)

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O23	0.043(9)	0.037(8)	0.028(7)	-0.003(5)	-0.010(6)	0.000(7)
O24	0.073(9)	0.018(6)	0.022(6)	-0.002(5)	-0.008(7)	-0.009(7)
O25	0.056(9)	0.014(7)	0.028(7)	0.008(5)	0.007(6)	0.009(6)
O26	0.042(8)	0.028(7)	0.026(7)	0.004(6)	-0.015(6)	-0.005(6)
O27	0.065(9)	0.024(7)	0.029(8)	-0.004(6)	0.005(7)	-0.005(6)
N1	0.038(10)	0.047(9)	0.029(9)	0.007(7)	-0.016(8)	-0.015(8)
N2	0.027(9)	0.049(9)	0.032(9)	-0.010(7)	-0.007(8)	-0.016(8)
N3	0.057(11)	0.045(10)	0.029(9)	-0.005(8)	-0.008(8)	0.020(9)
N4	0.081(14)	0.049(11)	0.056(12)	0.010(9)	-0.031(11)	-0.003(10)
N5	0.048(11)	0.050(11)	0.038(10)	0.003(8)	0.003(8)	-0.008(8)
N6	0.033(9)	0.037(10)	0.039(10)	-0.009(8)	-0.002(8)	0.021(8)
N7	0.064(15)	0.047(12)	0.039(11)	-0.001(9)	0.005(10)	0.033(10)
N8	0.058(8)	0.063(8)	0.036(8)	0.014(7)	-0.002(7)	0.005(7)
N9	0.048(11)	0.031(9)	0.012(8)	0.003(7)	-0.003(8)	-0.005(8)
N10	0.051(11)	0.063(11)	0.034(9)	-0.025(8)	0.004(8)	-0.004(9)
N11	0.041(7)	0.042(7)	0.017(6)	-0.001(6)	-0.002(6)	-0.009(6)
N12	0.055(11)	0.031(9)	0.036(10)	0.016(7)	-0.020(8)	-0.006(8)
N13	0.035(10)	0.018(8)	0.047(10)	-0.003(7)	0.005(8)	-0.009(7)
N14	0.052(10)	0.035(9)	0.015(7)	0.014(7)	0.016(7)	0.002(9)
N15	0.052(8)	0.026(7)	0.018(7)	0.003(6)	-0.006(6)	0.002(6)
N16	0.069(12)	0.010(9)	0.034(10)	0.009(7)	0.010(8)	0.013(8)
N17	0.067(9)	0.044(8)	0.035(8)	-0.005(7)	0.007(7)	0.003(7)
N18	0.080(13)	0.040(10)	0.021(9)	0.013(7)	-0.006(10)	0.011(11)
C1	0.038(7)	0.030(7)	0.038(7)	-0.006(6)	0.004(6)	-0.001(6)
C2	0.043(9)	0.034(8)	0.043(8)	-0.001(7)	0.009(7)	0.005(8)
C3	0.064(16)	0.044(13)	0.059(14)	-0.001(11)	0.028(12)	-0.021(12)
C4	0.080(11)	0.088(11)	0.066(10)	0.000(8)	0.018(8)	-0.009(9)
C5	0.12(2)	0.056(16)	0.060(16)	0.011(13)	-0.005(15)	0.018(15)
C6	0.027(8)	0.038(8)	0.024(8)	0.002(7)	-0.001(7)	0.010(7)
C7	0.039(9)	0.049(8)	0.028(8)	-0.017(7)	-0.017(7)	0.001(7)
C8	0.082(18)	0.054(14)	0.041(14)	-0.018(11)	0.001(12)	-0.004(13)
C9	0.087(19)	0.095(19)	0.060(16)	-0.034(14)	0.000(15)	-0.035(16)

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C10	0.12(2)	0.054(14)	0.049(14)	-0.024(11)	0.014(14)	0.032(16)
C11	0.009(10)	0.028(11)	0.054(15)	0.010(11)	-0.007(10)	0.006(9)
C12	0.047(9)	0.028(8)	0.028(8)	0.005(7)	-0.011(7)	0.012(7)
C13	0.058(14)	0.045(12)	0.018(10)	-0.007(10)	-0.014(10)	0.001(11)
C14	0.061(16)	0.063(14)	0.048(13)	0.015(11)	0.010(13)	0.014(13)
C15	0.15(2)	0.053(14)	0.013(11)	-0.005(10)	-0.007(13)	-0.001(16)
C16	0.074(18)	0.039(14)	0.026(12)	-0.015(9)	-0.003(11)	-0.034(15)
C17	0.071(17)	0.045(14)	0.052(14)	0.004(11)	-0.006(12)	0.011(12)
C18	0.097(12)	0.051(9)	0.091(10)	0.006(10)	-0.010(11)	0.014(8)
C19	0.117(15)	0.043(11)	0.089(11)	-0.005(10)	-0.010(12)	0.005(11)
C20	0.080(10)	0.070(9)	0.097(9)	0.001(8)	-0.015(8)	0.004(7)
C21	0.035(8)	0.029(8)	0.020(7)	-0.008(7)	0.002(7)	0.000(7)
C22	0.078(17)	0.063(15)	0.025(11)	0.010(10)	-0.017(11)	0.007(13)
C23	0.041(12)	0.045(12)	0.046(12)	0.008(11)	0.010(10)	0.001(11)
C24	0.065(15)	0.058(15)	0.069(15)	-0.018(13)	0.025(12)	-0.014(13)
C25	0.064(15)	0.049(13)	0.063(15)	-0.003(11)	0.015(12)	-0.004(12)
C26	0.032(13)	0.071(17)	0.072(18)	-0.026(15)	0.002(13)	0.001(12)
C27	0.058(13)	0.018(10)	0.019(10)	-0.006(8)	0.006(10)	0.005(9)
C28	0.087(17)	0.069(16)	0.027(12)	-0.033(11)	-0.008(12)	0.025(14)
C29	0.065(10)	0.066(10)	0.055(10)	-0.018(8)	0.008(8)	0.017(8)
C30	0.053(9)	0.064(9)	0.041(8)	-0.002(8)	0.016(8)	-0.004(8)
C31	0.07(2)	0.08(2)	0.047(14)	-0.008(16)	0.003(14)	-0.034(17)
C32	0.054(17)	0.14(3)	0.071(18)	0.000(17)	0.009(14)	0.024(17)
C33	0.070(11)	0.088(11)	0.086(11)	0.003(9)	-0.004(9)	-0.001(9)
C34	0.160(17)	0.162(17)	0.146(17)	0.011(10)	0.003(10)	-0.007(10)
C35	0.044(9)	0.038(9)	0.025(8)	0.005(7)	0.007(7)	0.002(8)
C36	0.091(19)	0.085(18)	0.040(14)	0.020(13)	0.028(14)	-0.018(15)
C37	0.051(13)	0.032(11)	0.026(11)	-0.001(10)	-0.019(12)	0.005(11)
C38	0.063(14)	0.032(11)	0.037(11)	-0.005(10)	0.020(10)	0.002(11)
C39	0.041(9)	0.091(12)	0.071(12)	-0.027(9)	0.023(9)	-0.001(10)
C40	0.052(11)	0.112(14)	0.085(13)	-0.042(11)	0.036(10)	-0.014(11)
C41	0.053(12)	0.094(13)	0.096(15)	-0.018(10)	0.014(11)	0.006(11)

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C42	0.047(14)	0.034(11)	0.022(12)	0.014(9)	0.013(12)	-0.002(11)
C43	0.055(15)	0.038(12)	0.033(12)	-0.010(9)	-0.017(10)	-0.009(10)
C44	0.041(13)	0.039(12)	0.035(12)	-0.005(10)	-0.009(10)	-0.018(10)
C45	0.11(2)	0.067(16)	0.035(13)	-0.006(11)	-0.014(14)	0.006(15)
C46	0.073(18)	0.063(16)	0.065(16)	-0.026(13)	-0.009(14)	0.004(14)
C47	0.042(7)	0.038(7)	0.038(7)	0.005(5)	-0.009(6)	-0.005(6)
C48	0.050(6)	0.039(7)	0.055(7)	0.012(5)	-0.016(6)	-0.007(6)
C49	0.050(6)	0.043(8)	0.067(8)	0.017(6)	-0.018(7)	-0.004(6)
C50	0.069(10)	0.069(12)	0.099(10)	0.038(9)	-0.042(10)	-0.008(10)
C51	0.061(10)	0.051(11)	0.087(9)	0.002(9)	0.005(9)	-0.014(9)
C52	0.033(9)	0.042(9)	0.024(8)	0.007(7)	-0.005(7)	0.001(8)
C53	0.068(15)	0.019(10)	0.015(10)	0.006(8)	0.003(10)	-0.016(10)
C54	0.062(15)	0.036(12)	0.048(13)	0.029(10)	-0.016(12)	-0.021(11)
C55	0.033(12)	0.056(14)	0.066(14)	0.010(11)	-0.009(11)	0.007(11)
C56	0.033(13)	0.082(16)	0.040(13)	0.008(11)	0.002(11)	0.006(12)
C57	0.033(8)	0.027(8)	0.025(8)	0.010(7)	-0.006(7)	0.003(7)
C58	0.053(9)	0.037(8)	0.031(8)	0.010(7)	-0.003(7)	0.005(8)
C59	0.064(15)	0.045(13)	0.018(10)	0.001(9)	0.006(10)	0.035(12)
C60	0.083(17)	0.044(13)	0.030(12)	0.013(10)	0.014(11)	-0.007(13)
C61	0.063(16)	0.063(15)	0.064(15)	-0.022(12)	0.000(13)	0.001(13)
C62	0.038(8)	0.044(9)	0.030(8)	-0.007(8)	-0.011(7)	-0.003(7)
C63	0.055(14)	0.035(12)	0.020(10)	-0.001(9)	-0.012(10)	0.006(10)
C64	0.049(9)	0.032(8)	0.028(8)	-0.011(7)	0.001(7)	0.006(7)
C65	0.12(2)	0.054(14)	0.044(14)	0.005(11)	0.019(15)	0.007(15)
C66	0.11(2)	0.035(13)	0.039(13)	-0.007(10)	-0.020(13)	-0.015(13)
C67	0.027(12)	0.053(15)	0.043(13)	-0.005(12)	-0.007(10)	-0.005(11)
C68	0.066(10)	0.049(9)	0.054(9)	0.018(8)	0.003(8)	0.003(8)
C69	0.053(16)	0.056(15)	0.080(19)	-0.016(14)	0.013(14)	-0.010(12)
C70	0.088(11)	0.070(10)	0.071(10)	-0.010(8)	-0.005(9)	0.004(9)
C71	0.081(9)	0.055(12)	0.062(12)	0.003(10)	-0.004(12)	0.015(13)
C72	0.084(9)	0.090(10)	0.094(10)	0.012(8)	-0.003(8)	0.001(9)
Gd3	0.0487(6)	0.0359(5)	0.0225(4)	0.0011(4)	-0.0008(5)	-0.0041(5)

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O30	0.055(9)	0.034(8)	0.027(7)	0.016(6)	-0.006(6)	0.007(7)
N30	0.058(12)	0.049(12)	0.026(11)	0.007(9)	-0.009(9)	-0.016(10)
O31	0.056(9)	0.057(9)	0.022(7)	0.009(6)	-0.001(6)	-0.001(7)
O32	0.076(10)	0.047(8)	0.029(8)	-0.010(7)	0.011(8)	-0.004(8)
O40	0.070(10)	0.031(7)	0.025(7)	-0.013(6)	0.015(7)	-0.008(7)
N40	0.041(12)	0.051(11)	0.021(9)	0.000(9)	0.017(9)	-0.005(10)
O41	0.066(9)	0.022(7)	0.038(7)	-0.001(6)	0.013(7)	-0.017(7)
O42	0.050(9)	0.076(10)	0.042(8)	-0.004(8)	0.011(7)	-0.019(8)
O50	0.057(9)	0.029(7)	0.029(7)	-0.002(6)	-0.004(6)	-0.010(7)
N50	0.041(8)	0.042(8)	0.025(7)	-0.008(7)	-0.007(6)	0.003(7)
O51	0.081(11)	0.020(7)	0.063(9)	0.000(6)	-0.004(9)	-0.018(7)
O52	0.064(7)	0.048(7)	0.037(6)	0.006(6)	-0.018(6)	0.007(6)
O60	0.064(9)	0.035(8)	0.043(8)	-0.016(6)	0.004(7)	-0.004(7)
N60	0.068(14)	0.033(11)	0.033(10)	0.000(9)	0.002(10)	0.018(10)
O61	0.036(8)	0.046(8)	0.029(7)	0.002(6)	0.007(6)	-0.016(6)
O62	0.098(11)	0.033(8)	0.069(9)	-0.008(8)	0.011(9)	-0.007(9)
O70	0.052(8)	0.042(7)	0.026(7)	0.013(6)	-0.009(6)	-0.002(6)
N70	0.052(8)	0.038(8)	0.046(8)	0.008(7)	-0.012(7)	0.000(7)
O71	0.061(9)	0.041(8)	0.043(8)	-0.004(6)	-0.003(7)	0.007(7)
O72	0.082(11)	0.071(11)	0.087(12)	0.025(9)	-0.058(10)	0.002(9)
Cl1	0.081(4)	0.057(4)	0.078(4)	0.009(3)	0.001(4)	0.006(3)
O33	0.082(6)	0.101(11)	0.114(11)	0.031(9)	-0.013(8)	0.003(6)
O34	0.132(12)	0.106(12)	0.082(6)	-0.006(6)	-0.002(8)	0.015(10)
O35	0.117(11)	0.097(9)	0.107(9)	0.047(8)	-0.015(10)	-0.010(8)
O36	0.102(9)	0.087(9)	0.095(10)	0.004(7)	-0.015(10)	0.033(7)
Cl2	0.087(4)	0.061(4)	0.104(5)	0.010(3)	-0.012(4)	-0.016(3)
O43	0.108(8)	0.165(15)	0.183(16)	0.022(13)	-0.052(10)	-0.005(8)
O44	0.118(12)	0.102(11)	0.119(9)	0.036(7)	-0.002(9)	-0.031(10)
O45	0.182(14)	0.059(10)	0.124(11)	-0.002(7)	0.015(10)	-0.009(9)
O46	0.150(12)	0.069(8)	0.109(12)	-0.001(7)	-0.010(11)	-0.042(8)
Cl3	0.138(7)	0.175(8)	0.055(4)	0.003(5)	0.051(5)	0.016(6)
O53	0.231(17)	0.246(15)	0.082(10)	0.052(11)	0.008(12)	-0.032(16)

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O54	0.165(13)	0.238(17)	0.064(8)	-0.005(10)	0.017(9)	0.072(14)
O55	0.256(18)	0.212(12)	0.118(14)	-0.020(10)	0.084(15)	0.069(14)
O56	0.149(8)	0.263(18)	0.157(15)	-0.070(15)	0.080(10)	-0.014(12)
Cl4	0.198(9)	0.169(9)	0.109(6)	0.017(6)	-0.006(7)	0.032(7)
O63	0.253(17)	0.220(16)	0.186(16)	-0.016(14)	0.041(17)	0.057(15)
O64	0.216(17)	0.200(13)	0.128(13)	0.046(11)	-0.042(15)	-0.006(13)
O65	0.213(12)	0.207(18)	0.129(14)	-0.013(15)	0.012(13)	-0.009(12)
O66	0.222(18)	0.206(17)	0.103(7)	0.022(10)	0.001(12)	0.022(16)
Cl5	0.185(7)	0.160(7)	0.170(7)	-0.009(6)	0.041(6)	0.026(6)
O73	0.198(16)	0.197(17)	0.174(13)	-0.059(11)	0.022(10)	0.067(14)
O74	0.264(19)	0.211(16)	0.238(18)	0.007(13)	0.109(15)	0.007(14)
O75	0.231(19)	0.204(14)	0.200(17)	-0.046(12)	0.007(15)	0.010(13)
O76	0.186(14)	0.232(18)	0.176(17)	-0.002(15)	0.037(11)	0.053(12)
O1W	0.084(8)	0.062(7)	0.055(7)	0.003(6)	0.026(6)	0.011(7)
O2W	0.149(12)	0.152(12)	0.167(12)	0.016(9)	0.009(9)	0.018(9)
N2S	0.090(15)	0.127(17)	0.100(13)	0.042(13)	-0.008(14)	0.006(11)
C9S	0.079(14)	0.118(17)	0.096(13)	0.015(13)	-0.018(13)	-0.002(11)
C10S	0.085(15)	0.111(17)	0.106(15)	-0.005(15)	-0.010(14)	0.000(12)
N3S	0.160(11)	0.161(12)	0.156(12)	-0.001(9)	-0.024(9)	0.013(9)
C11S	0.165(15)	0.173(16)	0.168(15)	-0.017(14)	-0.027(13)	0.005(14)
C12S	0.169(19)	0.19(2)	0.173(17)	-0.023(17)	-0.028(19)	-0.009(19)
N4S	0.115(17)	0.21(2)	0.27(3)	0.02(2)	0.06(3)	0.04(3)
C13S	0.113(17)	0.20(2)	0.27(3)	0.02(2)	0.07(3)	0.03(3)
C14S	0.113(18)	0.20(2)	0.28(3)	0.02(2)	0.07(3)	0.03(3)

The general temperature factor expression:

$$\exp\left(-2\pi^2\left(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl\right)\right)$$

Table 3. Bond Lengths (Å)

atom	atom	distance	atom	atom	distance
Gd1	O12	2.416(11)	Gd1	O14	2.430(12)
Gd1	O10	2.431(11)	Gd1	O8	2.437(12)
Gd1	O6	2.443(12)	Gd1	O4	2.447(12)
Gd1	O1	2.491(11)	Gd1	O2	2.502(13)
Gd1	O3	2.528(10)	Gd1	Ni2	3.513(3)
Gd1	Ni1	3.513(2)	Gd1	Ni3	3.522(2)
Gd2	O26	2.422(11)	Gd2	O16	2.450(11)
Gd2	O18	2.468(11)	Gd2	O3	2.472(10)
Gd2	O20	2.474(13)	Gd2	O1	2.473(10)
Gd2	O22	2.482(11)	Gd2	O24	2.485(11)
Gd2	O2	2.505(11)	Gd2	Ni6	3.530(2)
Ni1	O6	2.015(11)	Ni1	N7	2.041(17)
Ni1	N2	2.061(13)	Ni1	O4	2.062(10)
Ni1	N1	2.073(14)	Ni1	O9	2.109(13)
Ni2	O10	2.032(12)	Ni2	O12	2.037(12)
Ni2	N5	2.050(16)	Ni2	N8	2.063(16)
Ni2	N4	2.069(16)	Ni2	O7	2.116(11)
Ni3	O8	2.022(11)	Ni3	N3	2.039(14)
Ni3	O14	2.047(11)	Ni3	N6	2.051(14)
Ni3	N9	2.093(16)	Ni3	O13	2.095(13)
Ni4	O18	2.025(11)	Ni4	O16	2.045(11)
Ni4	N11	2.070(13)	Ni4	N10	2.094(14)
Ni4	N16	2.109(15)	Ni4	O21	2.112(12)
Ni5	O22	2.016(11)	Ni5	N12	2.042(15)
Ni5	O20	2.049(11)	Ni5	N13	2.057(13)
Ni5	N17	2.074(17)	Ni5	O25	2.084(11)
Ni6	O24	2.034(11)	Ni6	O26	2.039(11)
Ni6	N14	2.055(12)	Ni6	N18	2.08(2)
Ni6	N15	2.106(13)	Ni6	O19	2.110(12)
O1	H1A	0.9900	O1	H1B	0.9900

atom	atom	distance	atom	atom	distance
O2	H2B	0.9900	O2	H2C	0.9900
O3	H3B	0.9900	O3	H3C	0.9900
O4	C1	1.31(2)	O5	C1	1.22(2)
O6	C6	1.25(2)	O7	C6	1.24(2)
O8	C11	1.30(2)	O9	C11	1.20(2)
O10	C16	1.27(2)	O11	C16	1.26(2)
O12	C21	1.29(2)	O13	C21	1.21(2)
O14	C26	1.35(2)	O15	C26	1.26(2)
O16	C37	1.27(2)	O17	C37	1.203(19)
O18	C42	1.25(2)	O19	C42	1.237(19)
O20	C47	1.28(2)	O21	C47	1.18(2)
O22	C52	1.25(2)	O23	C52	1.23(2)
O24	C57	1.259(19)	O25	C57	1.203(19)
O26	C62	1.33(2)	O27	C62	1.25(2)
N1	C2	1.51(2)	N2	C7	1.49(2)
N3	C12	1.51(2)	N4	C17	1.48(2)
N5	C22	1.54(2)	N6	C27	1.46(2)
N7	C31	1.04(3)	N8	C33	1.13(3)
N9	C35	1.10(2)	N10	C38	1.50(2)
N11	C43	1.49(2)	N12	C48	1.45(2)
N13	C53	1.46(2)	N14	C58	1.51(2)
N15	C63	1.50(2)	N16	C67	1.06(2)
N17	C69	1.11(2)	N18	C71	1.10(3)
C1	C2	1.52(2)	C2	C3	1.54(2)
C2	H2A	1.0000	C3	C4	1.56(3)
C3	C5	1.58(3)	C3	H3A	1.0000
C4	H4A	0.9800	C4	H4B	0.9800
C4	H4C	0.9800	C5	H5A	0.9800
C5	H5B	0.9800	C5	H5C	0.9800
C6	C7	1.56(2)	C7	C8	1.53(2)
C7	H7A	1.0000	C8	C10	1.53(3)
C8	C9	1.55(3)	C8	H8A	1.0000

atom	atom	distance	atom	atom	distance
C9	H9A	0.9800	C9	H9B	0.9800
C9	H9C	0.9800	C10	H10A	0.9800
C10	H10B	0.9800	C10	H10C	0.9800
C11	C12	1.54(2)	C12	C13	1.52(2)
C12	H12A	1.0000	C13	C14	1.50(3)
C13	C15	1.53(3)	C13	H13A	1.0000
C14	H14A	0.9800	C14	H14B	0.9800
C14	H14C	0.9800	C15	H15A	0.9800
C15	H15B	0.9800	C15	H15C	0.9800
C16	C17	1.53(3)	C17	C18	1.61(3)
C17	H17A	1.0000	C18	C19	1.45(3)
C18	C20	1.48(3)	C18	H18A	1.0000
C19	H19A	0.9800	C19	H19B	0.9800
C19	H19C	0.9800	C20	H20A	0.9800
C20	H20B	0.9800	C20	H20C	0.9800
C21	C22	1.57(3)	C22	C23	1.45(2)
C22	H22A	1.0000	C23	C24	1.53(2)
C23	C25	1.56(2)	C23	H23A	1.0000
C24	H24A	0.9800	C24	H24B	0.9800
C24	H24C	0.9800	C25	H25A	0.9800
C25	H25B	0.9800	C25	H25C	0.9800
C26	C27	1.57(3)	C27	C28	1.53(2)
C27	H27A	1.0000	C28	C29	1.44(3)
C28	C30	1.57(3)	C28	H28A	1.0000
C29	H29A	0.9800	C29	H29B	0.9800
C29	H29C	0.9800	C30	H30A	0.9800
C30	H30B	0.9800	C30	H30C	0.9800
C31	C32	1.62(4)	C32	H32A	0.9800
C32	H32B	0.9800	C32	H32C	0.9800
C33	C34	1.58(4)	C34	H34A	0.9800
C34	H34B	0.9800	C34	H34C	0.9800
C35	C36	1.53(3)	C36	H36A	0.9800

atom	atom	distance	atom	atom	distance
C36	H36B	0.9800	C36	H36C	0.9800
C37	C38	1.58(3)	C38	C39	1.59(3)
C38	H38A	1.0000	C39	C40	1.48(3)
C39	C41	1.52(3)	C39	H39A	1.0000
C40	H40A	0.9800	C40	H40B	0.9800
C40	H40C	0.9800	C41	H41A	0.9800
C41	H41B	0.9800	C41	H41C	0.9800
C42	C43	1.53(3)	C43	C44	1.55(2)
C43	H43A	1.0000	C44	C45	1.48(3)
C44	C46	1.52(3)	C44	H44A	1.0000
C45	H45A	0.9800	C45	H45B	0.9800
C45	H45C	0.9800	C46	H46A	0.9800
C46	H46B	0.9800	C46	H46C	0.9800
C47	C48	1.53(2)	C48	C49	1.56(3)
C48	H48A	1.0000	C49	C51	1.47(3)
C49	C50	1.57(3)	C49	H49A	1.0000
C50	H50A	0.9800	C50	H50B	0.9800
C50	H50C	0.9800	C51	H51A	0.9800
C51	H51B	0.9800	C51	H51C	0.9800
C52	C53	1.58(2)	C53	C54	1.47(2)
C53	H53A	1.0000	C54	C55	1.53(2)
C54	C56	1.56(3)	C54	H54A	1.0000
C55	H55A	0.9800	C55	H55B	0.9800
C55	H55C	0.9800	C56	H56A	0.9800
C56	H56B	0.9800	C56	H56C	0.9800
C57	C58	1.57(2)	C58	C59	1.52(2)
C58	H58A	1.0000	C59	C60	1.53(3)
C59	C61	1.56(3)	C59	H59A	1.0000
C60	H60A	0.9800	C60	H60B	0.9800
C60	H60C	0.9800	C61	H61A	0.9800
C61	H61B	0.9800	C61	H61C	0.9800
C62	C63	1.50(2)	C63	C64	1.45(2)

atom	atom	distance	atom	atom	distance
C63	H63A	1.0000	C64	C66	1.49(3)
C64	C65	1.58(2)	C64	H64A	1.0000
C65	H65A	0.9800	C65	H65B	0.9800
C65	H65C	0.9800	C66	H66A	0.9800
C66	H66B	0.9800	C66	H66C	0.9800
C67	C68	1.50(3)	C68	H68A	0.9800
C68	H68B	0.9800	C68	H68C	0.9800
C69	C70	1.49(3)	C70	H70A	0.9800
C70	H70B	0.9800	C70	H70C	0.9800
C71	C72	1.55(3)	C72	H72A	0.9800
C72	H72B	0.9800	C72	H72C	0.9800
Gd3	O61	2.409(11)	Gd3	O71	2.425(12)
Gd3	O70	2.427(11)	Gd3	O50	2.432(11)
Gd3	O41	2.436(11)	Gd3	O60	2.466(12)
Gd3	O30	2.491(11)	Gd3	O40	2.504(11)
Gd3	O51	2.511(12)	Gd3	O31	2.519(12)
Gd3	N60	2.866(18)	Gd3	N70	2.875(18)
O30	N30	1.231(18)	N30	O32	1.239(19)
N30	O31	1.370(17)	O40	N40	1.273(17)
N40	O42	1.162(18)	N40	O41	1.299(17)
O50	N50	1.232(17)	N50	O52	1.242(17)
N50	O51	1.268(17)	O60	N60	1.268(18)
N60	O62	1.216(18)	N60	O61	1.293(18)
O70	N70	1.290(17)	N70	O72	1.211(18)
N70	O71	1.308(18)	Cl1	O33	1.400(12)
Cl1	O36	1.402(11)	Cl1	O35	1.420(12)
Cl1	O34	1.431(12)	Cl2	O46	1.402(12)
Cl2	O44	1.414(12)	Cl2	O43	1.423(13)
Cl2	O45	1.461(13)	Cl3	O53	1.287(15)
Cl3	O54	1.315(14)	Cl3	O56	1.331(15)
Cl3	O55	1.348(15)	Cl4	O66	1.519(16)
Cl4	O64	1.537(16)	Cl4	O65	1.574(16)

atom	atom	distance	atom	atom	distance
Cl4	O63	1.575(16)	Cl5	O73	1.531(17)
Cl5	O76	1.541(17)	Cl5	O75	1.558(17)
Cl5	O74	1.584(17)	N2S	C9S	1.10(2)
C9S	C10S	1.58(2)	C10S	H10D	0.9800
C10S	H10E	0.9800	C10S	H10F	0.9800
N3S	C11S	1.09(5)	C11S	C12S	1.58(5)
C12S	H12B	0.9800	C12S	H12C	0.9800
C12S	H12D	0.9800	N4S	C13S	1.10(2)
C13S	C14S	1.58(5)	C14S	H14D	0.9800
C14S	H14E	0.9800	C14S	H14F	0.9800
N5S	C15S	1.10(6)	C15S	C16S	1.58(6)
C16S	H16A	0.9800	C16S	H16B	0.9800
C16S	H16C	0.9800	N6S	C17S	1.10(6)
C17S	C18S	1.58(6)	C18S	H18B	0.9800
C18S	H18C	0.9800	C18S	H18D	0.9800
N1S	C7S	1.42(5)	N1S	C5S	1.42(5)
N1S	C1S	1.44(5)	N1S	C3S	1.46(5)
C1S	C2S	1.47(7)	C3S	C4S	1.47(7)
C5S	C6S	1.50(7)	C7S	C8S	1.46(7)

Table 4. Bond Angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
O12	Gd1	O14	68.8(4)	O12	Gd1	O10	68.0(4)
O14	Gd1	O10	120.0(4)	O12	Gd1	O8	74.7(4)
O14	Gd1	O8	67.9(4)	O10	Gd1	O8	133.0(4)
O12	Gd1	O6	75.9(3)	O14	Gd1	O6	133.6(4)
O10	Gd1	O6	69.5(3)	O8	Gd1	O6	74.6(4)
O12	Gd1	O4	134.6(3)	O14	Gd1	O4	119.1(4)
O10	Gd1	O4	120.8(4)	O8	Gd1	O4	69.5(4)
O6	Gd1	O4	68.4(3)	O12	Gd1	O1	137.5(4)
O14	Gd1	O1	130.5(3)	O10	Gd1	O1	70.1(4)
O8	Gd1	O1	144.1(4)	O6	Gd1	O1	95.8(3)
O4	Gd1	O1	74.8(4)	O12	Gd1	O2	143.2(4)
O14	Gd1	O2	75.1(4)	O10	Gd1	O2	128.6(4)
O8	Gd1	O2	98.4(4)	O6	Gd1	O2	138.2(4)
O4	Gd1	O2	70.5(4)	O1	Gd1	O2	65.5(4)
O12	Gd1	O3	95.9(3)	O14	Gd1	O3	71.8(3)
O10	Gd1	O3	73.5(3)	O8	Gd1	O3	139.3(4)
O6	Gd1	O3	142.5(3)	O4	Gd1	O3	129.5(3)
O1	Gd1	O3	65.4(3)	O2	Gd1	O3	65.4(3)
O12	Gd1	Ni2	34.3(3)	O14	Gd1	Ni2	97.7(3)
O10	Gd1	Ni2	34.2(3)	O8	Gd1	Ni2	102.4(3)
O6	Gd1	Ni2	64.5(3)	O4	Gd1	Ni2	132.6(3)
O1	Gd1	Ni2	104.3(3)	O2	Gd1	Ni2	153.4(3)
O3	Gd1	Ni2	88.0(2)	O12	Gd1	Ni1	103.5(2)
O14	Gd1	Ni1	131.3(3)	O10	Gd1	Ni1	97.9(2)
O8	Gd1	Ni1	63.8(3)	O6	Gd1	Ni1	33.9(3)
O4	Gd1	Ni1	35.0(2)	O1	Gd1	Ni1	88.8(2)
O2	Gd1	Ni1	105.5(3)	O3	Gd1	Ni1	154.2(2)
Ni2	Gd1	Ni1	98.41(6)	O12	Gd1	Ni3	63.9(3)
O14	Gd1	Ni3	34.4(3)	O10	Gd1	Ni3	131.6(3)
O8	Gd1	Ni3	33.9(3)	O6	Gd1	Ni3	102.7(2)

atom	atom	atom	angle	atom	atom	atom	angle
O4	Gd1	Ni3	97.2(3)	O1	Gd1	Ni3	155.5(3)
O2	Gd1	Ni3	90.0(3)	O3	Gd1	Ni3	106.2(2)
Ni2	Gd1	Ni3	98.13(6)	Ni1	Gd1	Ni3	97.70(6)
O26	Gd2	O16	119.5(4)	O26	Gd2	O18	69.7(4)
O16	Gd2	O18	67.2(3)	O26	Gd2	O3	74.4(3)
O16	Gd2	O3	131.5(3)	O18	Gd2	O3	144.0(3)
O26	Gd2	O20	132.5(3)	O16	Gd2	O20	68.7(4)
O18	Gd2	O20	72.9(4)	O3	Gd2	O20	138.8(3)
O26	Gd2	O1	130.8(4)	O16	Gd2	O1	72.0(4)
O18	Gd2	O1	138.9(4)	O3	Gd2	O1	66.5(4)
O20	Gd2	O1	96.7(3)	O26	Gd2	O22	121.3(4)
O16	Gd2	O22	119.0(4)	O18	Gd2	O22	131.7(3)
O3	Gd2	O22	71.7(3)	O20	Gd2	O22	67.4(4)
O1	Gd2	O22	73.5(4)	O26	Gd2	O24	67.7(4)
O16	Gd2	O24	133.5(4)	O18	Gd2	O24	75.0(4)
O3	Gd2	O24	95.1(4)	O20	Gd2	O24	75.1(4)
O1	Gd2	O24	142.0(4)	O22	Gd2	O24	69.1(3)
O26	Gd2	O2	71.9(4)	O16	Gd2	O2	74.6(4)
O18	Gd2	O2	98.4(4)	O3	Gd2	O2	66.2(4)
O20	Gd2	O2	142.8(4)	O1	Gd2	O2	65.7(4)
O22	Gd2	O2	129.9(4)	O24	Gd2	O2	138.8(4)
O26	Gd2	Ni6	34.0(3)	O16	Gd2	Ni6	130.8(3)
O18	Gd2	Ni6	64.0(2)	O3	Gd2	Ni6	88.1(2)
O20	Gd2	Ni6	102.4(2)	O1	Gd2	Ni6	154.6(3)
O22	Gd2	Ni6	98.5(3)	O24	Gd2	Ni6	34.3(2)
O2	Gd2	Ni6	105.9(3)	O26	Gd2	Gd1	92.2(3)
O16	Gd2	Gd1	92.0(2)	O18	Gd2	Gd1	137.4(2)
O3	Gd2	Gd1	39.5(2)	O20	Gd2	Gd1	135.3(2)
O1	Gd2	Gd1	38.6(2)	O22	Gd2	Gd1	90.8(2)
O24	Gd2	Gd1	134.6(3)	O2	Gd2	Gd1	39.0(3)
Ni6	Gd2	Gd1	119.77(5)	O6	Ni1	N7	92.8(6)
O6	Ni1	N2	84.3(5)	N7	Ni1	N2	89.2(7)

atom	atom	atom	angle	atom	atom	atom	angle
O6	Ni1	O4	84.8(5)	N7	Ni1	O4	90.5(6)
N2	Ni1	O4	169.1(5)	O6	Ni1	N1	166.8(5)
N7	Ni1	N1	90.0(7)	N2	Ni1	N1	108.6(5)
O4	Ni1	N1	82.3(5)	O6	Ni1	O9	88.4(4)
N7	Ni1	O9	177.9(6)	N2	Ni1	O9	89.2(5)
O4	Ni1	O9	91.4(4)	N1	Ni1	O9	89.3(5)
O6	Ni1	Gd1	42.5(3)	N7	Ni1	Gd1	98.1(5)
N2	Ni1	Gd1	126.4(4)	O4	Ni1	Gd1	42.9(3)
N1	Ni1	Gd1	124.3(4)	O9	Ni1	Gd1	83.9(3)
O10	Ni2	O12	83.5(5)	O10	Ni2	N5	167.6(5)
O12	Ni2	N5	84.5(5)	O10	Ni2	N8	88.4(6)
O12	Ni2	N8	92.4(6)	N5	Ni2	N8	89.1(6)
O10	Ni2	N4	83.9(6)	O12	Ni2	N4	166.9(6)
N5	Ni2	N4	108.2(7)	N8	Ni2	N4	91.0(7)
O10	Ni2	O7	89.3(4)	O12	Ni2	O7	88.6(4)
N5	Ni2	O7	93.5(5)	N8	Ni2	O7	177.3(6)
N4	Ni2	O7	87.4(6)	O10	Ni2	Gd1	42.3(3)
O12	Ni2	Gd1	41.9(3)	N5	Ni2	Gd1	126.2(4)
N8	Ni2	Gd1	96.5(5)	N4	Ni2	Gd1	125.1(5)
O7	Ni2	Gd1	82.6(3)	O8	Ni3	N3	84.9(5)
O8	Ni3	O14	83.8(5)	N3	Ni3	O14	168.6(5)
O8	Ni3	N6	168.1(5)	N3	Ni3	N6	106.7(6)
O14	Ni3	N6	84.6(5)	O8	Ni3	N9	91.6(5)
N3	Ni3	N9	92.4(6)	O14	Ni3	N9	88.8(5)
N6	Ni3	N9	90.4(6)	O8	Ni3	O13	88.7(5)
N3	Ni3	O13	89.5(6)	O14	Ni3	O13	89.4(5)
N6	Ni3	O13	88.9(5)	N9	Ni3	O13	178.1(5)
O8	Ni3	Gd1	42.2(4)	N3	Ni3	Gd1	126.5(4)
O14	Ni3	Gd1	42.2(3)	N6	Ni3	Gd1	125.9(4)
N9	Ni3	Gd1	95.6(4)	O13	Ni3	Gd1	83.3(4)
O18	Ni4	O16	83.9(4)	O18	Ni4	N11	83.4(5)
O16	Ni4	N11	167.2(5)	O18	Ni4	N10	166.8(5)

atom	atom	atom	angle	atom	atom	atom	angle
O16	Ni4	N10	83.8(5)	N11	Ni4	N10	108.6(6)
O18	Ni4	N16	94.7(5)	O16	Ni4	N16	89.2(5)
N11	Ni4	N16	94.1(6)	N10	Ni4	N16	89.9(6)
O18	Ni4	O21	86.6(4)	O16	Ni4	O21	91.2(5)
N11	Ni4	O21	85.8(5)	N10	Ni4	O21	88.8(5)
N16	Ni4	O21	178.6(6)	O22	Ni5	N12	167.5(5)
O22	Ni5	O20	85.1(5)	N12	Ni5	O20	82.9(6)
O22	Ni5	N13	82.1(5)	N12	Ni5	N13	109.5(6)
O20	Ni5	N13	166.3(5)	O22	Ni5	N17	92.6(6)
N12	Ni5	N17	91.6(7)	O20	Ni5	N17	93.2(5)
N13	Ni5	N17	92.3(6)	O22	Ni5	O25	91.3(5)
N12	Ni5	O25	84.9(5)	O20	Ni5	O25	88.7(4)
N13	Ni5	O25	86.6(5)	N17	Ni5	O25	175.8(6)
O24	Ni6	O26	84.4(4)	O24	Ni6	N14	80.9(5)
O26	Ni6	N14	165.3(5)	O24	Ni6	N18	93.0(6)
O26	Ni6	N18	90.7(5)	N14	Ni6	N18	89.6(5)
O24	Ni6	N15	167.1(5)	O26	Ni6	N15	83.1(5)
N14	Ni6	N15	111.5(5)	N18	Ni6	N15	90.6(6)
O24	Ni6	O19	88.7(5)	O26	Ni6	O19	90.5(4)
N14	Ni6	O19	89.7(5)	N18	Ni6	O19	178.0(6)
N15	Ni6	O19	87.9(5)	O24	Ni6	Gd2	43.5(3)
O26	Ni6	Gd2	41.7(3)	N14	Ni6	Gd2	123.9(4)
N18	Ni6	Gd2	98.7(4)	N15	Ni6	Gd2	123.7(4)
O19	Ni6	Gd2	83.3(3)	Gd2	O1	Gd1	103.0(4)
Gd2	O1	H1A	111.2	Gd1	O1	H1A	111.2
Gd2	O1	H1B	111.2	Gd1	O1	H1B	111.2
H1A	O1	H1B	109.1	Gd1	O2	Gd2	101.8(4)
Gd1	O2	H2B	111.4	Gd2	O2	H2B	111.4
Gd1	O2	H2C	111.4	Gd2	O2	H2C	111.4
H2B	O2	H2C	109.3	Gd2	O3	Gd1	102.0(4)
Gd2	O3	H3B	111.4	Gd1	O3	H3B	111.4
Gd2	O3	H3C	111.4	Gd1	O3	H3C	111.4

atom	atom	atom	angle	atom	atom	atom	angle
H3B	O3	H3C	109.2	C1	O4	Ni1	114.4(10)
C1	O4	Gd1	143.5(10)	Ni1	O4	Gd1	102.0(5)
C6	O6	Ni1	115.7(11)	C6	O6	Gd1	139.0(11)
Ni1	O6	Gd1	103.6(5)	C6	O7	Ni2	127.4(11)
C11	O8	Ni3	116.5(11)	C11	O8	Gd1	138.4(11)
Ni3	O8	Gd1	103.9(5)	C11	O9	Ni1	125.8(11)
C16	O10	Ni2	113.8(12)	C16	O10	Gd1	141.9(12)
Ni2	O10	Gd1	103.5(5)	C21	O12	Ni2	115.8(11)
C21	O12	Gd1	139.1(11)	Ni2	O12	Gd1	103.8(5)
C21	O13	Ni3	126.6(13)	C26	O14	Ni3	113.1(13)
C26	O14	Gd1	143.1(13)	Ni3	O14	Gd1	103.4(5)
C37	O16	Ni4	116.5(11)	C37	O16	Gd2	138.3(11)
Ni4	O16	Gd2	103.9(4)	C42	O18	Ni4	116.5(12)
C42	O18	Gd2	138.5(11)	Ni4	O18	Gd2	103.9(4)
C42	O19	Ni6	126.5(12)	C47	O20	Ni5	114.8(12)
C47	O20	Gd2	138.8(11)	Ni5	O20	Gd2	102.7(5)
C47	O21	Ni4	128.4(13)	C52	O22	Ni5	116.3(11)
C52	O22	Gd2	138.3(11)	Ni5	O22	Gd2	103.4(5)
C57	O24	Ni6	119.3(11)	C57	O24	Gd2	134.5(11)
Ni6	O24	Gd2	102.3(4)	C57	O25	Ni5	125.8(11)
C62	O26	Ni6	112.9(11)	C62	O26	Gd2	142.0(11)
Ni6	O26	Gd2	104.3(5)	C2	N1	Ni1	106.2(10)
C7	N2	Ni1	108.8(10)	C12	N3	Ni3	108.3(10)
C17	N4	Ni2	106.3(12)	C22	N5	Ni2	110.0(11)
C27	N6	Ni3	107.7(10)	C31	N7	Ni1	171(2)
C33	N8	Ni2	167(2)	C35	N9	Ni3	169.7(15)
C38	N10	Ni4	107.7(10)	C43	N11	Ni4	108.4(10)
C48	N12	Ni5	107.4(11)	C53	N13	Ni5	109.4(10)
C58	N14	Ni6	107.9(9)	C63	N15	Ni6	106.1(9)
C67	N16	Ni4	165.9(17)	C69	N17	Ni5	168(2)
C71	N18	Ni6	170(2)	O5	C1	O4	120.5(16)
O5	C1	C2	123.6(17)	O4	C1	C2	115.8(16)

atom	atom	atom	angle	atom	atom	atom	angle
N1	C2	C1	110.2(15)	N1	C2	C3	114.1(15)
C1	C2	C3	110.9(15)	N1	C2	H2A	107.1
C1	C2	H2A	107.1	C3	C2	H2A	107.1
C2	C3	C4	109.2(17)	C2	C3	C5	110.8(17)
C4	C3	C5	115.1(18)	C2	C3	H3A	107.1
C4	C3	H3A	107.1	C5	C3	H3A	107.1
C3	C4	H4A	109.5	C3	C4	H4B	109.5
H4A	C4	H4B	109.5	C3	C4	H4C	109.5
H4A	C4	H4C	109.5	H4B	C4	H4C	109.5
C3	C5	H5A	109.5	C3	C5	H5B	109.5
H5A	C5	H5B	109.5	C3	C5	H5C	109.5
H5A	C5	H5C	109.5	H5B	C5	H5C	109.5
O7	C6	O6	124.8(16)	O7	C6	C7	116.4(17)
O6	C6	C7	118.8(17)	N2	C7	C8	114.1(16)
N2	C7	C6	112.1(14)	C8	C7	C6	113.8(16)
N2	C7	H7A	105.2	C8	C7	H7A	105.2
C6	C7	H7A	105.2	C10	C8	C7	111.1(17)
C10	C8	C9	115.0(18)	C7	C8	C9	109.6(17)
C10	C8	H8A	107.0	C7	C8	H8A	107.0
C9	C8	H8A	107.0	C8	C9	H9A	109.5
C8	C9	H9B	109.5	H9A	C9	H9B	109.5
C8	C9	H9C	109.5	H9A	C9	H9C	109.5
H9B	C9	H9C	109.5	C8	C10	H10A	109.5
C8	C10	H10B	109.5	H10A	C10	H10B	109.5
C8	C10	H10C	109.5	H10A	C10	H10C	109.5
H10B	C10	H10C	109.5	O9	C11	O8	126.5(16)
O9	C11	C12	118.1(18)	O8	C11	C12	115.4(17)
N3	C12	C13	113.0(14)	N3	C12	C11	114.9(15)
C13	C12	C11	108.9(15)	N3	C12	H12A	106.5
C13	C12	H12A	106.5	C11	C12	H12A	106.5
C14	C13	C12	112.4(15)	C14	C13	C15	110.6(16)
C12	C13	C15	113.1(16)	C14	C13	H13A	106.8

atom	atom	atom	angle	atom	atom	atom	angle
C12	C13	H13A	106.8	C15	C13	H13A	106.8
C13	C14	H14A	109.5	C13	C14	H14B	109.5
H14A	C14	H14B	109.5	C13	C14	H14C	109.5
H14A	C14	H14C	109.5	H14B	C14	H14C	109.5
C13	C15	H15A	109.5	C13	C15	H15B	109.5
H15A	C15	H15B	109.5	C13	C15	H15C	109.5
H15A	C15	H15C	109.5	H15B	C15	H15C	109.5
O11	C16	O10	125.7(17)	O11	C16	C17	116(2)
O10	C16	C17	118(2)	N4	C17	C16	112.0(17)
N4	C17	C18	112.8(18)	C16	C17	C18	114.5(19)
N4	C17	H17A	105.5	C16	C17	H17A	105.5
C18	C17	H17A	105.5	C19	C18	C20	116(2)
C19	C18	C17	113.7(19)	C20	C18	C17	109(2)
C19	C18	H18A	105.5	C20	C18	H18A	105.5
C17	C18	H18A	105.5	C18	C19	H19A	109.5
C18	C19	H19B	109.5	H19A	C19	H19B	109.5
C18	C19	H19C	109.5	H19A	C19	H19C	109.5
H19B	C19	H19C	109.5	C18	C20	H20A	109.5
C18	C20	H20B	109.5	H20A	C20	H20B	109.5
C18	C20	H20C	109.5	H20A	C20	H20C	109.5
H20B	C20	H20C	109.5	O13	C21	O12	125.9(17)
O13	C21	C22	115.8(17)	O12	C21	C22	118.1(16)
C23	C22	N5	111.5(17)	C23	C22	C21	111.2(16)
N5	C22	C21	110.6(16)	C23	C22	H22A	107.8
N5	C22	H22A	107.8	C21	C22	H22A	107.8
C22	C23	C24	114.6(16)	C22	C23	C25	113.2(16)
C24	C23	C25	111.5(15)	C22	C23	H23A	105.5
C24	C23	H23A	105.5	C25	C23	H23A	105.5
C23	C24	H24A	109.5	C23	C24	H24B	109.5
H24A	C24	H24B	109.5	C23	C24	H24C	109.5
H24A	C24	H24C	109.5	H24B	C24	H24C	109.5
C23	C25	H25A	109.5	C23	C25	H25B	109.5

atom	atom	atom	angle	atom	atom	atom	angle
H25A	C25	H25B	109.5	C23	C25	H25C	109.5
H25A	C25	H25C	109.5	H25B	C25	H25C	109.5
O15	C26	O14	121.4(18)	O15	C26	C27	124.2(18)
O14	C26	C27	114(2)	N6	C27	C28	117.7(15)
N6	C27	C26	112.2(14)	C28	C27	C26	110.0(16)
N6	C27	H27A	105.3	C28	C27	H27A	105.3
C26	C27	H27A	105.3	C29	C28	C27	110.8(18)
C29	C28	C30	112.2(18)	C27	C28	C30	111.2(15)
C29	C28	H28A	107.5	C27	C28	H28A	107.5
C30	C28	H28A	107.5	C28	C29	H29A	109.5
C28	C29	H29B	109.5	H29A	C29	H29B	109.5
C28	C29	H29C	109.5	H29A	C29	H29C	109.5
H29B	C29	H29C	109.5	C28	C30	H30A	109.5
C28	C30	H30B	109.5	H30A	C30	H30B	109.5
C28	C30	H30C	109.5	H30A	C30	H30C	109.5
H30B	C30	H30C	109.5	N7	C31	C32	176(3)
C31	C32	H32A	109.5	C31	C32	H32B	109.5
H32A	C32	H32B	109.5	C31	C32	H32C	109.5
H32A	C32	H32C	109.5	H32B	C32	H32C	109.5
N8	C33	C34	173(3)	C33	C34	H34A	109.5
C33	C34	H34B	109.5	H34A	C34	H34B	109.5
C33	C34	H34C	109.5	H34A	C34	H34C	109.5
H34B	C34	H34C	109.5	N9	C35	C36	177(2)
C35	C36	H36A	109.5	C35	C36	H36B	109.5
H36A	C36	H36B	109.5	C35	C36	H36C	109.5
H36A	C36	H36C	109.5	H36B	C36	H36C	109.5
O17	C37	O16	126.2(18)	O17	C37	C38	117.4(16)
O16	C37	C38	116.4(16)	N10	C38	C37	112.7(13)
N10	C38	C39	113.1(16)	C37	C38	C39	108.9(15)
N10	C38	H38A	107.3	C37	C38	H38A	107.3
C39	C38	H38A	107.3	C40	C39	C41	114(2)
C40	C39	C38	108.2(17)	C41	C39	C38	111.0(18)

atom	atom	atom	angle	atom	atom	atom	angle
C40	C39	H39A	107.8	C41	C39	H39A	107.8
C38	C39	H39A	107.8	C39	C40	H40A	109.5
C39	C40	H40B	109.5	H40A	C40	H40B	109.5
C39	C40	H40C	109.5	H40A	C40	H40C	109.5
H40B	C40	H40C	109.5	C39	C41	H41A	109.5
C39	C41	H41B	109.5	H41A	C41	H41B	109.5
C39	C41	H41C	109.5	H41A	C41	H41C	109.5
H41B	C41	H41C	109.5	O19	C42	O18	126.3(18)
O19	C42	C43	115.8(17)	O18	C42	C43	117.7(16)
N11	C43	C42	113.7(14)	N11	C43	C44	113.5(15)
C42	C43	C44	109.8(16)	N11	C43	H43A	106.5
C42	C43	H43A	106.5	C44	C43	H43A	106.5
C45	C44	C46	111.7(17)	C45	C44	C43	112.6(17)
C46	C44	C43	111.1(15)	C45	C44	H44A	107.0
C46	C44	H44A	107.0	C43	C44	H44A	107.0
C44	C45	H45A	109.5	C44	C45	H45B	109.5
H45A	C45	H45B	109.5	C44	C45	H45C	109.5
H45A	C45	H45C	109.5	H45B	C45	H45C	109.5
C44	C46	H46A	109.5	C44	C46	H46B	109.5
H46A	C46	H46B	109.5	C44	C46	H46C	109.5
H46A	C46	H46C	109.5	H46B	C46	H46C	109.5
O21	C47	O20	123.3(18)	O21	C47	C48	121.4(19)
O20	C47	C48	114.9(18)	N12	C48	C47	113.2(15)
N12	C48	C49	111.3(16)	C47	C48	C49	112.1(17)
N12	C48	H48A	106.6	C47	C48	H48A	106.6
C49	C48	H48A	106.6	C51	C49	C48	115.2(18)
C51	C49	C50	113.5(18)	C48	C49	C50	109.7(17)
C51	C49	H49A	105.9	C48	C49	H49A	105.9
C50	C49	H49A	105.9	C49	C50	H50A	109.5
C49	C50	H50B	109.5	H50A	C50	H50B	109.5
C49	C50	H50C	109.5	H50A	C50	H50C	109.5
H50B	C50	H50C	109.5	C49	C51	H51A	109.5

atom	atom	atom	angle	atom	atom	atom	angle
C49	C51	H51B	109.5	H51A	C51	H51B	109.5
C49	C51	H51C	109.5	H51A	C51	H51C	109.5
H51B	C51	H51C	109.5	O23	C52	O22	125.3(17)
O23	C52	C53	119.0(17)	O22	C52	C53	115.6(17)
N13	C53	C54	113.3(14)	N13	C53	C52	108.1(14)
C54	C53	C52	111.6(16)	N13	C53	H53A	107.9
C54	C53	H53A	107.9	C52	C53	H53A	107.9
C53	C54	C55	113.9(18)	C53	C54	C56	115.8(16)
C55	C54	C56	105.1(15)	C53	C54	H54A	107.2
C55	C54	H54A	107.2	C56	C54	H54A	107.2
C54	C55	H55A	109.5	C54	C55	H55B	109.5
H55A	C55	H55B	109.5	C54	C55	H55C	109.5
H55A	C55	H55C	109.5	H55B	C55	H55C	109.5
C54	C56	H56A	109.5	C54	C56	H56B	109.5
H56A	C56	H56B	109.5	C54	C56	H56C	109.5
H56A	C56	H56C	109.5	H56B	C56	H56C	109.5
O25	C57	O24	128.8(16)	O25	C57	C58	117.7(15)
O24	C57	C58	113.5(15)	N14	C58	C59	113.2(14)
N14	C58	C57	109.7(14)	C59	C58	C57	115.4(15)
N14	C58	H58A	105.9	C59	C58	H58A	105.9
C57	C58	H58A	105.9	C58	C59	C60	115.4(16)
C58	C59	C61	113.8(17)	C60	C59	C61	112.3(16)
C58	C59	H59A	104.6	C60	C59	H59A	104.6
C61	C59	H59A	104.6	C59	C60	H60A	109.5
C59	C60	H60B	109.5	H60A	C60	H60B	109.5
C59	C60	H60C	109.5	H60A	C60	H60C	109.5
H60B	C60	H60C	109.5	C59	C61	H61A	109.5
C59	C61	H61B	109.5	H61A	C61	H61B	109.5
C59	C61	H61C	109.5	H61A	C61	H61C	109.5
H61B	C61	H61C	109.5	O27	C62	O26	121.3(16)
O27	C62	C63	119.8(16)	O26	C62	C63	118.3(16)
C64	C63	C62	113.5(15)	C64	C63	N15	116.0(15)

atom	atom	atom	angle	atom	atom	atom	angle
C62	C63	N15	110.2(15)	C64	C63	H63A	105.4
C62	C63	H63A	105.4	N15	C63	H63A	105.4
C63	C64	C66	112.7(17)	C63	C64	C65	111.0(15)
C66	C64	C65	106.9(16)	C63	C64	H64A	108.7
C66	C64	H64A	108.7	C65	C64	H64A	108.7
C64	C65	H65A	109.5	C64	C65	H65B	109.5
H65A	C65	H65B	109.5	C64	C65	H65C	109.5
H65A	C65	H65C	109.5	H65B	C65	H65C	109.5
C64	C66	H66A	109.5	C64	C66	H66B	109.5
H66A	C66	H66B	109.5	C64	C66	H66C	109.5
H66A	C66	H66C	109.5	H66B	C66	H66C	109.5
N16	C67	C68	176(2)	C67	C68	H68A	109.5
C67	C68	H68B	109.5	H68A	C68	H68B	109.5
C67	C68	H68C	109.5	H68A	C68	H68C	109.5
H68B	C68	H68C	109.5	N17	C69	C70	176(3)
C69	C70	H70A	109.5	C69	C70	H70B	109.5
H70A	C70	H70B	109.5	C69	C70	H70C	109.5
H70A	C70	H70C	109.5	H70B	C70	H70C	109.5
N18	C71	C72	176(3)	C71	C72	H72A	109.5
C71	C72	H72B	109.5	H72A	C72	H72B	109.5
C71	C72	H72C	109.5	H72A	C72	H72C	109.5
H72B	C72	H72C	109.5	O61	Gd3	O71	86.1(4)
O61	Gd3	O70	123.9(4)	O71	Gd3	O70	53.2(4)
O61	Gd3	O50	80.6(4)	O71	Gd3	O50	159.2(4)
O70	Gd3	O50	123.5(4)	O61	Gd3	O41	75.0(4)
O71	Gd3	O41	121.2(4)	O70	Gd3	O41	156.0(4)
O50	Gd3	O41	70.5(4)	O61	Gd3	O60	52.8(4)
O71	Gd3	O60	76.6(4)	O70	Gd3	O60	78.8(4)
O50	Gd3	O60	82.6(4)	O41	Gd3	O60	124.5(4)
O61	Gd3	O30	141.4(4)	O71	Gd3	O30	78.2(4)
O70	Gd3	O30	72.5(4)	O50	Gd3	O30	121.9(4)
O41	Gd3	O30	83.5(4)	O60	Gd3	O30	149.5(4)

atom	atom	atom	angle	atom	atom	atom	angle
O61	Gd3	O40	70.6(4)	O71	Gd3	O40	70.4(5)
O70	Gd3	O40	117.1(4)	O50	Gd3	O40	119.1(4)
O41	Gd3	O40	50.9(4)	O60	Gd3	O40	115.3(4)
O30	Gd3	O40	70.9(4)	O61	Gd3	O51	108.1(4)
O71	Gd3	O51	120.3(5)	O70	Gd3	O51	72.7(4)
O50	Gd3	O51	50.9(4)	O41	Gd3	O51	118.4(4)
O60	Gd3	O51	69.4(4)	O30	Gd3	O51	110.3(4)
O40	Gd3	O51	169.3(5)	O61	Gd3	O31	149.0(4)
O71	Gd3	O31	123.8(4)	O70	Gd3	O31	84.7(4)
O50	Gd3	O31	72.6(4)	O41	Gd3	O31	81.5(4)
O60	Gd3	O31	135.4(4)	O30	Gd3	O31	52.2(4)
O40	Gd3	O31	109.1(4)	O51	Gd3	O31	66.2(4)
O61	Gd3	N60	26.6(4)	O71	Gd3	N60	80.9(4)
O70	Gd3	N60	101.8(5)	O50	Gd3	N60	80.1(4)
O41	Gd3	N60	99.9(5)	O60	Gd3	N60	26.2(4)
O30	Gd3	N60	157.1(4)	O40	Gd3	N60	93.5(4)
O51	Gd3	N60	88.1(4)	O31	Gd3	N60	150.5(4)
O61	Gd3	N70	107.4(4)	O71	Gd3	N70	26.9(4)
O70	Gd3	N70	26.5(4)	O50	Gd3	N70	147.3(4)
O41	Gd3	N70	142.0(4)	O60	Gd3	N70	78.2(4)
O30	Gd3	N70	71.6(4)	O40	Gd3	N70	93.1(4)
O51	Gd3	N70	97.3(5)	O31	Gd3	N70	103.6(4)
N60	Gd3	N70	93.4(5)	N30	O30	Gd3	98.4(10)
O30	N30	O32	126.7(15)	O30	N30	O31	115.8(16)
O32	N30	O31	117.3(17)	O30	N30	Gd3	57.1(9)
O32	N30	Gd3	176.2(13)	O31	N30	Gd3	58.9(9)
N30	O31	Gd3	93.3(11)	N40	O40	Gd3	97.6(10)
O42	N40	O40	123.2(16)	O42	N40	O41	125.4(17)
O40	N40	O41	111.3(16)	O42	N40	Gd3	179.1(12)
O40	N40	Gd3	57.1(9)	O41	N40	Gd3	54.2(9)
N40	O41	Gd3	100.1(11)	N50	O50	Gd3	98.1(10)
O50	N50	O52	123.6(16)	O50	N50	O51	116.4(15)

atom	atom	atom	angle	atom	atom	atom	angle
O52	N50	O51	120.0(16)	O50	N50	Gd3	56.8(8)
O52	N50	Gd3	172.2(11)	O51	N50	Gd3	60.6(8)
N50	O51	Gd3	93.3(10)	N60	O60	Gd3	94.8(11)
O62	N60	O60	124.4(18)	O62	N60	O61	120.1(17)
O60	N60	O61	115.6(15)	O62	N60	Gd3	176.4(14)
O60	N60	Gd3	59.0(9)	O61	N60	Gd3	56.6(8)
N60	O61	Gd3	96.8(10)	N70	O70	Gd3	96.5(10)
O72	N70	O70	120.5(16)	O72	N70	O71	125.6(16)
O70	N70	O71	113.6(15)	O72	N70	Gd3	177.4(13)
O70	N70	Gd3	57.0(8)	O71	N70	Gd3	57.0(8)
N70	O71	Gd3	96.1(10)	O33	Cl1	O36	111.0(8)
O33	Cl1	O35	110.9(8)	O36	Cl1	O35	110.2(8)
O33	Cl1	O34	108.4(8)	O36	Cl1	O34	108.2(8)
O35	Cl1	O34	108.2(8)	O46	Cl2	O44	111.5(8)
O46	Cl2	O43	112.1(9)	O44	Cl2	O43	110.8(9)
O46	Cl2	O45	108.0(8)	O44	Cl2	O45	108.2(8)
O43	Cl2	O45	106.0(9)	O53	Cl3	O54	114.4(11)
O53	Cl3	O56	113.5(11)	O54	Cl3	O56	106.8(9)
O53	Cl3	O55	107.3(10)	O54	Cl3	O55	108.4(11)
O56	Cl3	O55	106.0(11)	O66	Cl4	O64	112.8(10)
O66	Cl4	O65	109.5(9)	O64	Cl4	O65	111.3(9)
O66	Cl4	O63	109.3(9)	O64	Cl4	O63	108.1(9)
O65	Cl4	O63	105.5(9)	O73	Cl5	O76	112.2(9)
O73	Cl5	O75	111.0(10)	O76	Cl5	O75	110.0(10)
O73	Cl5	O74	107.5(10)	O76	Cl5	O74	108.3(9)
O75	Cl5	O74	107.7(9)	N2S	C9S	C10S	169(3)
C9S	C10S	H10D	109.5	C9S	C10S	H10E	109.5
H10D	C10S	H10E	109.5	C9S	C10S	H10F	109.5
H10D	C10S	H10F	109.5	H10E	C10S	H10F	109.5
N3S	C11S	C12S	166(5)	C11S	C12S	H12B	109.5
C11S	C12S	H12C	109.5	H12B	C12S	H12C	109.5
C11S	C12S	H12D	109.5	H12B	C12S	H12D	109.5

atom	atom	atom	angle	atom	atom	atom	angle
H12C	C12S	H12D	109.5	N4S	C13S	C14S	169(5)
C13S	C14S	H14D	109.5	C13S	C14S	H14E	109.5
H14D	C14S	H14E	109.5	C13S	C14S	H14F	109.5
H14D	C14S	H14F	109.5	H14E	C14S	H14F	109.5
N5S	C15S	C16S	177(5)	C15S	C16S	H16A	109.5
C15S	C16S	H16B	109.5	H16A	C16S	H16B	109.5
C15S	C16S	H16C	109.5	H16A	C16S	H16C	109.5
H16B	C16S	H16C	109.5	N6S	C17S	C18S	155(6)
C17S	C18S	H18B	109.5	C17S	C18S	H18C	109.5
H18B	C18S	H18C	109.5	C17S	C18S	H18D	109.5
H18B	C18S	H18D	109.5	H18C	C18S	H18D	109.5
C7S	N1S	C5S	111(3)	C7S	N1S	C1S	110(3)
C5S	N1S	C1S	109(3)	C7S	N1S	C3S	109(3)
C5S	N1S	C3S	109(3)	C1S	N1S	C3S	108(3)
N1S	C1S	C2S	88(2)	N1S	C3S	C4S	87(2)
N1S	C5S	C6S	87(2)	N1S	C7S	C8S	89(2)

Table 5. Special Distances (Å)

atom	atom	distance	atom	atom	distance
Gd1	Gd2	5.886(2)	Gd1	Ni1	3.513(2)
Gd1	Ni2	3.513(3)	Gd1	Ni3	3.522(2)
Gd2	Ni4	3.548(2)	Gd2	Ni5	3.541(2)
Gd2	Ni6	3.530(2)	Ni1	Ni2	5.319(4)
Ni2	Ni3	5.314(4)	Ni3	Ni1	5.297(3)
Ni4	Ni5	5.307(3)	Ni5	Ni6	5.328(4)
Ni6	Ni4	5.329(4)			

Structure Factor Table for

$TEA[Gd_2\{Ni(val)_2\}_6(H_2O)_3(NO_3)_3(CH_3CN)_3](ClO_4)_4$ (**4**)

Table 1. Atomic coordinates, U_{eq} and occupancy

atom	x	y	z	U_{eq}	occ
Gd(1)	0.12404(2)	0.1240	0.1240	0.03897(3)	0.3333
Gd(2)	0.02941(2)	0.0294	0.0294	0.03748(3)	0.3333
Ni(1)	0.17977(5)	0.24887(5)	0.07009(5)	0.0490(3)	1.0000
Ni(2)	0.06159(5)	0.01378(5)	-0.11198(5)	0.0487(3)	1.0000
Cl(1)	0.4263(2)	-0.0107(3)	0.1943(2)	0.135(2)	1.0000
Cl(2)	0.2882(2)	0.2882	0.2882	0.108(1)	0.3333
O(1)	0.1361(3)	0.2247(2)	0.1376(3)	0.049(2)	1.0000
O(2)	0.1066(3)	0.2541(3)	0.2211(3)	0.059(2)	1.0000
O(3)	0.1638(3)	0.1700(2)	0.0425(2)	0.046(2)	1.0000
O(4)	0.1843(3)	0.1120(3)	-0.0266(3)	0.059(2)	1.0000
O(5)	0.0438(3)	-0.0364(2)	-0.0469(2)	0.047(2)	1.0000
O(6)	0.0262(3)	-0.1252(3)	-0.0251(3)	0.062(2)	1.0000
O(7)	0.0621(2)	0.0756(2)	-0.0545(2)	0.043(2)	1.0000
O(8)	0.0665(3)	0.1683(3)	-0.0473(3)	0.057(2)	1.0000
O(9)	0.0459(2)	0.1308(2)	0.0530(2)	0.042(1)	1.0000
O(10)	0.1450(3)	-0.0010(3)	-0.0899(3)	0.069(2)	1.0000
O(11)	0.1788(5)	0.0027(8)	-0.1720(6)	0.171(6)	1.0000
O(12)	0.2337(4)	-0.0082(7)	-0.1083(8)	0.166(7)	1.0000
O(13)	0.413(1)	0.0399(10)	0.2207(8)	0.26(1)	1.0000
O(14)	0.3735(9)	-0.050(1)	0.197(1)	0.28(1)	1.0000
O(15)	0.420(1)	-0.003(1)	0.1408(7)	0.33(1)	1.0000
O(16)	0.4722(7)	-0.026(1)	0.2180(9)	0.31(1)	1.0000
O(17)	0.288(1)	0.270(1)	0.3412(8)	0.23(1)	1.0000
O(18)	0.2554(6)	0.2554	0.2554	0.194(6)	0.3333
N(1)	0.1894(4)	0.3220(3)	0.1146(4)	0.063(3)	1.0000
N(2)	0.2232(4)	0.2559(4)	-0.0039(4)	0.060(2)	1.0000
N(3)	0.0556(4)	-0.0589(4)	-0.1560(4)	0.070(3)	1.0000
N(4)	0.0785(4)	0.0766(4)	-0.1652(3)	0.063(3)	1.0000
N(5)	0.1066(4)	0.2777(4)	0.0302(4)	0.072(3)	1.0000
N(6)	0.1866(4)	-0.0036(5)	-0.1225(5)	0.079(3)	1.0000

atom	x	y	z	U_{eq}	occ
N(7)	0.4059(9)	0.4059	0.4059	0.122(4)	0.3333
C(1)	0.1612(5)	0.3177(4)	0.1698(5)	0.060(3)	1.0000
C(2)	0.1306(4)	0.2616(4)	0.1777(4)	0.054(3)	1.0000
C(3)	0.1213(6)	0.3648(5)	0.1838(5)	0.071(3)	1.0000
C(4)	0.0772(6)	0.3709(6)	0.1435(7)	0.099(5)	1.0000
C(5)	0.1549(8)	0.4192(6)	0.1862(9)	0.129(7)	1.0000
C(6)	0.2035(5)	0.2106(4)	-0.0397(4)	0.057(3)	1.0000
C(7)	0.1840(4)	0.1590(4)	-0.0058(4)	0.048(2)	1.0000
C(8)	0.2455(5)	0.1930(5)	-0.0871(5)	0.072(4)	1.0000
C(9)	0.2577(9)	0.2442(7)	-0.1236(7)	0.132(7)	1.0000
C(10)	0.3012(6)	0.1706(7)	-0.0618(7)	0.098(5)	1.0000
C(11)	0.0356(5)	-0.1043(4)	-0.1218(4)	0.067(3)	1.0000
C(12)	0.0362(4)	-0.0885(4)	-0.0592(4)	0.051(3)	1.0000
C(13)	0.072(2)	-0.1588(7)	-0.1315(6)	0.21(1)	1.0000
C(14)	0.143(2)	-0.145(2)	-0.134(2)	0.45(3)	1.0000
C(15)	0.047(3)	-0.1780(10)	-0.1893(9)	0.35(2)	1.0000
C(16)	0.0939(5)	0.1283(4)	-0.1350(4)	0.059(3)	1.0000
C(17)	0.0719(4)	0.1244(4)	-0.0752(4)	0.049(2)	1.0000
C(18)	0.0797(7)	0.1815(5)	-0.1648(5)	0.086(4)	1.0000
C(19)	0.0169(10)	0.1846(9)	-0.1756(8)	0.150(8)	1.0000
C(20)	0.1121(10)	0.1865(6)	-0.2202(6)	0.127(7)	1.0000
C(21)	0.075(1)	0.291(1)	0.003(2)	0.28(2)	1.0000
C(22)	0.015(2)	0.276(2)	-0.009(2)	0.274(10)	1.0000
C(23)	0.4553	0.4136	0.4255	0.206(5)	0.3333
C(24)	0.4993	0.4333	0.4646	0.284(3)	0.3333
C(25)	0.392(2)	0.438(2)	0.371(2)	0.30(3)	1.0000
C(26)	0.341(3)	0.440(4)	0.347(2)	0.49(5)	1.0000
H(1)	0.0136	0.1475	0.0685	0.0500	1.0000
H(2)	0.0572	0.1514	0.0210	0.0500	1.0000
H(3)	0.2278	0.3290	0.1201	0.0763	1.0000
H(4)	0.1733	0.3519	0.0941	0.0763	1.0000
H(5)	0.2162	0.2909	-0.0206	0.0718	1.0000

atom	x	y	z	U_{eq}	occ
H(6)	0.2620	0.2519	0.0027	0.0718	1.0000
H(7)	0.0309	-0.0538	-0.1861	0.0834	1.0000
H(8)	0.0916	-0.0684	-0.1698	0.0834	1.0000
H(9)	0.1091	0.0660	-0.1881	0.0757	1.0000
H(10)	0.0470	0.0837	-0.1874	0.0757	1.0000
H(11)	0.1898	0.3189	0.1971	0.0705	1.0000
H(12)	0.1052	0.3580	0.2195	0.0841	1.0000
H(13)	0.0540	0.4011	0.1539	0.1180	1.0000
H(14)	0.0934	0.3785	0.1079	0.1180	1.0000
H(15)	0.0563	0.3377	0.1416	0.1180	1.0000
H(16)	0.1841	0.4154	0.2128	0.1527	1.0000
H(17)	0.1710	0.4260	0.1505	0.1527	1.0000
H(18)	0.1315	0.4490	0.1961	0.1527	1.0000
H(19)	0.1709	0.2248	-0.0579	0.0699	1.0000
H(20)	0.2289	0.1647	-0.1095	0.0877	1.0000
H(21)	0.2743	0.2725	-0.1017	0.1573	1.0000
H(22)	0.2831	0.2338	-0.1527	0.1573	1.0000
H(23)	0.2244	0.2575	-0.1399	0.1573	1.0000
H(24)	0.2939	0.1391	-0.0385	0.1180	1.0000
H(25)	0.3262	0.1598	-0.0904	0.1180	1.0000
H(26)	0.3183	0.1988	-0.0395	0.1180	1.0000
H(27)	-0.0017	-0.1118	-0.1319	0.0775	1.0000
H(28)	0.0622	-0.1861	-0.1040	0.2405	1.0000
H(29)	0.1608	-0.1796	-0.1378	0.5115	1.0000
H(30)	0.1495	-0.1204	-0.1610	0.5115	1.0000
H(31)	0.1517	-0.1303	-0.0972	0.5115	1.0000
H(32)	0.0072	-0.1832	-0.1861	0.4275	1.0000
H(33)	0.0527	-0.1486	-0.2163	0.4275	1.0000
H(34)	0.0636	-0.2105	-0.2017	0.4275	1.0000
H(35)	0.1333	0.1279	-0.1321	0.0705	1.0000
H(36)	0.0897	0.2118	-0.1416	0.1024	1.0000
H(37)	0.0077	0.2177	-0.1944	0.1899	1.0000

atom	x	y	z	U_{eq}	occ
H(38)	0.0056	0.1532	-0.1977	0.1899	1.0000
H(39)	-0.0027	0.1829	-0.1410	0.1899	1.0000
H(40)	0.1512	0.1861	-0.2126	0.1536	1.0000
H(41)	0.1032	0.1562	-0.2438	0.1536	1.0000
H(42)	0.1029	0.2205	-0.2380	0.1536	1.0000
H(43)	-0.0080	0.2787	0.0189	0.3613	1.0000
H(44)	0.0065	0.3076	-0.0370	0.3613	1.0000
H(45)	0.0147	0.2439	-0.0306	0.3613	1.0000
H(46)	0.3998	0.4709	0.3860	0.3878	1.0000
H(47)	0.4137	0.4261	0.3417	0.3878	1.0000
H(48)	0.3121	0.4567	0.3730	0.4918	1.0000
H(49)	0.3429	0.4733	0.3187	0.4918	1.0000
H(50)	0.3260	0.4117	0.3287	0.4918	1.0000

$$Ueq = \frac{1}{3}\left(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha\right)$$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Gd(1)	0.0390(2)	0.0390	0.0390	0.0015(2)	0.0015	0.0015
Gd(2)	0.0375(2)	0.0375	0.0375	0.0030(2)	0.0030	0.0030
Ni(1)	0.0558(7)	0.0410(6)	0.0502(6)	-0.0040(5)	0.0065(5)	0.0000(5)
Ni(2)	0.0579(7)	0.0464(6)	0.0417(6)	0.0028(5)	0.0103(5)	0.0009(5)
Cl(1)	0.145(4)	0.174(5)	0.085(3)	0.084(4)	0.019(3)	0.027(3)
Cl(2)	0.103(6)	0.1109	0.1109	-0.006(7)	-0.0073	-0.0073
O(1)	0.056(4)	0.044(3)	0.047(3)	-0.004(3)	0.000(3)	-0.004(3)
O(2)	0.072(4)	0.055(4)	0.050(4)	-0.001(3)	0.016(3)	-0.006(3)
O(3)	0.059(3)	0.040(3)	0.038(3)	-0.009(3)	0.011(3)	0.002(2)
O(4)	0.075(4)	0.049(4)	0.052(3)	-0.010(3)	0.022(4)	-0.004(3)
O(5)	0.059(4)	0.037(3)	0.046(3)	0.000(3)	0.007(3)	-0.003(2)
O(6)	0.086(5)	0.045(3)	0.053(3)	-0.006(4)	-0.002(4)	0.002(3)
O(7)	0.052(3)	0.040(3)	0.036(3)	0.003(3)	0.008(3)	0.004(2)
O(8)	0.084(5)	0.040(3)	0.047(3)	0.005(3)	0.006(3)	0.006(3)
O(9)	0.046(3)	0.040(3)	0.041(3)	0.009(2)	0.008(2)	0.004(2)
O(10)	0.054(4)	0.076(5)	0.075(5)	0.010(4)	0.018(4)	-0.002(4)
O(11)	0.101(8)	0.31(2)	0.107(9)	0.05(1)	0.064(7)	0.06(1)
O(12)	0.061(7)	0.20(2)	0.24(2)	0.023(8)	0.021(8)	0.00(1)
O(13)	0.33(3)	0.29(3)	0.17(2)	0.21(3)	-0.04(2)	-0.04(2)
O(14)	0.17(2)	0.26(3)	0.42(4)	-0.01(2)	0.10(2)	0.08(3)
O(15)	0.44(4)	0.45(4)	0.10(1)	0.17(3)	0.05(2)	0.12(2)
O(16)	0.13(1)	0.59(5)	0.22(2)	0.16(2)	0.07(1)	0.17(3)
O(17)	0.24(2)	0.31(3)	0.15(1)	-0.02(2)	0.01(2)	0.03(2)
O(18)	0.19(4)	0.1972	0.1972	-0.04(4)	-0.0498	-0.0498
N(1)	0.072(5)	0.046(4)	0.073(6)	-0.009(4)	0.011(5)	-0.006(4)
N(2)	0.075(5)	0.049(4)	0.057(5)	-0.017(4)	0.012(4)	-0.002(4)
N(3)	0.091(7)	0.061(5)	0.058(5)	-0.002(5)	0.011(5)	-0.004(4)
N(4)	0.083(6)	0.059(5)	0.046(4)	0.000(5)	0.011(4)	0.004(4)
N(5)	0.078(6)	0.069(6)	0.068(6)	0.011(5)	-0.007(5)	0.000(5)
N(6)	0.061(6)	0.090(7)	0.085(7)	0.015(5)	0.033(6)	-0.005(6)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(7)	0.10(3)	0.1308	0.1308	0.03(3)	0.0280	0.0280
C(1)	0.078(7)	0.041(5)	0.061(6)	-0.006(5)	-0.002(5)	-0.005(5)
C(2)	0.054(5)	0.050(5)	0.056(5)	0.009(4)	-0.001(5)	0.004(4)
C(3)	0.080(7)	0.061(6)	0.072(7)	0.007(6)	0.011(6)	-0.020(5)
C(4)	0.085(9)	0.073(8)	0.14(1)	0.021(7)	0.020(9)	-0.015(9)
C(5)	0.14(1)	0.060(8)	0.19(2)	0.004(9)	0.02(1)	-0.05(1)
C(6)	0.079(7)	0.046(5)	0.046(5)	-0.016(5)	0.007(5)	0.009(4)
C(7)	0.051(5)	0.043(5)	0.050(5)	-0.003(4)	0.009(4)	0.002(4)
C(8)	0.077(7)	0.081(8)	0.059(6)	-0.027(6)	0.024(6)	-0.009(6)
C(9)	0.18(2)	0.11(1)	0.10(1)	-0.04(1)	0.06(1)	0.03(1)
C(10)	0.069(8)	0.10(1)	0.12(1)	-0.019(7)	0.041(8)	-0.030(9)
C(11)	0.096(8)	0.053(5)	0.051(5)	-0.009(6)	0.001(6)	-0.004(5)
C(12)	0.059(6)	0.049(5)	0.045(5)	0.004(4)	0.000(4)	-0.005(4)
C(13)	0.49(5)	0.069(9)	0.052(8)	0.04(2)	0.04(2)	-0.014(7)
C(14)	0.37(5)	0.27(4)	0.70(10)	0.22(4)	-0.41(7)	-0.32(6)
C(15)	0.9(1)	0.11(2)	0.09(1)	-0.06(4)	0.03(3)	-0.07(1)
C(16)	0.079(7)	0.050(5)	0.047(5)	0.000(5)	0.016(5)	0.008(4)
C(17)	0.057(5)	0.048(5)	0.042(4)	-0.002(4)	0.002(4)	0.001(4)
C(18)	0.13(1)	0.068(7)	0.055(6)	0.015(8)	0.018(7)	0.021(6)
C(19)	0.19(2)	0.15(2)	0.11(1)	0.12(2)	0.02(1)	0.04(1)
C(20)	0.22(2)	0.082(9)	0.083(9)	0.00(1)	0.05(1)	0.037(8)
C(21)	0.25(3)	0.23(3)	0.37(5)	0.17(3)	-0.21(3)	-0.20(3)
C(25)	0.27(6)	0.28(5)	0.36(8)	0.00(5)	-0.03(5)	0.11(5)
C(26)	0.4(1)	0.9(2)	0.19(4)	-0.3(1)	-0.07(5)	-0.04(7)

The general temperature factor expression:

$$\exp\left(-2\pi^2\left(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl\right)\right)$$

Table 3. Bond Lengths (Å)

atom	atom	distance	atom	atom	distance
Gd(1)	O(1)	2.457(6)	Gd(1)	O(1)[1)]	2.457(6)
Gd(1)	O(1)[2)]	2.457(6)	Gd(1)	O(3)	2.442(5)
Gd(1)	O(3)[1)]	2.442(5)	Gd(1)	O(3)[2)]	2.442(5)
Gd(1)	O(9)	2.542(6)	Gd(1)	O(9)[1)]	2.542(6)
Gd(1)	O(9)[2)]	2.542(6)	Gd(2)	O(5)	2.446(6)
Gd(2)	O(5)[1)]	2.446(6)	Gd(2)	O(5)[2)]	2.446(6)
Gd(2)	O(7)	2.431(5)	Gd(2)	O(7)[1)]	2.431(5)
Gd(2)	O(7)[2)]	2.431(5)	Gd(2)	O(9)	2.532(6)
Gd(2)	O(9)[1)]	2.532(6)	Gd(2)	O(9)[2)]	2.532(6)
Ni(1)	O(1)	2.016(6)	Ni(1)	O(2)[2)]	2.098(7)
Ni(1)	O(3)	2.043(6)	Ni(1)	N(1)	2.069(8)
Ni(1)	N(2)	2.066(9)	Ni(1)	N(5)	2.12(1)
Ni(2)	O(5)	2.020(6)	Ni(2)	O(6)[1)]	2.128(7)
Ni(2)	O(7)	2.029(6)	Ni(2)	O(10)	2.103(7)
Ni(2)	N(3)	2.047(9)	Ni(2)	N(4)	2.020(8)
Cl(1)	O(13)	1.41(2)	Cl(1)	O(14)	1.58(2)
Cl(1)	O(15)	1.31(2)	Cl(1)	O(16)	1.29(2)
Cl(2)	O(17)	1.34(2)	Cl(2)	O(17)[1)]	1.34(2)
Cl(2)	O(17)[2)]	1.34(2)	Cl(2)	O(18)	1.36(3)
O(1)	C(2)	1.32(1)	O(2)	C(2)	1.20(1)
O(3)	C(7)	1.29(1)	O(4)	C(7)	1.23(1)
O(5)	C(12)	1.30(1)	O(6)	C(12)	1.23(1)
O(7)	C(17)	1.29(1)	O(8)	C(17)	1.26(1)
O(9)	H(1)	0.950	O(9)	H(2)	0.953
O(10)	N(6)	1.27(1)	O(11)	N(6)	1.21(2)
O(12)	N(6)	1.19(2)	N(1)	C(1)	1.49(1)
N(1)	H(3)	0.946	N(1)	H(4)	0.954
N(2)	C(6)	1.47(1)	N(2)	H(5)	0.947
N(2)	H(6)	0.951	N(3)	C(11)	1.45(1)
N(3)	H(7)	0.943	N(3)	H(8)	0.954

atom	atom	distance	atom	atom	distance
N(4)	C(16)	1.48(1)	N(4)	H(9)	0.952
N(4)	H(10)	0.941	N(5)	C(21)	1.04(2)
N(7)	C(23)	1.29(3)	N(7)	C(23)[1)]	1.29(3)
N(7)	C(23)[2)]	1.29(3)	N(7)	C(25)	1.18(4)
N(7)	C(25)[1)]	1.18(4)	N(7)	C(25)[2)]	1.18(4)
C(1)	C(2)	1.55(1)	C(1)	C(3)	1.52(2)
C(1)	H(11)	0.950	C(3)	C(4)	1.44(2)
C(3)	C(5)	1.54(2)	C(3)	H(12)	0.954
C(4)	H(13)	0.947	C(4)	H(14)	0.957
C(4)	H(15)	0.944	C(5)	H(16)	0.954
C(5)	H(17)	0.954	C(5)	H(18)	0.940
C(6)	C(7)	1.55(1)	C(6)	C(8)	1.58(1)
C(6)	H(19)	0.958	C(8)	C(9)	1.54(2)
C(8)	C(10)	1.57(2)	C(8)	H(20)	0.956
C(9)	H(21)	0.946	C(9)	H(22)	0.961
C(9)	H(23)	0.947	C(10)	H(24)	0.957
C(10)	H(25)	0.948	C(10)	H(26)	0.956
C(11)	C(12)	1.55(1)	C(11)	C(13)	1.59(3)
C(11)	H(27)	0.946	C(13)	C(14)	1.75(5)
C(13)	C(15)	1.58(4)	C(13)	H(28)	0.956
C(14)	H(29)	0.936	C(14)	H(30)	0.888
C(14)	H(31)	0.982	C(15)	H(32)	0.959
C(15)	H(33)	0.970	C(15)	H(34)	0.929
C(16)	C(17)	1.53(1)	C(16)	C(18)	1.50(2)
C(16)	H(35)	0.950	C(18)	C(19)	1.53(3)
C(18)	C(20)	1.55(2)	C(18)	H(36)	0.948
C(19)	H(37)	0.939	C(19)	H(38)	0.963
C(19)	H(39)	0.957	C(20)	H(40)	0.959
C(20)	H(41)	0.947	C(20)	H(42)	0.948
C(21)	C(22)	1.51(5)	C(22)	H(43)	0.867
C(22)	H(44)	1.039	C(22)	H(45)	0.937
C(23)	C(23)[1)]	1.265	C(23)	C(23)[2)]	1.265

atom	atom	distance	atom	atom	distance
C(23)	C(24)	1.491	C(23)	C(25)[2)]	1.37(5)
C(23)	H(46)[2)]	0.980	C(25)	C(26)	1.34(7)
C(25)	H(46)	0.898	C(25)	H(47)	0.922
C(26)	H(48)	1.029	C(26)	H(49)	1.048
C(26)	H(50)	0.883			

Symmetry operations

(1) Z,X,Y

(2) Y,Z,X

Table 4. Bond Angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
O(1)	Gd(1)	O(1)$^{1)}$	74.8(2)	O(1)	Gd(1)	O(1)$^{2)}$	74.8(2)
O(1)	Gd(1)	O(3)	67.4(2)	O(1)	Gd(1)	O(3)$^{1)}$	69.5(2)
O(1)	Gd(1)	O(3)$^{2)}$	133.2(2)	O(1)	Gd(1)	O(9)	96.5(2)
O(1)	Gd(1)	O(9)$^{1)}$	142.9(2)	O(1)	Gd(1)	O(9)$^{2)}$	138.7(2)
O(1)$^{1)}$	Gd(1)	O(1)$^{2)}$	74.8(2)	O(1)$^{1)}$	Gd(1)	O(3)	133.2(2)
O(1)$^{1)}$	Gd(1)	O(3)$^{1)}$	67.4(2)	O(1)$^{1)}$	Gd(1)	O(3)$^{2)}$	69.5(2)
O(1)$^{1)}$	Gd(1)	O(9)	138.7(2)	O(1)$^{1)}$	Gd(1)	O(9)$^{1)}$	96.5(2)
O(1)$^{1)}$	Gd(1)	O(9)$^{2)}$	142.9(2)	O(1)$^{2)}$	Gd(1)	O(3)	69.5(2)
O(1)$^{2)}$	Gd(1)	O(3)$^{1)}$	133.2(2)	O(1)$^{2)}$	Gd(1)	O(3)$^{2)}$	67.4(2)
O(1)$^{2)}$	Gd(1)	O(9)	142.9(2)	O(1)$^{2)}$	Gd(1)	O(9)$^{1)}$	138.7(2)
O(1)$^{2)}$	Gd(1)	O(9)$^{2)}$	96.5(2)	O(3)	Gd(1)	O(3)$^{1)}$	119.94(1)
O(3)	Gd(1)	O(3)$^{2)}$	119.94(1)	O(3)	Gd(1)	O(9)	73.8(2)
O(3)	Gd(1)	O(9)$^{1)}$	130.4(2)	O(3)	Gd(1)	O(9)$^{2)}$	71.7(2)
O(3)$^{1)}$	Gd(1)	O(3)$^{2)}$	119.94(1)	O(3)$^{1)}$	Gd(1)	O(9)	71.7(2)
O(3)$^{1)}$	Gd(1)	O(9)$^{1)}$	73.8(2)	O(3)$^{1)}$	Gd(1)	O(9)$^{2)}$	130.4(2)
O(3)$^{2)}$	Gd(1)	O(9)	130.4(2)	O(3)$^{2)}$	Gd(1)	O(9)$^{1)}$	71.7(2)
O(3)$^{2)}$	Gd(1)	O(9)$^{2)}$	73.8(2)	O(9)	Gd(1)	O(9)$^{1)}$	66.1(2)
O(9)	Gd(1)	O(9)$^{2)}$	66.1(2)	O(9)$^{1)}$	Gd(1)	O(9)$^{2)}$	66.1(2)
O(5)	Gd(2)	O(5)$^{1)}$	73.3(2)	O(5)	Gd(2)	O(5)$^{2)}$	73.3(2)
O(5)	Gd(2)	O(7)	68.2(2)	O(5)	Gd(2)	O(7)$^{1)}$	132.0(2)
O(5)	Gd(2)	O(7)$^{2)}$	69.0(2)	O(5)	Gd(2)	O(9)	140.1(2)
O(5)	Gd(2)	O(9)$^{1)}$	142.3(2)	O(5)	Gd(2)	O(9)$^{2)}$	97.2(2)
O(5)$^{1)}$	Gd(2)	O(5)$^{2)}$	73.3(2)	O(5)$^{1)}$	Gd(2)	O(7)	69.0(2)
O(5)$^{1)}$	Gd(2)	O(7)$^{1)}$	68.2(2)	O(5)$^{1)}$	Gd(2)	O(7)$^{2)}$	132.0(2)
O(5)$^{1)}$	Gd(2)	O(9)	97.2(2)	O(5)$^{1)}$	Gd(2)	O(9)$^{1)}$	140.1(2)
O(5)$^{1)}$	Gd(2)	O(9)$^{2)}$	142.3(2)	O(5)$^{2)}$	Gd(2)	O(7)	132.0(2)
O(5)$^{2)}$	Gd(2)	O(7)$^{1)}$	69.0(2)	O(5)$^{2)}$	Gd(2)	O(7)$^{2)}$	68.2(2)
O(5)$^{2)}$	Gd(2)	O(9)	142.3(2)	O(5)$^{2)}$	Gd(2)	O(9)$^{1)}$	97.2(2)
O(5)$^{2)}$	Gd(2)	O(9)$^{2)}$	140.1(2)	O(7)	Gd(2)	O(7)$^{1)}$	119.92(1)
O(7)	Gd(2)	O(7)$^{2)}$	119.92(1)	O(7)	Gd(2)	O(9)	72.3(2)

atom	atom	atom	angle	atom	atom	atom	angle
O(7)	Gd(2)	O(9)[1)]	130.8(2)	O(7)	Gd(2)	O(9)[2)]	73.5(2)
O(7)[1)]	Gd(2)	O(7)[2)]	119.92(1)	O(7)[1)]	Gd(2)	O(9)	73.5(2)
O(7)[1)]	Gd(2)	O(9)[1)]	72.3(2)	O(7)[1)]	Gd(2)	O(9)[2)]	130.8(2)
O(7)[2)]	Gd(2)	O(9)	130.8(2)	O(7)[2)]	Gd(2)	O(9)[1)]	73.5(2)
O(7)[2)]	Gd(2)	O(9)[2)]	72.3(2)	O(9)	Gd(2)	O(9)[1)]	66.4(2)
O(9)	Gd(2)	O(9)[2)]	66.4(2)	O(9)[1)]	Gd(2)	O(9)[2)]	66.4(2)
O(1)	Ni(1)	O(2)[2)]	90.9(3)	O(1)	Ni(1)	O(3)	84.0(2)
O(1)	Ni(1)	N(1)	83.5(3)	O(1)	Ni(1)	N(2)	167.7(3)
O(1)	Ni(1)	N(5)	91.5(3)	O(2)[2)]	Ni(1)	O(3)	90.0(3)
O(2)[2)]	Ni(1)	N(1)	87.6(3)	O(2)[2)]	Ni(1)	N(2)	87.5(3)
O(2)[2)]	Ni(1)	N(5)	177.7(4)	O(3)	Ni(1)	N(1)	167.3(3)
O(3)	Ni(1)	N(2)	83.8(3)	O(3)	Ni(1)	N(5)	90.0(3)
N(1)	Ni(1)	N(2)	108.5(3)	N(1)	Ni(1)	N(5)	92.8(4)
N(2)	Ni(1)	N(5)	90.2(4)	O(5)	Ni(2)	O(6)[1)]	89.6(3)
O(5)	Ni(2)	O(7)	85.0(2)	O(5)	Ni(2)	O(10)	84.5(3)
O(5)	Ni(2)	N(3)	82.8(3)	O(5)	Ni(2)	N(4)	168.2(3)
O(6)[1)]	Ni(2)	O(7)	90.3(3)	O(6)[1)]	Ni(2)	O(10)	173.7(3)
O(6)[1)]	Ni(2)	N(3)	88.5(4)	O(6)[1)]	Ni(2)	N(4)	89.9(3)
O(7)	Ni(2)	O(10)	86.9(3)	O(7)	Ni(2)	N(3)	167.7(3)
O(7)	Ni(2)	N(4)	83.2(3)	O(10)	Ni(2)	N(3)	93.1(4)
O(10)	Ni(2)	N(4)	95.4(4)	N(3)	Ni(2)	N(4)	109.0(4)
O(13)	Cl(1)	O(14)	108(1)	O(13)	Cl(1)	O(15)	107(1)
O(13)	Cl(1)	O(16)	104(1)	O(14)	Cl(1)	O(15)	92(1)
O(14)	Cl(1)	O(16)	119(1)	O(15)	Cl(1)	O(16)	124(1)
O(17)	Cl(2)	O(17)[1)]	107(1)	O(17)	Cl(2)	O(17)	107(1)
O(17)	Cl(2)	O(18)	111(1)	O(17)[1)]	Cl(2)	O(17)	107(1)
O(17)[1)]	Cl(2)	O(18)	111(1)	O(17)[2)]	Cl(2)	O(18)	111(1)
Gd(1)	O(1)	Ni(1)	103.8(2)	Gd(1)	O(1)	C(2)	138.3(6)
Ni(1)	O(1)	C(2)	116.6(6)	Ni(1)[1)]	O(2)	C(2)	127.1(7)
Gd(1)	O(3)	Ni(1)	103.4(2)	Gd(1)	O(3)	C(7)	141.1(6)
Ni(1)	O(3)	C(7)	114.4(5)	Gd(2)	O(5)	Ni(2)	102.9(2)
Gd(2)	O(5)	C(12)	140.6(6)	Ni(2)	O(5)	C(12)	115.5(6)

atom	atom	atom	angle	atom	atom	atom	angle
Ni(2)[2)]	O(6)	C(12)	125.0(6)	Gd(2)	O(7)	Ni(2)	103.2(2)
Gd(2)	O(7)	C(17)	142.3(5)	Ni(2)	O(7)	C(17)	113.7(5)
Gd(1)	O(9)	Gd(2)	101.8(2)	Gd(1)	O(9)	H(1)	111.6
Gd(1)	O(9)	H(2)	111.5	Gd(2)	O(9)	H(1)	111.4
Gd(2)	O(9)	H(2)	111.2	H(1)	O(9)	H(2)	109.3
Ni(2)	O(10)	N(6)	126.9(8)	Ni(1)	N(1)	C(1)	110.5(6)
Ni(1)	N(1)	H(3)	109.5	Ni(1)	N(1)	H(4)	109.1
C(1)	N(1)	H(3)	109.4	C(1)	N(1)	H(4)	109.0
H(3)	N(1)	H(4)	109.5	Ni(1)	N(2)	C(6)	106.3(6)
Ni(1)	N(2)	H(5)	110.4	Ni(1)	N(2)	H(6)	110.2
C(6)	N(2)	H(5)	110.6	C(6)	N(2)	H(6)	109.7
H(5)	N(2)	H(6)	109.7	Ni(2)	N(3)	C(11)	111.8(6)
Ni(2)	N(3)	H(7)	109.1	Ni(2)	N(3)	H(8)	108.5
C(11)	N(3)	H(7)	109.1	C(11)	N(3)	H(8)	108.7
H(7)	N(3)	H(8)	109.7	Ni(2)	N(4)	C(16)	111.4(6)
Ni(2)	N(4)	H(9)	108.7	Ni(2)	N(4)	H(10)	109.2
C(16)	N(4)	H(9)	108.4	C(16)	N(4)	H(10)	109.0
H(9)	N(4)	H(10)	110.0	Ni(1)	N(5)	C(21)	168(2)
O(10)	N(6)	O(11)	118(1)	O(10)	N(6)	O(12)	125(1)
O(11)	N(6)	O(12)	116(1)	C(23)	N(7)	C(23)[1)]	58(1)
C(23)	N(7)	C(23)[2)]	58(1)	C(23)	N(7)	C(25)	115(3)
C(23)	N(7)	C(25)[1)]	117(3)	C(23)	N(7)	C(25)[2)]	67(2)
C(23)[1)]	N(7)	C(23)[2)]	58(1)	C(23)[1)]	N(7)	C(25)	67(2)
C(23)[1)]	N(7)	C(25)[1)]	115(3)	C(23)[1)]	N(7)	C(25)[2)]	117(3)
C(23)[2)]	N(7)	C(25)	117(3)	C(23)[2)]	N(7)	C(25)[1)]	67(2)
C(23)[2)]	N(7)	C(25)[2)]	115(3)	C(25)	N(7)	C(25)[1)]	116(2)
C(25)	N(7)	C(25)[2)]	116(2)	C(25)[1)]	N(7)	C(25)[2)]	116(2)
N(1)	C(1)	C(2)	112.7(8)	N(1)	C(1)	C(3)	115.7(9)
N(1)	C(1)	H(11)	106.4	C(2)	C(1)	C(3)	108.7(9)
C(2)	C(1)	H(11)	106.5	C(3)	C(1)	H(11)	106.3
O(1)	C(2)	O(2)	125.6(9)	O(1)	C(2)	C(1)	116.6(9)
O(2)	C(2)	C(1)	117.7(9)	C(1)	C(3)	C(4)	112.9(10)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	C(3)	C(5)	108(1)	C(1)	C(3)	H(12)	109.1
C(4)	C(3)	C(5)	108(1)	C(4)	C(3)	H(12)	108.8
C(5)	C(3)	H(12)	109.0	C(3)	C(4)	H(13)	109.5
C(3)	C(4)	H(14)	108.7	C(3)	C(4)	H(15)	109.8
H(13)	C(4)	H(14)	109.2	H(13)	C(4)	H(15)	110.3
H(14)	C(4)	H(15)	109.4	C(3)	C(5)	H(16)	109.2
C(3)	C(5)	H(17)	109.0	C(3)	C(5)	H(18)	110.0
H(16)	C(5)	H(17)	108.7	H(16)	C(5)	H(18)	109.9
H(17)	C(5)	H(18)	109.9	N(2)	C(6)	C(7)	112.4(8)
N(2)	C(6)	C(8)	114.5(8)	N(2)	C(6)	H(19)	105.5
C(7)	C(6)	C(8)	110.9(8)	C(7)	C(6)	H(19)	106.1
C(8)	C(6)	H(19)	106.7	O(3)	C(7)	O(4)	123.8(8)
O(3)	C(7)	C(6)	115.0(8)	O(4)	C(7)	C(6)	121.0(8)
C(6)	C(8)	C(9)	108(1)	C(6)	C(8)	C(10)	111.0(10)
C(6)	C(8)	H(20)	109.2	C(9)	C(8)	C(10)	109(1)
C(9)	C(8)	H(20)	109.2	C(10)	C(8)	H(20)	109.3
C(8)	C(9)	H(21)	109.7	C(8)	C(9)	H(22)	109.1
C(8)	C(9)	H(23)	110.1	H(21)	C(9)	H(22)	108.9
H(21)	C(9)	H(23)	110.1	H(22)	C(9)	H(23)	108.8
C(8)	C(10)	H(24)	109.9	C(8)	C(10)	H(25)	110.6
C(8)	C(10)	H(26)	109.8	H(24)	C(10)	H(25)	109.0
H(24)	C(10)	H(26)	108.3	H(25)	C(10)	H(26)	109.1
N(3)	C(11)	C(12)	111.5(8)	N(3)	C(11)	C(13)	110(1)
N(3)	C(11)	H(27)	108.1	C(12)	C(11)	C(13)	109(1)
C(12)	C(11)	H(27)	107.7	C(13)	C(11)	H(27)	108.7
O(5)	C(12)	O(6)	124.6(9)	O(5)	C(12)	C(11)	117.2(8)
O(6)	C(12)	C(11)	118.1(8)	C(11)	C(13)	C(14)	112(1)
C(11)	C(13)	C(15)	99(2)	C(11)	C(13)	H(28)	109.6
C(14)	C(13)	C(15)	113(2)	C(14)	C(13)	H(28)	112.8
C(15)	C(13)	H(28)	108.5	C(13)	C(14)	H(29)	106.4
C(13)	C(14)	H(30)	109.0	C(13)	C(14)	H(31)	104.0
H(29)	C(14)	H(30)	116.6	H(29)	C(14)	H(31)	108.0

atom	atom	atom	angle	atom	atom	atom	angle
H(30)	C(14)	H(31)	112.1	C(13)	C(15)	H(32)	110.0
C(13)	C(15)	H(33)	108.5	C(13)	C(15)	H(34)	111.1
H(32)	C(15)	H(33)	107.1	H(32)	C(15)	H(34)	110.5
H(33)	C(15)	H(34)	109.6	N(4)	C(16)	C(17)	108.8(8)
N(4)	C(16)	C(18)	114.9(9)	N(4)	C(16)	H(35)	105.9
C(17)	C(16)	C(18)	114.8(9)	C(17)	C(16)	H(35)	105.9
C(18)	C(16)	H(35)	105.7	O(7)	C(17)	O(8)	122.3(8)
O(7)	C(17)	C(16)	118.6(8)	O(8)	C(17)	C(16)	119.0(8)
C(16)	C(18)	C(19)	110(1)	C(16)	C(18)	C(20)	111(1)
C(16)	C(18)	H(36)	108.4	C(19)	C(18)	C(20)	110(1)
C(19)	C(18)	H(36)	108.2	C(20)	C(18)	H(36)	108.5
C(18)	C(19)	H(37)	110.8	C(18)	C(19)	H(38)	109.4
C(18)	C(19)	H(39)	109.6	H(37)	C(19)	H(38)	109.3
H(37)	C(19)	H(39)	109.8	H(38)	C(19)	H(39)	107.8
C(18)	C(20)	H(40)	109.2	C(18)	C(20)	H(41)	110.0
C(18)	C(20)	H(42)	109.8	H(40)	C(20)	H(41)	109.0
H(40)	C(20)	H(42)	108.9	H(41)	C(20)	H(42)	109.9
N(5)	C(21)	C(22)	137(5)	C(21)	C(22)	H(43)	116.7
C(21)	C(22)	H(44)	98.4	C(21)	C(22)	H(45)	108.4
H(43)	C(22)	H(44)	108.6	H(43)	C(22)	H(45)	118.6
H(44)	C(22)	H(45)	103.3	N(7)	C(23)	C(23)[1)]	60.6(8)
N(7)	C(23)	C(23)[2)]	60.6(8)	N(7)	C(23)	C(24)	158.0(8)
N(7)	C(23)	C(25)[2)]	52(1)	N(7)	C(23)	H(46)[2)]	91.5
C(23)[1)]	C(23)	C(23)[2)]	60.0000(3)	C(23)[1)]	C(23)	C(24)	106.9327(4)
C(23)[1)]	C(23)	C(25)[2)]	106(2)	C(23)[1)]	C(23)	H(46)[2)]	127.5
C(23)[2)]	C(23)	C(24)	97.6299(7)	C(23)[2)]	C(23)	C(25)[2)]	104(2)
C(23)[2)]	C(23)	H(46)[2)]	144.4	C(24)	C(23)	C(25)[2)]	145(1)
C(24)	C(23)	H(46)[2)]	109.9	C(25)[2)]	C(23)	H(46)[2)]	40.8
N(7)	C(25)	C(23)[1)]	60(2)	N(7)	C(25)	C(26)	126(6)
N(7)	C(25)	H(46)	103.2	N(7)	C(25)	H(47)	100.6
C(23)[1)]	C(25)	C(26)	147(7)	C(23)[1)]	C(25)	H(46)	45.5
C(23)[1)]	C(25)	H(47)	109.0	C(26)	C(25)	H(46)	109.3

atom	atom	atom	angle	atom	atom	atom	angle
C(26)	C(25)	H(47)	101.1	H(46)	C(25)	H(47)	117.0
C(25)	C(26)	H(48)	111.3	C(25)	C(26)	H(49)	106.2
C(25)	C(26)	H(50)	124.1	H(48)	C(26)	H(49)	96.7
H(48)	C(26)	H(50)	108.2	H(49)	C(26)	H(50)	106.7

Symmetry operations

(2) Z,X,Y

(2) Y,Z,X

Table 5. Special Distances (Å)

atom	atom	distance	atom	atom	distance
Gd(1)	Ni(1)	3.530(1)	Gd(1)	Ni(1)[1)]	3.530(1)
Gd(1)	Ni(1)[2)]	3.530(1)	Gd(1)	Gd(2)	3.937(1)
Gd(2)	Ni(2)	3.503(1)	Gd(2)	Ni(2)[1)]	3.503(1)
Gd(2)	Ni(2)[2)]	3.503(1)	Ni(1)	Ni(1)[1)]	5.304(2)
Ni(1)	Ni(1)[2)]	5.304(2)	Ni(2)	Ni(2)[1)]	5.275(2)
Ni(2)	Ni(2)[2)]	5.275(2)			

Symmetry operations

(3) Z,X,Y (2) Y,Z,X