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Re-refinement of dineodymium tris[sulfate(VI)] tetrahydrate

Suwadee Jiajaroen,[a]* Chatphorn Theppitak,[b] Sakchai Laksee[c] and Kittipong Chainok[d]

[a]Division of Science and Mathematic, Faculty of Science and Technology, Rajamangala University of Technology Tawan-ok, Bangpra, Sriracha, Chonburi, 20110, Thailand, [b]Chulabhorn Research Institute, Lak Si, Bangkok 10210, Thailand, [c]Thailand Institute of Nuclear Technology (Public, Organization), Nakhon Nayok 26120, Thailand, and [d]Thammasat University Research Unit in Multifunctional Crystalline Materials and Applications (TU-MCMA), Faculty of Science and Technology, Thammasat, University, Khlong Luang, Pathum Thani, 12121, Thailand. *Correspondence e-mail: suwadee_ji@rmutto.ac.th

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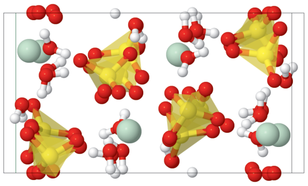
The crystal structure of the title compound, poly[tetraaquatri-μ-sulfato-dineodymium], $[Nd_2(SO_4)_3(H_2O)_4]_n$, was re-refined from modern CCD-based single-crystal X-ray diffraction data. In comparison with the original report [Bede (1987). *Jiegou Huaxue*, **6**, 70–74], the re-refinement shows improved precision and accuracy, with all hydrogen atoms being located. The crystal structure comprises two crystallographically independent Nd^{III} sites. One adopts a capped square-antiprismatic and the other a square-antiprismatic coordination environment. The cations are interconnected by bridging sulfato ligands into a framework structure that is reinforced by classical O—H···O hydrogen-bonding interactions of medium to weak strengths.

3D view



Structure description

Coordination networks comprising lanthanide metal ions have attracted considerable interest in recent decades due to their structural complexity and functional properties in optical and magnetic materials, resulting from their unpaired electrons in *f*-orbitals (Patra & Pal, 2025; Mautner *et al.*, 2021; Cui *et al.*, 2012; Eliseeva & Bünzli, 2010). Since lanthanide ions favour hard donor atoms, a variety of organic ligands with oxygen atoms have been used extensively for the creation of different lanthanide coordination networks. Among them, polycarboxylic acids, particularly aromatic dicarboxylic acids like terephthalic acid (H_2bdc) and its derivatives, have been extensively used as bridging linkers in the formation of lanthanide coordination networks (He *et al.*, 2020; Bai *et al.*, 2016), demonstrating significant luminescent properties (Alexander *et al.*, 2025). Furthermore, negatively charged polyatomic ions or oxyanions such as nitrate, sulfate, or

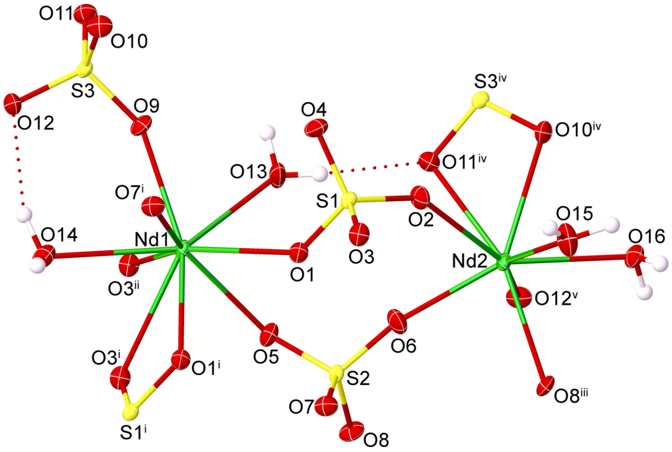


Figure 1

The asymmetric unit of $[Nd_2(SO_4)_3(H_2O)_4]$ expanded to show the full coordination spheres of the Nd atoms. Displacement ellipsoids are drawn at the 50% probability level; hydrogen-bonding interactions are shown as dashed lines. [Symmetry codes: (i) $-x + 1, -y + 1, -z + 1$; (ii) $x, y - 1, z$; (iii) $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$; (iv) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$; (v) $x + \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$.]

Table 1

Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O13—H13$A\cdots$O4^{i}	0.82 (2)	2.10 (4)	2.838 (4)	149 (5)
O13—H13$B\cdots$O11^{ii}	0.82 (2)	2.01 (3)	2.776 (4)	156 (6)
O14—H14$A\cdots$O8^{iii}	0.83 (2)	2.52 (6)	3.038 (4)	121 (6)
O14—H14$A\cdots$O12	0.83 (2)	2.36 (6)	2.933 (4)	127 (6)
O14—H14$B\cdots$O5^{iv}	0.84 (2)	1.96 (2)	2.785 (4)	166 (5)
O15—H15$A\cdots$O10^{v}	0.84 (2)	2.03 (3)	2.798 (4)	151 (6)
O15—H15$B\cdots$O5^{vi}	0.84 (2)	2.54 (6)	3.141 (4)	130 (7)
O15—H15$B\cdots$O13^{vi}	0.84 (2)	2.47 (5)	3.194 (4)	145 (7)
O16—H16$A\cdots$O4^{v}	0.82 (2)	2.02 (3)	2.799 (4)	157 (6)
O16—H16$B\cdots$O10^{v}	0.84 (2)	1.87 (2)	2.676 (4)	162 (5)

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

carbonate are effective as linkers in the construction of neutral coordination networks (Yimklan *et al.*, 2024; Guo *et al.*, 2023). These networks display intriguing magnetic features attributable to the diverse coordination modes of oxyanions that connect the lanthanide cations in close proximity.

In the context given above, we reacted neodymium chloride with 1-(4-carboxyphenyl)-5-mercapto-1*H*-tetrazole (cmt) under solvothermal conditions. This reaction unexpectedly yielded crystals of the inorganic title compound $[Nd_2(SO_4)_3(H_2O)_4]$ (Fig. 1). The sulfate anion was probably generated from the decomposition of cmt under the solvothermal conditions. A search of the Inorganic Crystal Structure Database (ICSD; Zagorac *et al.*, 2019) revealed that the crystal structure of this compound has been determined previously (collection code 68006; Bede, 1987). Isotypic lanthanide (*Ln*) crystal structures are reported for *Ln* = Ce (240937; Xu, 2008; 417417; Casari & Langer, 2007), *Ln* = Pr (422431; Kazmierczak & Hoeppe, 2011), *Ln* = La (68005; Bede, 1987), and *Ln* = Eu (420715; Choi *et al.*, 2010). The current re-refinement of $[Nd_2(SO_4)_3(H_2O)_4]$ provides improved precision of atomic coordinates and displacement parameters and more accurate bond lengths and bond angles. All hydrogen-atom positions were located from difference-Fourier maps and refined, allowing a more reliable description of the hydrogen-bonding interactions between water molecules and sulfate anions (Table 1).

The asymmetric unit comprises two Nd^{III} cations (Nd1 and Nd2), three sulfate anions (S1–S3), and four coordinating water molecules (O13–O16) (Fig.1). The shapes of the coordination polyhedra around the Nd^{III} cations were calculated using the *SHAPE* program (Llunell *et al.*, 2013). The Nd1 site exhibits a distorted capped square-antiprismatic (CSAPR-9) $[NdO_9]$ coordination environment, comprising seven oxygen atoms from six different sulfate anions and two oxygen atoms from the coordinating water molecules. The Nd2 site has a distorted square-antiprismatic (SAPR-8) $[NdO_8]$ coordination environment defined by six oxygen atoms from five distinct sulfate anions and two oxygen atoms from the coordinating water molecules. The Nd—O bond lengths range from 2.318 (3) to 2.676 (3) Å, while the O—Nd—O bond angles vary from 53.94 (8) to 150.36 (8)°. Bond lengths of the tetrahedral sulfate groups are in typical ranges [1.446 (3)–1.503 (2) Å].

Each Nd1 site is connected through μ_4-κ^2O,O':κO:$\kappa O'$:$\kappa O''$ bridging sulfato ligands, forming a double chain parallel to [010]. Nd1 and Nd2 sites are interlinked to generate a sheet structure extending parallel (100) through μ_4-κ^2O,O':κO:$\kappa O'$:$\kappa O''$ and μ_4-κO:$\kappa O'$:$\kappa O''$:$\kappa O'''$ bridging sulfato ligands (Fig. 2). These sheets are interconnected *via* another sulfato ligand in a μ_3-κ^2O,O':κO:$\kappa O'$ bridging mode along [001] (Fig. 3). Hydrogen-bonding interactions of medium to weak strengths between water molecules and sulfate O atoms, including two bifurcated hydrogen bonds (Table 1), consolidate the packing.

Fig. 4 shows the infrared spectrum of the title compound. The broad absorption bands observed at around 3016 and

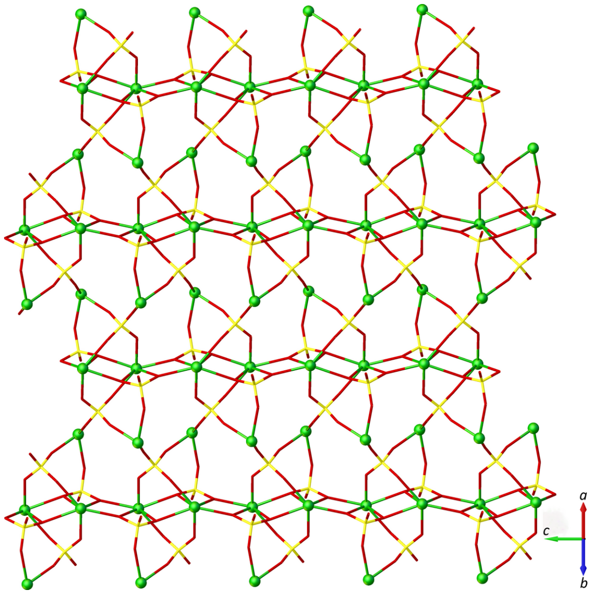


Figure 2

The (100) sheet in the title compound in a view along [101]. Water molecules are omitted for clarity.

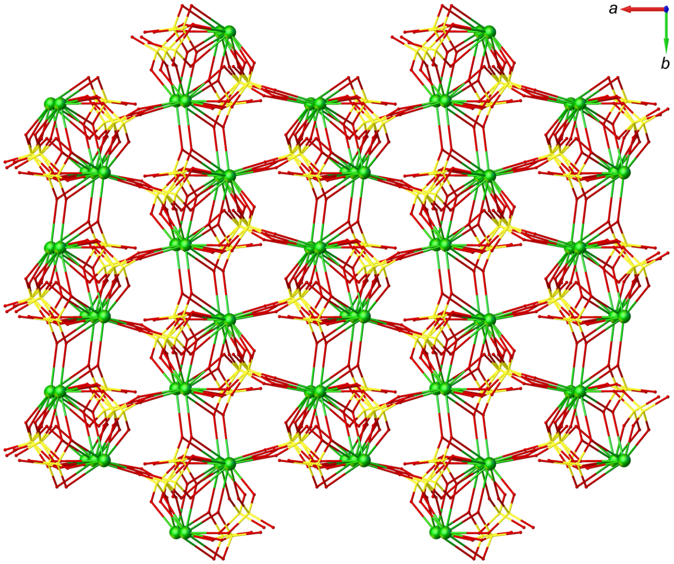


Figure 3
The crystal structure of the title compound in a viewe along [001].

3502 cm^{-1} correspond to O—H stretching vibrations of coordinating water molecules. The strong bands in the 972–1074 cm^{-1} region signify the vibration modes of the sulfate groups.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Nd_2(SO_4)_3(H_2O)_4]$
M_r	648.72
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, b, c (Å)	13.0092 (6), 7.2033 (3), 13.2968 (6)
β (°)	92.388 (2)
V (Å^3)	1244.95 (10)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	8.84
Crystal size (mm)	0.20 × 0.08 × 0.08
Data collection	
Diffractometer	Bruker D8 QUEST CMOS
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.578, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	24828, 3099, 2819
R_{int}	0.066
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.668
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.023, 0.059, 1.09
No. of reflections	3099
No. of parameters	223
No. of restraints	8
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.19, −1.63

Computer programs: *APEX4* and *SAINT* (Bruker, 2021), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

Synthesis and crystallization

All reagents were of analytical grade and were used as received without further purification. A mixture solution of $NdCl_3 \cdot 6H_2O$ (35.9 mg, 0.1 mmol) and cmt (22.2 mg, 0.1 mmol) in mixed EtOH (3 ml) and H_2O (2 ml) solution was added into a 15 ml Teflon lined reactor. The mixture solution was stirred at room temperature for 10 min, sealed in a stainless steel autoclave and heated in an oven at 428 K under autogenous pressure for 24 h. After cooling to room temperature and filtration, pink crystals were obtained in 45% yield (16.2 mg) based on $NdCl_3 \cdot 6H_2O$.

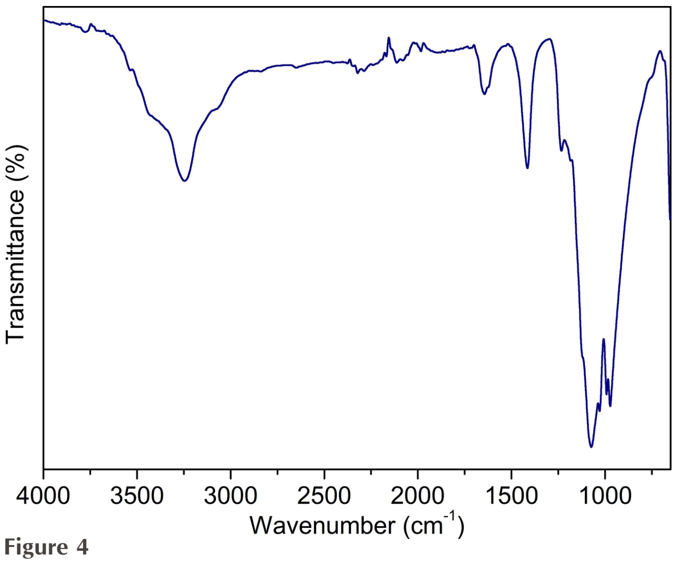


Figure 4
IR spectrum of the title compound.

An infrared (IR) spectrum was recorded on a Perkin-Elmer model Spectrum 100 spectrometer in the ATR mode, in the range of 650–4000 cm^{-1}.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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full crystallographic data

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Re-refinement of dineodymium tris[sulfate(VI)] tetrahydrate

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Poly[tetraaquatri-μ-sulfato-dineodymium]

Crystal data

$[Nd_2(SO_4)_3(H_2O)_4]$
M_r = 648.72
Monoclinic, $P2_1/n$
a = 13.0092 (6) Å
b = 7.2033 (3) Å
c = 13.2968 (6) Å
β = 92.388 (2)°
V = 1244.95 (10) Å^3
Z = 4

$F(000)$ = 1216
D_x = 3.461 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9967 reflections
θ = 3.1–28.4°
μ = 8.84 mm^{-1}
T = 296 K
Plate, pink
0.20 × 0.08 × 0.08 mm

Data collection

Bruker D8 QUEST CMOS diffractometer
Radiation source: sealed x-ray tube
Graphite monochromator
Detector resolution: 7.39 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
$T_{\min}$ = 0.578, $T_{\max}$ = 0.746

24828 measured reflections
3099 independent reflections
2819 reflections with $I > 2\sigma(I)$
R_{int} = 0.066
$\theta_{\max}$ = 28.4°, $\theta_{\min}$ = 3.1°
$h = -17 \rightarrow 17$
$k = -9 \rightarrow 9$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.059
S = 1.09
3099 reflections
223 parameters
8 restraints
Hydrogen site location: difference Fourier map
All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0257P)^2 + 2.3205P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$ = 0.001
$\Delta\rho_{\max}$ = 1.19 e Å^{-3}
$\Delta\rho_{\min}$ = −1.62 e Å^{-3}
Extinction correction: SHELXL-2019/1 (Sheldrick, 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00229 (13)

Special details

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

Refinement. The H atoms bound to O atoms were located from difference Fourier maps and were refined with distance restraints of O—H = 0.84 ± 0.02 Å and with $U_{\text{iso}}(H) = 1.5U_{\text{eq}}(O)$.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Nd1	0.41471 (2)	0.25908 (2)	0.46486 (2)	0.01048 (7)
Nd2	0.57353 (2)	0.73670 (2)	0.14948 (2)	0.01158 (7)
S1	0.40088 (6)	0.76256 (10)	0.36613 (6)	0.01053 (17)
S2	0.65392 (6)	0.39592 (11)	0.34841 (6)	0.01083 (16)
S3	0.13844 (6)	0.11067 (11)	0.45661 (6)	0.01159 (16)
O1	0.45540 (18)	0.5984 (3)	0.41346 (18)	0.0138 (5)
O2	0.4361 (2)	0.7922 (4)	0.26405 (19)	0.0179 (5)
O3	0.43662 (19)	0.9222 (3)	0.43036 (18)	0.0153 (5)
O4	0.2906 (2)	0.7380 (3)	0.3657 (2)	0.0187 (6)
O5	0.5769 (2)	0.2568 (3)	0.3787 (2)	0.0166 (6)
O6	0.6119 (2)	0.4962 (4)	0.26066 (18)	0.0205 (5)
O7	0.67762 (18)	0.5244 (4)	0.43216 (19)	0.0164 (5)
O8	0.74692 (19)	0.2962 (4)	0.3207 (2)	0.0177 (5)
O9	0.23938 (18)	0.1645 (4)	0.42137 (19)	0.0190 (5)
O10	0.0759 (2)	0.2808 (3)	0.4724 (2)	0.0175 (5)
O11	0.07797 (18)	0.0010 (3)	0.38166 (18)	0.0171 (5)
O12	0.15163 (19)	0.0109 (4)	0.55274 (18)	0.0187 (5)
O13	0.3728 (2)	0.2806 (5)	0.2807 (2)	0.0267 (7)
H13A	0.317 (3)	0.244 (7)	0.256 (4)	0.042 (18)*
H13B	0.389 (5)	0.369 (6)	0.246 (4)	0.062 (19)*
O14	0.3584 (2)	0.1111 (4)	0.6308 (2)	0.0214 (6)
H14A	0.297 (2)	0.126 (11)	0.644 (5)	0.08 (2)*
H14B	0.372 (4)	−0.003 (3)	0.637 (4)	0.039 (14)*
O15	0.5499 (2)	1.0738 (4)	0.1648 (2)	0.0247 (6)
H15A	0.549 (4)	1.152 (7)	0.117 (3)	0.052 (17)*
H15B	0.527 (6)	1.160 (8)	0.200 (5)	0.09 (3)*
O16	0.63068 (19)	0.8621 (4)	−0.01063 (19)	0.0177 (5)
H16A	0.677 (3)	0.805 (7)	−0.038 (4)	0.049 (17)*
H16B	0.628 (4)	0.978 (3)	−0.018 (4)	0.032 (13)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Nd1	0.00967 (11)	0.01244 (11)	0.00959 (10)	−0.00025 (6)	0.00351 (7)	−0.00079 (6)
Nd2	0.00989 (11)	0.01386 (11)	0.01126 (11)	0.00054 (6)	0.00388 (7)	0.00217 (6)
S1	0.0091 (4)	0.0129 (4)	0.0097 (4)	0.0001 (3)	0.0029 (3)	−0.0006 (3)
S2	0.0096 (4)	0.0135 (4)	0.0097 (4)	0.0012 (3)	0.0044 (3)	0.0012 (3)
S3	0.0092 (4)	0.0148 (4)	0.0111 (4)	−0.0004 (3)	0.0030 (3)	0.0006 (3)
O1	0.0142 (11)	0.0119 (11)	0.0155 (12)	0.0019 (9)	0.0029 (9)	0.0004 (9)
O2	0.0202 (13)	0.0238 (13)	0.0101 (12)	0.0023 (11)	0.0041 (10)	0.0014 (10)
O3	0.0185 (12)	0.0128 (11)	0.0149 (12)	0.0001 (9)	0.0035 (9)	−0.0026 (9)
O4	0.0110 (13)	0.0247 (14)	0.0205 (14)	−0.0014 (9)	0.0008 (10)	0.0004 (10)
O5	0.0161 (14)	0.0160 (13)	0.0184 (13)	−0.0021 (9)	0.0069 (10)	0.0003 (9)
O6	0.0239 (13)	0.0247 (13)	0.0131 (12)	0.0039 (11)	0.0017 (10)	0.0056 (10)
O7	0.0150 (12)	0.0191 (12)	0.0151 (11)	0.0016 (10)	0.0022 (9)	−0.0039 (10)

O8	0.0106 (12)	0.0228 (12)	0.0202 (13)	0.0033 (10)	0.0055 (10)	−0.0045 (11)
O9	0.0103 (11)	0.0267 (14)	0.0204 (13)	−0.0013 (10)	0.0064 (9)	0.0019 (11)
O10	0.0174 (13)	0.0160 (12)	0.0193 (13)	0.0037 (10)	0.0021 (10)	−0.0055 (10)
O11	0.0152 (12)	0.0187 (12)	0.0172 (12)	−0.0010 (10)	−0.0008 (9)	−0.0028 (10)
O12	0.0182 (12)	0.0251 (13)	0.0128 (11)	−0.0025 (10)	0.0006 (9)	0.0058 (10)
O13	0.0252 (16)	0.0401 (17)	0.0146 (14)	−0.0146 (13)	−0.0022 (12)	0.0111 (12)
O14	0.0161 (13)	0.0179 (13)	0.0308 (15)	0.0013 (10)	0.0073 (11)	0.0047 (12)
O15	0.0394 (17)	0.0172 (13)	0.0181 (14)	0.0021 (12)	0.0067 (12)	0.0023 (11)
O16	0.0168 (12)	0.0198 (13)	0.0171 (12)	0.0001 (10)	0.0078 (10)	0.0012 (11)

Geometric parameters (Å, º)

Nd1—O1	2.598 (2)	S1—O3	1.495 (3)
Nd1—O1^{i}	2.510 (2)	S1—O4	1.446 (3)
Nd1—O3^{ii}	2.489 (2)	S2—O5	1.484 (3)
Nd1—O3^{i}	2.676 (3)	S2—O6	1.459 (3)
Nd1—O5	2.443 (3)	S2—O7	1.471 (3)
Nd1—O7^{i}	2.427 (2)	S2—O8	1.467 (2)
Nd1—O9	2.427 (2)	S3—O9	1.465 (2)
Nd1—O13	2.491 (3)	S3—O10	1.490 (3)
Nd1—O14	2.584 (3)	S3—O11	1.473 (3)
Nd2—O2	2.430 (2)	S3—O12	1.470 (3)
Nd2—O6	2.318 (3)	O13—H13A	0.82 (2)
Nd2—O8^{iii}	2.392 (2)	O13—H13B	0.82 (2)
Nd2—O10^{iv}	2.499 (3)	O14—H14A	0.83 (2)
Nd2—O11^{iv}	2.621 (2)	O14—H14B	0.84 (2)
Nd2—O12^{v}	2.445 (2)	O15—H15A	0.84 (2)
Nd2—O15	2.457 (3)	O15—H15B	0.84 (2)
Nd2—O16	2.456 (2)	O16—H16A	0.82 (2)
S1—O1	1.503 (2)	O16—H16B	0.837 (19)
S1—O2	1.466 (3)		

O1^{i}—Nd1—O1	69.25 (9)	O15—Nd2—O10^{iv}	80.31 (9)
O1^{i}—Nd1—O3^{i}	53.94 (8)	O15—Nd2—O11^{iv}	123.88 (9)
O1—Nd1—O3^{i}	116.43 (7)	O16—Nd2—O10^{iv}	69.32 (8)
O1^{i}—Nd1—O14	79.94 (8)	O16—Nd2—O11^{iv}	110.74 (8)
O3^{ii}—Nd1—O1^{i}	116.01 (8)	O16—Nd2—O15	75.62 (9)
O3^{ii}—Nd1—O1	147.43 (8)	O1—S1—Nd1^{i}	49.11 (10)
O3^{ii}—Nd1—O3^{i}	62.25 (10)	O2—S1—Nd1^{i}	113.62 (11)
O3^{ii}—Nd1—O13	84.36 (10)	O2—S1—O1	110.01 (14)
O3^{ii}—Nd1—O14	78.11 (8)	O2—S1—O3	108.37 (15)
O5—Nd1—O1^{i}	74.56 (9)	O3—S1—Nd1^{i}	55.51 (10)
O5—Nd1—O1	72.16 (7)	O3—S1—O1	103.63 (15)
O5—Nd1—O3^{ii}	78.41 (8)	O4—S1—Nd1^{i}	134.98 (12)
O5—Nd1—O3^{i}	67.75 (8)	O4—S1—O1	110.87 (14)
O5—Nd1—O13	72.38 (10)	O4—S1—O2	111.26 (17)
O5—Nd1—O14	132.77 (9)	O4—S1—O3	112.42 (15)
O7^{i}—Nd1—O1	69.80 (8)	O6—S2—O5	108.43 (17)

O7$^{\text{i}}$—Nd1—O1$^{\text{i}}$	73.09 (8)	O6—S2—O7	110.72 (16)
O7$^{\text{i}}$—Nd1—O3$^{\text{i}}$	112.57 (8)	O6—S2—O8	109.10 (15)
O7$^{\text{i}}$—Nd1—O3$^{\text{ii}}$	142.58 (8)	O7—S2—O5	110.01 (15)
O7$^{\text{i}}$—Nd1—O5	136.61 (8)	O8—S2—O5	108.09 (15)
O7$^{\text{i}}$—Nd1—O9	80.36 (8)	O8—S2—O7	110.42 (15)
O7$^{\text{i}}$—Nd1—O13	114.92 (10)	O9—S3—Nd2$^{\text{vi}}$	123.73 (11)
O7$^{\text{i}}$—Nd1—O14	67.57 (8)	O9—S3—O10	109.19 (16)
O9—Nd1—O1$^{\text{i}}$	150.36 (8)	O9—S3—O11	112.71 (15)
O9—Nd1—O1	113.64 (8)	O9—S3—O12	109.51 (15)
O9—Nd1—O3$^{\text{i}}$	129.70 (8)	O10—S3—Nd2$^{\text{vi}}$	50.12 (11)
O9—Nd1—O3$^{\text{ii}}$	78.24 (9)	O11—S3—Nd2$^{\text{vi}}$	54.81 (10)
O9—Nd1—O5	135.06 (9)	O11—S3—O10	104.88 (15)
O9—Nd1—O13	67.55 (9)	O12—S3—Nd2$^{\text{vi}}$	126.40 (10)
O9—Nd1—O14	77.92 (9)	O12—S3—O10	108.93 (16)
O13—Nd1—O1$^{\text{i}}$	136.23 (9)	O12—S3—O11	111.46 (15)
O13—Nd1—O1	73.83 (9)	Nd1$^{\text{i}}$—O1—Nd1	110.75 (9)
O13—Nd1—O3$^{\text{i}}$	131.76 (9)	S1—O1—Nd1$^{\text{i}}$	103.97 (12)
O13—Nd1—O14	143.79 (9)	S1—O1—Nd1	138.78 (14)
O14—Nd1—O1	132.89 (8)	S1—O2—Nd2	145.36 (17)
O14—Nd1—O3$^{\text{i}}$	65.08 (8)	Nd1$^{\text{vii}}$—O3—Nd1$^{\text{i}}$	117.75 (10)
O2—Nd2—O10$^{\text{iv}}$	79.18 (9)	S1—O3—Nd1$^{\text{vii}}$	145.10 (15)
O2—Nd2—O11$^{\text{iv}}$	68.74 (8)	S1—O3—Nd1$^{\text{i}}$	97.07 (12)
O2—Nd2—O12$^{\text{v}}$	141.50 (9)	S2—O5—Nd1	136.75 (14)
O2—Nd2—O15	71.81 (9)	S2—O6—Nd2	160.63 (18)
O2—Nd2—O16	137.73 (9)	S2—O7—Nd1$^{\text{i}}$	137.62 (14)
O6—Nd2—O2	82.39 (9)	S2—O8—Nd2$^{\text{viii}}$	148.89 (17)
O6—Nd2—O8$^{\text{iii}}$	81.12 (9)	S3—O9—Nd1	147.58 (16)
O6—Nd2—O10$^{\text{iv}}$	130.49 (9)	S3—O10—Nd2$^{\text{vi}}$	102.64 (13)
O6—Nd2—O11$^{\text{iv}}$	75.94 (9)	S3—O11—Nd2$^{\text{vi}}$	97.84 (12)
O6—Nd2—O12$^{\text{v}}$	72.98 (9)	S3—O12—Nd2$^{\text{ix}}$	141.08 (16)
O6—Nd2—O15	135.23 (9)	Nd1—O13—H13A	121 (4)
O6—Nd2—O16	139.71 (9)	Nd1—O13—H13B	124 (5)
O8$^{\text{iii}}$—Nd2—O2	127.28 (9)	H13A—O13—H13B	105 (6)
O8$^{\text{iii}}$—Nd2—O10$^{\text{iv}}$	144.39 (8)	Nd1—O14—H14A	116 (5)
O8$^{\text{iii}}$—Nd2—O11$^{\text{iv}}$	149.90 (9)	Nd1—O14—H14B	115 (3)
O8$^{\text{iii}}$—Nd2—O12$^{\text{v}}$	78.09 (9)	H14A—O14—H14B	108 (6)
O8$^{\text{iii}}$—Nd2—O15	86.19 (10)	Nd2—O15—H15A	126 (4)
O8$^{\text{iii}}$—Nd2—O16	75.46 (9)	Nd2—O15—H15B	146 (6)
O10$^{\text{iv}}$—Nd2—O11$^{\text{iv}}$	54.56 (8)	H15A—O15—H15B	86 (6)
O12$^{\text{v}}$—Nd2—O10$^{\text{iv}}$	94.64 (9)	Nd2—O16—H16A	117 (4)
O12$^{\text{v}}$—Nd2—O11$^{\text{iv}}$	76.73 (8)	Nd2—O16—H16B	116 (3)
O12$^{\text{v}}$—Nd2—O15	145.15 (9)	H16A—O16—H16B	119 (5)
O12$^{\text{v}}$—Nd2—O16	70.43 (9)		

Nd1$^{\text{i}}$—S1—O1—Nd1	146.9 (2)	O5—S2—O8—Nd2$^{\text{viii}}$	−118.4 (3)
Nd1$^{\text{i}}$—S1—O2—Nd2	31.0 (3)	O6—S2—O5—Nd1	−75.7 (3)
Nd1$^{\text{i}}$—S1—O3—Nd1$^{\text{vii}}$	176.3 (3)	O6—S2—O7—Nd1$^{\text{i}}$	60.9 (3)
Nd2$^{\text{vi}}$—S3—O9—Nd1	141.0 (2)	O6—S2—O8—Nd2$^{\text{viii}}$	123.9 (3)

Nd2$^{\text{vi}}$—S3—O12—Nd2$^{\text{ix}}$	39.3 (3)	O7—S2—O5—Nd1	45.6 (3)
O1—S1—O2—Nd2	−22.0 (3)	O7—S2—O6—Nd2	21.7 (5)
O1—S1—O3—Nd1$^{\text{vii}}$	−173.3 (2)	O7—S2—O8—Nd2$^{\text{viii}}$	2.0 (4)
O1—S1—O3—Nd1$^{\text{i}}$	10.33 (13)	O8—S2—O5—Nd1	166.2 (2)
O2—S1—O1—Nd1	−108.7 (2)	O8—S2—O6—Nd2	−100.1 (5)
O2—S1—O1—Nd1$^{\text{i}}$	104.40 (15)	O8—S2—O7—Nd1$^{\text{i}}$	−178.1 (2)
O2—S1—O3—Nd1$^{\text{vii}}$	69.8 (3)	O9—S3—O10—Nd2$^{\text{vi}}$	118.38 (14)
O2—S1—O3—Nd1$^{\text{i}}$	−106.50 (13)	O9—S3—O11—Nd2$^{\text{vi}}$	−116.20 (14)
O3—S1—O1—Nd1	135.65 (19)	O9—S3—O12—Nd2$^{\text{ix}}$	−147.5 (2)
O3—S1—O1—Nd1$^{\text{i}}$	−11.28 (14)	O10—S3—O9—Nd1	86.7 (3)
O3—S1—O2—Nd2	90.6 (3)	O10—S3—O11—Nd2$^{\text{vi}}$	2.48 (15)
O4—S1—O1—Nd1$^{\text{i}}$	−132.11 (14)	O10—S3—O12—Nd2$^{\text{ix}}$	93.1 (3)
O4—S1—O1—Nd1	14.8 (3)	O11—S3—O9—Nd1	−157.1 (3)
O4—S1—O2—Nd2	−145.3 (3)	O11—S3—O10—Nd2$^{\text{vi}}$	−2.64 (16)
O4—S1—O3—Nd1$^{\text{i}}$	130.11 (13)	O11—S3—O12—Nd2$^{\text{ix}}$	−22.1 (3)
O4—S1—O3—Nd1$^{\text{vii}}$	−53.6 (3)	O12—S3—O9—Nd1	−32.5 (4)
O5—S2—O6—Nd2	142.4 (5)	O12—S3—O10—Nd2$^{\text{vi}}$	−122.07 (14)
O5—S2—O7—Nd1$^{\text{i}}$	−58.9 (3)	O12—S3—O11—Nd2$^{\text{vi}}$	120.19 (13)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O13—H13*A*···O4$^{\text{vi}}$	0.82 (2)	2.10 (4)	2.838 (4)	149 (5)
O13—H13*B*···O11$^{\text{iv}}$	0.82 (2)	2.01 (3)	2.776 (4)	156 (6)
O14—H14*A*···O8$^{\text{ix}}$	0.83 (2)	2.52 (6)	3.038 (4)	121 (6)
O14—H14*A*···O12	0.83 (2)	2.36 (6)	2.933 (4)	127 (6)
O14—H14*B*···O5$^{\text{x}}$	0.84 (2)	1.96 (2)	2.785 (4)	166 (5)
O15—H15*A*···O10$^{\text{xi}}$	0.84 (2)	2.03 (3)	2.798 (4)	151 (6)
O15—H15*B*···O5$^{\text{vii}}$	0.84 (2)	2.54 (6)	3.141 (4)	130 (7)
O15—H15*B*···O13$^{\text{vii}}$	0.84 (2)	2.47 (5)	3.194 (4)	145 (7)
O16—H16*A*···O4$^{\text{xi}}$	0.82 (2)	2.02 (3)	2.799 (4)	157 (6)
O16—H16*B*···O10$^{\text{xi}}$	0.84 (2)	1.87 (2)	2.676 (4)	162 (5)

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