

Poly[(μ_4 -benzene-1,3,5-tricarboxylato)-bis(dimethyl sulfoxide- κ O)-neodymium(III)]

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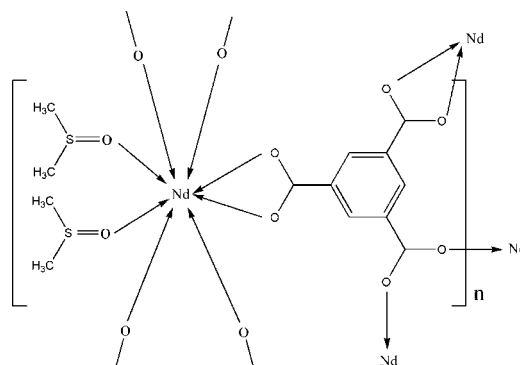
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 Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(\text{C}–\text{C}) = 0.009$ Å; R factor = 0.039; wR factor = 0.082; data-to-parameter ratio = 13.6.

The asymmetric unit of the title compound, $[\text{Nd}(\text{C}_9\text{H}_3\text{O}_6)(\text{C}_2\text{H}_6\text{OS})_2]_n$, contains one Nd^{3+} ion, one benzene-1,3,5-tricarboxylic ligand and two coordinating dimethyl sulfoxide molecules. The Nd^{3+} ion is coordinated by six O atoms from four carboxylate groups of the benzene-1,3,5-tricarboxylate ligands and two O atoms from two dimethyl sulfoxide molecules. The metal-organic cluster formed upon symmetry expansion of the asymmetric unit consists of two metal atoms and four benzene-1,3,5-tricarboxylate groups, creating a paddle-wheel-type building block arrangement. The remaining coordination sites are occupied by additional benzene-1,3,5-tricarboxylate groups and dimethyl sulfoxide molecules, forming a three-dimensional polymeric rare earth metal-organic framework structure.

Related literature

For metal-organic framework structures with adsorption, catalytic and fluorescence properties, see: Sun *et al.* (2006); Ravon *et al.* (2008); Allendorf *et al.* (2009). For isostructural rare earth complexes, see: Thirumurugan & Natarajan (2004); For rare earth coordination polymers, see: Guo *et al.* (2006).



Experimental

Crystal data

 $[\text{Nd}(\text{C}_9\text{H}_3\text{O}_6)(\text{C}_2\text{H}_6\text{OS})_2]$
 $M_r = 507.61$

 Monoclinic, $P2_1/n$
 $a = 10.380$ (2) Å

 $b = 10.752$ (3) Å

 $c = 16.025$ (4) Å

 $\beta = 106.419$ (4)°

 $V = 1715.6$ (7) Å³
 $Z = 4$

 Mo $K\alpha$ radiation

 $\mu = 3.31$ mm⁻¹
 $T = 273$ K

 $0.50 \times 0.40 \times 0.40$ mm

Data collection

Bruker APEX CCD diffractometer

Absorption correction: multi-scan

(SADABS; Sheldrick, 2008)

 $T_{\min} = 0.289$, $T_{\max} = 0.351$

8925 measured reflections

3008 independent reflections

 2453 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.049$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.082$
 $S = 0.98$

3008 reflections

221 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 1.92$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.83$ e Å⁻³

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JJ2108).

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supporting information

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Poly[(μ_4 -benzene-1,3,5-tricarboxylato)bis(dimethyl sulfoxide- κO)neodymium(III)]

Zhongyue Li and Kun Liu

S1. Comment

Metal-organic framework design and construction is currently a flourishing field of research owing to the intriguing molecular topologies and the potentially exploitable adsorption (Sun *et al.*, 2006), catalytic (Ravon *et al.*, 2008) and fluorescence (Allendorf *et al.*, 2009) properties of these types of compounds. As functional metal centers, rare earth metals are attracting more attention from synthetic chemists for their unusual coordination properties and special chemical characteristics arising from interactions with the 4f electrons and the propensity to form isostructural complexes (Thirumurugan & Natarajan, 2004). Many coordination polymers utilizing the rare earth elements have been synthesized (Guo *et al.*, 2006).

The title compound poly[(benzene-1,3,5-tricarboxylato)bis(dimethyl sulfoxide)neodymium(III)]_n represents a rare-earth three-dimensional metal-organic framework structure (Fig. 1). In this compound, the asymmetric unit, Nd(C₉H₃O₆)(C₂H₆OS)₂, contains one eight-coordinated Nd³⁺ ion, one benzene-1,3,5-tricarboxylate ligand and two coordinated dimethyl sulfoxide molecules, without any guest molecule. Each of two metal center Nd³⁺ ions in a formed cluster is coordinated with six oxygen atoms from four carboxylate groups of the 1,3,5- benzenetricarboxylic ligands and two oxygen atoms from two terminal dimethyl sulfoxide molecules. Upon symmetry expansion of the asymmetric unit, the metal organic cluster formed therefore consists of two metal centers and four benzene-1,3,5-tricarboxylate groups creating a paddle-wheel type building block arrangement. The remaining coordination sites are occupied by additional benzene-1,3,5-tricarboxylate groups and dimethyl sulfoxide molecules forming a polymeric rare earth three-dimensional metal-organic framework structure.

S2. Experimental

All reagents were of analytical grade. A mixture of neodymium nitrate (40 mg, 0.10 mmol) and benzene-1,3,5-tricarboxylate acid (10 mg, 0.05 mmol) was dissolved in *N,N*-dimethylformamide (15 ml) and dimethyl sulfoxide (10 ml) at room temperature. Two drops of NaOH (aq, 2 M) was added, followed by some nitric acid (aq, 2 M) until the solution is clear. This mixture was placed at 55°C for 20 days giving rise to purple rod crystals suitable for *x*-ray crystallographic analysis.

S3. Refinement

H atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å (aromatic C), C—H = 0.96 Å (methyl C) and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. S1 and S2 have been restrained with $DFIX = 0.02$.

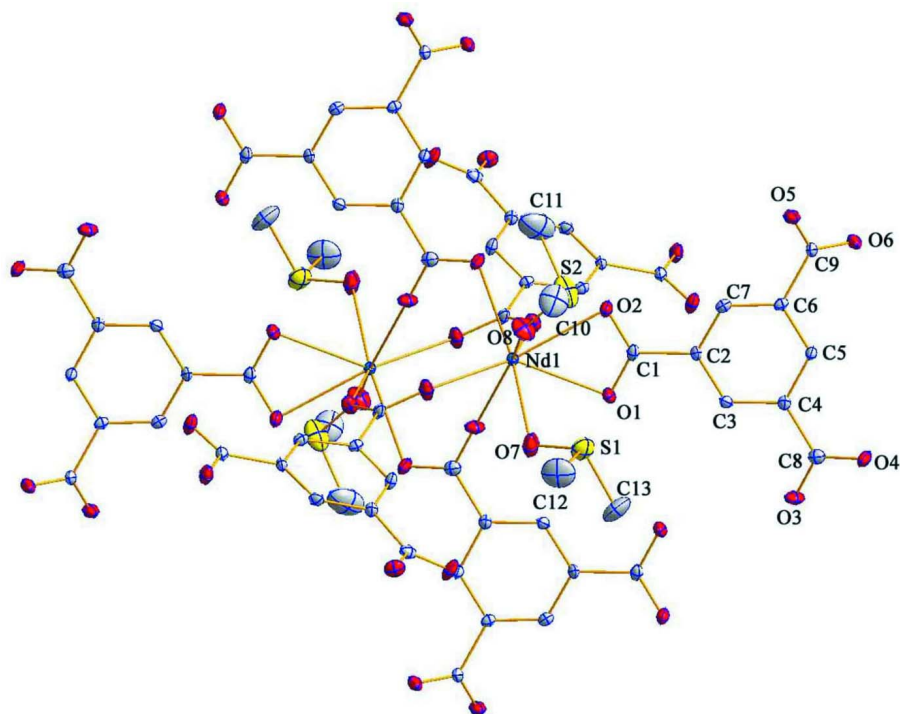


Figure 1

Molecular structure of (I) showing the atom-numbering scheme of the asymmetric unit and symmetry expanded metal-organic framework structure. Displacement ellipsoids are drawn at the 30% probability level.

Poly[(μ_4 -benzene-1,3,5-tricarboxylato)bis(dimethyl sulfoxide- κ O) neodymium(III)]

Crystal data

[Nd(C₉H₃O₆)(C₂H₆OS)₂]

$M_r = 507.61$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 10.380$ (2) Å

$b = 10.752$ (3) Å

$c = 16.025$ (4) Å

$\beta = 106.419$ (4)°

$V = 1715.6$ (7) Å³

$Z = 4$

$F(000) = 996$

$D_x = 1.965$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2282 reflections

$\theta = 2.3$ – 24.8°

$\mu = 3.31$ mm⁻¹

$T = 273$ K

Rod, purple

$0.50 \times 0.40 \times 0.40$ mm

Data collection

Bruker APEX CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 8.33 pixels mm⁻¹

phi and ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 2008)

$T_{\min} = 0.289$, $T_{\max} = 0.351$

8925 measured reflections

3008 independent reflections

2453 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.049$

$\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.1^\circ$

$h = -11 \rightarrow 12$

$k = -10 \rightarrow 12$

$l = -18 \rightarrow 19$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.082$
 $S = 0.98$
 3008 reflections
 221 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0335P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 1.92 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.83 \text{ e } \text{\AA}^{-3}$

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Nd1	0.36554 (3)	0.12931 (3)	0.02773 (2)	0.01539 (12)
S1	0.0680 (2)	0.2768 (2)	-0.08861 (14)	0.0492 (6)
S2	0.3373 (3)	0.4585 (2)	0.08367 (18)	0.0664 (8)
O1	0.1446 (4)	0.0876 (4)	0.0571 (3)	0.0280 (11)
O2	0.2784 (4)	0.2139 (4)	0.1508 (3)	0.0301 (11)
O3	-0.3430 (4)	0.0586 (4)	0.0532 (3)	0.0297 (11)
O4	-0.4178 (4)	0.1981 (4)	0.1279 (3)	0.0360 (12)
O5	0.0801 (4)	0.4650 (4)	0.3619 (3)	0.0268 (11)
O6	-0.0472 (4)	0.3271 (4)	0.4070 (3)	0.0309 (11)
O7	0.1768 (5)	0.1920 (5)	-0.1004 (3)	0.0462 (14)
O8	0.3616 (5)	0.3615 (4)	0.0214 (3)	0.0476 (14)
C1	0.1662 (6)	0.1639 (5)	0.1191 (4)	0.0204 (15)
C2	0.0514 (6)	0.1983 (6)	0.1562 (4)	0.0179 (14)
C3	-0.0760 (6)	0.1517 (5)	0.1195 (4)	0.0196 (14)
H3	-0.0916	0.0987	0.0719	0.024*
C4	-0.1821 (6)	0.1837 (6)	0.1535 (4)	0.0190 (14)
C5	-0.1545 (6)	0.2560 (5)	0.2286 (4)	0.0202 (15)
H5	-0.2228	0.2735	0.2540	0.024*
C6	-0.0262 (6)	0.3024 (5)	0.2661 (4)	0.0165 (13)
C7	0.0737 (6)	0.2764 (5)	0.2272 (4)	0.0196 (14)
H7	0.1579	0.3123	0.2494	0.024*
C8	-0.3236 (6)	0.1436 (6)	0.1090 (4)	0.0223 (15)
C9	0.0043 (6)	0.3722 (6)	0.3517 (4)	0.0204 (14)
C10	0.3202 (10)	0.6008 (7)	0.0260 (7)	0.080 (3)
H10A	0.3911	0.6083	-0.0013	0.121*

H10B	0.3251	0.6687	0.0657	0.121*
H10C	0.2350	0.6025	-0.0176	0.121*
C11	0.4971 (10)	0.4797 (10)	0.1533 (7)	0.106 (4)
H11A	0.5345	0.4005	0.1752	0.159*
H11B	0.4922	0.5318	0.2010	0.159*
H11C	0.5531	0.5186	0.1224	0.159*
C12	0.0497 (10)	0.3915 (8)	-0.1710 (6)	0.075 (3)
H12A	0.1285	0.4430	-0.1580	0.113*
H12B	-0.0275	0.4420	-0.1733	0.113*
H12C	0.0383	0.3515	-0.2262	0.113*
C13	-0.0810 (8)	0.1947 (9)	-0.1314 (7)	0.079 (3)
H13A	-0.0857	0.1672	-0.1892	0.119*
H13B	-0.1561	0.2478	-0.1333	0.119*
H13C	-0.0832	0.1239	-0.0953	0.119*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Nd1	0.01401 (19)	0.01665 (19)	0.01629 (19)	0.00024 (16)	0.00554 (13)	-0.00076 (15)
S1	0.0391 (12)	0.0561 (14)	0.0477 (14)	0.0094 (11)	0.0047 (10)	0.0119 (10)
S2	0.102 (2)	0.0324 (12)	0.082 (2)	-0.0009 (13)	0.0536 (17)	-0.0043 (12)
O1	0.024 (3)	0.037 (3)	0.027 (3)	-0.002 (2)	0.012 (2)	-0.012 (2)
O2	0.019 (3)	0.037 (3)	0.037 (3)	-0.004 (2)	0.014 (2)	-0.011 (2)
O3	0.032 (3)	0.024 (3)	0.028 (3)	-0.003 (2)	0.001 (2)	-0.009 (2)
O4	0.014 (3)	0.049 (3)	0.045 (3)	-0.001 (2)	0.008 (2)	-0.017 (3)
O5	0.031 (3)	0.028 (3)	0.023 (3)	-0.011 (2)	0.009 (2)	-0.006 (2)
O6	0.033 (3)	0.039 (3)	0.025 (3)	-0.011 (2)	0.015 (2)	-0.013 (2)
O7	0.032 (3)	0.065 (4)	0.045 (4)	0.019 (3)	0.017 (3)	0.012 (3)
O8	0.071 (4)	0.023 (3)	0.053 (4)	-0.001 (3)	0.025 (3)	-0.009 (2)
C1	0.019 (4)	0.023 (4)	0.021 (4)	0.001 (3)	0.010 (3)	0.004 (3)
C2	0.016 (3)	0.024 (4)	0.015 (3)	-0.002 (3)	0.008 (3)	0.000 (3)
C3	0.020 (3)	0.023 (4)	0.015 (3)	0.002 (3)	0.003 (3)	-0.003 (3)
C4	0.017 (3)	0.023 (3)	0.019 (4)	0.000 (3)	0.007 (3)	0.000 (3)
C5	0.014 (3)	0.023 (4)	0.025 (4)	-0.002 (3)	0.009 (3)	-0.005 (3)
C6	0.015 (3)	0.015 (3)	0.018 (4)	0.002 (3)	0.002 (3)	0.001 (3)
C7	0.015 (3)	0.021 (3)	0.021 (4)	-0.001 (3)	0.002 (3)	0.000 (3)
C8	0.025 (4)	0.021 (4)	0.020 (4)	-0.004 (3)	0.004 (3)	0.004 (3)
C9	0.015 (3)	0.028 (4)	0.019 (4)	0.001 (3)	0.007 (3)	-0.006 (3)
C10	0.091 (8)	0.038 (6)	0.118 (10)	0.004 (5)	0.038 (7)	-0.004 (5)
C11	0.112 (10)	0.112 (10)	0.072 (9)	0.054 (8)	-0.009 (7)	-0.003 (7)
C12	0.098 (8)	0.054 (6)	0.065 (7)	0.008 (5)	0.009 (6)	0.035 (5)
C13	0.029 (5)	0.106 (8)	0.092 (9)	-0.007 (5)	-0.001 (5)	-0.004 (7)

Geometric parameters (Å, °)

Nd1—O3 ⁱ	2.376 (4)	C1—C2	1.519 (8)
Nd1—O6 ⁱⁱ	2.403 (4)	C2—C3	1.381 (8)
Nd1—O5 ⁱⁱⁱ	2.451 (4)	C2—C7	1.380 (8)

Nd1—O4 ^{iv}	2.478 (4)	C3—C4	1.401 (8)
Nd1—O7	2.497 (5)	C3—H3	0.9300
Nd1—O8	2.498 (4)	C4—C5	1.394 (8)
Nd1—O1	2.509 (4)	C4—C8	1.503 (8)
Nd1—O2	2.559 (4)	C5—C6	1.390 (8)
Nd1—C1	2.878 (6)	C5—H5	0.9300
S1—O7	1.505 (5)	C6—C7	1.381 (8)
S1—C13	1.744 (8)	C6—C9	1.515 (8)
S1—C12	1.777 (8)	C7—H7	0.9300
S2—O8	1.513 (5)	C10—H10A	0.9600
S2—C11	1.733 (10)	C10—H10B	0.9600
S2—C10	1.770 (9)	C10—H10C	0.9600
O1—C1	1.258 (7)	C11—H11A	0.9600
O2—C1	1.253 (7)	C11—H11B	0.9600
O3—C8	1.255 (7)	C11—H11C	0.9600
O3—Nd1 ⁱ	2.376 (4)	C12—H12A	0.9600
O4—C8	1.249 (7)	C12—H12B	0.9600
O4—Nd1 ^v	2.478 (4)	C12—H12C	0.9600
O5—C9	1.253 (7)	C13—H13A	0.9600
O5—Nd1 ^{vi}	2.451 (4)	C13—H13B	0.9600
O6—C9	1.255 (7)	C13—H13C	0.9600
O6—Nd1 ^{vii}	2.403 (4)		
O3 ⁱ —Nd1—O6 ⁱⁱ	74.21 (15)	O1—C1—C2	118.9 (5)
O3 ⁱ —Nd1—O5 ⁱⁱⁱ	75.39 (15)	O2—C1—Nd1	62.7 (3)
O6 ⁱⁱ —Nd1—O5 ⁱⁱⁱ	131.26 (14)	O1—C1—Nd1	60.5 (3)
O3 ⁱ —Nd1—O4 ^{iv}	122.58 (15)	C2—C1—Nd1	170.6 (4)
O6 ⁱⁱ —Nd1—O4 ^{iv}	89.06 (16)	C3—C2—C7	119.2 (5)
O5 ⁱⁱⁱ —Nd1—O4 ^{iv}	76.48 (15)	C3—C2—C1	120.5 (5)
O3 ⁱ —Nd1—O7	81.22 (16)	C7—C2—C1	120.3 (5)
O6 ⁱⁱ —Nd1—O7	70.85 (15)	C2—C3—C4	120.6 (6)
O5 ⁱⁱⁱ —Nd1—O7	139.05 (16)	C2—C3—H3	119.7
O4 ^{iv} —Nd1—O7	144.05 (17)	C4—C3—H3	119.7
O3 ⁱ —Nd1—O8	146.04 (16)	C5—C4—C3	118.7 (6)
O6 ⁱⁱ —Nd1—O8	77.17 (15)	C5—C4—C8	120.3 (5)
O5 ⁱⁱⁱ —Nd1—O8	138.39 (15)	C3—C4—C8	121.0 (5)
O4 ^{iv} —Nd1—O8	74.30 (16)	C6—C5—C4	120.8 (5)
O7—Nd1—O8	72.36 (17)	C6—C5—H5	119.6
O3 ⁱ —Nd1—O1	89.81 (14)	C4—C5—H5	119.6
O6 ⁱⁱ —Nd1—O1	139.36 (15)	C7—C6—C5	118.8 (5)
O5 ⁱⁱⁱ —Nd1—O1	76.81 (14)	C7—C6—C9	121.2 (5)
O4 ^{iv} —Nd1—O1	129.95 (14)	C5—C6—C9	119.9 (5)
O7—Nd1—O1	69.90 (15)	C2—C7—C6	121.6 (6)
O8—Nd1—O1	100.41 (15)	C2—C7—H7	119.2
O3 ⁱ —Nd1—O2	136.16 (14)	C6—C7—H7	119.2
O6 ⁱⁱ —Nd1—O2	147.93 (15)	O4—C8—O3	122.4 (6)
O5 ⁱⁱⁱ —Nd1—O2	76.07 (14)	O4—C8—C4	118.6 (5)
O4 ^{iv} —Nd1—O2	81.29 (14)	O3—C8—C4	119.1 (6)

O7—Nd1—O2	99.90 (15)	O5—C9—O6	126.3 (6)
O8—Nd1—O2	70.79 (15)	O5—C9—C6	118.4 (5)
O1—Nd1—O2	51.48 (13)	O6—C9—C6	115.3 (5)
O3 ⁱ —Nd1—C1	114.43 (16)	S2—C10—H10A	109.5
O6 ⁱⁱ —Nd1—C1	150.90 (16)	S2—C10—H10B	109.5
O5 ⁱⁱⁱ —Nd1—C1	77.15 (15)	H10A—C10—H10B	109.5
O4 ^{iv} —Nd1—C1	106.46 (17)	S2—C10—H10C	109.5
O7—Nd1—C1	82.76 (16)	H10A—C10—H10C	109.5
O8—Nd1—C1	83.44 (16)	H10B—C10—H10C	109.5
O1—Nd1—C1	25.87 (15)	S2—C11—H11A	109.5
O2—Nd1—C1	25.79 (15)	S2—C11—H11B	109.5
O7—S1—C13	104.9 (4)	H11A—C11—H11B	109.5
O7—S1—C12	104.7 (4)	S2—C11—H11C	109.5
C13—S1—C12	99.3 (5)	H11A—C11—H11C	109.5
O8—S2—C11	102.0 (4)	H11B—C11—H11C	109.5
O8—S2—C10	105.2 (4)	S1—C12—H12A	109.5
C11—S2—C10	99.2 (5)	S1—C12—H12B	109.5
C1—O1—Nd1	93.7 (4)	H12A—C12—H12B	109.5
C1—O2—Nd1	91.5 (4)	S1—C12—H12C	109.5
C8—O3—Nd1 ⁱ	168.4 (4)	H12A—C12—H12C	109.5
C8—O4—Nd1 ^v	109.4 (4)	H12B—C12—H12C	109.5
C9—O5—Nd1 ^{vi}	132.6 (4)	S1—C13—H13A	109.5
C9—O6—Nd1 ^{vii}	145.7 (4)	S1—C13—H13B	109.5
S1—O7—Nd1	120.2 (3)	H13A—C13—H13B	109.5
S2—O8—Nd1	131.7 (3)	S1—C13—H13C	109.5
O2—C1—O1	122.5 (5)	H13A—C13—H13C	109.5
O2—C1—C2	118.6 (5)	H13B—C13—H13C	109.5
O3 ⁱ —Nd1—O1—C1	162.7 (4)	O7—Nd1—C1—O2	-131.4 (4)
O6 ⁱⁱ —Nd1—O1—C1	-132.2 (4)	O8—Nd1—C1—O2	-58.4 (4)
O5 ⁱⁱⁱ —Nd1—O1—C1	87.7 (4)	O1—Nd1—C1—O2	170.7 (6)
O4 ^{iv} —Nd1—O1—C1	28.3 (4)	O3 ⁱ —Nd1—C1—O1	-19.0 (4)
O7—Nd1—O1—C1	-116.5 (4)	O6 ⁱⁱ —Nd1—C1—O1	82.6 (5)
O8—Nd1—O1—C1	-49.8 (4)	O5 ⁱⁱⁱ —Nd1—C1—O1	-86.2 (4)
O2—Nd1—O1—C1	5.1 (3)	O4 ^{iv} —Nd1—C1—O1	-157.7 (4)
O3 ⁱ —Nd1—O2—C1	-38.5 (4)	O7—Nd1—C1—O1	57.9 (4)
O6 ⁱⁱ —Nd1—O2—C1	118.6 (4)	O8—Nd1—C1—O1	130.8 (4)
O5 ⁱⁱⁱ —Nd1—O2—C1	-89.2 (4)	O2—Nd1—C1—O1	-170.7 (6)
O4 ^{iv} —Nd1—O2—C1	-167.4 (4)	O2—C1—C2—C3	175.7 (6)
O7—Nd1—O2—C1	49.1 (4)	O1—C1—C2—C3	-3.3 (9)
O8—Nd1—O2—C1	116.3 (4)	O2—C1—C2—C7	-4.5 (9)
O1—Nd1—O2—C1	-5.2 (3)	O1—C1—C2—C7	176.5 (6)
C13—S1—O7—Nd1	-123.4 (4)	C7—C2—C3—C4	0.4 (9)
C12—S1—O7—Nd1	132.5 (4)	C1—C2—C3—C4	-179.8 (5)
O3 ⁱ —Nd1—O7—S1	144.9 (3)	C2—C3—C4—C5	-4.5 (9)
O6 ⁱⁱ —Nd1—O7—S1	-138.8 (4)	C2—C3—C4—C8	174.1 (5)
O5 ⁱⁱⁱ —Nd1—O7—S1	89.5 (4)	C3—C4—C5—C6	4.1 (9)
O4 ^{iv} —Nd1—O7—S1	-79.4 (4)	C8—C4—C5—C6	-174.5 (5)

O8—Nd1—O7—S1	-56.7 (3)	C4—C5—C6—C7	0.5 (9)
O1—Nd1—O7—S1	51.9 (3)	C4—C5—C6—C9	-175.2 (6)
O2—Nd1—O7—S1	9.4 (3)	C3—C2—C7—C6	4.4 (9)
C1—Nd1—O7—S1	28.7 (3)	C1—C2—C7—C6	-175.4 (5)
C11—S2—O8—Nd1	87.3 (5)	C5—C6—C7—C2	-4.9 (9)
C10—S2—O8—Nd1	-169.6 (4)	C9—C6—C7—C2	170.7 (6)
O3 ⁱ —Nd1—O8—S2	157.4 (3)	Nd1 ^v —O4—C8—O3	-6.6 (7)
O6 ⁱⁱ —Nd1—O8—S2	-169.6 (4)	Nd1 ^v —O4—C8—C4	171.9 (4)
O5 ⁱⁱⁱ —Nd1—O8—S2	-29.9 (5)	Nd1 ⁱ —O3—C8—O4	-105 (2)
O4 ^{iv} —Nd1—O8—S2	-76.9 (4)	Nd1 ⁱ —O3—C8—C4	76 (2)
O7—Nd1—O8—S2	116.7 (4)	C5—C4—C8—O4	16.2 (9)
O1—Nd1—O8—S2	51.9 (4)	C3—C4—C8—O4	-162.4 (6)
O2—Nd1—O8—S2	9.2 (4)	C5—C4—C8—O3	-165.3 (6)
C1—Nd1—O8—S2	32.3 (4)	C3—C4—C8—O3	16.1 (9)
Nd1—O2—C1—O1	9.6 (6)	Nd1 ^{vi} —O5—C9—O6	-14.0 (10)
Nd1—O2—C1—C2	-169.4 (5)	Nd1 ^{vi} —O5—C9—C6	168.5 (4)
Nd1—O1—C1—O2	-9.8 (7)	Nd1 ^{vii} —O6—C9—O5	32.1 (11)
Nd1—O1—C1—C2	169.2 (5)	Nd1 ^{vii} —O6—C9—C6	-150.3 (5)
O3 ⁱ —Nd1—C1—O2	151.7 (3)	C7—C6—C9—O5	43.1 (8)
O6 ⁱⁱ —Nd1—C1—O2	-106.7 (5)	C5—C6—C9—O5	-141.3 (6)
O5 ⁱⁱⁱ —Nd1—C1—O2	84.5 (4)	C7—C6—C9—O6	-134.6 (6)
O4 ^{iv} —Nd1—C1—O2	13.0 (4)	C5—C6—C9—O6	40.9 (8)

Symmetry codes: (i) $-x, -y, -z$; (ii) $x+1/2, -y+1/2, z-1/2$; (iii) $-x+1/2, y-1/2, -z+1/2$; (iv) $x+1, y, z$; (v) $x-1, y, z$; (vi) $-x+1/2, y+1/2, -z+1/2$; (vii) $x-1/2, -y+1/2, z+1/2$.