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Poly[tris(dimethylformamide)(μ_3 -2,4,6-triiodobenzene-1,3,5-tricarboxylato)-samarium(III)]

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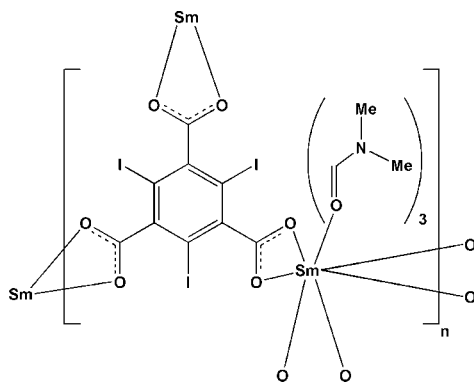
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Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.021; wR factor = 0.049; data-to-parameter ratio = 20.2.

In the title compound, $[\text{Sm}(\text{C}_9\text{I}_3\text{O}_6)(\text{C}_3\text{H}_7\text{NO})_3]_n$, the Sm^{III} atom is coordinated by nine O atoms, *viz.* six carboxylate O atoms from three 2,4,6-triiodobenzene-1,3,5-tricarboxylate (I_3BTC) ligands and three O atoms from three *N,N*-dimethylformamide (DMF) molecules. Each I_3BTC ligand bridges three Sm^{III} atoms, generating a three-dimensional metal-organic framework structure. The asymmetric unit contains one Sm^{III} ion and one I_3BTC anion, both situated on a threefold axis, and one DMF molecule in a general position.

Related literature

For applications of compounds with metal-organic framework structures (MOFs), see: Nakanishi & Tanaka (2007); Phan *et al.* (2010); Suib *et al.* (2008). For related structures, see: Daiguebonne *et al.* (2002); Han *et al.* (2012); Lu *et al.* (2008); Serre *et al.* (2004).



Experimental

Crystal data

$[\text{Sm}(\text{C}_9\text{I}_3\text{O}_6)(\text{C}_3\text{H}_7\text{NO})_3]$
 $M_r = 954.43$
 Cubic, $P2_13$
 $a = 14.1341$ (16) Å
 $V = 2823.6$ (6) Å³

$Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 5.41$ mm⁻¹
 $T = 295$ K
 $0.16 \times 0.15 \times 0.15$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2005)
 $T_{\text{min}} = 0.478$, $T_{\text{max}} = 0.498$

5119 measured reflections
 2143 independent reflections
 2026 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.020$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.021$
 $wR(F^2) = 0.049$
 $S = 1.03$
 2143 reflections
 106 parameters
 H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.72$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.62$ e Å⁻³
 Absolute structure: Flack (1983),
 943 Friedel pairs
 Flack parameter: 0.02 (2)

Data collection: APEX2 (Bruker, 2005); cell refinement: SAINT (Bruker, 2005); data reduction: SAINT; program(s) used to solve structure: SIR97 (Altomare *et al.*, 1999); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: WinGX (Farrugia, 2012).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5378).

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supporting information

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Poly[tris(dimethylformamide)(μ_3 -2,4,6-triiodobenzene-1,3,5-tricarboxylato)samarium(III)]

Bin Yan, Daopeng Sheng and Yanzhao Yang

S1. Comment

Metal-organic framework (MOF) compounds have attracted considerable interest because of their potential applications in a variety of areas, including catalysis, shape-selective adsorption, gas storage, photochemistry, and materials with magnetic properties (Nakanishi *et al.*, 2007; Phan *et al.*, 2010; Suib *et al.*, 2008). The design and synthesis of MOFs with great potential for chemical and structural diversity, is one of the major current challenges in inorganic chemistry. To the best of our knowledge, MOF structure of the I₃BTC ligand is not reported so far. The I₃BTC ligand, besides three iodine atoms at the 2,4,6-sites of benzene ring, is same as 1,3,5- benzenetricarboxylic acid (H₃BTC). Although the coordinated ability of carbonylic O atoms is influenced by the electronic properties of iodine atoms to some extent, its coordinated mode is almost no change (Daiguebonne *et al.*, 2002). In recent years, the construction of MOFs based on H₃BTC ligand has been widely investigated owing to their fascinating coordination modes (Han *et al.*, 2012; Lu *et al.*, 2008; Serre *et al.*, 2004). Herein we report the hydrothermal synthesis and crystal structure of the title compound (I).

In (I), the asymmetric unit contains one Sm^{III} ion and one I₃BTC anion, both situated on a threefold axis, and one DMF molecule in general position. As shown in Fig. 1, each Sm center is coordinated by nine O atoms -six carboxylate O atoms from three ligands and three O atoms from three DMF molecules. The Sm1–O bond lengths fall in the range of 2.446 (3)–2.562 (3) Å, and the O–Sm–O angles varying from 51.702 (88)–142.712 (91)°, thus falling in the expected region. Each ligand I₃BTC bridges three Sm atoms to produce a three-dimensional metal organic framework structure, while coordinated solvent molecules (DMF) exist among the pore canals by coordinating O atoms to central metal ions.

S2. Experimental

The title compound was prepared by the solvothermal reaction of Sm(NO₃)₃·6H₂O (100 mg), 2,4,6-triiodobenzene-1,3,5-tricarboxylic acid (100 mg), DMF (4 ml) and ethanol (4 ml) at 90 °C for 72 h. The autoclave was subsequently allowed to cool to room temperature. After washing with ethanol, colourless block crystals were obtained.

S3. Refinement

All H atoms were placed in geometrically calculated positions (C–H = 0.93–0.96 %A), and refined using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2\text{--}1.5 U_{\text{eq}}(\text{C})$.

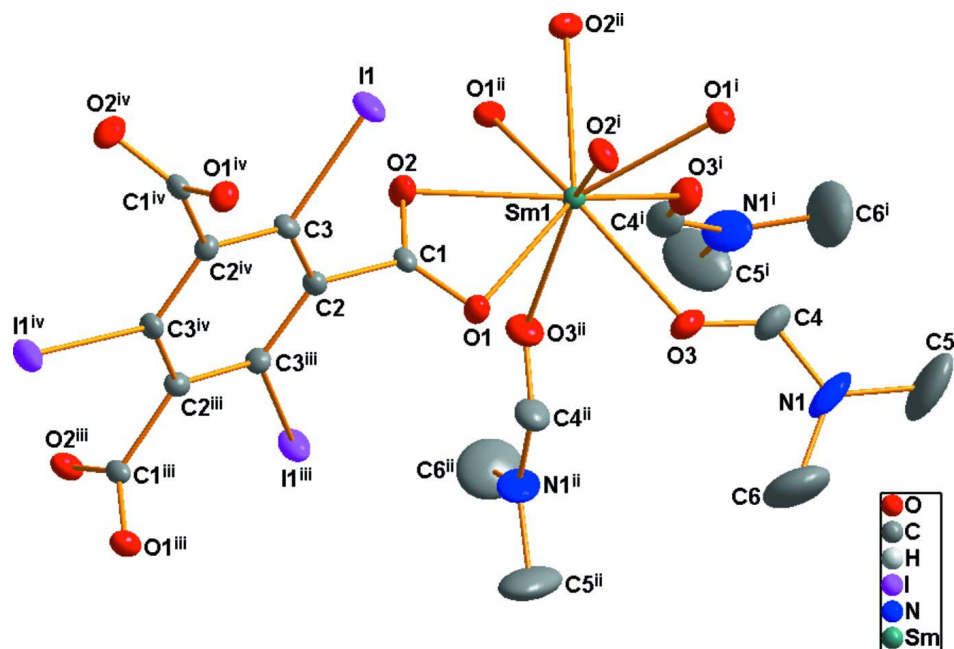


Figure 1

A portion of the crystal structure of (I) showing the coordination environment of Sm1, 30% probability displacement ellipsoids and atomic numbering [symmetry codes: (i) $1 - x, 1/2 + y, 3/2 - z$; (ii) $3/2 - x, 1 - y, -1/2 + z$; (iii) $3/2 - x, 1 - y, -1/2 + z$; (iv) $1/2 - x, -y, 1/2 + z$].

Poly[tris(dimethylformamide)(μ_3 -2,4,6-triiodobenzene-1,3,5-tricarboxylato)samarium(III)]

Crystal data

[Sm(C₉I₃O₆)(C₃H₇NO)₃]

$M_r = 954.43$

Cubic, $P2_13$

Hall symbol: P 2ac 2ab 3

$a = 14.1341$ (16) Å

$V = 2823.6$ (6) Å³

$Z = 4$

$F(000) = 1772$

$D_x = 2.245$ Mg m⁻³

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

Cell parameters from 2685 reflections

$\theta = 3.2$ – 27.2°

$\mu = 5.41$ mm⁻¹

$T = 295$ K

Prism, yellow

$0.16 \times 0.15 \times 0.15$ mm

Data collection

Bruker APEXII CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(SADABS; Bruker, 2005)

$T_{\min} = 0.478$, $T_{\max} = 0.498$

5119 measured reflections

2143 independent reflections

2026 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.020$

$\theta_{\max} = 27.4^\circ$, $\theta_{\min} = 3.2^\circ$

$h = -12 \rightarrow 7$

$k = 0 \rightarrow 18$

$l = -16 \rightarrow 12$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.021$

$wR(F^2) = 0.049$

$S = 1.03$

2143 reflections

106 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

$$w = 1/[\sigma^2(F_o^2) + (0.0236P)^2]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.002$$

$$\Delta\rho_{\max} = 0.72 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.62 \text{ e } \text{\AA}^{-3}$$

Extinction correction: *SHELXL97* (Sheldrick,
2008), $F_c^* = kFc[1 + 0.001x Fc^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.00049 (7)

Absolute structure: Flack (1983), 943 Friedel
pairs

Absolute structure parameter: 0.02 (2)

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. *SHELXTL* (Sheldrick, 2008)

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O2	0.9837 (2)	-0.17185 (19)	0.4744 (2)	0.0341 (7)
C1	0.9099 (3)	-0.1640 (3)	0.4268 (3)	0.0219 (8)
C2	0.8710 (2)	-0.2536 (3)	0.3796 (3)	0.0227 (8)
C3	0.9151 (3)	-0.2914 (3)	0.2996 (3)	0.0236 (8)
C4	0.8963 (4)	0.2099 (3)	0.4875 (4)	0.0464 (12)
H4	0.9575	0.2290	0.5023	0.056*
C5	0.8521 (6)	0.3734 (5)	0.5058 (7)	0.125 (4)
H5A	0.8541	0.4090	0.4479	0.187*
H5B	0.9125	0.3772	0.5367	0.187*
H5C	0.8042	0.3990	0.5465	0.187*
C6	0.7318 (5)	0.2501 (7)	0.4593 (7)	0.126 (4)
H6A	0.7297	0.1860	0.4370	0.189*
H6B	0.7099	0.2918	0.4103	0.189*
H6C	0.6920	0.2564	0.5139	0.189*
I1	1.03806 (2)	-0.22509 (2)	0.248693 (19)	0.03739 (10)
N1	0.8303 (4)	0.2748 (3)	0.4848 (4)	0.0687 (14)
O1	0.8674 (2)	-0.08834 (19)	0.4139 (2)	0.0304 (6)
O3	0.8828 (2)	0.1250 (2)	0.4717 (2)	0.0428 (8)
Sm1	0.999507 (13)	0.000493 (13)	0.500493 (13)	0.01931 (8)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0346 (17)	0.0259 (14)	0.0419 (17)	0.0000 (12)	-0.0116 (13)	-0.0055 (12)
C1	0.0222 (19)	0.0212 (19)	0.0224 (19)	-0.0053 (15)	0.0077 (15)	-0.0030 (15)
C2	0.0207 (19)	0.022 (2)	0.025 (2)	-0.0016 (15)	-0.0020 (14)	-0.0003 (15)

C3	0.0211 (19)	0.026 (2)	0.0234 (19)	-0.0046 (15)	0.0047 (15)	0.0007 (15)
C4	0.050 (3)	0.042 (3)	0.047 (3)	0.022 (2)	0.000 (2)	0.005 (2)
C5	0.170 (9)	0.061 (5)	0.143 (8)	0.061 (5)	-0.040 (7)	-0.039 (5)
C6	0.072 (5)	0.147 (10)	0.160 (9)	0.056 (6)	-0.011 (5)	-0.011 (6)
I1	0.03269 (16)	0.04066 (18)	0.03881 (18)	-0.01484 (12)	0.01194 (11)	-0.00927 (13)
N1	0.086 (4)	0.053 (3)	0.067 (3)	0.046 (3)	0.003 (3)	-0.007 (2)
O1	0.0303 (16)	0.0243 (15)	0.0365 (17)	0.0005 (12)	-0.0038 (13)	-0.0024 (12)
O3	0.0369 (18)	0.0390 (19)	0.053 (2)	0.0154 (14)	0.0044 (15)	0.0053 (16)
Sm1	0.01931 (8)	0.01931 (8)	0.01931 (8)	0.00093 (7)	0.00093 (7)	-0.00093 (7)

Geometric parameters (Å, °)

O2—C1	1.245 (5)	C5—H5C	0.9600
O2—Sm1	2.474 (3)	C6—N1	1.480 (10)
C1—O1	1.240 (5)	C6—H6A	0.9600
C1—C2	1.534 (5)	C6—H6B	0.9600
C1—Sm1	2.844 (4)	C6—H6C	0.9600
C2—C3 ⁱ	1.393 (5)	O1—Sm1	2.562 (3)
C2—C3	1.397 (5)	O3—Sm1	2.446 (3)
C3—C2 ⁱⁱ	1.393 (5)	Sm1—O3 ⁱⁱⁱ	2.446 (3)
C3—I1	2.101 (4)	Sm1—O3 ^{iv}	2.446 (3)
C4—O3	1.236 (6)	Sm1—O2 ^{iv}	2.474 (3)
C4—N1	1.309 (6)	Sm1—O2 ⁱⁱⁱ	2.474 (3)
C4—H4	0.9300	Sm1—O1 ⁱⁱⁱ	2.562 (3)
C5—N1	1.458 (9)	Sm1—O1 ^{iv}	2.562 (3)
C5—H5A	0.9600	Sm1—C1 ^{iv}	2.844 (4)
C5—H5B	0.9600	Sm1—C1 ⁱⁱⁱ	2.844 (4)
C1—O2—Sm1	93.9 (2)	O3 ^{iv} —Sm1—O1	73.51 (10)
O1—C1—O2	124.2 (4)	O2 ^{iv} —Sm1—O1	133.46 (10)
O1—C1—C2	118.3 (3)	O2—Sm1—O1	51.69 (9)
O2—C1—C2	117.5 (3)	O2 ⁱⁱⁱ —Sm1—O1	71.50 (9)
O1—C1—Sm1	64.2 (2)	O3 ⁱⁱⁱ —Sm1—O1 ⁱⁱⁱ	77.37 (10)
O2—C1—Sm1	60.20 (19)	O3—Sm1—O1 ⁱⁱⁱ	73.51 (10)
C2—C1—Sm1	173.6 (2)	O3 ^{iv} —Sm1—O1 ⁱⁱⁱ	142.72 (11)
C3 ⁱ —C2—C3	118.3 (4)	O2 ^{iv} —Sm1—O1 ⁱⁱⁱ	71.50 (9)
C3 ⁱ —C2—C1	121.2 (3)	O2—Sm1—O1 ⁱⁱⁱ	133.46 (10)
C3—C2—C1	120.5 (3)	O2 ⁱⁱⁱ —Sm1—O1 ⁱⁱⁱ	51.69 (9)
C2 ⁱⁱ —C3—C2	121.7 (4)	O1—Sm1—O1 ⁱⁱⁱ	118.13 (3)
C2 ⁱⁱ —C3—I1	119.9 (3)	O3 ⁱⁱⁱ —Sm1—O1 ^{iv}	73.51 (10)
C2—C3—I1	118.4 (3)	O3—Sm1—O1 ^{iv}	142.72 (11)
O3—C4—N1	124.4 (5)	O3 ^{iv} —Sm1—O1 ^{iv}	77.37 (10)
O3—C4—H4	117.8	O2 ^{iv} —Sm1—O1 ^{iv}	51.69 (9)
N1—C4—H4	117.8	O2—Sm1—O1 ^{iv}	71.50 (9)
N1—C5—H5A	109.5	O2 ⁱⁱⁱ —Sm1—O1 ^{iv}	133.46 (10)
N1—C5—H5B	109.5	O1—Sm1—O1 ^{iv}	118.13 (3)
H5A—C5—H5B	109.5	O1 ⁱⁱⁱ —Sm1—O1 ^{iv}	118.13 (3)
N1—C5—H5C	109.5	O3 ⁱⁱⁱ —Sm1—C1	152.70 (11)

H5A—C5—H5C	109.5	O3—Sm1—C1	103.10 (11)
H5B—C5—H5C	109.5	O3 ^{iv} —Sm1—C1	77.91 (10)
N1—C6—H6A	109.5	O2 ^{iv} —Sm1—C1	110.46 (10)
N1—C6—H6B	109.5	O2—Sm1—C1	25.90 (10)
H6A—C6—H6B	109.5	O2 ⁱⁱⁱ —Sm1—C1	77.28 (10)
N1—C6—H6C	109.5	O1—Sm1—C1	25.84 (10)
H6A—C6—H6C	109.5	O1 ⁱⁱⁱ —Sm1—C1	128.98 (10)
H6B—C6—H6C	109.5	O1 ^{iv} —Sm1—C1	95.43 (10)
C4—N1—C5	120.9 (6)	O3 ⁱⁱⁱ —Sm1—C1 ^{iv}	77.91 (10)
C4—N1—C6	120.8 (6)	O3—Sm1—C1 ^{iv}	152.70 (11)
C5—N1—C6	118.3 (5)	O3 ^{iv} —Sm1—C1 ^{iv}	103.10 (11)
C1—O1—Sm1	89.9 (2)	O2 ^{iv} —Sm1—C1 ^{iv}	25.90 (10)
C4—O3—Sm1	124.4 (3)	O2—Sm1—C1 ^{iv}	77.28 (10)
O3 ⁱⁱⁱ —Sm1—O3	75.35 (12)	O2 ⁱⁱⁱ —Sm1—C1 ^{iv}	110.46 (10)
O3 ⁱⁱⁱ —Sm1—O3 ^{iv}	75.35 (12)	O1—Sm1—C1 ^{iv}	128.98 (10)
O3—Sm1—O3 ^{iv}	75.35 (12)	O1 ⁱⁱⁱ —Sm1—C1 ^{iv}	95.43 (10)
O3 ⁱⁱⁱ —Sm1—O2 ^{iv}	82.62 (10)	O1 ^{iv} —Sm1—C1 ^{iv}	25.84 (10)
O3—Sm1—O2 ^{iv}	141.85 (10)	C1—Sm1—C1 ^{iv}	103.16 (9)
O3 ^{iv} —Sm1—O2 ^{iv}	128.50 (10)	O3 ⁱⁱⁱ —Sm1—C1 ⁱⁱⁱ	103.10 (11)
O3 ⁱⁱⁱ —Sm1—O2	141.85 (10)	O3—Sm1—C1 ⁱⁱⁱ	77.91 (10)
O3—Sm1—O2	128.50 (10)	O3 ^{iv} —Sm1—C1 ⁱⁱⁱ	152.70 (11)
O3 ^{iv} —Sm1—O2	82.62 (10)	O2 ^{iv} —Sm1—C1 ⁱⁱⁱ	77.28 (10)
O2 ^{iv} —Sm1—O2	87.46 (10)	O2—Sm1—C1 ⁱⁱⁱ	110.46 (10)
O3 ⁱⁱⁱ —Sm1—O2 ⁱⁱⁱ	128.50 (10)	O2 ⁱⁱⁱ —Sm1—C1 ⁱⁱⁱ	25.90 (10)
O3—Sm1—O2 ⁱⁱⁱ	82.62 (10)	O1—Sm1—C1 ⁱⁱⁱ	95.43 (10)
O3 ^{iv} —Sm1—O2 ⁱⁱⁱ	141.85 (10)	O1 ⁱⁱⁱ —Sm1—C1 ⁱⁱⁱ	25.84 (10)
O2 ^{iv} —Sm1—O2 ⁱⁱⁱ	87.46 (10)	O1 ^{iv} —Sm1—C1 ⁱⁱⁱ	128.98 (10)
O2—Sm1—O2 ⁱⁱⁱ	87.46 (10)	C1—Sm1—C1 ⁱⁱⁱ	103.16 (9)
O3 ⁱⁱⁱ —Sm1—O1	142.72 (11)	C1 ^{iv} —Sm1—C1 ⁱⁱⁱ	103.16 (9)
O3—Sm1—O1	77.37 (10)		
Sm1—O2—C1—O1	-5.3 (4)	C1—O1—Sm1—O3 ^{iv}	-96.3 (2)
Sm1—O2—C1—C2	173.3 (3)	C1—O1—Sm1—O2 ^{iv}	31.5 (3)
O1—C1—C2—C3 ⁱ	-76.0 (5)	C1—O1—Sm1—O2	-2.7 (2)
O2—C1—C2—C3 ⁱ	105.3 (4)	C1—O1—Sm1—O2 ⁱⁱⁱ	99.1 (2)
Sm1—C1—C2—C3 ⁱ	172 (2)	C1—O1—Sm1—O1 ⁱⁱⁱ	122.17 (19)
O1—C1—C2—C3	104.2 (4)	C1—O1—Sm1—O1 ^{iv}	-31.0 (3)
O2—C1—C2—C3	-74.4 (5)	C1—O1—Sm1—C1 ^{iv}	-2.6 (3)
Sm1—C1—C2—C3	-8 (3)	C1—O1—Sm1—C1 ⁱⁱⁱ	109.2 (3)
C3 ⁱ —C2—C3—C2 ⁱⁱ	2.2 (7)	O1—C1—Sm1—O3 ⁱⁱⁱ	88.8 (3)
C1—C2—C3—C2 ⁱⁱ	-178.0 (3)	O2—C1—Sm1—O3 ⁱⁱⁱ	-86.3 (3)
C3 ⁱ —C2—C3—I1	-177.81 (18)	C2—C1—Sm1—O3 ⁱⁱⁱ	-156 (2)
C1—C2—C3—I1	2.0 (5)	O1—C1—Sm1—O3	5.5 (3)
O3—C4—N1—C5	179.1 (7)	O2—C1—Sm1—O3	-169.7 (2)
O3—C4—N1—C6	-1.6 (9)	C2—C1—Sm1—O3	120 (2)
O2—C1—O1—Sm1	5.1 (4)	O1—C1—Sm1—O3 ^{iv}	77.1 (2)
C2—C1—O1—Sm1	-173.4 (3)	O2—C1—Sm1—O3 ^{iv}	-98.1 (2)
N1—C4—O3—Sm1	-170.0 (4)	C2—C1—Sm1—O3 ^{iv}	-168 (2)

C4—O3—Sm1—O3 ⁱⁱⁱ	33.2 (4)	O1—C1—Sm1—O2 ^{iv}	-156.1 (2)
C4—O3—Sm1—O3 ^{iv}	111.6 (4)	O2—C1—Sm1—O2 ^{iv}	28.8 (2)
C4—O3—Sm1—O2 ^{iv}	-23.6 (5)	C2—C1—Sm1—O2 ^{iv}	-41 (2)
C4—O3—Sm1—O2	179.4 (4)	O1—C1—Sm1—O2	175.1 (4)
C4—O3—Sm1—O2 ⁱⁱⁱ	-99.8 (4)	C2—C1—Sm1—O2	-70 (2)
C4—O3—Sm1—O1	-172.4 (4)	O1—C1—Sm1—O2 ⁱⁱⁱ	-73.7 (2)
C4—O3—Sm1—O1 ⁱⁱⁱ	-47.7 (4)	O2—C1—Sm1—O2 ⁱⁱⁱ	111.1 (3)
C4—O3—Sm1—O1 ^{iv}	67.3 (4)	C2—C1—Sm1—O2 ⁱⁱⁱ	41 (2)
C4—O3—Sm1—C1	-174.9 (4)	O2—C1—Sm1—O1	-175.1 (4)
C4—O3—Sm1—C1 ^{iv}	21.3 (5)	C2—C1—Sm1—O1	115 (2)
C4—O3—Sm1—C1 ⁱⁱⁱ	-74.0 (4)	O1—C1—Sm1—O1 ⁱⁱⁱ	-73.78 (19)
C1—O2—Sm1—O3 ⁱⁱⁱ	132.2 (2)	O2—C1—Sm1—O1 ⁱⁱⁱ	111.1 (2)
C1—O2—Sm1—O3	12.9 (3)	C2—C1—Sm1—O1 ⁱⁱⁱ	41 (2)
C1—O2—Sm1—O3 ^{iv}	77.5 (2)	O1—C1—Sm1—O1 ^{iv}	152.9 (2)
C1—O2—Sm1—O2 ^{iv}	-153.2 (2)	O2—C1—Sm1—O1 ^{iv}	-22.3 (2)
C1—O2—Sm1—O2 ⁱⁱⁱ	-65.6 (3)	C2—C1—Sm1—O1 ^{iv}	-92 (2)
C1—O2—Sm1—O1	2.7 (2)	O1—C1—Sm1—C1 ^{iv}	177.9 (2)
C1—O2—Sm1—O1 ⁱⁱⁱ	-91.8 (3)	O2—C1—Sm1—C1 ^{iv}	2.8 (3)
C1—O2—Sm1—O1 ^{iv}	156.6 (2)	C2—C1—Sm1—C1 ^{iv}	-67 (2)
C1—O2—Sm1—C1 ^{iv}	-177.2 (3)	O1—C1—Sm1—C1 ⁱⁱⁱ	-75.0 (3)
C1—O2—Sm1—C1 ⁱⁱⁱ	-77.76 (18)	O2—C1—Sm1—C1 ⁱⁱⁱ	109.90 (18)
C1—O1—Sm1—O3 ⁱⁱⁱ	-130.8 (2)	C2—C1—Sm1—C1 ⁱⁱⁱ	40 (2)
C1—O1—Sm1—O3	-174.6 (3)		

Symmetry codes: (i) $-y+1/2, -z, x-1/2$; (ii) $z+1/2, -x+1/2, -y$; (iii) $-z+3/2, -x+1, y+1/2$; (iv) $-y+1, z-1/2, -x+3/2$.