Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Poly[[hexaaqua(μ_2-fumarato-$\kappa^4O^1,O^{1'}:O^4,O^{4'}$)bis($\mu_3$-maleato-$\kappa^4O^1,O^{1'}:O^4:O^{4'}$)disamarium(III)] hexahydrate]

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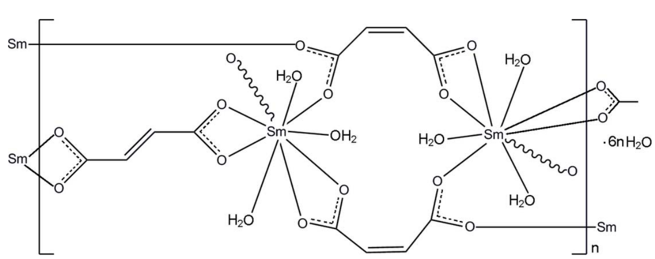
Received 5 October 2010; accepted 4 November 2010

Key indicators: single-crystal X-ray study; T = 290 K; mean σ(C–C) = 0.006 Å; R factor = 0.017; wR factor = 0.066; data-to-parameter ratio = 17.9.

In the title coordination polymer, {[$Sm_2(C_4H_2O_4)_3(H_2O)_6$]·6$H_2O$}$_n$, the Sm^{III} ion is nine-coordinated by four O atoms from three different maleate ligands, two O atoms from one fumarate ligand and three O atoms from three water molecules. The fumarate ligand lies on an inversion center. Adjacent Sm^{III} ions are bridged by the maleate and fumarate ligands, forming a layer parallel to (011). The layers are further linked by intermolecular O—H···O hydrogen bonds into a three-dimensional supramolecular network.

Related literature

For the structures of transition metal complexes with malonate ligands, see: Li *et al.* (2006); Ye *et al.* (2007); Zhu *et al.* (2007). For a related structure, see: Hansson & Thörnqwist (1975).



Experimental

Crystal data

[$Sm_2(C_4H_2O_4)_3(H_2O)_6$]·6$H_2O$
M_r = 859.08
Triclinic, $P\bar{1}$
a = 6.150 (3) Å
b = 10.679 (6) Å
c = 11.214 (6) Å
α = 69.99 (3)°
β = 79.64 (2)°
γ = 89.74 (2)°
V = 679.4 (6) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 4.38 mm^{-1}
T = 290 K
0.08 × 0.07 × 0.06 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.732, T_{max} = 0.782
6707 measured reflections
3071 independent reflections
2950 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.017
$wR(F^2)$ = 0.066
S = 1.00
3071 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7B···O6^{i}	0.85	1.88	2.680 (4)	156
O7—H7A···O11^{ii}	0.85	1.95	2.774 (5)	164
O8—H8A···O11^{iii}	0.85	1.94	2.770 (5)	164
O8—H8B···O10^{ii}	0.85	1.97	2.792 (5)	164
O9—H9A···O7^{iv}	0.85	2.10	2.893 (4)	155
O9—H9B···O3^{iv}	0.85	1.97	2.808 (4)	168
O10—H10A···O1^{v}	0.85	1.97	2.783 (4)	160
O10—H10B···O12	0.85	1.95	2.761 (5)	159
O11—H11B···O12	0.85	1.93	2.775 (5)	171
O11—H11A···O10^{iv}	0.85	1.95	2.755 (5)	157
O12—H12A···O4^{vi}	0.85	1.87	2.705 (5)	168
O12—H12B···O5^{ii}	0.89	1.98	2.744 (5)	142

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *PLATON* (Spek, 2009).

This work was supported financially by the National Basic Research Program of China (grant No. 2007CB808003) and the National Natural Science Foundation of China (grant Nos. 20973082, 20921003, 20703019).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2363).

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supplementary materials

Acta Cryst. (2010). E**66**, m1540 [**doi:10.1107/S1600536810045204**]

Poly[[hexaaqua(μ_2-fumarato-$\kappa^4O^1,O^{1'}:O^4,O^{4'}$)bis($\mu_3$-maleato-$\kappa^4O^1,O^{1'}:O^4:O^{4'}$)disamarium(III)] hexahydrate]

B. Li and **L.-X. Wu**

Comment

Diacids have been widely used to form metal–organic frameworks. Recently, we reported several compounds based on malonate ligand and different transition metal ions (Li *et al.*, 2006; Ye *et al.*, 2007; Zhu *et al.*, 2007). Hererin, we report the crystal structure of the title compound based on maleate ligand.

The structure of the title compound is shown in Fig. 1. The bond lengths and angles are normal and comparable with those reported for a similar structure (Hansson & Thörnqwist, 1975). The Sm^{III} ion is nine-coordinated by four O atoms from three maleate ligands, two O atoms from one fumarate ligand and three coordinated water molecules. The two carboxylate groups of the fumarate ligand and one of the carboxylate groups of the maleate ligand exhibit a chelating coordination mode, while the other carboxylate group of the maleate ligand binds Sm^{III} ions in a bidentate bridging mode. Adjacent Sm^{III} ions are bridged by the maleate and fumarate ligands, forming a layer parallel to (0 1 1) (Fig. 2). Additionally, abundant O—H···O hydrogen bonds stabilize the crystal structure of the title compound (Table 1).

Experimental

Maleic acid and $Sm(NO_3)_3$ of analytical grade are used without further purification. $Sm(NO_3)_3$ (67.24 mg, 0.2 mmol) and maleic acid (69.64 mg, 0.6 mmol) were dissolved in water (10 ml), and the pH value was adjusted to about 3 using a dilute NaOH solution. The mixture was stirred for half an hour and then filtered. The filtrate was allowed to stand at room temperature for two weeks, giving colorless block-shaped crystals.

Refinement

C-bound H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding atoms, with $U_{iso}(H) = 1.2\ U_{eq}(C)$. H atoms of the water molecules were initially located in a difference Fourier map, but were idealized and refined as riding atoms, with O—H = 0.85 Å and $U_{iso}(H) = 1.5U_{eq}(O)$.

Figures

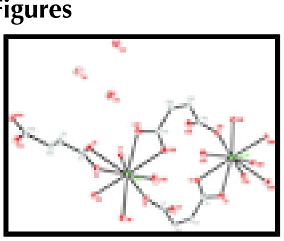

Fig. 1. The asymmetric unit of the title compound, with the symmetry-related atoms to complete the Sm coordination. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry codes: (A) -*x*, 1-*y*, 1-*z*; (B) 2-*x*, 2-*y*, -*z*; (C) 1+*x*, *y*, *z*; (D) 1-*x*, 2-*y*, -*z*.]

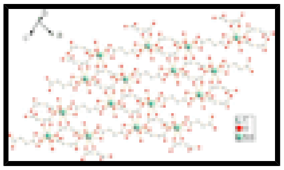
Fig. 2. Crystal packing diagram of the title cmopound, showing the two-dimensional network.

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Crystal data

$[Sm_2(C_4H_2O_4)_3(H_2O)_6]\cdot6H_2O$	$Z = 1$
$M_r = 859.08$	$F(000) = 418$
Triclinic, $P\overline{1}$	$D_x = 2.100$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 6.150$ (3) Å	Cell parameters from 6497 reflections
$b = 10.679$ (6) Å	$\theta = 3.3$–27.5°
$c = 11.214$ (6) Å	$\mu = 4.38$ mm^{-1}
$\alpha = 69.99$ (3)°	$T = 290$ K
$\beta = 79.64$ (2)°	Block, colorless
$\gamma = 89.74$ (2)°	0.08 × 0.07 × 0.06 mm
$V = 679.4$ (6) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	3071 independent reflections
Radiation source: rotation anode	2950 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.018$
ω scans	$\theta_{max} = 27.5°$, $\theta_{min} = 3.3°$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$h = -7\rightarrow7$
$T_{min} = 0.732$, $T_{max} = 0.782$	$k = -13\rightarrow13$
6707 measured reflections	$l = -14\rightarrow13$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.017$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.066$	H-atom parameters constrained
$S = 1.00$	$w = 1/[\sigma^2(F_o^2) + (0.0342P)^2 + 3.0041P]$ where $P = (F_o^2 + 2F_c^2)/3$
3071 reflections	$(\Delta/\sigma)_{max} < 0.001$
172 parameters	$\Delta\rho_{max} = 0.58$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.58$ e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
C1	0.6917 (6)	1.1675 (4)	0.0453 (3)	0.0173 (7)
C2	0.7911 (7)	1.3067 (4)	0.0028 (4)	0.0256 (8)
H2	0.7026	1.3681	0.0269	0.031*
C3	0.9922 (7)	1.3525 (4)	−0.0657 (4)	0.0291 (9)
H3	1.0311	1.4423	−0.0853	0.035*
C4	1.1596 (6)	1.2717 (4)	−0.1134 (3)	0.0190 (7)
C5	0.2343 (6)	0.6379 (4)	0.4136 (3)	0.0176 (7)
C6	0.0980 (7)	0.5175 (4)	0.5083 (4)	0.0254 (8)
H6	0.1523	0.4658	0.5807	0.031*
O1	0.6917 (5)	1.0926 (3)	0.1584 (3)	0.0230 (6)
O2	0.6003 (5)	1.1329 (4)	−0.0303 (3)	0.0321 (7)
O3	1.1332 (4)	1.1467 (3)	−0.0770 (3)	0.0211 (5)
O4	1.3316 (5)	1.3327 (3)	−0.1921 (3)	0.0326 (7)
O5	0.4186 (5)	0.6652 (3)	0.4363 (3)	0.0253 (6)
O6	0.1671 (4)	0.7103 (3)	0.3142 (3)	0.0224 (5)
O7	0.8126 (4)	0.8515 (3)	0.3427 (3)	0.0223 (5)
H7B	0.8962	0.7909	0.3325	0.033*
H7A	0.8156	0.8534	0.4176	0.033*
O8	0.3684 (5)	0.9438 (3)	0.4042 (3)	0.0289 (6)
H8A	0.3148	1.0200	0.3882	0.043*
H8B	0.3346	0.9100	0.4861	0.043*
O9	0.1952 (4)	1.0193 (3)	0.1778 (3)	0.0236 (6)
H9A	0.0669	0.9933	0.2236	0.035*
H9B	0.1633	1.0477	0.1027	0.035*
O10	0.8053 (6)	0.1975 (3)	0.3360 (3)	0.0339 (7)
H10A	0.7981	0.1545	0.2853	0.051*
H10B	0.7485	0.2727	0.3128	0.051*
O11	0.2212 (5)	0.1916 (3)	0.3961 (3)	0.0322 (7)
H11B	0.3085	0.2599	0.3771	0.048*
H11A	0.1137	0.2035	0.3560	0.048*
O12	0.5308 (6)	0.4066 (3)	0.3112 (3)	0.0384 (8)
H12A	0.5696	0.4872	0.2639	0.058*
H12B	0.5062	0.4142	0.3894	0.058*
Sm1	0.50414 (3)	0.869449 (17)	0.223642 (16)	0.01447 (7)

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0152 (16)	0.0201 (17)	0.0163 (16)	0.0006 (13)	0.0001 (12)	−0.0074 (13)
C2	0.028 (2)	0.0164 (17)	0.029 (2)	0.0044 (15)	0.0018 (16)	−0.0079 (15)
C3	0.035 (2)	0.0138 (17)	0.033 (2)	−0.0033 (15)	0.0089 (17)	−0.0089 (16)
C4	0.0210 (17)	0.0184 (16)	0.0152 (16)	−0.0009 (14)	−0.0014 (13)	−0.0038 (13)
C5	0.0164 (16)	0.0167 (16)	0.0163 (16)	0.0012 (13)	−0.0015 (13)	−0.0023 (13)
C6	0.0252 (19)	0.0207 (18)	0.0224 (18)	−0.0066 (15)	0.0005 (15)	0.0002 (15)

O1	0.0281 (14)	0.0196 (13)	0.0172 (12)	−0.0039 (11)	−0.0035 (11)	−0.0013 (10)
O2	0.0257 (15)	0.051 (2)	0.0247 (15)	−0.0029 (14)	−0.0051 (12)	−0.0194 (14)
O3	0.0207 (13)	0.0153 (12)	0.0247 (13)	−0.0003 (10)	−0.0003 (10)	−0.0055 (10)
O4	0.0282 (15)	0.0187 (14)	0.0409 (18)	−0.0034 (12)	0.0135 (13)	−0.0076 (13)
O5	0.0186 (13)	0.0246 (14)	0.0274 (14)	−0.0048 (11)	−0.0072 (11)	−0.0006 (11)
O6	0.0169 (12)	0.0215 (13)	0.0219 (13)	−0.0008 (10)	−0.0043 (10)	0.0017 (10)
O7	0.0154 (12)	0.0271 (14)	0.0234 (13)	0.0044 (10)	−0.0063 (10)	−0.0062 (11)
O8	0.0423 (17)	0.0262 (15)	0.0168 (13)	0.0084 (13)	−0.0019 (12)	−0.0074 (11)
O9	0.0168 (12)	0.0270 (14)	0.0216 (13)	0.0030 (11)	−0.0029 (10)	−0.0021 (11)
O10	0.0396 (18)	0.0385 (18)	0.0292 (16)	0.0048 (14)	−0.0105 (13)	−0.0168 (14)
O11	0.0342 (17)	0.0299 (16)	0.0337 (16)	0.0009 (13)	−0.0113 (13)	−0.0101 (13)
O12	0.051 (2)	0.0229 (15)	0.0373 (18)	−0.0064 (14)	−0.0083 (15)	−0.0057 (13)
Sm1	0.01201 (10)	0.01535 (10)	0.01502 (10)	−0.00140 (6)	−0.00158 (6)	−0.00444 (7)

Geometric parameters (Å, °)

C1—O1	1.247 (5)	O9—H9A	0.8500
C1—O2	1.249 (5)	O9—H9B	0.8500
C1—C2	1.493 (5)	O10—H10A	0.8500
C2—C3	1.328 (6)	O10—H10B	0.8501
C2—H2	0.9300	O11—H11B	0.8500
C3—C4	1.484 (5)	O11—H11A	0.8500
C3—H3	0.9300	O12—H12A	0.8500
C4—O3	1.256 (5)	O12—H12B	0.8944
C4—O4	1.265 (5)	Sm1—O1	2.464 (3)
C5—O6	1.258 (5)	Sm1—O2^{ii}	2.377 (3)
C5—O5	1.262 (5)	Sm1—O3^{iii}	2.566 (3)
C5—C6	1.496 (5)	Sm1—O4^{iii}	2.486 (3)
C6—C6^{i}	1.327 (8)	Sm1—O5	2.593 (3)
C6—H6	0.9300	Sm1—O6	2.512 (3)
O7—H7B	0.8500	Sm1—O7	2.480 (3)
O7—H7A	0.8499	Sm1—O8	2.432 (3)
O8—H8A	0.8500	Sm1—O9	2.489 (3)
O8—H8B	0.8500		
O1—C1—O2	122.4 (4)	O2^{ii}—Sm1—O7	145.71 (10)
O1—C1—C2	118.2 (3)	O8—Sm1—O7	73.67 (10)
O2—C1—C2	119.2 (4)	O1—Sm1—O7	71.50 (10)
C3—C2—C1	127.1 (4)	O2^{ii}—Sm1—O4^{iii}	76.01 (12)
C3—C2—H2	116.4	O8—Sm1—O4^{iii}	137.15 (11)
C1—C2—H2	116.4	O1—Sm1—O4^{iii}	126.86 (10)
C2—C3—C4	125.2 (4)	O7—Sm1—O4^{iii}	80.70 (11)
C2—C3—H3	117.4	O2^{ii}—Sm1—O9	71.17 (11)
C4—C3—H3	117.4	O8—Sm1—O9	69.13 (10)
O3—C4—O4	120.7 (3)	O1—Sm1—O9	77.68 (10)
O3—C4—C3	121.5 (3)	O7—Sm1—O9	136.11 (10)
O4—C4—C3	117.7 (3)	O4^{iii}—Sm1—O9	143.16 (11)

O3—C4—Sm1^{iii}	62.2 (2)	O2^{ii}—Sm1—O6	79.19 (10)
O4—C4—Sm1^{iii}	58.6 (2)	O8—Sm1—O6	84.11 (11)
C3—C4—Sm1^{iii}	175.8 (3)	O1—Sm1—O6	152.27 (10)
O6—C5—O5	120.8 (3)	O7—Sm1—O6	121.53 (9)
O6—C5—C6	121.1 (3)	O4^{iii}—Sm1—O6	80.77 (10)
O5—C5—C6	118.1 (3)	O9—Sm1—O6	77.11 (10)
C6^{i}—C6—C5	121.8 (5)	O2^{ii}—Sm1—O3^{iii}	74.78 (10)
C6^{i}—C6—H6	119.1	O8—Sm1—O3^{iii}	140.72 (10)
C5—C6—H6	119.1	O1—Sm1—O3^{iii}	76.69 (9)
C1—O1—Sm1	115.9 (2)	O7—Sm1—O3^{iii}	71.03 (10)
C1—O2—Sm1^{ii}	161.0 (3)	O4^{iii}—Sm1—O3^{iii}	51.38 (9)
C4—O3—Sm1^{iii}	92.2 (2)	O9—Sm1—O3^{iii}	130.71 (9)
C4—O4—Sm1^{iii}	95.7 (2)	O6—Sm1—O3^{iii}	129.48 (9)
C5—O5—Sm1	92.2 (2)	O2^{ii}—Sm1—O5	121.78 (11)
C5—O6—Sm1	96.1 (2)	O8—Sm1—O5	70.25 (11)
Sm1—O7—H7B	110.4	O1—Sm1—O5	134.92 (9)
Sm1—O7—H7A	131.5	O7—Sm1—O5	70.75 (9)
H7B—O7—H7A	106.8	O4^{iii}—Sm1—O5	69.11 (11)
Sm1—O8—H8A	118.2	O9—Sm1—O5	115.51 (9)
Sm1—O8—H8B	137.9	O6—Sm1—O5	50.82 (9)
H8A—O8—H8B	102.8	O3^{iii}—Sm1—O5	112.47 (9)
Sm1—O9—H9A	118.7	O2^{ii}—Sm1—C4^{iii}	74.35 (11)
Sm1—O9—H9B	120.7	O8—Sm1—C4^{iii}	146.16 (11)
H9A—O9—H9B	100.2	O1—Sm1—C4^{iii}	101.68 (11)
H10A—O10—H10B	113.0	O7—Sm1—C4^{iii}	73.74 (10)
H11B—O11—H11A	115.2	O4^{iii}—Sm1—C4^{iii}	25.73 (10)
H12A—O12—H12B	100.4	O9—Sm1—C4^{iii}	144.26 (10)
O2^{ii}—Sm1—O8	139.41 (11)	O6—Sm1—C4^{iii}	105.51 (11)
O2^{ii}—Sm1—O1	103.29 (11)	O3^{iii}—Sm1—C4^{iii}	25.66 (9)
O8—Sm1—O1	76.25 (10)	O5—Sm1—C4^{iii}	90.53 (11)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H7B···O6^{iv}	0.85	1.88	2.680 (4)	156
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O11—H11B···O12	0.85	1.93	2.775 (5)	171
O11—H11A···O10^{vii}	0.85	1.95	2.755 (5)	157
O12—H12A···O4^{iii}	0.85	1.87	2.705 (5)	168
O12—H12B···O5^{v}	0.89	1.98	2.744 (5)	142

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

Fig. 1

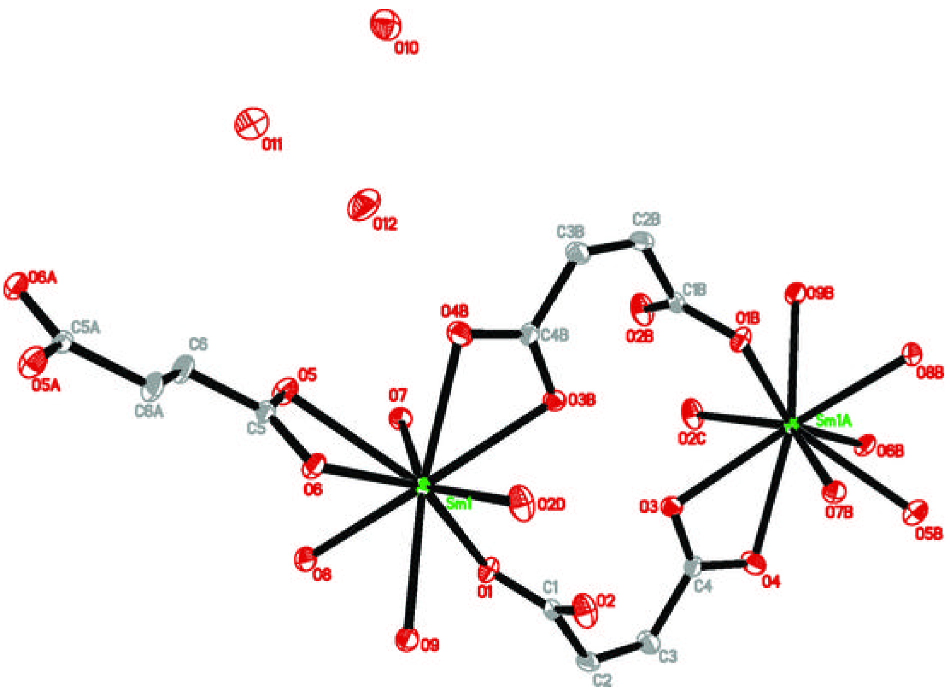
O10
O11
O12
O6A
C5A
O5A
C6A
C6
C5
O5
O6
O7
O4B
C4B
O3B
C3B
C2B
C1B
O2B
O1B
O9B
O8B
Sm1A
O2C
O6B
O7B
O5B
O3
O4
C4
C3
C2
C1
O2
O1
Sm1
O2D
O8
O9

Fig. 2