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Poly[diaqua(μ_6-benzene-1,2,4,5-tetracarboxylato)-(μ_6-2,5-dicarboxybenzene-1,4-dicarboxylato)-disamarium]

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Key indicators

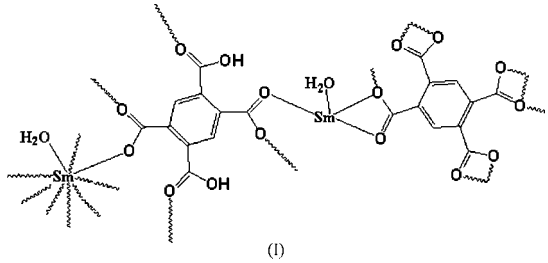
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.010 Å
R factor = 0.032
wR factor = 0.081
Data-to-parameter ratio = 9.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $[Sm_2(C_{10}H_2O_8)(C_{10}H_4O_8)(H_2O)_2]_n$ or $[Sm_2(btec)(H_2btec)(H_2O)_2]_n$, was synthesized hydrothermally by the reaction of Sm_2O_3 with 1,2,4,5-benzenetetracarboxylic acid (H_4btec). The Sm atom is coordinated by nine O atoms, three from H_2btec^{2-}, five from $btec^{4-}$ and one from a coordinated water molecule. Sm—O distances range from 2.376 (3) to 2.558 (5) Å.

Comment

Recently, the construction of supramolecular architectures has received much attention owing to their intriguing structural features and properties as new classes of materials (Fujita *et al.*, 1994, Hagrman *et al.*, 1999). We are interested in using H_4btec (1,2,4,5-benzenetetracarboxylic acid) to construct coordination polymers because of its well established coordination chemistry. We report here the synthesis and crystal structure of the title compound, (I). Two kinds of carboxylate ligands, *viz*. H_2btec^{2-} and $btec^{4-}$, are present in the structure. The Sm atom is coordinated by nine O atoms, three from H_2btec^{2-}, five from $btec^{4-}$ and one from a coordinated water molecule. This leads to the formation of a three-dimensional structure. The compound is isostructural with its neodymium analogue (Sun *et al.*, 2002).



(I)

Experimental

Sm_2O_3 (0.19 g, 0.5 mmol), H_4btec (0.127 g, 0.5 mmol) and 18% HCl (0.5 ml) were mixed in H_2O (10 ml) and heated at 433 K for 3 d in a sealed 25 ml Teflon-lined stainless steel vessel under autogenous pressure. After cooling to room temperature at 5 K h^{-1}, yellow crystals of (I) were isolated, washed with water and dried in air.

Crystal data

$[Sm_2(C_{10}H_2O_8)(C_{10}H_4O_8)(H_2O)_2]$
M_r = 839
Triclinic, $P\overline{1}$
a = 6.3222 (8) Å
b = 9.2626 (11) Å
c = 9.4421 (12) Å
α = 88.316 (2)°
β = 73.963 (2)°
γ = 76.626 (2)°
V = 516.65 (11) Å^3
Z = 1
D_x = 2.697 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2333 reflections
θ = 2.3–25.2°
μ = 5.73 mm^{-1}
T = 293 (2) K
Prism, yellow
0.40 × 0.30 × 0.15 mm

Data collection

Siemens SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.138, T_{max} = 0.423
2737 measured reflections
1846 independent reflections
1734 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 25.2°
$h = -7 \rightarrow 7$
$k = -10 \rightarrow 11$
$l = -11 \rightarrow 6$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.081
S = 1.13
1846 reflections
185 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0335P)^2 + 5.4125P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.27 e Å^{-3}
$\Delta\rho_{min}$ = −1.41 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sm1—O7^{i}	2.313 (5)	Sm1—O2	2.474 (5)
Sm1—O8^{ii}	2.378 (5)	Sm1—O6	2.479 (5)
Sm1—O1*W*	2.384 (5)	Sm1—O1	2.525 (5)
Sm1—O3^{iii}	2.442 (5)	Sm1—O4^{iii}	2.558 (5)
Sm1—O4^{iv}	2.455 (5)		
O7^{i}—Sm1—O8^{ii}	76.05 (18)	O3^{iii}—Sm1—O6	157.56 (17)
O7^{i}—Sm1—O1*W*	139.2 (2)	O4^{iv}—Sm1—O6	86.79 (17)
O8^{ii}—Sm1—O1*W*	66.60 (19)	O2—Sm1—O6	71.21 (16)
O7^{i}—Sm1—O3^{iii}	80.50 (18)	O7^{i}—Sm1—O1	73.66 (18)
O8^{ii}—Sm1—O3^{iii}	72.76 (17)	O8^{ii}—Sm1—O1	136.72 (17)
O1*W*—Sm1—O3^{iii}	102.7 (2)	O1*W*—Sm1—O1	146.62 (19)
O7^{i}—Sm1—O4^{iv}	146.00 (18)	O3^{iii}—Sm1—O1	72.35 (16)
O8^{ii}—Sm1—O4^{iv}	136.90 (17)	O4^{iv}—Sm1—O1	81.04 (17)
O1*W*—Sm1—O4^{iv}	70.57 (19)	O2—Sm1—O1	51.99 (16)
O3^{iii}—Sm1—O4^{iv}	113.20 (16)	O6—Sm1—O1	123.08 (16)
O7^{i}—Sm1—O2	73.30 (19)	O7^{i}—Sm1—O4^{iii}	128.62 (18)
O8^{ii}—Sm1—O2	141.78 (18)	O8^{ii}—Sm1—O4^{iii}	102.63 (17)
O1*W*—Sm1—O2	130.1 (2)	O1*W*—Sm1—O4^{iii}	77.08 (19)
O3^{iii}—Sm1—O2	122.87 (16)	O3^{iii}—Sm1—O4^{iii}	51.85 (16)
O4^{iv}—Sm1—O2	73.28 (17)	O4^{iv}—Sm1—O4^{iii}	62.38 (18)
O7^{i}—Sm1—O6	88.32 (19)	O2—Sm1—O4^{iii}	114.21 (17)
O8^{ii}—Sm1—O6	85.73 (17)	O6—Sm1—O4^{iii}	143.04 (17)
O1*W*—Sm1—O6	73.5 (2)	O1—Sm1—O4^{iii}	74.35 (16)

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O1^{v}	0.82	2.07	2.891 (8)	175
O5—H5*A*···O2	0.90	1.67	2.558 (7)	168

Symmetry code: (v) $-x, -y, -z+2$.

The C-bound H atoms were positioned geometrically and refined as riding on their parent atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The carboxyl H atoms were located in a difference Fourier map and refined isotropically. The maximum and minimum residual electron-density peaks lie 0.92 and 0.93 Å, respectively, from atom Sm1.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART* and *SAINT* (Siemens, 1994); data reduction: *SAINT* and *XPREP* in *SHELXTL* (Siemens, 1994); program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

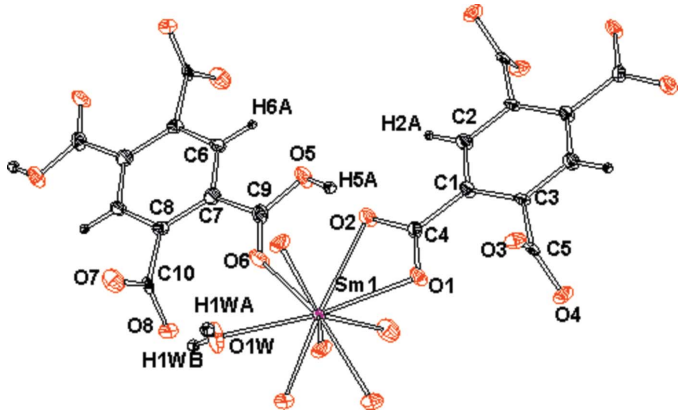


Figure 1
Part of the polymeric structure of the title complex, showing the atom-labelling scheme and with displacement ellipsoids drawn at the 40% probability level.

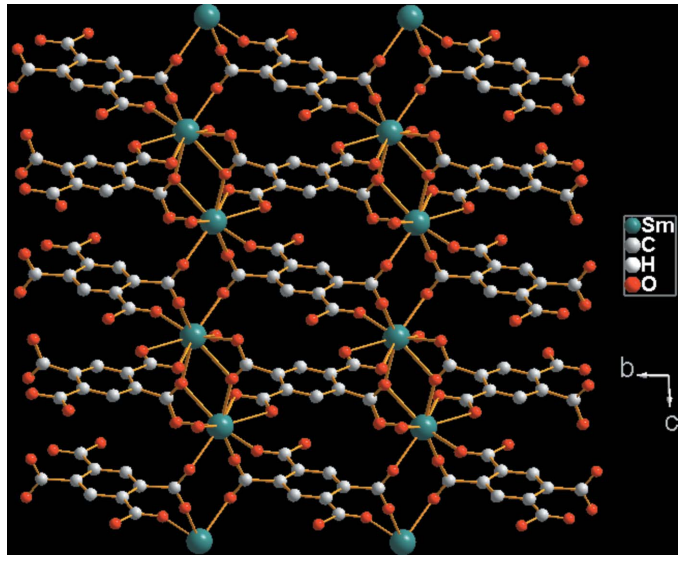


Figure 2
The three-dimensional packing of the title complex. H atoms have been omitted.

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