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Samarium(III) formate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(O–C) = 0.010 Å
R factor = 0.027
wR factor = 0.061
Data-to-parameter ratio = 8.0

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

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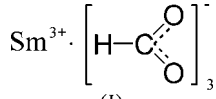
The title compound, poly[samarium(III)-tri-μ-formato], $[Sm(HCO_2)_3]_n$, is isostructural with numerous lanthanide formates and comprises a three-dimensional framework assembled from SmO_9 polyhedra and HCO_2^- anions. The Sm atom lies on a site of 3m symmetry and is coordinated by nine O atoms in a typical coordination geometry. The formate anions lie on mirror planes.

Comment

The title compound, (I), is isostructural with numerous lanthanide formates, including those of La, Ce, Tb, Tm (Bolotovsky *et al.*, 1990) and Gd (Kistaiah *et al.*, 1981), as well as that of the actinide U (Chadha *et al.*, 1980). Unit-cell data have been reported previously for $Sm(HCO_2)_3$ (Mayer *et al.*, 1962), although the compound was described in that case as a fractional hydrate and atomic coordinates were not determined.



(I)

As shown in Fig. 1, the Sm atom lies on a site of 3m symmetry and is coordinated by nine O atoms from the HCO_2^- anions, which lie on mirror planes. The Sm environment has typical geometrical parameters (Table 1). The C—O distances within the anions are 1.235 (16) and 1.259 (16) Å and the O—C—O angle is 125.8 (13)°. Each C atom makes three C—O—Sm linkages through one μ_1-bound O atom (O1) and one μ_2 bridging O atom (O2). Three Sm atoms and three HCO_2^- anions are connected, forming six-membered rings, which are connected by further HCO_2^- anions, generating a three-dimensional framework (Fig. 2). The distance between adjacent Sm atoms is 4.006 (3) Å.

Experimental

Colourless needle-like crystals of the title compound were synthesized hydrothermally from a mixture of Sm_2O_3, HCO_2H, H_2O, tetramethylammonium hydroxide (TMAOH) and dimethylformamide. In a typical synthesis, Sm_2O_3 (0.15 g) was dissolved in a mixed solvent of dimethyl formamide (1.08 g) and water (10.0 g), followed by addition of HCO_2H (0.57 g) and 10% TMAOH (1.08 g) with constant stirring. The mixture was kept in a 25 ml Teflon-lined steel autoclave at 453 K for 10 d. The autoclave was slowly cooled to room temperature, and the product was then filtered, washed with distilled water, and dried at room temperature. Although the final product did not contain TMAOH, this was needed for preparation of the title compound.

Crystal data

$[Sm(HCO_2)_3]$
M_r = 285.40
Trigonal, *R*3*m*
a = 10.503 (3) Å
c = 4.006 (3) Å
V = 382.7 (3) Å^3
Z = 3
D_x = 3.715 Mg m^{-3}
Mo *Kα* radiation
μ = 11.47 mm^{-1}
T = 293 (2) K
Block, colourless
0.06 × 0.04 × 0.04 mm

Data collection

Bruker APEXII CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.546, T_{max} = 0.657
825 measured reflections
201 independent reflections
201 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 29.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.061
S = 1.10
201 reflections
25 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0348P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.007
$\Delta\rho_{max}$ = 1.95 e Å^{-3}
$\Delta\rho_{min}$ = −1.25 e Å^{-3}
Absolute structure: Flack (1983), 69 Friedel pairs
Flack parameter: 0.01 (9)

Table 1
Selected geometric parameters (Å, °).

Sm1—O1	2.409 (10)	Sm1—O2^{ii}	2.529 (9)
Sm1—O2^{i}	2.543 (9)		
O1—Sm1—O1^{iii}	119.93 (2)	O2^{vi}—Sm1—O2^{ii}	64.4 (3)
O1—Sm1—O2^{i}	126.2 (3)	O2^{iv}—Sm1—O2^{v}	144.27 (13)
O1—Sm1—O2^{iv}	129.4 (3)	O2^{ii}—Sm1—O2^{v}	104.3 (3)
O1—Sm1—O2^{v}	71.0 (2)	O2^{v}—Sm1—O2^{vii}	64.0 (3)
O1—Sm1—O2^{ii}	73.3 (2)		

Symmetry codes: (i) $x-\frac{1}{3}, y+\frac{1}{3}, z-\frac{2}{3}$; (ii) $-y+\frac{2}{3}, x-y-\frac{2}{3}, z+\frac{1}{3}$; (iii) $-y+1, x-y, z$; (iv) $x-\frac{1}{3}, y+\frac{1}{3}, z+\frac{1}{3}$; (v) $-y+\frac{2}{3}, x-y-\frac{2}{3}, z-\frac{2}{3}$; (vi) $-x+y+\frac{5}{3}, -x+\frac{4}{3}, z+\frac{1}{3}$; (vii) $-x+y+\frac{5}{3}, -x+\frac{4}{3}, z-\frac{2}{3}$.

The maximum and minimum peaks in the difference density are located at 0.95 and 0.87 Å, respectively, from Sm1. The H atom was located in a difference Fourier map, and refined with an isotropic displacement parameter, with the C1—H1 and O1/O2···H1 distances restrained to be 0.96 (2) and 1.88 (2) Å, respectively.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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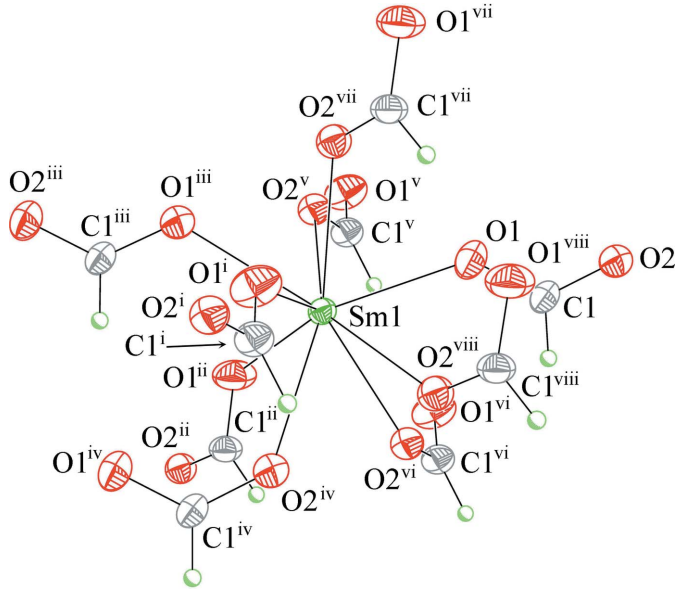

Figure 1
The coordination geometry of Sm1, showing displacement ellipsoids drawn at the 70% probability level. H atoms are shown as spheres of arbitrary radius. [Symmetry codes: (i) $-y+1, x-y, z$; (ii) $-x+y+1, -x+1, z$; (iii) $x-\frac{1}{3}, y+\frac{1}{3}, z-\frac{2}{3}$; (iv) $x-\frac{1}{3}, y+\frac{1}{3}, z+\frac{1}{3}$; (v) $-y+\frac{2}{3}, x-y-\frac{2}{3}, z-\frac{2}{3}$; (vi) $-y+\frac{2}{3}, x-y-\frac{2}{3}, z+\frac{1}{3}$; (vii) $-x+y+\frac{5}{3}, -x+\frac{4}{3}, z-\frac{2}{3}$; (viii) $-x+y+\frac{5}{3}, -x+\frac{4}{3}, z+\frac{1}{3}$.]

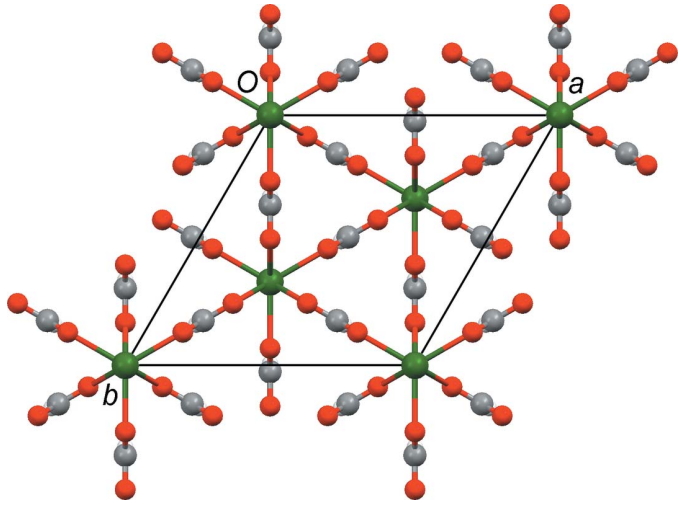

Figure 2
View along the *c* axis, showing the three-dimensional framework with six-membered rings.

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