Crystal structure of disamarium undeca-oxotetratellurate(IV), $\text{Sm}_2\text{Te}_4\text{O}_{11}$

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Abstract

$\text{O}_{11}\text{Sm}_2\text{Te}_4$, monoclinic, $C12/c1$ (no. 15),
 $a = 12.569(1)$ Å, $b = 5.1790(7)$ Å, $c = 16.211(2)$ Å,
 $\beta = 106.040(6)^\circ$, $V = 1014.2$ Å³, $Z = 4$,
 $R_{\text{gt}}(F) = 0.035$, $wR_{\text{ref}}(F^2) = 0.078$, $T = 298$ K.

Source of material

Single crystals of $\text{Sm}_2\text{Te}_4\text{O}_{11}$ were prepared from the reaction of Sm_2O_3 (Kojyundo Kagaku Co. Ltd.) and TeO_2 (Wako Chemical Co. Ltd.). The starting mixture of Sm_2O_3 and TeO_2 with a molar ratio of 1:4 was pressed into a shape of pellet and subsequently heated at 1073 K for two days in an Al_2O_3 crucible.

Discussion

$\text{Sm}_2\text{Te}_4\text{O}_{11}$ is isostructural with $\text{Ln}_2\text{Te}_4\text{O}_{11}$ ($\text{Ln} = \text{La} - \text{Lu}$) [1,2]. Detailed structural features were reported in the single crystal studies for $\text{Pr}_2\text{Te}_4\text{O}_{11}$ [3], $\text{Nd}_2\text{Te}_4\text{O}_{11}$ [4], $\text{Ho}_2\text{Te}_4\text{O}_{11}$ [5] and $\text{Er}_2\text{Te}_4\text{O}_{11}$ [6]. The SmO_8 coordination polyhedron shows a distorted square antiprism, so as to form a polyhedral sheet parallel to the (001) plane. The $\text{Sm}-\text{O}$ distances range from 2.335(5) Å to 2.580(5) Å. The averaged distance of 2.437 Å in the SmO_8 coordination is comparable with those for $\text{Pr}-\text{O}$ (2.473 Å), $\text{Nd}-\text{O}$ (2.460 Å), $\text{Ho}-\text{O}$ (2.379 Å) and $\text{Er}-\text{O}$ (2.364 Å), when the lanthanoid contraction is considered. Te1 is coordinated to three shorter distances of 1.831(4) Å, 1.883(4) Å and 1.996(2) Å and a longer distance at 2.406(5) Å. Similar coordination feature was observed in the Te2 environment with the distances of 1.869(4) Å, 1.870(5) Å, 1.887(5) Å and 2.673(5) Å. The TeO_4 polyhedra are linked by sharing their corners to form the 'lone pair miscell' running parallel to the b axis. The bond valence calculation [7] supports the coordination of Te(IV) in the title compound.

Table 1. Data collection and handling.

Crystal:	pale yellow block, size $0.05 \times 0.05 \times 0.07$ mm
Wavelength:	Mo K_α radiation (0.71069 Å)
μ :	227.96 cm ⁻¹
Diffraction, scan mode:	Rigaku R-Axis RAPID IP, ω/ϕ
$2\theta_{\text{max}}$:	60.9°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	5590, 1538
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2\sigma(I_{\text{obs}})$, 1117
$N(\text{param})_{\text{refined}}$:	79
Programs:	SHELXL-97 [8], ATOMS [9]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sm	8f	0.11878(3)	0.24586(6)	0.53723(2)	0.0068(2)	0.0072(2)	0.0081(2)	0.0000(2)	0.0026(1)	0.0001(1)
Te(1)	8f	0.12052(4)	0.2266(1)	0.20161(3)	0.0084(2)	0.0090(2)	0.0079(2)	-0.0015(2)	0.0009(2)	0.0009(1)
Te(2)	8f	0.37091(3)	0.2792(1)	0.12768(2)	0.0066(2)	0.0073(2)	0.0070(2)	-0.0000(2)	0.0020(2)	-0.0004(1)
O(1)	8f	0.0267(4)	0.0911(9)	0.0995(3)	0.007(2)	0.012(2)	0.011(2)	-0.004(2)	0.001(2)	-0.006(2)
O(2)	8f	0.2061(4)	0.0410(9)	0.4435(3)	0.013(3)	0.011(2)	0.011(2)	-0.006(2)	0.005(2)	-0.008(2)
O(3)	8f	0.2502(4)	0.0646(8)	0.1293(3)	0.010(2)	0.011(2)	0.011(2)	-0.005(2)	0.003(2)	-0.003(2)
O(4)	8f	0.3520(4)	0.0551(9)	0.3290(3)	0.018(3)	0.011(2)	0.007(2)	0.004(2)	0.004(2)	0.000(2)
O(5)	8f	0.4283(4)	0.1185(9)	0.0460(3)	0.009(2)	0.011(2)	0.014(2)	-0.002(2)	0.002(2)	-0.005(2)
O(6)	4e	0	0.351(1)	1/4	0.016(4)	0.016(3)	0.017(3)	0	0.012(3)	0

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