Crystal structure of rubidium samarium dicarbonate, $\text{RbSm}(\text{CO}_3)_2$

I. Kutlu

Universität Hannover, Institut für Anorganische Chemie, Callinstr. 9, D-30167 Hannover, Germany

and G. Meyer

Universität zu Köln, Institut für Anorganische Chemie, Greinstr. 6, D-50939 Köln, Germany

Received August 14, 1997, transferred to 1st update of database ICSD in 1998, CSD-No. 409080

$\text{C}_2\text{O}_6\text{RbSm}$, monoclinic, $C12/c1$ (No. 15), $a = 8.819(1) \text{ \AA}$, $b = 9.336(1) \text{ \AA}$, $c = 7.099(1) \text{ \AA}$, $\beta = 111.51(1)^\circ$, $V = 543.7 \text{ \AA}^3$, $Z = 4$, $R(F) = 0.051$, $R_w(F^2) = 0.116$.

Table 1. Parameters used for the X-ray data collection

Crystal:	pale yellow, irregular, size $0.07 \times 0.1 \times 0.15 \text{ mm}$
Wavelength:	Mo $K\alpha$ radiation ($0.71073 \text{ \AA}$)
μ :	196.55 cm^{-1}
Diffractometer:	Stoe IPDS
Scan mode:	100 exposures, $\Delta\varphi = 1^\circ$
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	56°
$N(hkl)_{\text{unique}}$:	661
Criterion for I_o :	$I_o > 2 \sigma(I_o)$
$N(\text{param})_{\text{refined}}$:	48
Programs:	SHELXS-86, SHELXL-93

Source of material: A mixture of Rb_2CO_3 and $\text{SmCl}_3 \cdot 6\text{H}_2\text{O}$ (molar ratio 2.5:1, about 1 g in total) was added to 6 ml of frozen water in a steel autoclave with an inner volume of 13.5 cm^3 . The rest of the volume of the autoclave was filled with dry ice (solid CO_2 ; approximately 7 g). Single crystals were obtained after 4 weeks at 648 K. As they are insensitive to moisture, the basic mother liquor may be removed with water from the crystals (see ref. 1).

$\text{RbSm}(\text{CO}_3)_2$ crystallizes in the same structure type as, for example, $\text{KDy}(\text{CO}_3)_2$ (see ref. 2). The polyhedra $[\text{Rb}-\mu_1-(\text{CO}_3)_4-\mu_2-(\text{CO}_3)_2]$ and $[\text{Sm}-\mu_1-(\text{CO}_3)_4-\mu_2-(\text{CO}_3)_2]$ with average Rb–O and Sm–O distances of 299.8(8) pm and 238.7(8) pm, respectively, are each connected to zig-zag chains and by further O-ligand atoms of the carbonate ligands in a way that each chain is surrounded by four unlike chains.

Table 2. Final atomic coordinates and displacement parameters (in $\text{\AA}^2$)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Rb(1)	4e	1/2	0.6083(2)	1/4	0.0154(7)	0.0187(8)	0.0220(8)	0	0.0032(6)	0
Sm(1)	4e	0	0.59877(7)	1/4	0.0053(4)	0.0058(4)	0.0068(4)	0	–0.0009(3)	0
C(1)	8f	0.228(1)	0.378(1)	0.248(2)	0.014(5)	0.013(5)	0.026(7)	0.001(4)	0.012(5)	–0.001(4)
O(1)	8f	0.253(1)	0.4782(9)	0.379(1)	0.017(4)	0.023(5)	0.019(4)	0.002(3)	0.000(3)	–0.004(3)
O(2)	8f	0.085(1)	0.3788(9)	0.102(1)	0.014(4)	0.018(4)	0.016(4)	0.001(3)	0.000(3)	0.001(3)
O(3)	8f	0.329(1)	0.281(1)	0.264(2)	0.025(5)	0.026(5)	0.035(5)	0.012(4)	0.004(4)	–0.006(4)

References

1. Kutlu, I.: Komplexe Acetate und Carbonate der Seltenen Erden. Dissertation, Universität Hannover, Germany 1997.
2. Kutlu, I.; Kalz, H.-J.; Wartchow, R.; Ehrhardt, H.; Seidel, H.; Meyer, G.: Kalium-Lanthanoid-Carbonate, $\text{KM}(\text{CO}_3)_2$ (M = Nd, Gd, Dy, Ho, Yb). *Z. Anorg. Allg. Chem.* **623** (1997) 1753–1758.
3. Sheldrick, G. M.: Phase Annealing in SHELX-90: Direct Methods for Large Structures. *Acta Crystallogr. A* **46** (1990) 467–473.
4. Sheldrick, G. M.: SHELXL-93. Program for refining crystal structures. University of Göttingen, Germany 1993.