Crystal structure of rubidium samarium dicarbonate, $RbSm(CO_3)_2$

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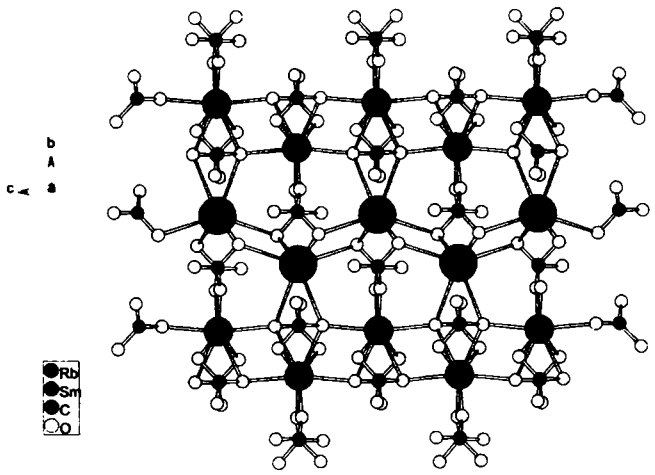

C_2O_6RbSm, monoclinic, $C12/c1$ (No. 15), a =8.819(1) Å, b =9.336(1) Å, c =7.099(1) Å, β =111.51(1)°, V =543.7 Å^3, Z =4, $R(F)$ =0.051, $R_w(F^2)$ =0.116.

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

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

Source of material: A mixture of Rb_2CO_3 and $SmCl_3 \cdot 6H_2O$ (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).

$RbSm(CO_3)_2$ crystallizes in the same structure type as, for example, $KDy(CO_3)_2$ (see ref. 2). The polyhedra [Rb-μ_1-$(CO_3)_4$-μ_2-$(CO_3)_2$] and [Sm-μ_1-$(CO_3)_4$-μ_2-$(CO_3)_2$] 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-ligator atoms of the carbonate ligands in a way that each chain is surrounded by four unlike chains.

References

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Table 2. Final atomic coordinates and displacement parameters (in Å^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)