Crystal structure of caesium gadolinium dicarbonate, $CsGd(CO_3)_2$

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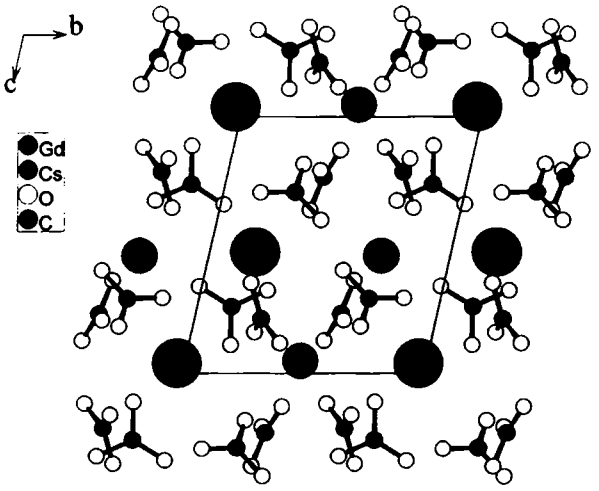

Source of material: A mixture of Cs_2CO_3 and $GdCl_3 \cdot 6H_2O$ (molar ratio 2.5:1, about 1 g in total) was added to 6 ml of frozen water in a steel autoclave with an inner volume of 13.5 cm^3. The rest of the volume of the autoclave was filled with dry ice (solid CO_2; approximately 7 g). Single 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).

$CsGd(CO_3)_2$ crystallizes isostructurally with $CsPr(CO_3)_2$ (see ref. 2) in an ordered derivative structure of the mineral aragonite ($CaCO_3$). The Cs–O and Gd–O polyhedra are irregular. Coordination numbers, distance ranges and mean distances (in pm) are as follows: Cs1: 12 / 295.4(6) – 366.6(6) / 326.4(6); Cs2: 11 / 296.0(6) – 351.4(6) / 322.9(6); Gd1: 9 / 234.2(6) – 259.6(6) / 247.8(6); Gd2: 8 / 233.3(6) – 250.1(6) / 241.3(6).

C_2CsGdO_6, triclinic, $P\bar{1}$ (No. 2), a =8.453(2) Å, b =8.778(2) Å, c =8.779(2) Å, α =98.62(2)°, β =96.58(2)°, γ =115.30(2)°, V =570.5 $Å^3$, Z =4, $R(F)$ =0.037, $R_w(F^2)$ =0.091.

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

Crystal:	colorless, irregular, size 0.7 x 0.1 x 0.12 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	178.76 cm^{-1}
Diffractometer:	Stoe IPDS
Scan mode:	100 exposures, $\Delta\varphi = 1°$
$T_{measurement}$:	293 K
$2\theta_{max}$:	56.2°
$N(hkl)_{unique}$:	2558
Criterion for I_o:	$I_o > 2\,\sigma(I_o)$
$N(param)_{refined}$:	182
Programs:	SHELXS-86, SHELXL-93

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}
Gd(1)	2*i*	0.26104(5)	0.52195(5)	0.04854(4)	0.0057(2)	0.0099(2)	0.0064(2)	0.0026(2)	0.0029(2)	0.0020(2)
Gd(2)	2*i*	0.24185(5)	0.71362(5)	0.54156(4)	0.0056(2)	0.0093(2)	0.0060(2)	0.0019(2)	0.0024(2)	0.0018(2)
Cs(1)	2*i*	0.24276(7)	0.03044(7)	0.03970(6)	0.0135(3)	0.0161(3)	0.0158(3)	0.0046(2)	0.0042(3)	0.0042(2)
Cs(2)	2*i*	0.23930(7)	0.18780(8)	0.52709(7)	0.0108(3)	0.0213(3)	0.0175(3)	0.0080(3)	0.0037(3)	0.0054(2)
O(1)	2*i*	0.5050(8)	0.4433(8)	0.1281(7)	0.015(3)	0.022(3)	0.010(3)	0.009(3)	0.005(3)	0.009(3)
O(2)	2*i*	0.7232(8)	0.3809(8)	0.2071(7)	0.011(3)	0.022(3)	0.013(3)	0.007(3)	0.006(3)	0.005(3)
O(3)	2*i*	0.4645(8)	0.6254(9)	0.6383(7)	0.013(3)	0.031(4)	0.015(3)	0.009(3)	0.007(3)	0.011(3)
O(4)	2*i*	0.0475(8)	0.6255(8)	0.1169(7)	0.008(3)	0.022(3)	0.011(3)	0.008(3)	0.005(3)	0.001(2)
O(5)	2*i*	0.1349(8)	0.2592(8)	0.8393(7)	0.012(3)	0.021(3)	0.008(3)	0.010(3)	–0.002(3)	0.000(2)
O(6)	2*i*	0.0939(8)	0.8011(8)	0.3521(6)	0.009(3)	0.019(3)	0.005(3)	0.006(3)	–0.002(3)	–0.004(2)
O(7)	2*i*	0.6084(8)	0.2750(8)	0.6764(7)	0.009(3)	0.012(3)	0.013(3)	0.002(2)	0.004(3)	0.006(2)
O(8)	2*i*	0.5548(8)	0.1739(8)	0.8896(7)	0.014(3)	0.016(3)	0.011(3)	0.003(3)	0.006(3)	0.003(3)
O(9)	2*i*	0.5275(8)	0.0113(8)	0.3393(7)	0.016(3)	0.019(3)	0.014(3)	–0.001(3)	0.008(3)	–0.001(3)
O(10)	2*i*	0.0647(8)	0.4294(8)	0.4016(7)	0.013(3)	0.015(3)	0.013(3)	0.003(3)	0.007(3)	0.000(2)
O(11)	2*i*	0.1058(8)	0.8472(7)	0.7060(7)	0.012(3)	0.012(3)	0.013(3)	0.001(3)	0.011(3)	0.002(2)
O(12)	2*i*	0.1202(8)	0.3046(8)	0.1822(7)	0.018(3)	0.015(3)	0.015(3)	0.006(3)	0.013(3)	0.007(3)
C(1)	2*i*	0.585(1)	0.400(1)	0.232(1)	0.015(4)	0.010(4)	0.009(4)	0.002(4)	0.007(4)	0.003(3)
C(2)	2*i*	0.005(1)	0.725(1)	0.213(1)	0.012(4)	0.008(4)	0.012(4)	0.003(3)	0.004(4)	0.004(3)
C(3)	2*i*	0.543(1)	0.141(1)	0.740(1)	0.005(4)	0.012(4)	0.009(4)	0.001(3)	–0.002(3)	–0.001(3)
C(4)	2*i*	0.029(1)	0.296(1)	0.291(1)	0.010(4)	0.011(4)	0.012(4)	0.007(3)	0.002(4)	0.004(3)

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