Crystal structure of a new alkaline-cadmium carbonate $Li_2RbCd(CO_3)_2F$, $C_2CdFLi_2O_6Rb$

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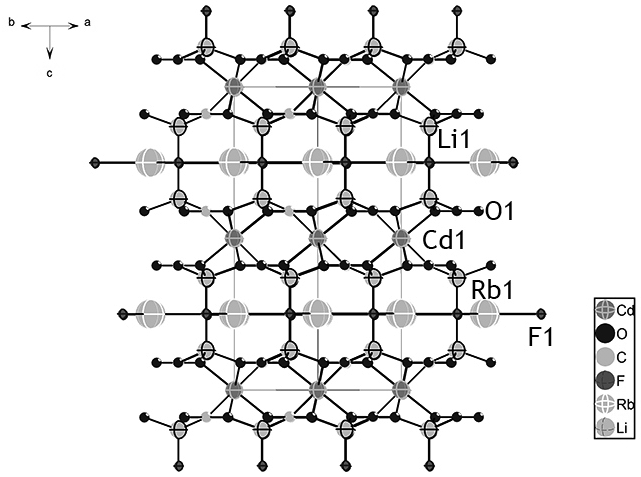

Abstract

$C_2CdFLi_2O_6Rb$, hexagonal, $P6_3/m$ (no. 176), a = 4.915(4) Å, c = 15.45(1) Å, V = 323.3 Å^3, Z = 2, $R_{gt(F)}$ = 0.0242, $wR_{ref(F^2)}$ = 0.0571, T = 293 K.

Table 1. Data collection and handling.

Crystal:	colourless prisms, size 0.10×0.10×0.10 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	108.59 cm^{-1}
Diffractometer, scan mode:	Mercury70 (2x2 bin mode), CCD Profile fitting
$2\theta_{max}$:	54.8°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	2332, 258
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 233
$N(param)_{refined}$:	22
Programs:	SHELX [7], PLATON [8]

Source of material

Single crystal of $Li_2RbCd(CO_3)_2F$ was synthesized under a subcritical hydrothermal condition. A mixture of Rb_2CO_3 (4.6 g, 0.02 mol), LiF (0.312 g, 0.012 mol), $CdCl_2{\cdot}5H_2O$ (0.912 g, 0.004 mol), and H_2O (5.0 mL) was sealed in an autoclave equipped with a Teflon liner (23mL) and heated at 493K for 5 days, followed by slow cooling to room temperature at a rate of 3K/h. The reaction product was washed with deionized water and then dried in air. A few colourless prism-shaped crystals of the title compound were obtained.

Experimental details

The structure of $Li_2RbCd(CO_3)_2F$ was solved by the direct methods. Then it was refined by full-matrix least-squares fitting on F^2 by SHELX-97 [7]. All nonhydrogen atoms were refined with anisotropic thermal parameters. The structure was verified using the ADDSYM algorithm from the program PLATON [8], and no higher symmetries were found.

Discussion

Owing to carbonates have potential application to optoelectronic and nonlinear optical devices [1, 2], they have attracted great attention of material scientists in recent years. As a result of intensive studies, many excellent carbonate crystals have been reported, including $ABCO_3F$ (A = K, Rb, Cs; B = Ca, Sr, Ba) [3], $CsNa_5Ca_5(CO_3)_8$, $Na_4La_2(CO_3)_5$ [4], $Na_3RE(CO_3)_3$ (RE = Y, Gd) [5], $Na_8Lu_2(CO_3)_6F_2$ and $Na_3Lu(CO_3)_2F_2$ [6]. It is worth noting that previous researches mainly focus on the alkaline-alkaline earth and alkaline-rare earth carbonate system. However, carbonates possessing a d^{10} cation like Cd^{2+} have rarely been studied. In the present work, the alkaline-cadmium systems were studied by hydrothermal method. As a result, we have obtained a new carbonate, $Li_2RbCd(CO_3)_2F$. The title structure is made up of alternately stacked layers of [$Li(CO_3)$] and [RbF] and all the adjacent [$Li(CO_3)$] are connected by [CdO_6] polyhedral, forming a complicated three-dimensional network. In the structure, all the atoms occupy one crystallographic position, respectively. The lithium atom is surrounded by the one F atom and three O atoms to form [LiO_3F] polyhedra. The cadmium atom is surrounded by six O atoms to form [CdO_6] polyhedra. In addition, the rubidium is connected by three F atoms and six O atoms to form [RbO_6F_3] polyhedra.

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Table 2. 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}
Cd(1)	2*b*	0	0	0	0.0083(2)	0.0083(2)	0.0096(4)	0.0041(1)	0	0
O(1)	12*i*	0.0727(7)	0.4033(6)	0.0900(2)	0.011(1)	0.010(1)	0.018(2)	0.004(1)	0.002(1)	–0.003(1)
C(1)	4*f*	$\frac{1}{3}$	$\frac{2}{3}$	0.0895(4)	0.012(2)	0.012(2)	0.001(3)	0.0057(9)	0	0
F(1)	2*d*	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$	0.019(2)	0.019(2)	0.011(3)	0.0092(9)	0	0
Rb(1)	2*a*	0	0	$\frac{1}{4}$	0.0157(3)	0.0157(3)	0.0128(5)	0.0079(2)	0	0
Li(1)	4*f*	$\frac{2}{3}$	$\frac{1}{3}$	0.1306(8)	0.006(3)	0.006(3)	0.018(6)	0.003(2)	0	0

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