Crystal structure of a new alkaline-cadmium carbonate Li$_2$RbCd(CO$_3$)$_2$F, C$_2$CdFLi$_2$O$_6$Rb

Jie Chen$^1$, Min Luo$^*$, II and Ning Ye$^{II}$

$^1$ College of Civil Engineering, Fujian University of Technology, Fuzhou 350108, Fujian Province, P. R. China
$^2$ Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, 155 W. Yangqiao Rd., Fuzhou 350002, Fujian Province, P. R. China

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Abstract

C$_2$CdFLi$_2$O$_6$Rb, 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.

Source of material

Single crystal of Li$_2$RbCd(CO$_3$)$_2$F was synthesized under a subcritical hydrothermal condition. A mixture of Rb$_2$CO$_3$ (4.6 g, 0.02 mol), CdCl$_2$·5H$_2$O (0.912 g, 0.004 mol), and H$_2$O (5.0 mL) was sealed in an autoclave equipped with a Teflon liner (23 mL) and heated at 493 K for 5 days, followed by slow cooling to room temperature at a rate of 3 K/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$_2$RbCd(CO$_3$)$_2$F 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$_3$F (A = K, Rb, Cs; B = Ca, Sr, Ba) [3], CsNa$_5$Ca$_5$(CO$_3$)$_8$, Na$_4$La$_2$(CO$_3$)$_5$ [4], Na$_3$RE(CO$_3$)$_3$(RE = Y, Gd) [5], Na$_8$Lu$_2$(CO$_3$)$_6$F$_2$ and Na$_3$Lu(CO$_3$)$_2$F$_2$ [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$_2$RbCd(CO$_3$)$_2$F. The title structure is made up of alternately stacked layers of [Li(CO$_3$)$_2$] and [RbF] and all the adjacent [Li(CO$_3$)$_2$] are connected by [CdO$_6$] polyhedra, 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$_3$F] 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$_6$F$_2$] polyhedra.
Table 2. Atomic coordinates and displacement parameters (in Å²).

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<th>Atom</th>
<th>Site</th>
<th>x</th>
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<th>z</th>
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<td>-0.003(1)</td>
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<td>½</td>
<td>½</td>
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<td>½</td>
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References