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The crystal structure of parisite-(Ce), $Ce_2CaF_2(CO_3)_3$

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ABSTRACT

The crystal structure of parisite–(Ce) was solved and refined to $R = 0.044$, $Rw = 0.037$ using three–dimensional X–ray diffraction data (XRD). In contrast to the putative hexagonal cell, weak XRD maxima on precession films demonstrate that the parisite–(Ce) is monoclinic with a space group *C*2/*c* or *Cc*.

The unit cell was refined as $a = 12.305(2)$, $b = 7.1053(5)$, $c = 28.250(5)$ Å, and $\beta = 98.257(14)°$. The structure refinement confirmed the space group *Cc*. Like bastnäsite and synchysite, parisite possesses a (001) layer structure, with layers of (Ca) and (CeF) separated by layers of carbonate groups. The [001] layer stacking sequence is … (Ca), (CO_3), (CeF), (CO_3), (CeF), (CO_3), (Ca), (CO_3), (CeF), (CO_3), (CeF), (CO_3)….

The parisite-(Ce) structure can be considered as two portions of the bastnäsite structure connected by a (Ca) layer. The insertion of a (Ca) layer would create long [001]* structure voids in the F columns if the bastnäsite portions stacked hexagonally; therefore, the two bastnäsite portions are offset along $[\bar{1}10]$ by $a/6(\sin 60°)$ (or $[\bar{1}00]$ in hexagonal cells, by $a/3$) such that the oxygen atoms of the vertical edges of the carbonate groups occupy the voids. Polytypism results because a bastnäsite portion can shift equally in two possible directions, ±120° from the previous offset vector. The parisite-(Ce) structure elucidated herein is the simplest and most common polytype possible, 2M. The polytype 6R, which was previously believed to be the most common, has not been found during our extensive study.