

LETTER

Crystal structure and Raman spectrum of hydroxyl-bästnasite-(Ce), CeCO₃(OH)

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ABSTRACT

Hydroxyl-bästnasite-(Ce), ideally CeCO₃(OH), had been regarded isostructural with bästnasite-(Ce), CeCO₃F, the dominant member of the bästnasite family that produces ~70% of the world's supply of rare-earth elements. Using single-crystal X-ray diffraction and Raman spectroscopy, our structural analysis on hydroxyl-bästnasite-(Ce) shows that the previous assumption is incorrect. The crystal structure of hydroxyl-bästnasite-(Ce) possesses $P\bar{6}$ symmetry with unit-cell parameters $a = 12.4112(2)$, $c = 9.8511(3)$ Å, and $V = 1314.2(1)$ Å³, in contrast to the space group $P\bar{6}2c$ and $a \approx 7.10$, $c \approx 9.76$ Å, and $V \approx 430$ Å³ for bästnasite-(Ce). Moreover, there are 6, 3, and 5 symmetrically-distinct CO₃ groups, Ce cations, and (OH/F) ions, respectively, in hydroxyl-bästnasite-(Ce), but 1, 1, and 2 in bästnasite-(Ce). The two structures, nevertheless, are similarly characterized by the layers of CO₃ groups alternating with the Ce-(OH/F) layers along the c direction. The Raman spectrum of hydroxyl-bästnasite-(Ce) is dominated by three strong bands at 1080, 1087, and 1098 cm⁻¹ in the CO₃ symmetrical stretching region, along with at least four bands in the OH stretching region. Our study further suggests that natural hydroxyl-bästnasite-(Nd) is most likely isotypic with hydroxyl-bästnasite-(Ce), rather than with bästnasite-(Ce), as previously proposed.

Keywords: Bästnasite, hydroxyl-bästnasite-(Ce), single-crystal X-ray diffraction, crystal structure, Raman spectra