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Heamanite-(Ce), $(K_{0.5}Ce_{0.5})TiO_3$, a new perovskite supergroup mineral found in diamond from Gahcho Kué, Canada

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Abstract

Heamanite-(Ce) (IMA 2020-001), ideally $(K_{0.5}Ce_{0.5})TiO_3$, is a new perovskite-group mineral found as an inclusion in a diamond from the Gahcho Kué mine in the Northwest Territories, Canada. It occurs as brown, translucent single crystals with an average maximum dimension of ~80 μm, associated with rutile and calcite. The luster is adamantine, and the fracture conchoidal. Heamanite-(Ce) is the K-analog of loparite-(Ce), ideally $(NaCe)Ti_2O_6$. The Mohs hardness is estimated to be 5½ by comparison to loparite-(Ce), and the calculated density is 4.73(1) g/cm^3. Electron microprobe wavelength-dispersive spectrometric analysis (average of 34 points) yielded: CaO 10.70, K_2O 7.38, Na_2O 0.16, Ce_2O_3 13.77, La_2O_3 8.22, Pr_2O_3 0.84, Nd_2O_3 1.59, SrO 6.69, BaO 2.96, ThO_2 0.36, PbO 0.15, TiO_2 45.77, Cr_2O_3 0.32, Al_2O_3 0.10, Fe_2O_3 0.09, Nb_2O_5 0.87, UO_3 0.01, total 99.98 wt%. The empirical formula, based on 3 O atoms, is: $[(K_{0.268}Na_{0.009})_{\Sigma 0.277}(Ce_{0.143}La_{0.086}Pr_{0.009}Nd_{0.016})_{\Sigma 0.254}(Ca_{0.326}Sr_{0.110}Ba_{0.033}Pb_{0.001})_{\Sigma 0.470}Th_{0.002}]_{\Sigma 1.003}(Ti_{0.979}Nb_{0.011}Cr_{0.007}Al_{0.003}Fe_{0.002})_{\Sigma 1.002}O_3$. The Goldschmidt tolerance factor for this formula is 1.003. Heamanite-(Ce) is cubic, space group $Pm\bar{3}m$, with unit-cell parameter a = 3.9129(9) Å, and volume V = 59.91(4) Å^3 (Z = 1). The crystal structure was solved using single-crystal X-ray diffraction data and refined to $R_1(F)$ = 2.61%. Heamanite-(Ce) has the aristotypic perovskite structure and adopts the same structure as isolueshite and tausonite. The six strongest diffraction lines are [d_{obs} in angstroms (I in percentages) (hkl)]: 2.764 (100) (110), 1.954 (41) (200), 1.596 (36) (211), 1.045 (16) (321), 1.236 (13) (310), and 1.382 (10) (220). The Raman spectrum of heamanite-(Ce) shows two broad bands at 560 and 787 cm^{-1}, with no bands observed above 1000 cm^{-1}. Heamanite-(Ce) is named after Larry Heaman, a renowned scientist in the field of radiometric dating applied to diamond-bearing kimberlites, mantle-derived eclogites, and lamprophyre dikes. The dominant REE should appear as a Levinson suffix, hence heamanite-(Ce).

Keywords: Heamanite-(Ce), new mineral, perovskite, crystal structure, loparite-(Ce), diamond inclusion, mantle, Gahcho Kué