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The crystal structure of painite $CaZrB[Al_9O_{18}]$ revisited

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Abstract

The crystal structure of the rare hexagonal mineral painite [a = 8.724(1), c = 8.464(2) Å] from Mogok (Myanmar), with the ideal composition $CaZrB[Al_9O_{18}]$, was re-determined by single-crystal X-ray diffraction. Structure refinements were performed in space groups $P6_3/m$ and $P6_3$. The centrosymmetric $P6_3/m$ model yielded excellent agreement (R_1 = 1.44%, 1189 reflections > 2σ I_{obs}, 54 parameters) with the observed diffraction data without any unusual atomic displacement parameters, thus the acentric $P6_3$ model was rejected. A previous structural study claimed that painite was non-centrosymmetric and differed from the related structures of jeremejevite $B_5[\square_3Al_6(OH)_3O_{15}]$ and fluoborite $B_3[Mg_9(F,OH)_9O_9]$ in having lower symmetry.

The structure of painite comprises a framework of AlO_6 octahedra that features two types of channels parallel to the **c** axis. One channel has a trigonal cross-section and is occupied by threefold coordinated B and Zr in sixfold prismatic coordination. The other channel has a hexagonal cross-section and is occupied by Ca. Chemical analysis by laser-ablation inductively-coupled plasma-mass spectrometry indicated that the crystal studied has significant substitution of Na for Ca (ca. 20%) charge-balanced by Ti^{4+} replacing octahedral Al leading to the formula $Ca_{0.77}Na_{0.19}Al_{8.80}Ti_{0.19}Cr_{0.03}V_{0.01}Zr_{0.94}Hf_{0.01}B_{1.06}O_{18}$.