

THE CRYSTAL STRUCTURE OF QINGHEIITE-(Fe²⁺), Na₂Fe²⁺MgAl(PO₄)₃, A NEW MINERAL OF THE WYLLIEITE GROUP

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Qingheiite-(Fe²⁺), ideally Na₂Fe²⁺MgAl(PO₄)₃, is a new mineral species from the Sebastião Cristino pegmatite, Minas Gerais, Brazil (1). Its empirical formula is $(\square_{0.65}\text{Na}_{0.35})(\text{Na}_{0.58}\text{Mn}^{2+}_{0.40}\text{Ca}_{0.02})(\text{Fe}^{2+}_{0.68}\text{Mn}^{2+}_{0.32})(\text{Mg}_{0.72}\text{Fe}^{3+}_{0.23}\text{Fe}^{2+}_{0.05})(\text{Al}_{0.62}\text{Fe}^{3+}_{0.38})[\text{PO}_4]_3$, and the single-crystal unit-cell parameters are $a = 11.910(2)$, $b = 12.383(3)$, $c = 6.372(1)$ Å, $\beta = 114.43(3)^\circ$, $V = 855.6(3)$ Å³, space group $P2_1/n$. Qingheiite-(Fe²⁺) is the Fe²⁺ analogue of qingheiite [Na₂MnMgAl(PO₄)₃], and belongs to the wyllieite group of minerals. The mineral species and name were approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (CNMNC-IMA) under the number 2009-076.

The crystal structure of qingheiite-(Fe²⁺) has been refined, based on single-crystal X-ray diffraction data, to $R_f = 2.91$ %. The basic structural unit is identical to that of other members of the wyllieite group, and consists of kinked chains of edge-sharing octahedra stacked parallel to {101}. These chains are formed by a succession of M(2a)-M(2b) octahedral pairs, linked by highly distorted M(1) octahedra. Equivalent chains are connected in the b direction by the P(1), P(2a) and P(2b) phosphate tetrahedra to form sheets oriented perpendicular to [010]. These interconnected sheets produce channels parallel to c , channels that contain the large X sites. The X(1a) site is a distorted octahedron, whereas the X(1b) site can be described as a very distorted cube. The morphology of the X(2) site corresponds to a very distorted gable disphenoid with a [7 + 1] coordination, similar to the X(2) site of rosemaryite (2) and to the A(2)' site of the alluaudite structure.

The structural features of qingheiite-(Fe²⁺) are compared to those of other wyllieite-type phosphates. In these minerals, Al is generally predominant on the M(2a) site, except in ferrowyllieite where this cation occurs on M(2b) (3). The morphologies and distortion coefficients of the X and M crystallographic sites are also compared among the different minerals of the wyllieite group.

References

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