# Crystal chemistry of the wyllieite group of phosphate minerals

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The wyllieite group of minerals contains Na-Mn-Fe-Mg-Al-bearing phosphates which occur in rare-elements granitic pegmatites; their crystal structure is topologically identical to the alluaudite structure. However, the ordering of cations in wyllieite-type phosphates induces a splitting of the M(2) and X(1) sites of alluaudite into the M(2a) M(2b) and X(1a) X(1b) sites, with a concurrent change of space group from $C2/c$ to $P2_1/n$. Three samples of minerals belonging to the wyllieite group were structurally investigated: wyllieite from the Buranga pegmatite, Rwanda (A), wyllieite from the Malpensata pegmatite, Italy (B), and qingheiite from the Santa Ana pegmatite, Argentina (C). Their crystal structures have been refined, based on single-crystal X-ray diffraction data, to $R_1$ = 2.72 % (A), 3.53 % (B), and 2.46 % (C); unit-cell parameters are: $a$ = 11.954(2), $b$ = 12.439(2), $c$ = 6.406(1) Å, $\beta$ = 114.54(1)° (A); $a$ = 11.983(1), $b$ = 12.423(1), $c$ = 6.381(1) Å, $\beta$ = 114.54(1)° (B); $a$ = 11.878(3), $b$ = 12.448(2), $c$ = 6.438(2) Å, $\beta$ = 114.49(1)° (C). The structure 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 slightly larger 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 A(2)' site of the alluaudite structure. The structural features of these phosphates are compared to those of other wyllieite-type phosphates: ferrorosemaryite, rosemaryite, and qingheiite-(FeII). These new structural data indicate that Al is predominant on the M(2a) site in the investigated samples, with Fe(II), Fe(III) or Mg on the M(2b) site. Variations of unit-cell parameters, of bond distances, and of distortion coefficients among members of the wyllieite group are discussed in detail.

**Keywords:** phosphate minerals, wyllieite group, crystal chemistry