The crystal structure of a new mineral hillite $Ca_2(Zn,Mg)[PO_4]_2 \cdot 2H_2O$.

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Hillite, ideally $Ca_2(Zn,Mg)[PO_4]_2 \cdot 2H_2O$, is the zincian analogue of collinsite. Both hillite and collinsite belongs to the fairfieldite group, which includes phosphates and arsenates with general formula $A_2M[TO_4]_2 \cdot 2H_2O$, where A = Ca, Na, M = Mg, Fe, Zn, Ni, Co, Mn and Cu, T = P, As. The new mineral was found in unmetamorphosed sediments of the Lower Cambrian Parachilna Formation at Reaphook Hill, South Australia. The single crystal of hillite do not exceed 50 μm in length; larger aggregates are inhomogeneous in terms of Zn:Mg ratio. The mineral is greenish and bluish to colourless, brittle with perfect cleavage along {010} and {001}. It is biaxial positive and non-pleochroic; D_{meas}=3.16(2)g/sm^3, D_{calc}=3.178g/sm^3.

The crystal structure of hillite $Ca_2(Zn_{0.62}Mg_{0.38})[PO_4]_2 \cdot 2H_2O$, triclinic, space group $P\bar{1}$, a 5.736(1), b 6.767(2), c 5.462(1)Å, α 97.41(2), β 108.59(2), γ 107.19(2)°, V=186.05(8)Å^3, Z=1, has been determined [automated single-crystal diffractometer, Mo$K\alpha$, graphite monochromator, imaging-plate aria detector system, T=293 K, 2928 reflections, wR$_2$=0.0998 for all 1078 unique reflections, R=0.0378 for 993 observed reflections with $I \geq 2\sigma(I)$]. The refinement of site occupancies showed that Zn and Mg are in the octahedral position at the centre of symmetry in the proportion 0.623(5):0.377(5). The positions of two independent H atoms were obtained from difference-Fourier syntheses and were refined under isotropic approximation. The geometric characteristics of hydrogen bonds are determined, and bond-valence analysis is made. Interatomic distances in hillite structure were analysed and compared with those of other members of the fairfieldite group.

The crystal structure of hillite consists of isolated $MO_4(H_2O)_2$ octahedra, which are connected by orthophosphate tetrahedra to form chains parallel to the c axis. Each tetrahedron shares two vertices with neighbouring octahedral along the chain, whereas the two other oxygen vertices co-ordinate a Ca^{2+} ion. In the a and b directions, these chains are held together by Ca atoms and hydrogen bonds.

According to the geometry of the hydrogen bonds the fairfieldite group of minerals can be divided into two subgroups (fairfieldite and collinsite). We consider the new mineral hillite as a member of the collinsite subgroup.