Synthesis and characterization of a new gallium fluoride hydrogen phosphate

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A new gallium fluoride hydrogen phosphate, \( \text{Ga}_3\text{F}_5(\text{HPO}_4)_2\cdot2\text{H}_2\text{O} \), was synthesized using a hydrothermal method. \( \text{Ga}_3\text{F}_5(\text{HPO}_4)_2\cdot2\text{H}_2\text{O} \) crystallizes in either the chiral space group, \( P4_122 \) or \( P4_322 \). The \( \text{Ga}^{3+} \) cation typically exhibits an octahedral coordination environment with oxide ligands, and the \( \text{PO}_4^{3-} \) anion has a rigid tetrahedral structure. The easy incorporation of fluoride into the framework can change the compositional ratio of the compound and extend band gaps in solid state materials because of its excellent ability to dissolve substances that are poorly soluble in water and its high electronegativity. Single crystal X-ray diffraction analysis reveals that the structure features a three-dimensional (3D) framework composed of 2D layers of corner-sharing \( \text{GaO}_2\text{F}_4 \) and \( \text{GaO}_4\text{F}_2 \) octahedra, which are further bridged by \( \text{PO}_4^3- \) tetrahedra. The isolated \( \text{F}^- \) anion is trapped in a cavity composed of water coordinated to gallium and phosphate groups, in which hydrogen is dislocated. The origin of the chirality of this material comes from the directionality of the hydrogen bonding between the isolated \( \text{F}^- \) anion and the hydrogen-dislocated phosphate groups. Detailed characterizations of the reported material are presented.

Figure 1. Ball-and-stick model of \( \text{Ga}_3\text{F}_5(\text{HPO}_4)_2\cdot2\text{H}_2\text{O} \) in the \( ab \)-plane (cyan, Ga; magenta, P; red, O; green, F; and white, H).