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Structural and vibrational properties of the Cu3Bi(SeO3)2O2Cl francisite at high-pressure

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In the last few decades, low-dimensional magnetic materials have attracted considerable attention in experimental and theoretical studies. They have been found to exhibit physical phenomena such as ferroelectricity, spin liquid, spin ice, and properties inherent to multiferroics. This makes them promising for practical applications in spintronics and quantum computing. Such compounds include materials based on Cu3R(SeO3)2O2X (R is a rare earth element, and X is Cl, Br), which are called francisites. The application of external pressure allows controlled changes in interatomic distances and valence angles in such compounds, which can significantly change their physical properties.

In our work we present the results of the study of the compound Cu3Bi(SeO3)2O2Cl by X-ray diffraction and Raman spectroscopy in a wide pressure range up to ~18 GPa at room temperature. It has found that the original orthorhombic crystal structure with the space group Pmmn is preserved up to 16 GPa. The lattice parameters, bond lengths and bulk modulus have been determined for this crystal structure phase. However, the Raman vibrational mode spectra show significant anomalies around 5 and 10 GPa. These pressure-induced effects can also lead to changes in the magnetic properties of this geometrically frustrated magnetic material.

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