Investigating Infrared Nonlinear Optical Chalcohalides with Distorted Ge3S9 Clusters

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Abstract: Nonlinear optical (NLO) materials in the infrared range are an essential part of the harmonic conversion process to expand the wavelength range of solid state lasers. Current IR NLO materials possess certain drawbacks that make them inefficient to produce high powered IR lasers. Strategies can be employed to design potential IR NLO materials that surpass the current commercial materials, including theoretical study of noncentrosymmetric (NCS) chalcogenides to find potential candidates, and the investigation of Ge3S9 clusters composed of multiple intrinsically distorted GeS4 tetrahedra combined to attempt to produce NCS crystal structures for NLO applications. Incorporation of halogens into sulfide compounds can also increase the band gap of the material and improve laser damage threshold. These strategies are combined and ignite our interest into one IR NLO candidate: KBa4Ge3S10Cl, derived from NaBa4Ge3S10Cl. Preliminary analysis on the compound has been performed, including solid state UV-Vis spectrophotometry to uncover optical properties and powder X-ray diffraction to confirm phase purity and crystal structure. Further investigations will be done on linear and nonlinear optical properties of this compound, as well as investigation into the synthesis of analogues to the compound and other new chalcohalides that incorporate Ge3S9 clusters.

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