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Density functional theory calculation of the optical properties and topological analysis of the electron density of MBi2B 2O7 (M = Ca,Zn) compounds

Abstract

The topology of the electron density for congruent melting oxyborate Bi2ZnOB2O6 and CaBi2B 2O7 is studied in light of the theory of atoms in molecules. All the electron density critical points in the unit cell are systematically calculated. What makes these compounds most interesting is a rich collection of B-O long-distance bond paths. We focus on the study of the asymmetric bonds and basins forming the anisotropic B2O5 groups in these compounds. B2O5 shows transferable contributions to the crystal, with long bond paths. We relate these observations to the strong behavior, which favorites its application to the second harmonic generation field. Wherefore, the analyses of bonding and related optical properties as well as the multipole moments of the CaBi2B 2O7 compounds are predicted for the first time. CaBi 2B2O7exhibits some uniaxial dielectric anisotropy resulting in a strong birefringence. We also report calculations of the complex second-order optical susceptibility dispersion for the principal tensor components and evaluate their intra-and inter-band contributions

Keywords

Atoms in Molecules; Topological analysis; Electron density measurement; Optical properties