

W0422

Chemical Bonding in Pentaerythritol at Very Low Temperature or at High Pressure: An Experimental and Theoretical Study. A.A. Pinkerton, E.A. Zhurova, V.G. Tsirelson, A.I. Stash, V.V. Zhurov, Dept. of Chem., Univ. of Toledo, Toledo, OH 43606; Mendeleev Univ. of Chem. Tech., Moscow, Russia; Karpov' Inst. of Phys. Chem., Moscow, Russia.

Chemical bonding in the pentaerythritol crystal based on the experimental electron density at 15(1)K, and theoretical calculations at the experimental molecular geometries obtained at room and low (15 K) temperatures has been analyzed and compared in terms of the topological analysis. Topological electron-density features corresponding to the high-pressure (1.15 GPa) geometry are also reported. In addition to the bond critical points (CPs) within the molecular layers, CPs between the atoms of different molecular layers have been located, and the bonding character of these relatively weak interactions discussed. Atomic charges and energies have been integrated over the atomic basins delimited by the zero-flux surfaces, and the intermolecular interaction energies have been calculated. The interaction between molecular layers in the crystal becomes stronger both at very low temperature and high pressure, as demonstrated by the more negative intermolecular interaction energies, higher electron density and energy density values at the CPs, and sharper electronic energy density profiles.