Journal of Materials Science, vol.48(10), 2013, pages 3805-3811

Electronic structure, density of electronic states, and the chemical bonding properties of 2,4-dihydroxyl hydrazone crystals ($C_{13}H_{11}N_3O_4$)

Abstract

Electronic crystal structure, bonding properties, and the electron charge densities of 2,4-dihydroxybenzaldehyde-4-nitrophenylhydrazone (2,4-DHNPH,$C_{13}H_{11}N_3O_4$) crystal are theoretically investigated. Calculations are performed with local density approximation; generalized gradient approximation, the Engel-Vosko generalized gradient approximation, and modified Becke-Johnson potential. We present the results of the total and partial (C, N, O, H atoms) density of states. Furthermore, the electronic charge density space distribution contours in the (1 1 0) crystallographic plane, which gives better insight picture of chemical bonding were calculated to understand the effect of hydrogen bonding on the crystal structure of 2,4-DHNP.

Keywords — Bonding property, electronic crystals, hydrogen bonds, crystallographic plane.