A Computational NMR Study of Boron Phosphide Nanotubes

Mahmoud Mirzaei

Young Researchers Club, Islamic Azad University, Shahr-e-Rey Branch, Shahr-e-Rey, Iran

Reprint requests to M. M.; E-mail: mdmirzaei@yahoo.com

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Structural properties of two representative (4,4) armchair and (6,0) zigzag boron phosphide nanotubes (BP-NTs) are studied by density functional theory (DFT) calculations. To this aim, both structures and also the equivalent layer-like structures are individually optimized; afterwards, the boron-11 and phosphorous-31 chemical shielding (CS) tensors are calculated in the optimized structures. The calculated energies indicate that tubular structures are stabilized and the CS tensors are divided into some layers based on equality of electronic properties in the structures. All computations are performed by Gaussian 98 program package.

Key words: Boron Phosphide; Nanotube; Density Functional Theory; Chemical Shielding.