عنوان مقاله:

Theoretical comparison of thermodynamic parameters, NMR analysis, electronic properties of Boron Nitride and Aluminum Nitride nanotubes

محل انتشار:

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خلاصه مقاله:

In this research, geometrical structures of armchair single walled boron nitride nanotube (SWBNNT) and armchair single walled aluminum nitride nanotube (SWAlNNT) were optimized by Density Functional Theory (DFT) in the gas phase, both having the same length of ۵ angstrom and n=۹, m=۹. B۳LYP/۶-۳۱G* level of theory have been used to determine and compare electronic properties, natural charge and chemical shielding tensors of nanotubes. The chemical shielding tensors were calculated using GIAO method to obtain structural information and dynamic behavior for optimal boron nitride and aluminum nitride nanotube structures. Also, thermodynamic functions for the boron nitride nanotube (۹, ۹-۵) and the aluminum nitride nanotube (۹, ۹-۵) in the gas phase were carried out with using the B۳LYP method and ۶-۳۱g* basis set. It is significant that all of NMR parameters and geometrical properties of both nanotubes .were determined in ۵ layers

کلمات کلیدی:

AlNNT, BNNT, Chemical shielding, DFT, Isotropic, Nanotube, NMR