عنوان مقاله:

The effects of F2 adsorption on NMR parameters of undoped and 3C-doped (8, 0) zigzag BPNTs

محل انتشار:

فصلنامه ارتباطات شیمی ایران, دوره 4, شماره 1 (سال: 1394)

تعداد صفحات اصل مقاله: 12

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خلاصه مقاله:

In this research, we studied the structure, properties and NMR parameters of interaction F2 gas with pristine and 3C-doped (8, 0) zigzag models of boron phosphide nanotubes (BPNTs). In order to reach these aims, we considered four different configurations for adsorption of F2gas on the outer and inner surfaces of BPNTs. The structures of all models were optimized by using density functional theory (DFT).The chemical shielding (CS) tensors at the sites of 11B and 31P nuclei were computed from the optimized structures and then the computed chemical shielding tensors were converted to isotropic chemical shielding (CSI) and anisotropic chemical shielding (CSA). Due to the donor electron effects of 3C doped atoms, the chemical shielding isotropic (CSI) of F2 gas on surface of BPNTs was significantly more than pristine models. The results showed that F2 adsorption on surface of nanotube was exothermic and 3C-doped decreased the adsorption energy values. The calculated results proved that the chemical activity of complex BPNTs/F2 has increased and hence the chemical stability of the nanotube has decreased.

کلمات کلیدی:

BPNTs; NMR; F2adsorption; 3C-doped