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THEORETICAL STUDY OF ELECTRONIC AND SPECTRAL PROPERTIES OF BORON NITRIDE AND ALUMINUM BORON NITRIDE NANOTUBES

Mehrnoosh khaleghian[1], F. Azarakhshi[2]

[1]Department of Chemistry, Islamshahr Branch, Islamic Azad University, Islamshahr, Iran

***Corresponding author- E-mail: Mehr_khaleghian@yahoo.com**

[2]Department of Chemistry, Varamin-Pishva Branch, Islamic Azad University, Varamin, Iran

E-mail: **fa_azarakhshi@yahoo.com**

Abstract: In this study, by using computational methods B3LYP 6-31g* and EPR-III, structure of B18N18 and Al6B12N18 optimized with application Gaussian software. The electronic, structural and spectral properties of B18N18 and Al6B12N18 have been examined**.** The results show that by replacing the lighter atoms with heavy atoms (Al) electron energy and dipole moment increases. Using output optimization, calculations Frequencies (FREQ) and Natural Bond Orbital (NBO) done for both structure. Frequencies calculations used to derive thermodynamic results and spectra of NBO calculations to determine the electron density of different levels, energy levels and related parameters such as ionization energy and electron energy, the share of hybrid and hybrid orbitals are performed.

Keywords: NBO, FREQ, B3LYP, EPR.

1. INTRODUCTION

Fullerene compounds as nano-structures that have special properties considered Late Twentieth Century. Boron nitride Fullerenes is also one of the most stable fullerene structures that in recent years due to their inherent capabilities and special properties compared to similar carbon compounds in the fields of scientific and theoretical research has been done on them. Carbon Fullerenes bonds are non-polar, while boron nitride fullerenes due to electronegativity difference between the atoms, are polar bonds and can have an effective interactions. After the discovery of C60 [1], carbon nano structures such as fullerene clusters, nanotubes, nano-capsules, cones and cubes have been reported [1-4]. Boron nitride Nanostructure has a band gap energy of about 6 eV it is expected that different electronic, optical and magnetic properties reveal [4]. Therefore, many studies on BN nanomaterials such as BN nanotubes [4,5], BN nanocapsules [4], BN clusters [3,4] and BN nanoparticles [6,7] have been reported, it is expected that these compounds to be useful for the electronics, semiconductor with high thermal stability and nanowires. The number of BN clusters and BN nano-rings have been studied using theoretical methods.