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(BN)n团簇的结构和稳定性

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摘要 用HF方法、密度泛函理论的B3LYP以及微扰理论的MP2方法，在6—31G(d)基组 水平上，对(BN)n(n=1-16)团簇的各种可能结构进行了优化．讨论了环状与笼状稳 定团簇的几何构型、自然键轨道(NBO）、振动频率、结合能、核独立化学位移 (NICS)和能量二次差分，得到了(BN)n(n＝1-16)团簇结构的稳定性信息．比较了 HF，B3LYP以及MP2三种理论方法对(BN)n团簇的适应性所表现出的差异．

关键词 密度泛函理论 簇状化合物 氮化硼 化学位移

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Structure and Stability of (BN)_n Clusters

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Abstract The structures of(BN)n(n. = l~16) clusters were studied by using Hartree-Fock (HF), B3LYP of density functional theory (DFT) and second order perturbation theory MP2 method with basis set of 6-31G(d). The geometries, natural bond orbital (NBO), electron structures, vibrational spectra, binding energies, nucleus independent chemical shirts (NICS) and energy secondaiy differences of ring and cage structures were discussed at the same level. The relationship between structure and stability was obtained. The results obtained from these three theoretical methods were also compared.

Key words DFT CLUSTER COMPOUND BORON NITRIDE CHEMICAL SHIFT

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