

研究论文

## 杂硼原子簇 $B_6X^-$ ( $X=N, P, As, Sb, Bi$ )稳定性和芳香性研究

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**摘要** 利用Gaussian 98程序, 采用从头算和密度泛函理论方法, 对 $B_6X^-$  ( $X=N, P, As, Sb, Bi$ )杂硼原子簇进行了理论研究, 优化得到了其稳定平衡构型, 讨论了其振动光谱和稳定性等, 通过自然键轨道(NBO)、分子轨道(MO)和核独立化学位移(NICS)分析, 确定这些杂硼原子簇都有离域的 $\pi$ 电子和 $\sigma$ 电子成键轨道, 满足 $4n+2$ 电子规则, 具有芳香性, 与纯 $B_6^-$ 或 $B_6^{2-}$ 原子簇呈反芳香性不同.

**关键词** [杂硼原子簇](#) [从头算](#) [密度泛函理论](#) [芳香性](#)

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## Stability and Aromaticity of $B_6X^-$ ( $X=N, P, As, Sb, Bi$ ) Clusters

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**Abstract** The geometries and chemical bonding of  $B_6X^-$  ( $X=N, P, As, Sb, Bi$ ) clusters have been investigated using *ab initio* and density functional theory computations with MP2, B3LYP and B3PW91 methods. Analytical gradients with the polarized split-valence basis sets (6-311+G\*) were used for B, N, P, and As. The relativistic effective core potential with the LANL2DZ basis set was chosen for Sb and Bi. It is seen that the very reasonable looking pyramidal minimum structure ( $C_{2v}$  symmetry) is the most stable. The analyses of molecular orbital, natural bond orbital, and nucleus-independent chemical shift for these quasi-pyramidal  $B_6X^-$  systems revealed a double-aromatic character ( $\pi$  and  $\sigma$ ), which had been reported to play an important role in the chemical bonding, structure, and stability of the pure boron clusters.

**Key words** [Hetero-polyboron cluster](#) [Ab initio calculation](#) [Density functional theory](#) [Aromaticity](#)

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