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研究论文

C_{30}卡宾三叶结分子结构与稳定性的理论研究

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摘要 三叶结分子是最简单的非平凡纽结分子, C_{30}卡宾三叶结分子是由一条闭合的$(C\equiv C—)_{15}$ sp杂化碳链组成的, 是具有D_3对称性的拓扑手性分子. 本文用密度泛函方法[DFT/RB3LYP/6-31G(D)]对分子结构和光谱性质进行了研究, 在优化构型的基础上通过自然键轨道(NBO)方法和轨道能级研究了它的共轭性、成键情况和稳定性, 并与平面型C_{30}卡宾环分子进行了比较. 计算结果表明三叶结分子的三叶弧上形成了非平面的C≡C共轭和扭曲的内螺旋结构, 交叉处具有弱成键作用, 且分子轨道也发生了扭曲; 三叶结分子比卡宾环的共轭性和赝Jahn-Teller效应都明显小, 而总能量高. 因此, 分子打结是一个能量升高的过程.

关键词 C_{30}卡宾三叶结 C_{30}卡宾环 振动光谱 自然键轨道(NBO) 轨道能级

分类号

Theoretical Studies on the Structure and Stability of C_{30} Carbyne Trefoil Knot

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Abstract The trefoil is known as the simplest nontrivial molecular knot. The C_{30} carbyne trefoil knot studied is intertwined by the sp hybridized $(C\equiv C—)_{15}$ chain, which is topologically chiral and belongs to D_3 point-group of symmetry. Density functional theory (DFT) calculations have been carried on the molecular knot at the RB3LYP/6-31G (D) levels. Based on the optimized geometry, the vibrational spectra, natural bond orbital (NBO) and orbital energy level analysis for C_{30} carbyne trefoil knot have been calculated at the same level, and compared with the cyclo-C_{30} carbyne molecule. The results show that the electronic structure possesses three primary attributes: C≡C nonplanar conjugated structure, inherently helical structure and highly strained crossing bonds, and the molecular orbitals are also twisted. Furthermore, the tied trefoil knot has less conjugation property and Jahn-Teller effect but higher total energy than the cyclo-C_{30} carbyne, that is, the process of “tied” could increase the energy of molecules.

Key words C_{30} carbyne trefoil knot cyclo-C_{30} carbyne vibrational spectrum natural bond orbital (NBO) orbital energy level

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