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论文

双噻唑苯二聚体自由基分子的极化率与二阶超极化率的理论研究

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摘要:

采用量子化学UMP2/6-31G(d,p)方法优化双噻唑苯二聚体自由基分子的几何结构, 以0.05 nm为单位步长拉长与缩短2分子片之间的距离, 选取5个点, 采用DFT UB3LYP/6-31G(d,p)方法, 对双噻唑苯二聚体自由基分子的极化率和二阶超极化率进行理论计算. 结果表明, 自由基体系的单重态为相对稳定状态. 在完全重叠的体系中, 在单、三重态时极化率都随着2分子片间距离的增大而增加; 三重态时二阶超极化率的绝对值随着2分子片间距离的增大而增大. 部分重叠的体系, 单重态时极化率随2分子片距离的增大而减小; 三重态时, 二阶超极化率的绝对值随着2分子片间距离的增大而增大.

关键词: 双噻唑苯二聚体自由基; 二阶超极化率; 分子片间距离

Theoretical Study on the Polarizability and the Second Hyperpolarizability of Benzo-bisdithiazolyl Dimer Radical

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Abstract:

The quantum chemistry UMP2/6-31G(d,p) method was used to optimize the structure of benzo-bisdithiazolyl dimer radical. Furthermore, the DFT UB3LYP/6-31G(d,p) approach was adopted to calculate the polarizability and the second hyperpolarizability of the five pointes of radical in which the interplanar distance was enlarged and shorten by a step of 0.05 nm. According to UMP2 calculations, the radical with singlet state is the stable one. For the vertical-stacking radical, the polarizabilities of the radical with singlet and triplet state increase with increasing the interplanar distance, while only the second hyperpolarizabilities of the radical with triplet state increases with increasing the interplanar distance. For the shifted-stacking radical, the polarizability of the radical with singlet decreases with increasing the interplanar distance, the absolute value of the second hyperpolarizability increases with increasing the interplanar distance for the radical with triplet shifted-stacking radical.

Keywords: Benzo-bisdithiazolyl dimer radical; Second hyperpolarizability; Interplanar distance

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