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论文

1,3-二氮杂蒽类衍生物电子结构和光谱性质的理论研究

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摘要:

对1,3-二氮杂蒽类衍生物采用密度泛函理论(DFT)在B3LYP/6-31G(*d*)的水平上进行了几何构型的全优化, 在此基础上探讨了分子结构和前线分子轨道能量等性质的变化规律, 采用含时密度泛函理论(TD-DFT)计算了分子的电子跃迁性质, 采用二维平面图和三维立体图来直观表示激发态的性质, 研究分子内电子转移特性. 跃迁密度矩阵的二维等高线图反映了电子-空穴相干性, 三维跃迁密度图反映了跃迁偶极矩的方向和强度, 三维电荷差异密度图说明了激发过程中分子内电子转移性质.

关键词: 1,3-二氮杂蒽 分子内电子转移 跃迁密度 电荷差异密度 电子-空穴相干性

Theoretical Studies on Electronic Structures and Spectroscopic Properties of 1,3-Diazaazulene Derivatives

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Abstract:

The geometries of four different kinds of 1,3-diazaazulene derivatives were fully optimized with Density Function Theory(DFT) at B3LYP/6-31G(*d*) level, on basis of which the energies of frontier molecular orbitals and the energy gap were investigated and the electronic transition properties were calculated with time-dependent DFT(TD-DFT) at the same level. The excited-state properties and the intra-molecular charge transfer(ICT) character were investigated with the two-dimensional(2D) and three-dimensional(3D) real space analysis methods. The electron-hole coherence is investigated with 2D contour plots of transition density matrix. The orientation and strengths of absorptive transition dipole moment are obtained by 3D transition density(TD). The ICT orientations are obtained with 3D charge difference density(CDD).

Keywords: 1,3-Diazaazulene derivative Intra-molecular charge transfer Transition density(TD) Charge difference density(CDD) Electron-hole coherence

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