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1,2方酸衍生物非线性光学性质的从头算研究

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摘要 用CPHF方法在abinitio/4-31G+pd水平上计算了四个1,2方酸衍生物分子的线性极化率,一阶和二阶超极化率.从电荷分布,跃迁偶极矩,前沿轨道性质等方面讨论了其结构与性能的关系.研究表明,四元环作为吸电基团(A),取代基作为供电基团(D),组成了D-A-D结构,取代基的性质对分子的非性光学系数有显著影响.

关键词 方酸 从头计算法 光学性质 非线性光学 结构与性能关系

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An ab initio study on nonlinear optical properties of squarates

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Abstract The linear polarizabilities, first and second hyperpolarizabilities of four squarates have been studied at initio/4-31G+pd leved by couple-perturbed Hartree-Fork (CPHF) method. A discussion of the relationships between their structures and properties has been done in terms of charge distributions, transition dipole moments, frontier orbitals, etc.. The calculations show that the squarates consist of the donor-acceptor-donor structures, where the four-membered rings act as electron-donating groups and the substituents as electron- withdrawing groups. Their molecular nonlinear optical susceptibilities strongly depend on the substituted effects.

Key words SQUARIC ACID AB INITIO CALCULATION OPTICAL PROPERTIES NON LINEAR OPTICS STRUCTURE AND PROPERTY CORRELATION

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