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巴比妥酸苯胺取代衍生物二阶非线性光学性质和电子光谱的**INDO/CI**研究

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摘要 利用量子化学密度泛函理论（DFT）B3LYP方法，在6-31G~*基组下对巴比妥酸苯胺取代衍生物体系BA1～BA5进行几何结构优化，以优化后的构型为基础，应用INDO/CI方法进行电子光谱计算，并结合实验数据进行了分析，同时应用完全态求 和（SOS）公式计算二阶非线性光学（NLO）系数β_μ,设计的系列体系中β_μ最 大值可达到65.47×10~(-30) esu。进一步探讨了体系的共轭性和烷基取代基链的长 度对二者的影响，结果表明，体系的共轭程度越高，烷基取代基的链长度越长，体 系β_μ值越大，而λ_max红移。

关键词 巴比妥酸 非线性光学 电子光谱学 密度泛函理论 取代基

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Theoretical Studies on Electronic Spectra and Second-order Nonlinear Optical Properties of Aniline Substituted Barbituric Acid Derivatives

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Abstract The structures of substituted aniline barbituric acid derivatives were optimized with DFT/B3LYP method at 6-31G* basis set. Based on the optimized structures, the electronic spectra were obtained by the INDO/CI method and were also compared with experiment values. The second-order nonlinear optical coefficientsβ_μwere calculated according to the sum-over states (SOS) formula. In addition, the influences of length of alkyl chain and conjugation degree of the designed systems on electronic spectra and second-order nonlinear optical coefficients were investigated. The results indicate that the higher the conjugation degree and the longer the alkyl chain, the largerλ_(max) and β_μ.

Key words barbituric acid NON LINEAR OPTICS ELECTRON SPECTROSCOPY DFT SUBSTITUENT GROUP

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