Chinese Journal of Chemistry 2006 24 (1): 119—123 ISSN: 0567-7351 CN: 31-1320/06

Full Papers

巴比妥酸葡萄糖基取代衍生物电子光谱和二阶非线性光学性质的理论研究

冯静东[1],颜力楷[1],苏忠民*,[a],阚玉和[a,b],兰亚乾[1],廖奕[1],朱玉兰[b,c]

[1]东北师范大学化学学院功能材料化学研究所，长春 130024

[2]淮阴师范学院化学系，江苏省低维材料化学重点建设实验室，淮安 223300

[3]延边大学理工学院化学系，延吉 133002

收稿日期 2004-10-29 修回日期 2005-9-19 网络版发布日期 接受日期

摘要 应用量子化学AM1半经验方法分别对巴比妥酸及硫代巴比妥酸的葡萄糖基系列取代衍生物$\mathbf{B}_{1\text{-}5}$和$\mathbf{T}_{1\text{-}5}$进行几何优化。基于优化后的稳定构型，利用INDO/CI方法计算其电子光谱。同时，根据完全态求和(SOS)公式计算其二阶非线性光学系数。结果显示，当葡萄糖基单元数增加时，无论是巴比妥酸衍生物还是硫代巴比妥酸衍生物，$|\beta_\mu|$均增大，尤其是硫代巴比妥酸衍生物增大更为显著，表明此种非共轭取代基同样可以改善材料的非线性光学性质。此外，随葡萄糖基链增长时，光谱的变化并不十分显著，且由于所有吸收带均在紫外光区内，因此推测所有体系均有望成为具有高度透明性的非线性光学侯选材料。

关键词 AM1,INDO/CI,电子光谱,二阶非线性光学性质

分类号

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

FENG Jing-Dong[1], YAN Li-Kai[1], SU Zhong-Min*,[1], , KAN Yu-He[1,2], LAN Ya-Qian[1], LIAO Yi[1], ZHU Yu-Lan[2,3]

[1] *Institute of Functional Material Chemistry, Faculty of Chemistry, Northeast Normal University, Changchun, Jilin 130024, China*

[2] *Department of Chemistry, Huaiyin Teachers College, Jiangsu Province Key Laboratory for Chemistry of Low-Dimensional Materials, Huaian 223300, China*

[3] *Department of Chemistry, Science and Engineering College, Yanbian University, Yanji, Jilin 133002, China*

Abstract AM1 semi-empirical method was used to optimize the barbituric acid derivatives substituted with glucosyl $\mathbf{B}_{1—5}$ (series **B**), and the thiobarbituric acid derivatives substituted with glucosyl $\mathbf{T}_{1—5}$ (series **T**). Based on the optimized structures, INDO/CI method was adopted to calculate the electronic spectra. Meanwhile, the second-order nonlinear optical (NLO) coefficients β_μ were calculated with the sum-over-state (SOS) formula. The results show that when the number of glucosyl units was increased, $|\beta_\mu|$ values of the barbituric and thiobarbituric acid derivatives were both enhanced, especially for thiobarbituric acid derivatives. It indicates that non-conjugated substituted group could also improve NLO properties of materials when the number of repeated units was increased. Additionally, the absorption bands appearing in UV area are consistent with the proper change of the number of glucosyl units, and consequently it can be concluded that the high transparencies of all systems were scarcely varied.

Key words AM1 INDO/CI electronic spectra second-order nonlinear optical property

DOI:

通讯作者 苏忠民 zmsu@nenu.edu.cn