[1]李雪梅,毛 焱,杨琼芬,等.含乙酰胺基链苯并菲盘状液晶分子的电子光谱与非线性光学性质[J].厦门大学学报(自然科学版),2013,52(05):665.[doi:10.6043/j.issn.0438-0479.2013.05.016]

LI Xue-mei*,MAO Yan,YANG Qiong-fen,et al.Electronic Spectra and Nonlinear Optical Properties of Triphenylene Discotic Liquid Crystals with Acetylamino Chain[J].Journal of Xiamen University(Natu [doi:10.6043/j.issn.0438-0479.2013.05.016]

点击复制

导航/NAVIGATE
本期目录/Table of Contents
下一篇/Next Article
上一篇/Previous Article

工具/TOOLS
引用本文的文章/References
下载 PDF/Download PDF(1964KB)
立即打印本文/Print Now
推荐给朋友/Recommend

含乙酰胺基链苯并菲盘状液晶分子的电子光性质(PDF)

分享到:

《厦门大学学报（自然科学版）》[ISSN:0438-0479/CN:35-1070/N] 卷: 52卷 期数: 2013年05期 页码: 665 栏目: 出版日期: 2013-08-15

Title: Electronic Spectra and Nonlinear Optical Properties of Triphenylene Discotic Liquid Crystals with Acetylamino Chain

作者: 李雪梅; 毛 焱; 杨琼芬; 张建平; 李 权

1.乐山师范学院物理与电子工程学院,四川 乐山 614000; 2.四川师范大学 化学与材料科学学院,先进功能材料四川省高校重点实验室,四川 成都 610066

Author(s): LI Xue-mei[1*]; MAO Yan[2]; YANG Qiong-fen[2]; ZHANG Jian-ping[1]; LI Quan[2]

1.School of Physics and Electronic Engineering,Leshan Normal University,Leshan 614000,China; 2.Key Laboratory of Advanced Functional Materials,Sichuan Province Higher Education System, College of Chemistry and Material Science,Sichuan Normal University,Chengdu 610066,China

关键词: 非线性光学; 含乙酰胺基链苯并菲; 密度泛函理论; 盘状液晶; 电子光谱

Keywords: nonlinear optics; acetylamino chain triphenylene; density functional theory; discotic liquid crystals; electronic spectra

分类号: O 641.12+1; O 561.2

DOI: 10.6043/j.issn.0438-0479.2013.05.016

文献标志码: -

摘要: 在密度泛函理论B3LYP/6-31G**理论水平上,计算含乙酰胺基链苯并菲分

子的电子吸收光谱和非线性光学性质.研究结果显示,该分子的最大吸收波长和最低能量跃迁吸收波长分别为282和334 nm,在近紫外区.该分子的二阶和三阶非线性光学性质计算值分别为235.60和1.11×10^{5}a.u..

Abstract: Organic π-conjugated molecular have received growing interests for electronic and opt-electronic applications,such as organic field-effect transistor,organic light-emitting diodes,organic photovoltaic cells and various types of sensors.Electronic absorption spectra and nonlinear optical properties of triphenylene derivatives with acetylamino chain have been calculated at B3LYP/6-31G** level.The studied results show that the maximum absorption wavelength and the lowest energy transition wavelength of triphenylene derivatives with acetylamino chain are 282 and 334 nm,belonging to the near UV absorption area,the calculation value of the second-order and the third-order non-linear optical properties are 235.60 and 1.11×10^{5}a.u.,respectively.

参考文献/References:

[1] Laschat S,Baro A,Steinke N,et al.Discotic liquid crystals:from tailor-made synthesis to plastic electronics[J].Angew Chem Int Ed,2007,46:4832-4887.

[2] Kumas S.Recent developments in the chemistry of triphenylene-based discotic liquid crystals[J].Liq Cryst,2004,31:1037-1059.

[3] 毛华香,何志群,张春秀.含柔性侧链苯并菲衍生物合成研究的进展[J].有机化学,2006,26:413-418.

[4] Ishihara S,Furuki Y,Takeoka S.A hydrogen-bonded supramolecular hexagonal columnar liquid crystal