

液晶与显示 2012, 27(1) 14-20 ISSN: CN:

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材料物理和化学

含偶氮基团的弯曲型分子的光谱特性研究

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摘要：偶氮连接基团($-N=N-$)有着特殊的热化学和光化学行为,在适当波长光的照射下,能发生可逆的顺反异构反应,从而发生吸收波长的变化。在分子设计、光定位、光致变色和热致变色等方面,偶氮连接基团的非线性光化学性质都有着潜在的应用价值。文章以含有偶氮基作为侧翼的弯曲型分子作为研究对象,比较了弯曲型和直线型分子的吸收光谱;并用计算机模拟计算了弯曲型分子的角度,发现分子弯曲角和紫外可见吸收光谱存在着密切的关系。

关键词：偶氮 分子弯曲角 紫外可见吸收

Spectral Characteristics of Bent-Core Azobenzen Monomers

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Abstract: The azo ($-N=N-$) linkage has the particular thermochemistry and actinochrome behavior, the azobenzene group can undergo reversible cis-trans isomerization under light irradiation and its nonlinear optical properties possess the potential applications in the aspects of molecular design, photofixation, photochromics, thermochromism, etc. The UV-Vis absorbance of sixteen bent-core or linear monomers containing azobenzene as side arms and substituted para/m-aminobenzoic acid as central units was studied. The angle of the bent-core molecules was simulated. The trans-form of azo compounds showed a strong band in the UV region (330–370 nm) and a weak band at 440–450 nm. It was found that it has a close relationship between the angle of the molecules and the UV-Vis absorption.

Keywords: azo angle of molecules UV-Vis absorption

收稿日期 2011-11-29 修回日期 2011-12-07 网络版发布日期 2012-02-15

基金项目:

国家自然科学基金(No.60878047, No.61108065)

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