激光技术 2014, 38(2) 205-209 DOI: 10.7510/jgjs.issn.1001-3806.2014.02.013 ISSN: 1001-3806 CN: 51-1125/TN

激光材料和光学元件

两种新型芴类衍生物的三光子吸收特性研究

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摘要： 为了研究分子结构对三光子吸收的影响，合成了两种新型芴类衍生物，分别是2，7-二（2-4（甲氧基苯基）乙炔基）-9，9-二辛基-9H-芴（A）和2-溴-7-（2-（4-甲氧基苯基）乙炔基）-9，9-二辛基-9H-芴（B），采用1064nm的Nd∶YAG激光器测试其三光子吸收截面的方法，得到了它们的三光子吸收截面分别高达（6.03±0.6）×$10^{-76}$$cm^6$·$s^2$/$photon^2$和（4.25±0.4）×$10^{-76}$$cm^6$·$s^2$/$photon^2$的结果，在高斯03软件下，用密度泛函方法对这两个分子进行了结构优化，并用含时密度泛函理论计算了它们的激发态能量和电子轨道。结果表明，分子内电荷转移方向对三光子吸收存在影响。

关键词： 非线性光学 三光子吸收截面 光限幅 芴类衍生物

Three-photon absorption characteristics in two novel fluorine-based derivatives

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Abstract: In order to study effect of molecular structure on three-photon absorption(3PA) characteristics, two novel fluorene-based derivatives: 2, 7-bis(2-(4-methoxyphenyl)ethynyl)-9,9-dioctyl-9H-fluorene(A) and 2-bromo-7-(2-(4-methoxyphenyl)ethynyl)-9,9-dioctyl-9H-fluorene(B) were synthesized. The 3PA cross-sections of both the compounds were tested by using a *Q*-switched Nd:YAG laser at 1064nm. The 3PA cross-sections were obtained, i.e., (6.03±0.6)×10^{-76} cm^6·s^2/$photon^2$ and (4.25±0.4)×$10^{-76}$$cm^6$·$s^2$/$photon^2$respectively. The geometries in the ground states and electronic structures of both the compounds were investigated by density functional theory methods and time-dependent density functional theory methods of Gaussian 03, and the impact on the three-photon absorption characteristics was analyzed.

Keywords: nonlinear optics three-photon absorption section optical limiting fluorine-based derivatives

收稿日期 2013-04-09 修回日期 2013-05-05 网络版发布日期 2014-01-06

DOI: 10.7510/jgjs.issn.1001-3806.2014.02.013

基金项目:

国家自然科学基金资助项目（11004048；61177004）

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