化学学报 1994 52 (4): 325-330 ISSN: 0567-7351 CN: 31-1320/06

酞菁铜分子的电子态和反饱和吸收

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收稿日期 修回日期 网络版发布日期 接受日期

摘要 用ROHF-INDO/SDCI方法结合实验研究了酞菁铜分子的电子的电子结构.紫外-可见光谱.
激发态分子动态学和反饱和吸收的微观机制.
对酞菁铜实现反饱和吸收的必要条件是最低四重态对激光的吸收截面必须大于基态对激光的吸收截面. 在波长为532nm的激光作用下.该条件得到了满足,故Cupc呈现反饱和吸收特征.理论分析与实验结果一致.

关键词 紫外分光光度法 量子化学 激发态 电子结构 酞菁 P 可见光谱

分类号 0641

The electronic states and reverse saturable absorption of copper phthalocyanine molecule

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Abstract The electronic structure, UV-visible spectrum, excited states mol. dynamics and micro-mechanism of reverse saturable absorption of the Cu phthalocyanine (CuPc) mol. were studied by using the ROHF-INDO/SDCI method associated with experiment The necessary condition of reverse saturable absorption of CuPc is that the lowest quadruple state absorption cross section must be larger than the ground state absorption cross section for laser radiation. This condition is satisfied when the wavelength of incident laser radiation is 532 nm for CuPc, so that reverse saturable absorption occurs. The theor. analyses are consistent with experimental results.

Key words ULTRAVIOLET SPECTROPHOTOMETRY QUANTUM CHEMISTRY EXCITED STATE ELECTRONIC STRUCTURE ZINC PHTHALOCYANINE VISIBLE SPECTRUM

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