Chinese Journal of Chemistry 2005 23 (10): 1430-1436 ISSN: 0567-7351 CN: 31-1320/06

Full Papers

吩噻嗪给体受体衍生物激发态的电荷转移

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收稿日期 2005-3-8 修回日期 2005-6-16 网络版发布日期 接受日期

摘要 合成了一系列的N10位取代的吩噻嗪给体受体衍生物，这些受体基团包括苯，苯甲醚，吡啶，萘，苯乙酮和苯甲腈。研究了不同极性溶剂中这些化合物的分子内的光诱导电荷转移现象。稳态荧光的溶剂化效应和较大的Stokes位移清楚表明，仅仅后四种吩噻嗪衍生物的激发态存在着分子内的电荷转移(ICT), 而苯和苯甲醚取代吩噻嗪不具有这种特性。修正过的Lippert-Mataga公式被用来分析Stokes位移值，从而获得激发态偶极矩。较大的激发态偶极矩说明这些给体受体衍生物体系内发生了完全的电子转移。在此吩噻嗪衍生物的体系里，荧光过渡态偶极矩主要由溶剂平衡的电荷转移态和基态间的作用所决定，因为它在不同极性的溶剂中缺乏明显的改变。随着N10位取代基电负性的增加，吩噻嗪衍生物的电子结构和分子构型将发生明显的变化。

关键词 吩噻嗪, 分子内电荷转移, 给体-受体, 偶极矩

分类号

Charge Transfer in Excited Donor-acceptor Phenothiazine Derivatives

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Abstract A series of *N*-bonded donor-acceptor derivatives of phenothiazine containing phenyl (PHPZ), anisyl (ANPZ), pyridyl (PYPZ), naphthyl (NAPZ), acetylphenyl (APPZ), and cyanophenyl (CPPZ) as an electron acceptor have been synthesized. Their photophysical properties were investigated in solvents of different polarities by absorption and emission techniques. These studies clearly revealed the existence of an intramolecular charge transfer (ICT) excited state in the latter four compounds. The solvent dependent Stokes shift values were analyzed by the modified Lippert-Mataga equation to obtain the excited state dipole moment values. The large excited state dipole moment suggests that the full (or nearly full) electron transfer take place in the A-D systems. In the system of A-D phenothiazine derivatives, the transition dipole moments M_{flu} were determined mainly by direct interactions between the solvent-equilibrated fluorescence ^{1}CT state and ground state because of their lack of significant change with increase of the solvent polarity. The electron structure and molecular conformation of phenothiazine derivatives will be significantly changed with the increase of the electron affinity of the N-10 substituent.

Key words phenothiazine intramolecular charge transfer donor-acceptor dipole moment

DOI:

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