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C_{60}富勒烯键联哌啶荒酸和**7-**氯代吩嗪的半经验计算和瞬态谱

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摘要 C_{60}富勒烯键联哌啶荒酸**1**和7-氯代吩嗪**2**是C_{60}富勒烯与二烯体经Diels-Alder环加成获得,
用纳秒激光光解技术研究了给电子基团键联C_{60}富勒烯衍生物的三线态物理特性.
在苯腈溶液中在近红外区通过瞬态谱观测了激发三线态.用半经验方法AM1计算了化合物**1**和**2**
的前线分子轨道HOMO 与 LUMO.关于化合物**1**和**2**的分子内电荷转移,
理论计算与纳秒时间分辨瞬态谱得出基本相符的结果.

关键词 富勒烯, 分子内电子转移, 瞬态谱

分类号

Combined Transient Spectra and Semiempirical Calculation of [60]Fullerenes Attached with Piperidinodithiocarboxylate and 7-Chloro-phenazine

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Abstract [60]Fullerenes attached with piperidinodithiocarboxylate dyad(**1**) and 7-chloro- 1,2,3,4-tetrahydrophenazine (**2**) were efficiently synthesized through Diels-Alder cycloaddition with dienes. The physical properties of the triplet states of these compounds, in which strong electron acceptor moieties were covalently attached to C_{60} cores, were investigated by nanosecond laser flash photolysis. The excited triplet states in benzonitrile have been evaluated by observing the transient absorption bands in the near-IR region. The HOMO and LUMO were calculated by semiempirical methods AM1, which could predict the intramolecular photoinduced electron transfer in **1** and **2**, and the nanosecond transient absorption spectra observed experimentally in solution were in excellent agreement with the calculated ones.

Key words fullerene computational chemistry transient spectra

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