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加成产物**HC60[CH2C(CH3)=CH2]**的电子结构和**UV**谱

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摘要 用INDO方法研究C60与2-甲基烯丙基氯化镁的加成产物HC60[CH2C(CH3)=CH2]的两种异构体的结构和UV谱, 表明1,2-加成产物具有Cs对称性, 1,4-加成产物具有C1对称性, 且前者比后者总能量低, 因而更易于形成。产物中2-甲基烯丙基与C60之间靠极性共价键连接, 并发生前者向后者的电子转移。以此优化构型为基础, 计算两种产物异构体的UV谱, 与实验值一致。同时对电子跃迁进行理论指认, 讨论了产物UV谱带红移的原因。

关键词 紫外分光光度法 电子结构 加成反应 微分重叠间忽略近似 电子转移 富勒烯 甲基烯丙基氯化镁

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Electronic structures and UV spectra for the additive products HC60[CH2C(CH3)=CH2]

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Abstract The structures and UV spectra of both of the isomers for the additive products HC60[CH2C(CH3)=CH2] resulted from C60 and CH2=C(CH3)CH2 MgCl have been investigated by the series of INDO methods. It is illustrated that the 1,2-additive product is of Cs symmetry and 1,4-additive product is of C1 symmetry, furthermore the total energy of the 1,2-isomer is lower than that of the 1,4-isomer thus the former is easier to obtain. The bond between CH2=(CH3)CH2 and C60 in the product belongs to the polar covalent bond and the electronic transmmission from the former to the latter has happened. Based on the optimised geometry, the UV spectra of both of the isomers have been calculated and are in agreement with the experimental results. Meanwhile the theoretical assignment for the electronic transition has been performed and the red shift of the UV peaks has been rationalized.

Key words ULTRAVIOLET SPECTROPHOTOMETRY ELECTRONIC STRUCTURE ADDITION REACTION INTERMEDIATE NEGLECT OF DIFFERENTIAL OVERLAP APPROXIMATION (IND FULLERENES

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