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研究论文

二芴及其衍生物的结构优化、前线轨道及其性质的理论研究

王继芬[1,2], 封继康[2]

1. 上海第二工业大学城市建设与环境工程学院, 上海 201209;
2. 吉林大学理论化学研究所, 理论化学计算国家重点实验室, 长春 130021

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摘要 采用DFT/B3LYP方法对系列二芴体系进行了全优化, 对其结构特征进行对比. 在此基础上, 得到各分子的最高占据轨道和最低空轨道能量关系及HOMO-LUMO能隙, 并分析其能隙与导电性的关系及预计其光谱特征. 对各分子的相关热力学性质进行了研究. 热力学参数表明各分子均较稳定, 其中化合物DFBT最稳定. 采用ZINDO和TD-DFT方法计算其吸收光谱, 分析结构特征对光谱性质的影响. 二芴中插入共轭程度高的结构后, 分子的共轭程度增加; HOMO-LUMO能隙变窄; 最低激发能降低, 导电性增强; 吸收光谱红移. 而接入扭曲的结构后, 共轭程度降低; HOMO-LUMO能隙变宽; 最低激发能有所升高, 导电性下降; 吸收光谱蓝移.

关键词 二芴衍生物 密度泛函理论 前线轨道 结构与性质

分类号 0641

Theoretical Studies of the Structure Optimization, Frontier Orbitals and Properties of Bifluorene and Its Derivatives

WANG Ji-Fen[1,2]*, FENG Ji-Kang[2]*

1. School of Urban Development and Environmental Engineering, Shanghai Second Polytechnic University, Shanghai 201209, China;
2. State Key Laboratory of Theoretical and Computational Chemistry, Institute of Theoretical Chemistry, Jilin University, Changchun 130021, China

Abstract The structures of bifluorene and its derivatives was optimized by the density functional theory with B3LYP/6-31G functional while their maximal absorption wavelength λ_{abs} were studied by employing the time dependent density functional theory(TD-DFT) and ZINDO. On the basis of fully optimized structures, the molecular orbitals of bifluorene and its derivatives DFE, DFA, DFBT, FDBO and FSCHD were analyzed by comparison. The derivatives DFE, DFA and DFBT were better conjugated and their HOMO-LUMO gaps were narrower than that of BF. So they were better conductor than BF. And the absorption spectra of them were red shifting. How-ever, FDBO and FSCHD were in the other way round. The thermochemical properties were studied in this paper and these properties were important to experiment. It is found that DFBT has the lowest total energy in these molecules from analyzing the thermochemical parameters.

Key words Bifluorene derivative Density functional theory Frontier orbital Structure and property

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通讯作者 封继康 Jikangf@yahoo.com