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论文

5,7′-(亚甲胺基)-二-8-羟基喹啉及其金属有机配合物的密度泛函和自然键轨道及电子密度拓扑理论研究

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摘要:

采用密度泛函理论, 在B3LYP/6-31G水平上对5,7′-(亚甲胺基)-二-羟基喹啉及其3种金属M(M=Zn, Mg, Be)有机配合物M(5,7′-Iminomethylq$_2$)$_2$的结构进行了全优化, 并用TDDFT方法计算了吸收光谱. 同时, 利用自然键轨道理论(NBO)和电子密度拓扑分析(AIM)方法对分子内氢键进行了分析. 结果表明, 光谱计算值与实验值基本符合, 该类化合物均具有较大的电子亲和能, 改变中心金属原子对配合物吸收光谱性质的影响不大. 和5,7′-Iminomethylq$_2$相比, M(5,7′-Iminomethylq$_2$)$_2$的吸收光谱产生明显红移. 5,7′-Iminomethylq$_2$及其M(5,7′-Iminomethylq$_2$)$_2$分子内存在较强的氢键, 可形成三元环, 五元环和六元环. 分子内氢键的存在使分子的稳定性增加.

关键词: 8-羟基喹啉衍生物; 氢键; 自然键轨道理论; 电子密度拓扑分析; 含时密度泛函; 光谱

Theory Studies of 5,7′-(Iminomethyl)-bis-8-hydroxyquinoline and Its Metal-organic Complexes *via* DFT, NBO and AIM

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Abstract:

The structures of 5,7′-(iminomethyl)-bis-8-hydroxyquinoline(5,7′-iminomethylq$_2$) and its metal-organic complexes M(5,7′-iminomethylq$_2$)$_2$(M=Zn, Mg, Be) were optimized at B3LYP/6-31G level. The absorption spectra based on the above structure were obtained by the time-dependent density functional theory TD-B3LYP with the 6-31G basis set. At the same time, dihydrogen bond in 5,7′-iminomethylq$_2$ and M(5,7′-iminomethylq$_2$)$_2$ were studied with NBO and AIM analysis. The calculated results of absorption spectrum for 5,7′-iminomethylq$_2$ has good agreement with the experimental data. All complexes are excellent electrontransporting materials, absorption spectrum wave bands of which can be tuned little by different metals on the ligand of 5,7′-(iminomethyl)-bis-8-hydroxyquinoline anion. The absorption of M(5,7′-iminomethylq$_2$)$_2$ have a substance red shift compared with that of 5,7′-iminomethylq$_2$. There are also hydrogen bonds in the molecules, which make the molecules more stable.

Keywords: Bis(8-hydroxyquinolinolinato) derivative; Hydrogen bond; NBO; AIM; Time-dependent density fonctional theory; Spectrum

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