

论文

2-苯基吡啶铱(III)配合物及其衍生物光谱性质的理论研究

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摘要:

采用密度泛函理论B3PW91和UB3PW91方法, 分别对4种Ir(III)配合物(ppy)<sub>2</sub>Ir(acac)(1, ppy=2-苯基吡啶, acac=乙酰丙酮)、(np<sub>y</sub>)<sub>2</sub>Ir(acac)(2, np<sub>y</sub>=2-萘-1-基吡啶)、(pq)<sub>2</sub>Ir(acac)(3, pq=2-苯基喹啉)和(bzq)<sub>2</sub>Ir(acac)(4, bzq=苯并喹啉)进行了基态和激发态的几何优化, 在此基础上用TD-DFT方法计算了吸收和发射光谱. 结果表明, 随着ppy配体上并苯环位置的变化, 参与最大吸收和发射的分子轨道能隙降低程度不同, 从而使配合物2, 3, 4的最大吸收和发射光谱都比配合物1发生红移, 其中在吡啶环上增加苯环对吸收光谱的影响最大. 这4个分子最大吸收波长的顺序为1<2<4<3, 而最大发射波长顺序则是1<4<3<2. 由于配合物2的两个苯环上H的强排斥作用降低了其共轭程度, 使分子发生很大程度的扭曲, 导致其斯托克位移最大.

关键词: 铱(III)配合物; 2-苯基吡啶; 吸收光谱; 发射光谱; 含时密度泛函理论

Theoretical Studies on Photophysical Properties of the 2-Phenylpyridine Iridium (III) Complex and Its Derivatives

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Abstract:

A series of iridium(III) complexes(C<sup>N</sup>)<sub>2</sub>Ir(acac) [C<sup>N</sup>=ppy, 1; C<sup>N</sup>=np<sub>y</sub>, 2; C<sup>N</sup>=pq, 3; C<sup>N</sup>=bzq, 4; ppy=2-phenylpyridine, np<sub>y</sub>=2-naphthalene-1-ylpyridine, pq= 2-phenylquinoline, bzq=benzoquinoline, acac=acetoylacetate] was investigated theoretically to probe their electronic structures and spectroscopic properties. Their ground and excited state geometries were fully optimized at B3PW91/LANL2DZ and UB3PW91/LANL2DZ levels, respectively. Then, by means of the TD-DFT method, the absorption and emission spectra of complexes 1—4 were calculated on the basis of the optimized ground and excited states geometries, respectively. The calculated results show that the position of phenyl group on the 2-phenylpyridine will decrease the energy gap to different extent, while the absorption and emission spectra of complexes 2, 3 and 4 are bathochromic shifted compared with complex 1. In addition, the addition of phenyl group on the pyridine significantly influences the absorption spectra. And the low lying absorption energies are in the order 1<2<4<3, but the emission spectra are in the order 1<4<3<2. The repulsion between the C6—H and C9—H of the complex 2 reduces the π-conjugation effect, which greatly affects its geometry relaxation between the ground and excited states, which results in the large Stokes shift.

Keywords: Iridium(III) complex; 2-Phenylpyridine; Absorption spectrum; Emission spectrum; Time dependent density functional theory(TD-DFT)

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