高效磷光[Ru(terpy)(phen)X]$^+$配合物结构和光谱性质的理论研究

Theoretical Studies on Structures and Spectroscopic Properties of Highly Efficient Phosphorescent [Ru(terpy)(phen)X]$^+$ Complexes

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中文关键词 混合配体Ru(II)配合物 电子结构 光谱特征 密度泛函计算 UB3LYP方法

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中文摘要

采用密度泛函方法研究了三个混合配体的Ru(II)配合物[Ru(terpy)(phen)X]$^+$ (terpy为2,2',6',20'-三联吡啶，phen为1,10-邻二氮杂菲，X为-C≡CH (1)、Cl (2)和CN(3))的几何结构、电子结构和光谱性质．分别在B3LYP/LanL2DZ UB3LYP/LanL2DZ水平下优化了它们的基态和激发态结构．在TD-DFT计算水平下结合极化连续介质模型得到了它们在CH3CN溶液中的吸收和发射光谱．计算得到的Ru-C、Ru-N和Ru-Cl基态

英文摘要

The ground and the lowest-lying triplet excited state geometries, electronic structures, and spectroscopic properties of three mixed-ligand Ru(II) complexes [Ru(terpy)(phen)X]$^+$(terpy=2,2',6',20'-terpyridine, phen=1,10-phenanthroline, and X=-C≡CH (1), X=Cl (2), X=CN (3)) were investigated theoretically using the density functional theory method. The ground and excited state geometries have been fully optimized at the B3LYP/LanL2DZ and UB3LYP/LanL2DZ levels, respectively. The absorption and emission spectra of the com-plexes in CH_3CN solutions were calculated by time-dependent density functional theory with the PCM solvent model. The calculated bond lengths of Ru-C, Ru-N, and Ru-Cl in the ground state agree well with the corresponding experimental results. The highest occupied molecular orbital were dominantly localized on the Ru atom and monodentate X ligand for 1 and 2, Ru atom and terpy ligand for 3, while the lowest unoccupied molecular orbital were π_*(terpy) type orbital. Therefore, the lowest-energy absorptions of 1 and 2 at 688 and 631 nm are attributed to a d_{yz}(Ru)+π/p(X)→π_*(terpy) transition with MLCT/XLCT (metal-to-ligand charge transfer/X ligand to terpy ligand charge transfer) character, whereas that of 3 at 529 nm is related to a d_{yz}(Ru)+π(terpy)→π_*(terpy) transition with MLCT and ILCT transition character. The calculated phosphorescence of three complexes at 1011 nm (1), 913 nm (2), and 838 nm (3) have similar transition properties to that of the lowest-lying absorption. It is shown that the lowest lying absorptions and emissions transition character of these Ru(II) complexes can be tuned by changing the electron-withdrawing ability of the monodentate ligand.

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