Title

Geometry optimization and UV/Vis spectra of organometallic chalcones functionalized with a benzo-15-crown-5 fragment: A DFT/TD-DFT investigation

Abstract

In this paper, we studied the structural and UV–visible absorption spectrum of the organometallic chalcones from ferrocene and cyrhetrene functionalized with a benzo-15-crown-5 fragment. The influence of different alkali and alkaline earth metal ions on geometric structures, frontier molecular orbitals character, gap energy and electronic absorption spectra of [(η5-C5H4C(O)CH = CH-4-benzo-15-crown5)MLn] (MLn = Fe(η5-C5H5) and Re(CO)3) has been theoretically studied by density functional theory (DFT) and time-dependent density functional theory (TDDFT) calculations with PBE0 and CAM-B3LYP hybrid functionals. Calculated geometric parameters of studied complexes are in good agreement with the available experimental values. The theoretical absorption spectra reproduce the main properties of the experimental spectra. Both alkali (Li+, Na+, K+, Rb+ and Cs+) and alkaline-earth (Be2+, Mg2+ and Ca2+) metal ions selective complexes have been theoretically identified. The calculated values the lowest energy band (λmax) of the crown ether derivatives to the alkaline earth metal cations increases from Be, Mg, and then Ca in the complexes [2 M], indicating that these absorption bands are associated to a transition from the HOMO to LUMO transition, which is assigned to metal-to-ligand charge transfer (MLCT).

Authors

Djouama H.; Djouama R.; MacLeod-Carey D.; Nafti N.

Author full names

Djouama, Hanane (58283758500); Djouama, Rabie (57214763557); MacLeod-Carey, Desmond (58063106100); Nafti, Narimane (58726352300)

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Affiliations

Applied Chemistry Laboratory, Faculty of Sciences, Chemistry Department, University of Mohamed Khider, Biskra, Algeria; LCPM Laboratory, Faculty of Sciences, Chemistry Department, University of Oran, 1 Ahmed Ben Bella, Oran, Algeria; Grupo de Química Inorgánica y Materiales Moleculares, Facultad de Ingenieria, Universidad Autonoma de Chile, El Llano Subercaseaux, Santiago, 2801, Chile

Authors with affiliations

Djouama H., Applied Chemistry Laboratory, Faculty of Sciences, Chemistry Department, University of Mohamed Khider, Biskra, Algeria; Djouama R., LCPM Laboratory, Faculty of Sciences, Chemistry Department, University of Oran, 1 Ahmed Ben Bella, Oran, Algeria; MacLeod-Carey D., Grupo de Química Inorgánica y Materiales Moleculares, Facultad de Ingenieria, Universidad Autonoma de Chile, El Llano Subercaseaux, Santiago, 2801, Chile; Nafti N., Applied Chemistry Laboratory, Faculty of Sciences, Chemistry Department, University of Mohamed Khider, Biskra, Algeria

Author Keywords

Absorption spectrum; Charge transfer; Crown ether; Geometric structures; Organometallic chalcones; TD-DFT

Index Keywords

Absorption spectroscopy; Alkaline earth metals; Crown ethers; Density functional theory; Electromagnetic wave absorption; Ethers; Geometry; Iron compounds; Ligands; Metal ions; Molecular orbitals; Orbits; Organometallics; Benzo-15-crown-5; Chalcones; Crown-ethers; Density-functional-theory; Functionalized; Geometric structure; Geometry optimization; Organometallic chalcone; TD-density functional theory; UV-Vis spectrum; Charge transfer

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Correspondence Address

H. Djouama; Applied Chemistry Laboratory, Faculty of Sciences, Chemistry Department, University of Mohamed Khider, Biskra, Algeria; email: h.djouama@univ-biskra.dz

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