

The role played by structural and energy parameters of β -Diketones derivatives as antenna ligands in Eu(III) complexes

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Abstract

Structural and energy parameters role of six β -diketone antennas (symmetry, bulkiness, quenching bonds, donor groups and coordination) were analyzed. Six β -diketone derivatives and its complexes $\text{Eu}(\text{Phen})(\text{X})_3$ and $\text{Gd}(\text{Phen})(\text{X})_3$ ($\text{X} = \beta$ -diketone), were synthesized, characterized, experimentally studied through photophysical characterization. To analyze the contribution of each antenna to the photophysical properties, TD-DFT calculations were performed. To elucidate the antennas/Eu(III) energy levels involved in the energy transfer process CASSCF calculations were performed. Two antenna ligands effectively feed the europium center. A ligand without symmetry, with donor groups, without quenching bonds, and capable to fulfill the energy requirements, is the best antenna ligand for these complexes.

Author keywords

Antenna effect

DFT lanthanides

Eu(III) complexes

photophysical characterization