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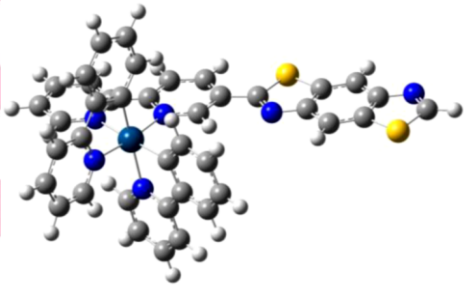
A DFT investigation on the effect of ligand substitution on photophysical properties of some new cyclometalated Ir(III) complexes

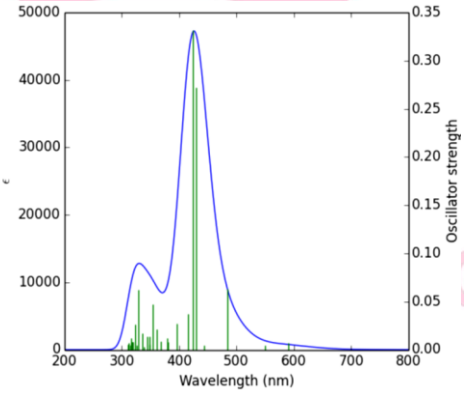
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Cyclometalated Ir(III) complexes has attracted considerable attention due to their applications in electroluminescence, photocatalysis, phosphorescent molecular probes [1] and their potential for solid-state lighting and display utilizations [2]. The complexes are more promising because of larger d-orbital splitting and strong spin-orbit coupling (SOC) effect [3]. Phosphorescent cyclometalated Ir(III) complexes usually represent high quantum yields and emissive metal to ligand charge transfer (^{3}MLCT) excited states. Ir(III) ion, due to the high SOC, facilitates the intersystem crossing of the excited states. Moreover, the forbidden $T_1 \rightarrow S_0$ transition is activated in these complexes [4].

Here, electronic structure of four new cyclometalated Ir(III) complexes are studied at DFT/B3LYP level of theory. Previously, the method has been successfully applied to investigate Ir(III) complexes [5]. The effect of functionalization of ancillary ligand by benzothiazole derivatives (as electron acceptor) and electron donor groups on the electronic structure of the complexes are investigated. It is well known that, the electrochemical and photophysical properties of these complexes could be tuned by functionalization of the ancillary ligand [4]. Photophysical properties of the compounds are studied by TDDFT method at the same level of theory.





Keywords: cyclometalated Ir(III) complexes, ancillary ligand, electron donor-acceptor, DFT

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