22nd Iranian Chemistry Conference, 23-25 August, 2023
University of Kurdistan

A fluorinated cyclometalated Pt(II) complex bearing a phosphine ligand: photophysical and theoretical investigations

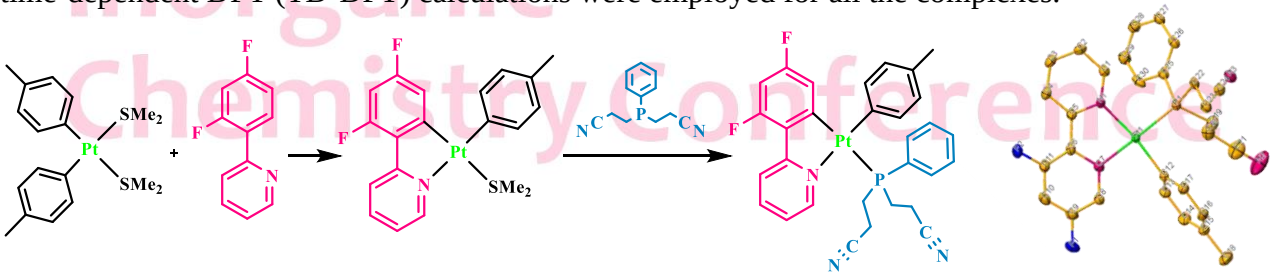
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In recent decades, numerous researchers have extensively explored luminescent cyclometalated platinum(II) complexes, and the number of publications in this area of study is growing. Various uses for the luminous cycloplatinated complexes include light-emitting devices, dye-sensitized solar cells, photoswitches, photocatalysts, and chemical or biological sensors [1]. The principal chromophore involved in producing room-temperature phosphorescence is the cyclometalated ligand. In addition, heavy metals like Pt induce high spin-orbit coupling and allow singlet-triplet intersystem crossing. The photophysical characteristics of such complexes are greatly influenced by the auxiliary ligands, in addition to the previously listed parameters. These ligands control the electron density at the metal center and, consequently, the degree of metal to ligand charge transfer (MLCT) in the lowest energy transition [2].

Herein, a heteroleptic cycloplatinated(II) complex [Pt(*p*-MeC_6H_4)(dfppy)($PPh(EtCN)_2$)], dfppy = 2-(2,4-difluorophenyl)pyridinate; and $PPh(EtCN)_2$ = bis(2-cyanoethyl)phenylphosphine, was synthesized and characterized. The complex exhibits greenish-blue phosphorescence under UV light at room temperature in the solid state, with mostly well-structured emission bands in the range of 450–490 nm (solid and CH_2Cl_2 fluid solution states, 298 and 77 K). Their emissions appear as structured bands, which indicates that the emissions mainly originate from the electronic transitions in the ligand with a small contribution of metal to ligand and/or ligand to ligand charge transfers. To rationalize the experimental photophysical data, density functional theory (DFT) and time-dependent DFT (TD-DFT) calculations were employed for all the complexes.



Scheme 1: Synthetic route for the preparation of the Pt(II) complex (left) and its crystal structure (right).

***Keywords*:** Phosphine; Cycloplatinated(II); Photophysics; Theoretical elucidation.

References

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