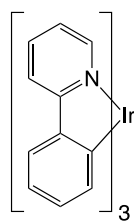


FIGURES FOR
Identifying TD-DFT Methods Towards Accurate Prediction of Emission Energies
for Iridium and Platinum Photoluminescent Complexes

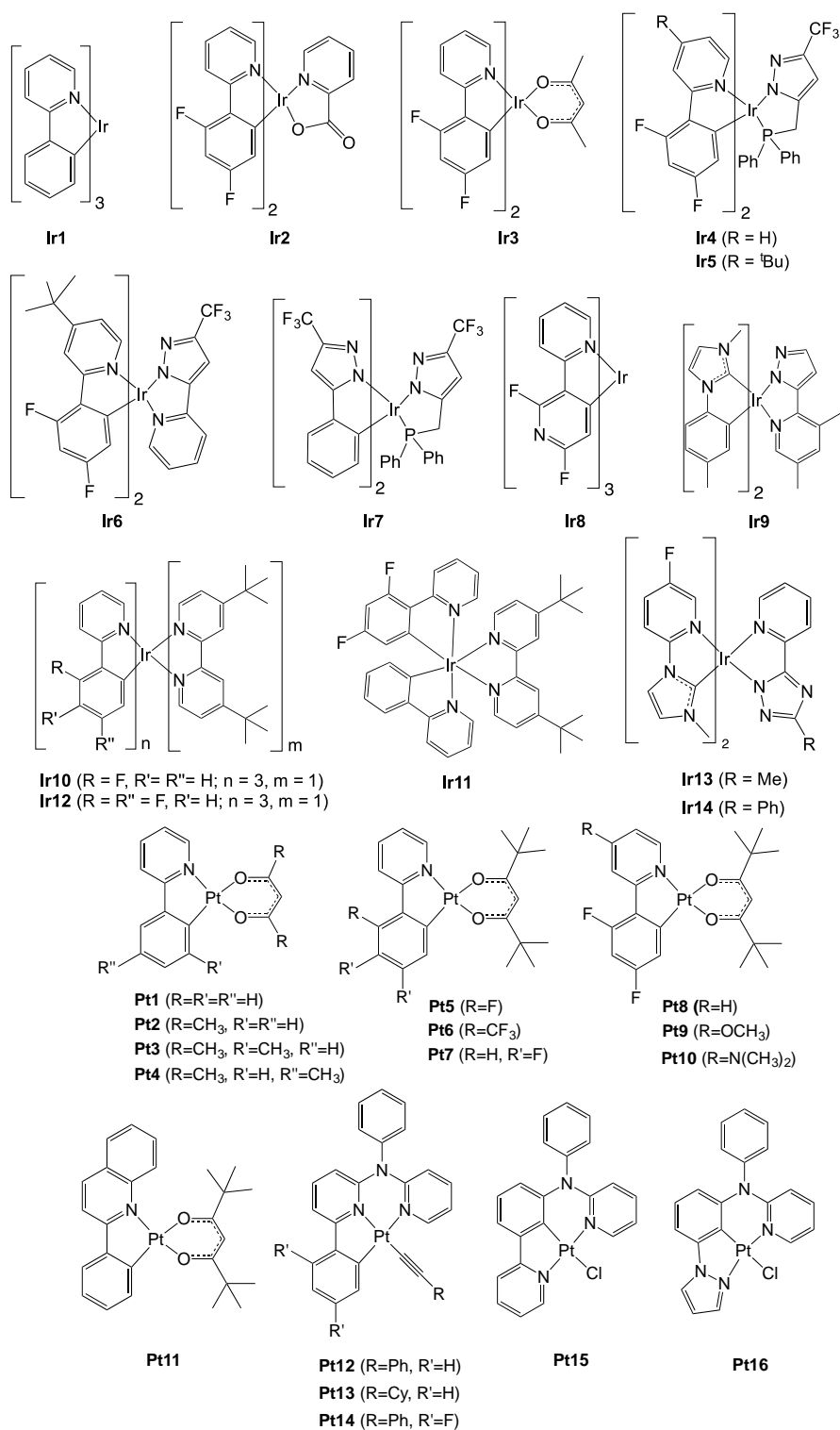
Glenn R. Morello



Ir(ppy)₃

Fig. 1 Structure of the green-emitting complex tris(2-phenylpyridine) iridium(III), Ir(ppy)₃, one of the first and most intensely studied OLED complexes.

Fig. 1 created with ChemDraw



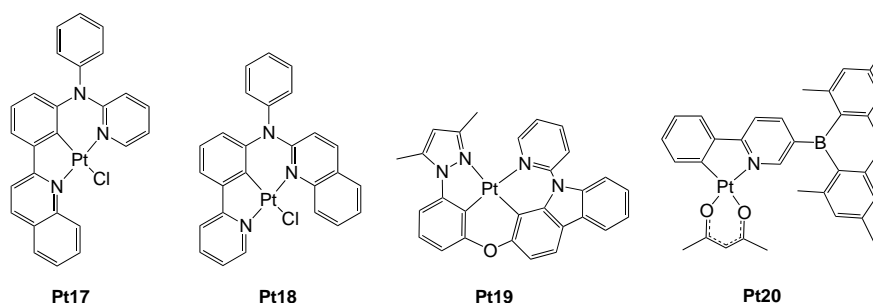


Fig. 2 Structures of OLED complexes studied in this work. See Supporting Information for references and experimentally determined emission values, λ_{em} , of all complexes at both 77 K and 298 K.

Fig. 2 created with ChemDraw

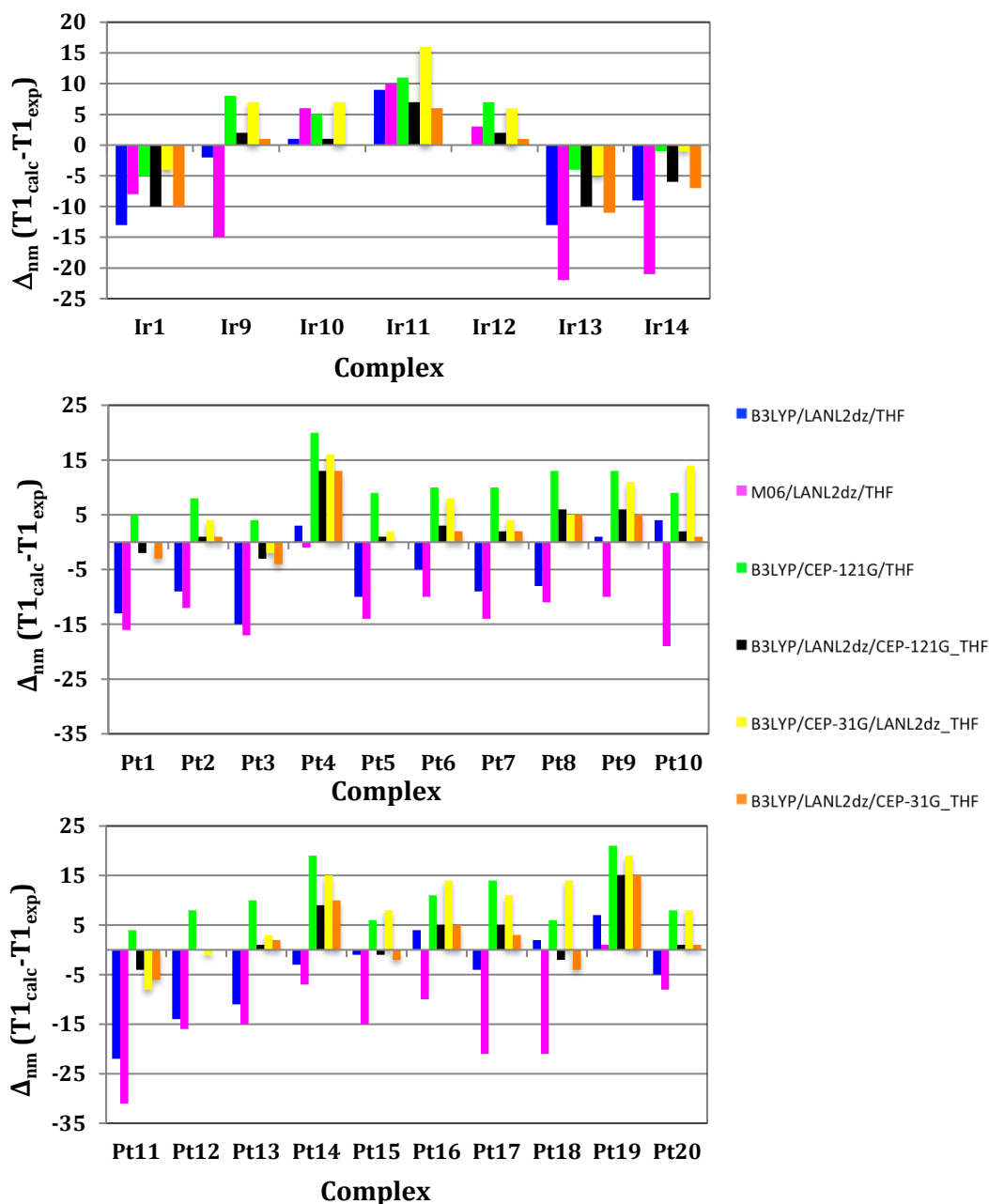


Fig. 3 Difference plots of $\Delta\lambda_{nm}$ for top performing basis sets used on iridium complexes (*top*) and platinum complexes (*middle* and *bottom*). Complete basis set data available in the Supporting Information.

Fig. 3 Plots created with Excel. Key taken as a screen shot from Xcel spreadsheet.