

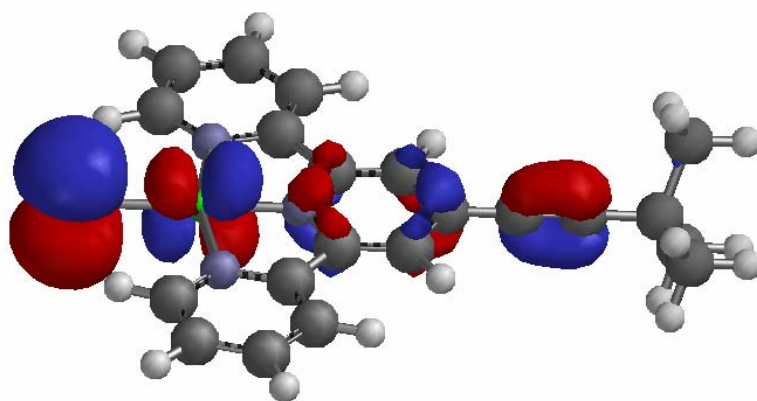
ESI for Room temperature photoluminescence from $[\text{Pt}(4'\text{-CCR-tpy})\text{Cl}]^+$ complexes

Maria L. Muro and Felix N. Castellano*

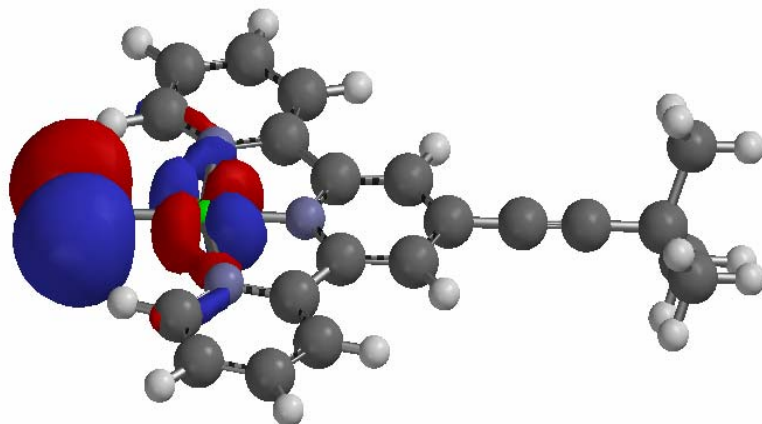
Department of Chemistry and Center for Photochemical Sciences, Bowling Green State University, Bowling Green, Ohio 43403, USA

Fig. S1 Representative molecular orbitals calculated for tBuCCtpyPtCl⁺ (1).

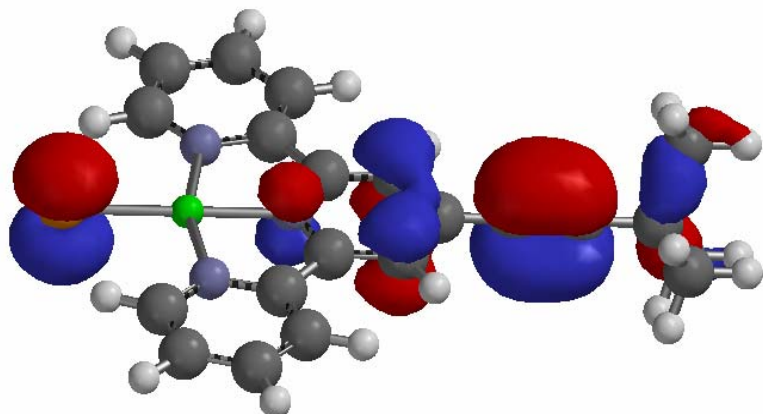
HOMO



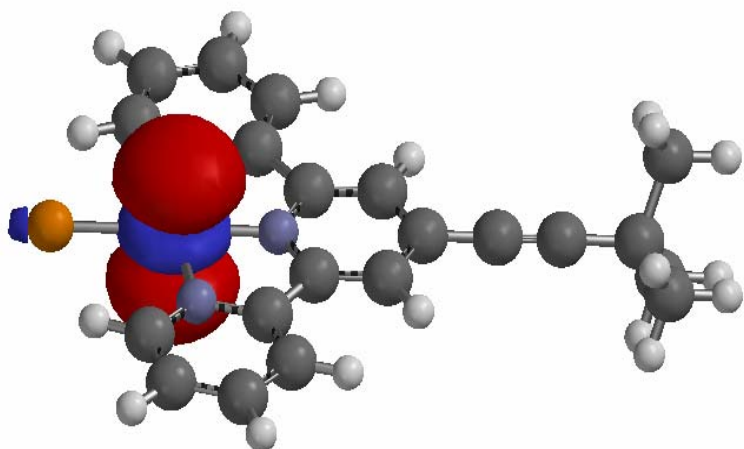
HOMO -1



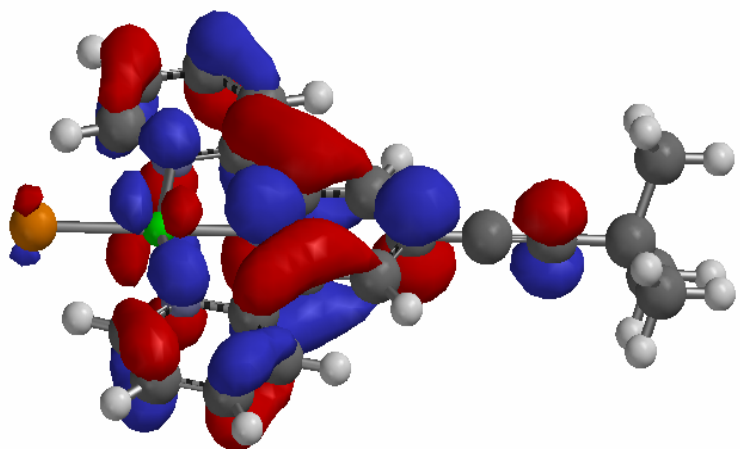
HOMO-2



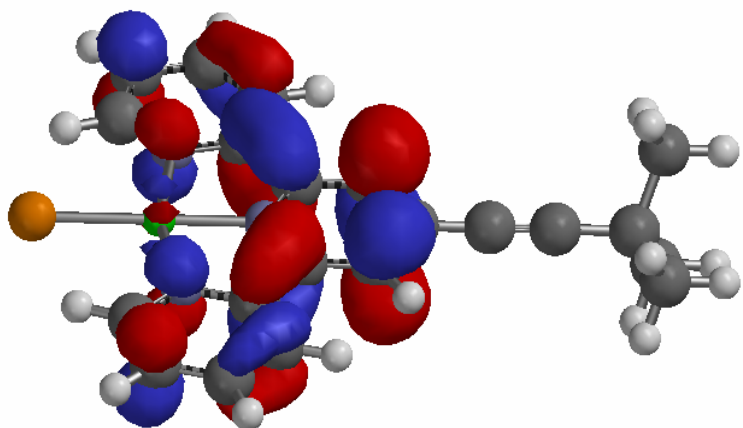
HOMO-3



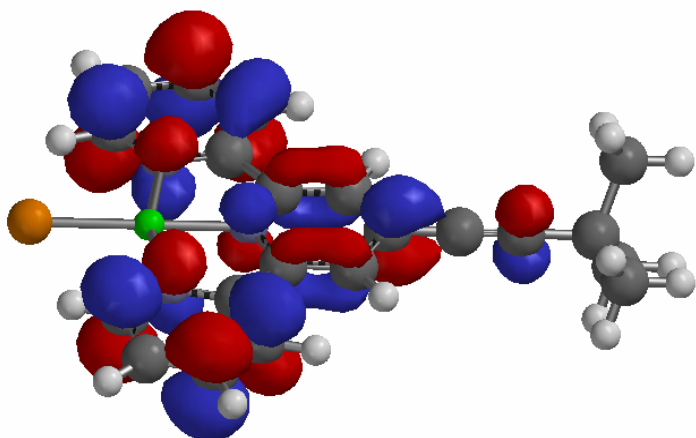
LUMO



LUMO+1



LUMO+2



LUMO+3

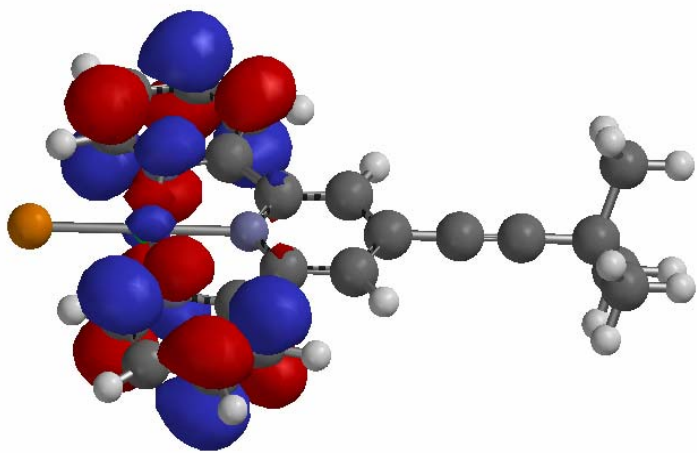
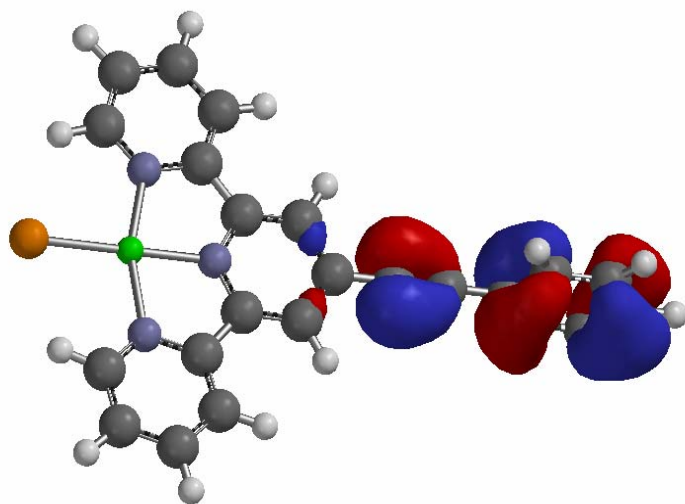
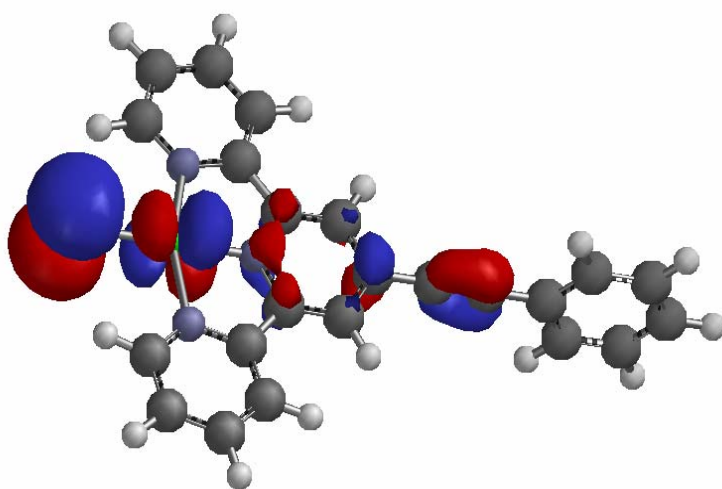


Fig. S2 Representative molecular orbitals calculated for PhCCtpyPtCl⁺ (**2**)

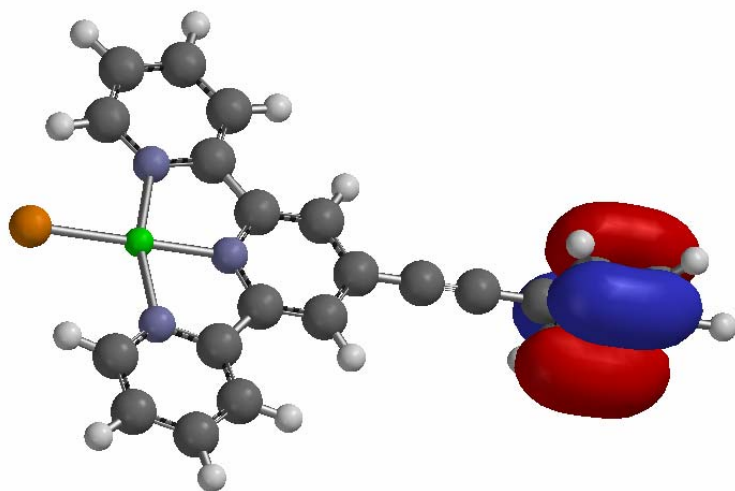
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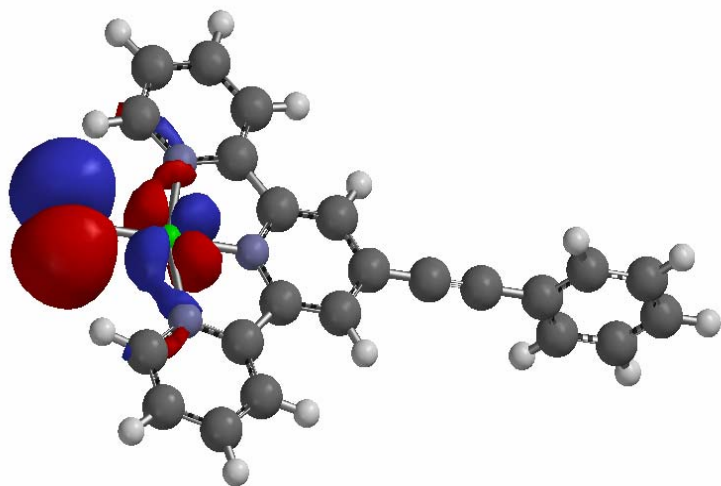
HOMO-1



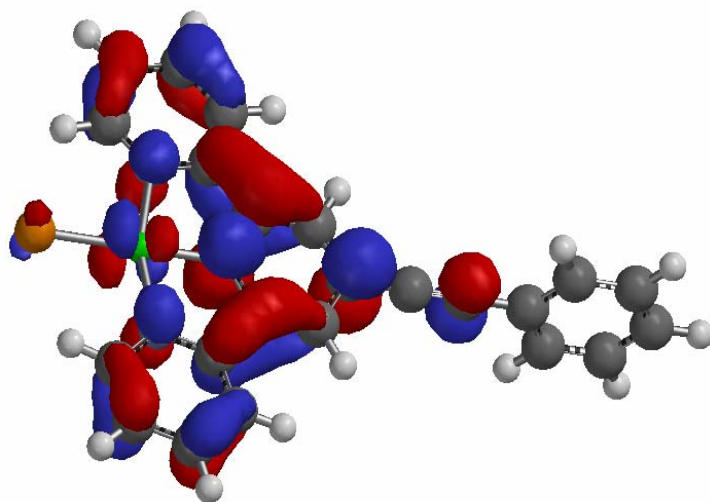
HOMO-2



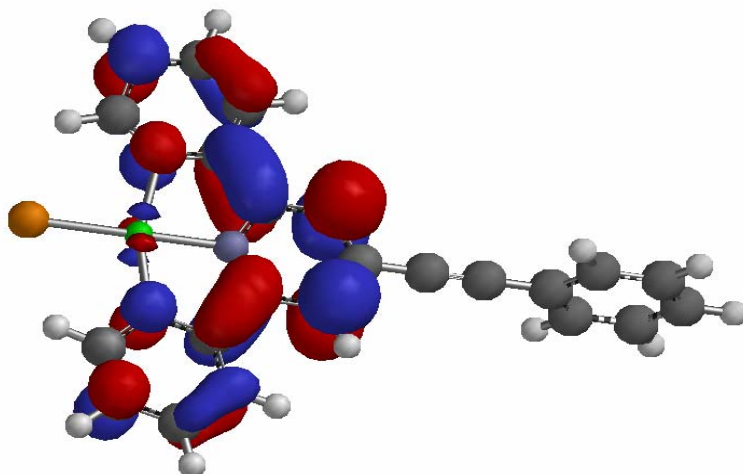
HOMO-3



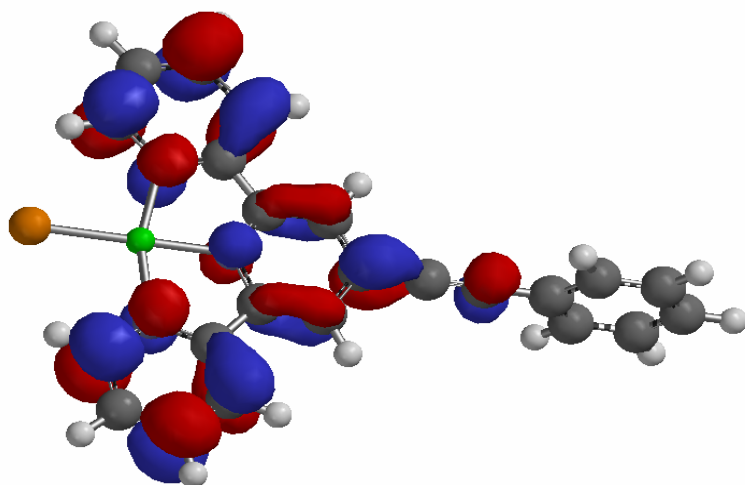
LUMO



LUMO+1



LUMO+2



LUMO+3

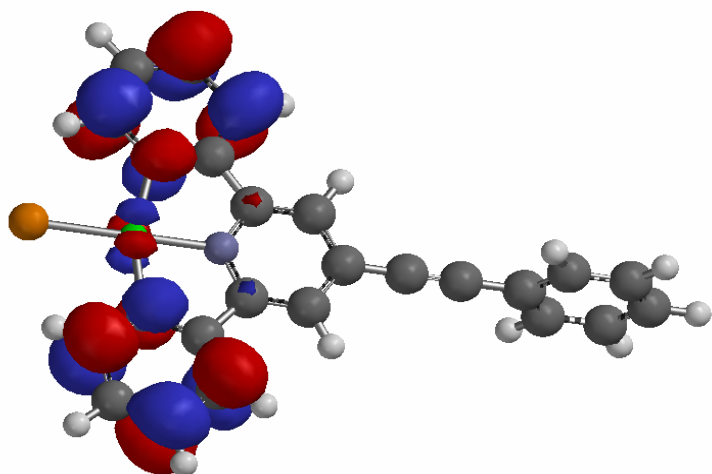
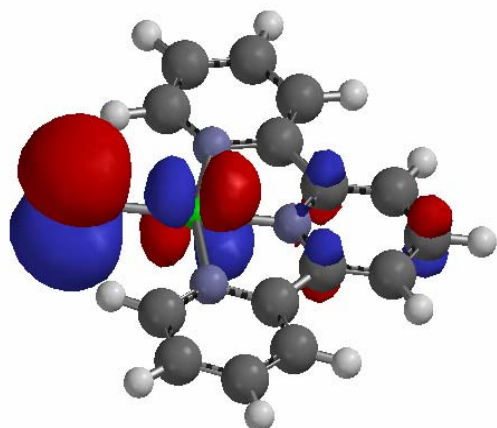
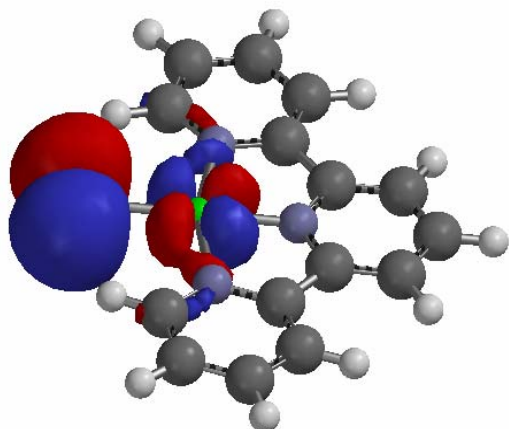


Fig. S3 Representative molecular orbitals calculated for tpyPtCl^+

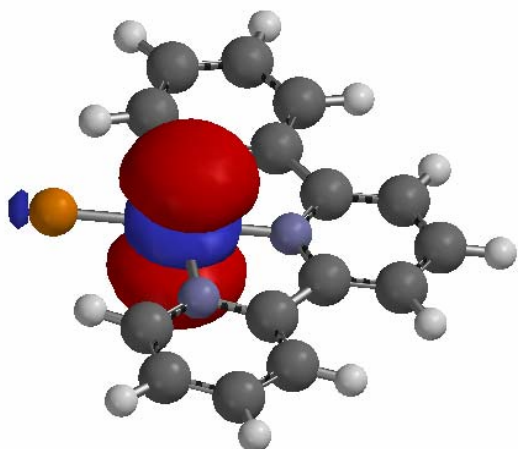
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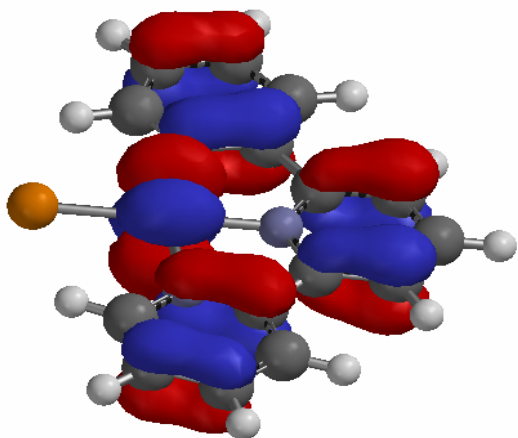
HOMO-1



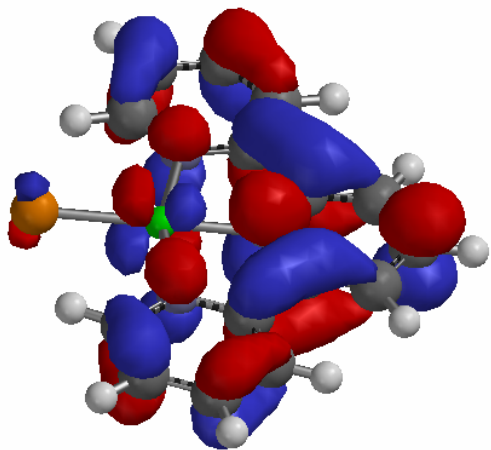
HOMO-2



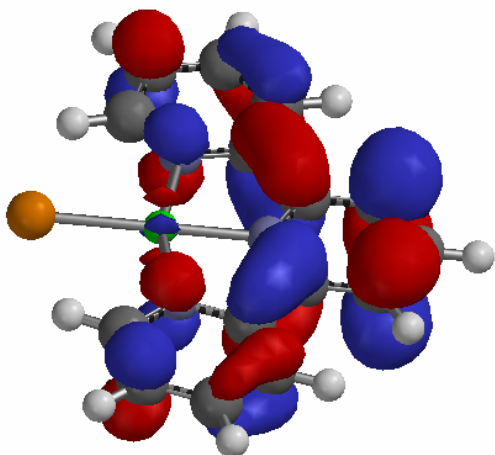
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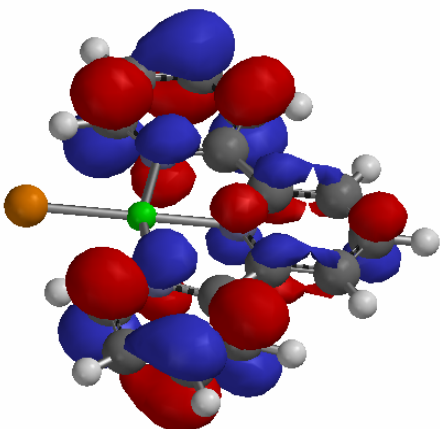
LUMO



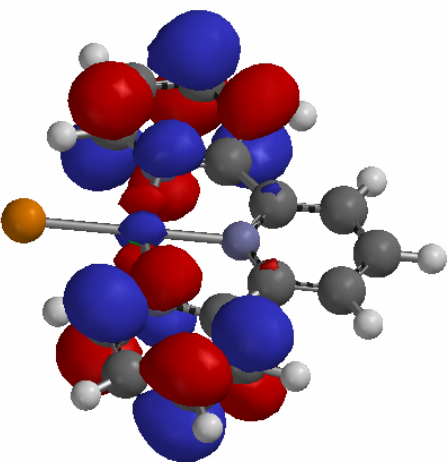
LUMO+1



LUMO+2



LUMO+3



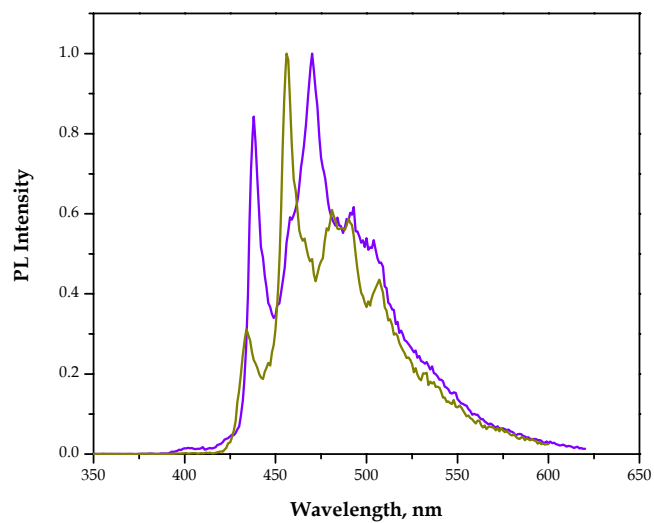


Fig. S4 Phosphorescence measurements in 4:1 EtOH/MeOH matrices at 77 K for 4'-C≡tBu-tpy (violet line) and 4'-C≡CPh-tpy (dark yellow line).