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Book of Abstracts

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Luminescent cyclometalated platinum(II) complexes with L^X chelating ligands: synthesis, optical properties and theoretical calculations

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Cyclometalated Pt^{II} compounds have brought considerable interest due to their exceptional photophysical properties, with high quantum photoluminescence yields, long lifetimes and easy emission modulation, which have been widely applied in OLEDs, chemosensing and bioimaging[1]. Their planar geometry allows Pt···Pt and/or π···π intermolecular interactions, able to produce extended linear chains and oligomeric nanostructures, which display rich polymorphism in solid state, and have been also employed as spectroscopic reporters of microenvironment changes, host−guest interactions, and chemo/biosensing applications.

Here, we present a series of luminescent Pt^{II} compounds based on 2-phenylbenzothiazole (PBT) as cyclometalated group and bidentate auxiliary ligands L^X, [Pt(PBT-κ*C,N*)(L^X)] [L^XH: PPh_2(*o*-PhCOOH) **2**, PPh_2(*o*-$PhSO_3H$) **3**, PPh_2{$(CH_2)_2$COOH} **4**, picolinic acid **5** and 3-aminopicolinic acid **6**], prepared starting from the DMSO solvate [Pt(PBT-κ*C,N*)Cl(DMSO)] **1**.

All complexes have been characterized, including by X-ray diffraction studies, and their photophysical properties examined in different media (solid state, solution, PS film for emission). Additional theoretical analysis have been carried out at DFT/TD−DFT level for selected complexes to study the electronic transitions of monomer molecules, and in the case of complex **5**, a dimer (**5_2**) have been studied to examine the Non-Covalent Interactions (NCI).

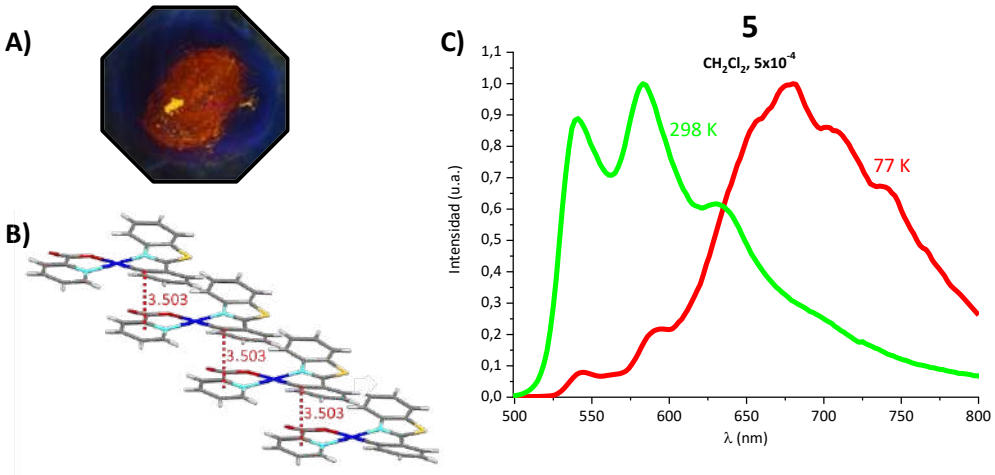

Figure 1. A) Microcrystalline (yellow) and ground (orange) solid of **5**; B) X-ray structure showing π···π interactions; C) emission spectra of **5** in CH_2Cl_2 (298 K and 77 K)

[1] Fleetham, T., Li, G., Li, J., *Advanced Materials*, **2017**, *29*, 1601861.