

SYNTHETIC AND OPTICAL STUDIES OF NEW CYCLOMETALATED Pt^{IV} COMPOUNDS WITH CHELATING N,N'-DONOR LIGANDS

D. Gómez de Segura, A. Corral-Zorzano, E. Lalinde and M.T. Moreno.

Departamento de Química – Centro de Investigación en Síntesis Química de La Rioja (CISQ), Universidad de La Rioja, C/ Madre De Dios nº 53, 26006, Logroño (La Rioja) España.

Email: daseguz@unirioja.es

In contrast to the numerous studies carried out on d⁶ (Ir^{III}, Ru^{II} or Os^{II}) and d⁸ phosphors (Pt^{II}, Au^{III}), the related on Pt^{IV} derivatives are scarce¹. Recently our group has published new series of neutral bis(cyclometalated)pentafluorophenyl Pt^{IV} complexes bearing Cl⁻ or CN⁻ as ancillary ligands². Benzothiazole has demonstrated to be a good platform employed as ligand to obtain yellow phosphorescent metal complexes with myriad applications as biosensing, optical devices, photocatalysis or chemotherapy.

In this topic, we present a new series of dicationic bis-cyclometalated Pt^{IV} compounds of type [Pt(pbt)₂(N[^]N)]Q₂, bearing 2-phenylbenzothiazole (pbt) as cyclometalating ligand and chelating N,N'-phenanthroline-based ligands (N[^]N = phen **4**, pyraphen **5**, NH₂-phen **6**), with two different counteranions (Q = PF₆, CF₃CO₂), using [Pt(pbt)₂Cl₂] **2** and [Pt(pbt)₂(OCOCF₃)₂] **3** as starting materials. The *trans*-N,N *cis*-C,C configuration was confirmed by X-Ray diffraction analysis of complexes **2**, **3** and **4-PF₆**. Optoelectronic properties in different media (solid state, solution and doped polymeric films) have been studied with the support of theoretical analysis at DFT/TD-DFT level for all complexes. Complexes **2** - **5** exhibit pbt-centered (³IL) emissions, whereas dual emission associated to two close different, ³IL'CT (L'=NH₂-phen) and ³IL(pbt), states was found for the NH₂-phen complex **6**.

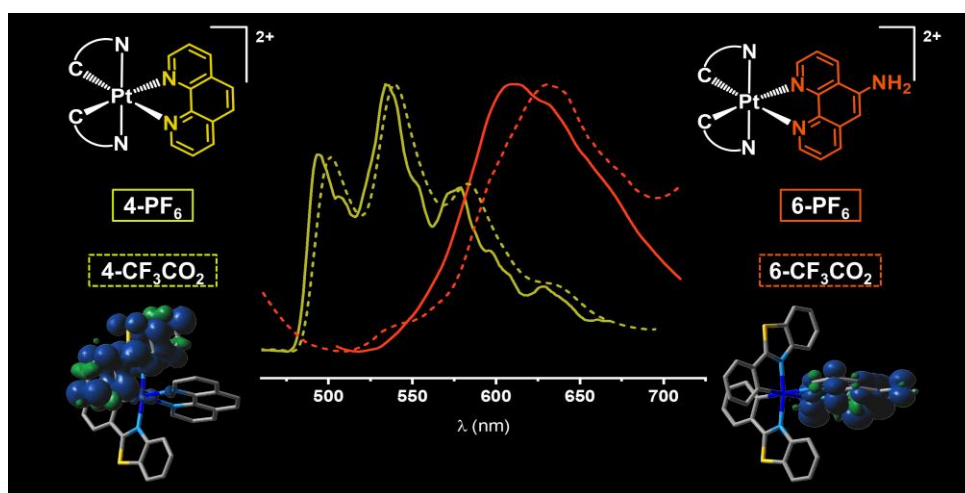


Figure 1: Structure, emission (CH₂Cl₂, 77 K) and spin density of the T₁ optimized state for **4** and **6**.

Acknowledgments: We thank Spanish Ministry of Science and Innovation (Project: PID2019-109742GB-I00) for financial support. D.G S is grateful to UR for a PhD grant.

References

1. Z. Feng, Y. Sun, X. Yang, G. Zhou, Novel Emission Color-Tuning Strategies in Heteroleptic Phosphorescent Ir(III) and Pt(II) Complexes, *Chemical Reviews*, **2019**, 19, 1710-1728.
2. E. Lalinde, R. Lara, I. P. López, M. T. Moreno, E. Alfaro-Arnedo, J. G. Pichel, S. Piñeiro-Hermida, Benzothiazole-Based Cycloplatinated Chromophores: Synthetic, Optical and Biological Studies, *Chemical European Journal*, **2018**, 24, 2440-2456.