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ABSTRACT BOOK

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Synthesis and Photophysical Properties of Cycloplatinated(II) Complexes Bearing Isocyanide and Alkynyl Ligands

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Cyclometalated platinum(II) complexes have gained increasing interest during the last years due to their rich chemistry and unique luminescent properties, making them suitable for light emitting diodes (OLEDs), photocatalysis, bioimaging or chemical sensors. However, there are very scarce antecedents of heteroleptic cycloplatinated(II) compounds with isocyanide and alkynyl ligands.[1]

To expand this research, we aimed to prepare a new family of luminescent cycloplatinated complexes with 2-(2,4-difluorophenyl)pyridine (dfppy, **a**) and 4-(2-pyridyl)benzaldehyde (ppy-CHO, **b**) as cyclometalating ligands. The alkynyl/*tert*-butyl isocyanide complexes [Pt(C^N)(C≡CR)(CN^{t}Bu)], bearing 4-ethynylanisole (**2**) and 2-ethynylthiophene (**3**) have obtained from the chloride derivatives [Pt(C^N)Cl(CN^{t}Bu)] (C^N = dfppy **1a**, ppy-CHO **1b**) using the Sonogashira protocol. These systems have been designed by taking into account features that could make these complexes interesting in biological studies.

The complexes have been fully characterized using NMR spectroscopy together with X-ray diffraction. Their optical properties have been studied in detail and interpreted with the help of TD-DFT calculations. The dfppy derivatives exhibit a mechanochromic behaviour, related to their strong tendency to form stacking structures or aggregates by Pt···Pt and/or π···π interactions.

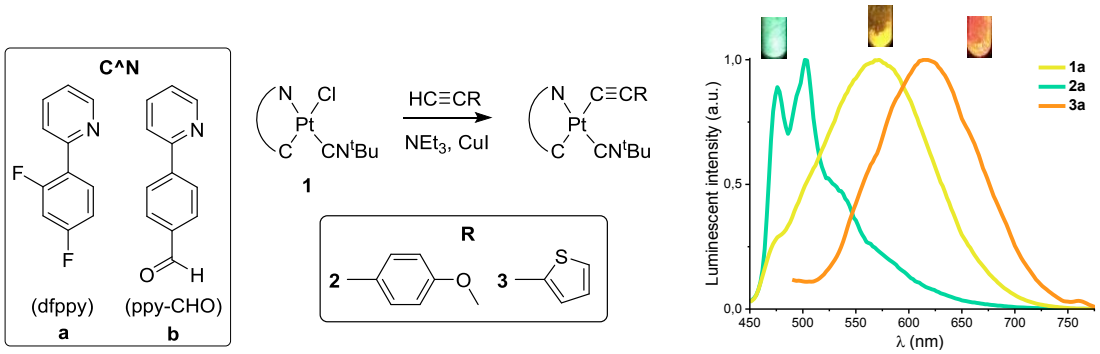

Figure 1. Scheme of the synthesis and selected emission spectra of dfppy derivatives.

References

[1] J. Forniés, V. Sicilia, P. Borja, J. M. Casas, A. Díez, E. Lalinde, C. Larraz, A. Martín, M. T. Moreno, *Chem. Asian J.*, **2012**, *7*, 2813-2823.