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BOOK OF ABSTRACTS

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Study of cycloplatinated complexes with isocyanide ligands: isomerism, optical properties and mechanochromism

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Platinum(II) cyclometalated derivatives have attracted a great interest due to their rich photophysical properties, with interesting applications as chemical sensors, photocatalysts or in light emitting diodes (OLEDs). The presence of planar ligands in these complexes improves the luminescence and the ability to form aggregates through the formation of Pt…Pt and/or π … π interactions. In this context, there are very scarce examples of heteroleptic complexes with isocyanide and alkynyl ligands.

In this work, we present the synthesis and characterization of a group of Pt(II) compounds featuring 2-phenylpyridine and 2-phenylquinoline as cyclometalated ligands and 2,6-dimethylphenyl isocyanide as auxiliary ligand. The p-tolylacetylide complexes [Pt(C^N)(C=CTol)(C=NXyI)] (C^N = ppy **3**, pq **4**) have been obtained from the chloride derivatives [Pt(C^N)CI(C=NXyI)] (C^N = ppy **1**, pq **2**). The isomerism of these compounds in which the isocyanide ligand can be trans to the nitrogen or to the carbon of the cyclometalated ligand has been determined by different techniques, as NMR and X-ray diffraction.

The photophysical properties (absorption and emission) of all complexes have been studied with the aid of theoretical calculations. Interestingly, the phenylpyridine derivatives exhibit mechanical stimuli responsive colour and luminescence changes correlated with the formation of different aggregates with $\pi \cdots \pi$ and/or Pt…Pt interactions.

