

Title: **Design of spin-cross-over heteroleptic Fe(II) coordination compounds based on gas absorption/desorption processes.**

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Departament of Inorganic chemistry and Organic chemistry, Inorganic section

This project has been fulfilled in the research Group of Magnetism and Functional Molecules (GMMF), at the University of Barcelona. The main purpose of this group is based on the synthesis and study of coordination compounds which present interesting physical properties such as magnetic and/or optical ones.

In this project, new heteroleptic complexes of Fe(II) have been designed with the finality that they can exhibit spin crossover behavior induced by absorption-desorption processes, in order to be applied as a chemical sensor for solvents or toxic gases. To achieve this goal, the organic ligand 2,6-bis(pyrazol-3-yl)pyridine (3-bpp) and its derivative 2,6-bis(5-(2-methoxyphenyl)pyrazol-3-yl)pyridine (H₂L) have been synthesized and thereafter reacted with different Fe(II) salts. Three heteroleptic complexes have been obtained and characterized: [Fe(3-bpp)(H₂L)](BF₄)₂·1.5Acetone exhibiting a LS configuration, [Fe(3-bpp)(H₂L)](BF₄)₂·EtOH which is in a LS state as well, and [Fe(3-bpp)(H₂L)](BF₄)₂·3Acetonitrile·H₂O which shows a HS configuration. Interestingly, the latter can be reversibly converted to its LS state at room temperature, most probably due to absorption-desorption of acetonitrile solvent molecules.

Keywords: coordination compounds, heteroleptic complexes, spin crossover, chemical sensor, organic ligand, LS state, HS configuration, homoleptic complex.