

*Title:* **Synthesis and design of heteroleptic spin-crossover compounds for their application as molecular switches.**

*Student:* Raquel Garcia Cabanas

*Date:* January 2019

*Supervisor/s:* Dr. David Aguilà Avilés

*Departament of Química Inorgànica i Orgànica (Secció de Químic Inorgànica)*

This project has been carried out within the Group of Magnetism and Functional Molecules (GMMF) at the University of Barcelona. The main objective of this research group is based on the synthesis and study of coordination compounds that present interesting physical properties.

In this case, the physical property around which the project has turned is the Spin CrossOver (SCO) and different iron (II) complexes have been designed. Homoleptic and heteroleptic compounds formed by Fe(II) and ligands based on 2,6-bis(pyrazol-3-yl)pyridine (3-bpp) and derivatives with functionalized extremes have been designed. These ligands have a favourable coordination environment to promote spin transition properties and the additional units can be used to coordinate other metal ions. Using the transition property of spin, the iron could be used as a switch to control the interaction between these new coordinated metals. Homoleptic compounds are formed by two equal ligands enveloping the iron while heteroleptic systems are based on two different ligands. This last case is interesting to facilitate the incorporation of additional ions. These potential heterometallic compounds may have very interesting applications, like in quantum computing, making the iron to act as a switch and coordinated external metals as quantum bits.

To achieve this objective, 3-bpp and different 3-bpp derivatives functionalized with pyridine groups and benzoic acid have been synthesized and characterized. Once the ligands have been obtained, the coordinating capacity to encapsulate Fe(II) has been studied.

**Keywords:** Spin Crossover, molecular magnetism, coordination chemistry, Fe(II) complexes, polypyrazolyl ligands, molecular switches.