

## Robust lanthanide complexes and their isotopologues for quantum information

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Keywords: Lanthanides, pyrazolylborate, isotopes, molecular magnetism, quantum information

**Description of the project:** This project is part of a large research consortium which goal is to investigate molecules, in particular paramagnetic complexes, as possible spin qubits, and assess their potential for quantum computing. To do so, lanthanide ions will be chosen as they provide various electronic spin together with the possibility to tune the nuclear spin through isotopic replacements. The ligand environment will provide the correct symmetry and hence electronic structure, help minimize the detrimental influence of other nuclear spins in order to engineer systems with long coherence times. Trispyrazolylborate ligands like L offer such possibilities, together with large denticity and hence large stability constants allowing the necessary study of the complexes in diluted conditions. A first target is then a series of mononuclear complexes with isotopically pure lanthanide centers such as Nd(III), Yb(III) etc..

Through multistep organic synthesis such ligands can also be modified to target dinuclear complexes with various spacers (from L') and hence controlled interactions between the distant lanthanide centers in order to provide two qubits gates. Modification of the ligands to allow grafting on adapted matrices will also be investigated.

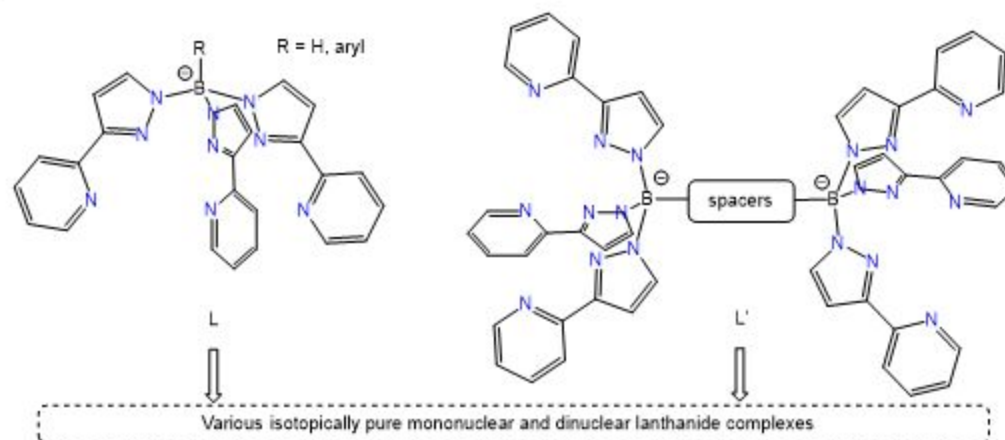


Fig. 1: Example of ligands for designing targeted lanthanide systems.

In this PEPR research project (France 2030 program), the PhD candidate will develop skills in the multistep synthesis of organic ligands, their association with lanthanide ions and their stable isotopes, the study of their optical and magnetic properties, and will benefit from interactions with specialists in various spectroscopies, in theoretical chemistry, and in quantum information processes.

**Candidate profile:** A motivated student with a very good knowledge in organic synthesis is required. Coordination chemistry skills together with interest for a multidisciplinary project going beyond chemistry will be appreciated. The University offers French courses for foreigners and hosts an international Erasmus Mundus program. Students will obtain their PhD degree within the 3 years of the financial support (starting date October 2025). Rennes is a medium size French city less one hour and half away from Paris, offering a relaxing life style with many cultural and sport activities.

Selected recent publications of the group related to the chemistry and isotopic enrichment developed in this project: 1) L. Norel et al. *Angew. Chem. Int. Ed.* **2018**, *57*, 1933-1938. 2) J. Flores Gonzalez et al. *Inorg. Chem. Front.* **2019**, *6*, 1081-1086. 3) J. Flores Gonzalez et al. *Inorg. Chem.* **2021**, *60*, 540-544. 4) F. Pointillart et al. *Chem. Commun.* **2023**, *59*, 8520-8531.