**University of Leicester**

**Chemistry GTA Studentship Project 2022**

**Section 1 – *Supervisor Information***

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| **First Supervisor (Name and Title)** | Dr Fabrizio Ortu |
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**Section 2 – *Project Information***

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| **Project Title** | Frustrated Lewis Pairs in Rare Earth Chemistry |
| **Project**  |
| *Background*Research into Frustrated Lewis Pair (FLP) chemistry has flourished over the last three decades. Their remarkable reactivity comes from the strong polarising capabilities generated by its isolated components (*i.e.* a Lewis acid and a Lewis base). This enables the activation of strategic molecules and substrates which would be otherwise fairly inert, such as H2 and CO2, thus creating essential building blocks to be exploited in catalytic reactions. Crucially, such transformations usually require expensive and toxic transition metals, whilst most FLP systems involve main group elements which are readily available and non-toxic.Very little attention has been given to the use of Rare Earth (RE) and Lanthanide (Ln) metals in FLP chemistry. REs are very strong Lewis acids, however they tend to have very high coordination numbers in their complexes (up to 12), where they try to maximise the number of electrostatic contacts. Because of this, it is extremely challenging to develop FLP systems with REs and these have been underdeveloped compared to main group elements.*The project*In this project, we will target the development of a new class of RE FLPs which will then be employed for the activation of small molecules, such as H2, CO and CO2. The main focus will be on using ligand design to fine tune the coordination chemistry of the RE metal centre and match it with the steric properties of various Lewis bases (*e.g.* amines, phosphines). The ambitious goal will be to deliver facile activation of target substrates and using the most abundant and cheap REs (e.g. La, Ce). To achieve these targets we will employ advanced anaerobic manipulation techniques (Schlenk line and glovebox), paired with the use state-of-the-art equipment and characterisation techniques (e.g. single crystal XRD, multinuclear NMR, EPR, electrochemistry). This project will offer a multi-faceted approach to the theme of green and sustainable chemistry by combining various aspects of synthetic f-element chemistry, spectroscopy and electrochemistry.  |
| **Methodology**  |
| All compounds will be synthesised following advanced anaerobic synthetic protocols used in organometallic and inorganic chemistry, including Schlenk line and glovebox techniques. As part of the project, the student will develop extensive knowledge of ligand design and its application in coordination chemistry, together with a variety of wet chemistry techniques. The synthetic work will be complemented by hands-on experience of a wide range of analytical and spectroscopic techniques, including single crystal X-ray crystallography, electrochemistry, multinuclear NMR spectroscopy, UV/vis/NIR and EPR. |