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| **Scheme: GTA** |  |

School of Chemistry PhD Project Proposal Form

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**Section 2 – *Project Information***

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| **Project Title** | Rare earth reagents for small molecule activation | |
| **Project Highlights:** | 1. | Activation of strategic small molecules (CO, CO2, H2, N2) |
| 2. | Rare earth multimetallic clusters |
| 3. | Applications in molecular magnetism and spintronics |
| **Project Description (max. 700 words; please include project background, aims and methodology) – for external advertising** | | |
| **Background.** Small molecule activation (SMA) is a pillar of the chemical industry. The activation and transformation of CO, CO2, H2 and N2 is vital for the industrial production of numerous commodity chemicals that sustain modern society (global market worth >$600 billion). Reagents and catalysts involved in these transformations classically require expensive, toxic and scarce metals, thus posing significant challenges towards the long-term sustainability of chemical manufacturing. To tackle these challenges, other approaches must be investigated, including the employment of earth-abundant and non-toxic metals – such as rare earth metals. Our research group studies the fundamental chemistry of main group and f-block metals and their application in sustainable synthesis. Most rare earth metals have very low toxicity and remarkable reactivity, which has already led to numerous applications in SMA.  **Aims.** As part of this project, we will develop new rare earth reagents stabilised using sterically demanding organometallic and nitrogen-based ligands. In preliminary work, we have already shown that such complexes can deliver facile activation of CO2 and CS2, leading to the transformation of these basic feedstocks into more complex organic molecules. We have also demonstrated that it is possible to use SMA to form multimetallic rare earth clusters, which are of great interest for their potential applications in molecular magnetism. In this project we will build on these exciting preliminary results and produce a large family on new rare earth compounds and test their reactivity with a range of small molecules, targeting both useful synthetic transformation and multimetallic clusters with interesting magnetic propertis.  **Methodology.** using *state-of-the-art* anaerobic methods (e.g. glovebox, Schlenk line) and a suite of characterisation techniques (multinuclear NMR, X-ray diffraction, UV-vis-NIR spectroscopy, photoluminescence). Additionally, this work will be complemented by comprehensive magnetic studies (EPR and SQUID) to evaluate potential applications of the new materials in molecular magnetism. | | |