

3.1 Publishable summary

According to our original proposal, the primary purpose of the project was to initiate a study about the coordination/activation chemistry of ammonia-borane ($\text{NH}_3\cdot\text{BH}_3$) and related adducts when reacted with different dinuclear transition metal complexes having metal-metal multiple bonds. These adducts are attracting much research interest in recent years as new materials for hydrogen storage, but also from their potential as precursors of new inorganic materials (i.e. polymers, ceramics, etc.) and as reducing and hydroborating reagents in organic chemistry. The main results obtained thanks to the EU funding of this project can be divided in three different areas:

- 1) **Research Outputs:** A wide range of dinuclear molybdenum and tungsten complexes were tested in reactions with various amine-borane adducts under thermal and photochemical activation. We have found that most of the tested complexes having bridging PR_2 ligands were essentially inactive in the catalytic dehydrogenation of these adducts. However, other readily accessible group 6 binuclear complexes having single ($[\text{M}_2\text{Cp}_2(\text{CO})_6]$) or triple ($[\text{Mo}_2\text{Cp}_2(\text{CO})_2(\text{L}_2)]$ [$\text{L}_2 = (\text{CO})_2$ and $\mu\text{-Ph}_2\text{PCH}_2\text{PPh}_2$]) metal-metal bonds are efficient catalysts for the dehydrogenation of a range of amine-borane adducts, including ammonia-borane, under mild thermal activation (333 K). To the best of our knowledge, these unsaturated complexes are the first compounds with multiple M-M bonds shown to be catalytically active in the dehydrogenation of amine-borane adducts. The most relevant results of this investigation have been collected in a recent publication (*Eur. J. Inorg. Chem.* **2013**, 4998). The work has also been presented as Final Project Thesis of two Master Students at the University of Oviedo (years 2012 and 2013), and as a poster in the 2013 national congress of the Spanish Royal Society of Chemistry.
- 2) **Researcher Development:** Thanks to the ERG grant, Dr. García-Vivó has been able to initiate and lead new independent research lines within the Host Institution, this allowing him to attain significant scientific independence. The funding has also been used to hire new research personnel (Master Students) who worked under his direct supervision, and which has provided him with an exceptional opportunity to improve his ability to mentor young researchers. During the time covered by the ERG grant Dr. García-Vivó he has also been involved in related projects in cooperation with other members of the host group, this allowing him to participate in the elaboration of different manuscripts and in the dissemination of these results in different congresses (including two oral presentations).
- 3) **Researcher Reintegration:** During this period, Dr. García-Vivó was able to secure a fellowship from his regional government, which covered his salary for two years (2011-2012). This allowed him to engage in teaching duties of undergraduate students for the Host Institution (Chemistry and Engineering Degrees). His current position is covered by research funds from the host group, but he has ongoing applications to secure a more permanent position within the Spanish research system. Surely, the research results and prestige gained through his successful participation in the ERG program will be a very favourable factor in terms of securing a long-term research position in Spain.