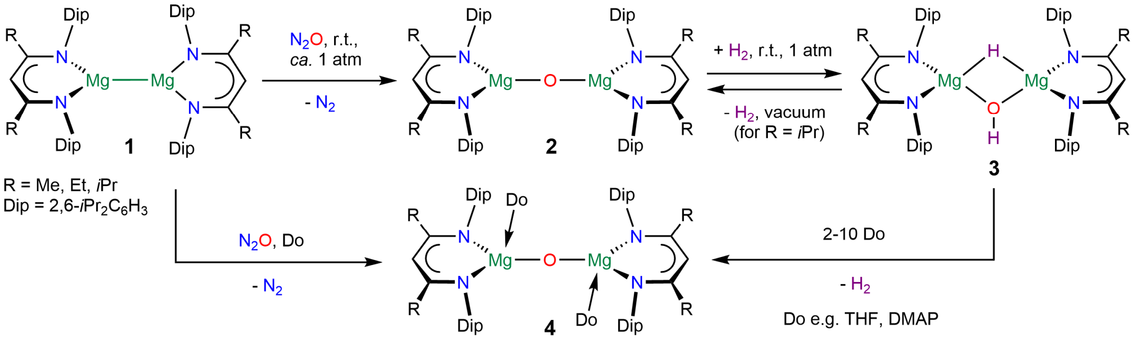
FACILE AND REVERSIBLE BOND ACTIVATION WITH LOW-COORDINATE MAGNESIUM OXIDE COMPLEXES

Samuel Thompson, Stuart Burnett, Rochelle Ferns, Tanja van Mourik,
Aidan P. McKay, Alexandra M. Z. Slawin, David B. Cordes, and Andreas Stasch

EaStCHEM School of Chemistry, University of St Andrews, St Andrews,
KY16 9ST, United Kingdom

Low oxidation state and low-coordinate main group complexes have in recent years been widely investigated for their unusual reactivity.[1,2] Dimagnesium(I) complexes (**1**) can be converted to low-coordinate magnesium oxide complexes (**2**) using nitrous oxide, see scheme. These highly reactive species have been found to readily activate dihydrogen under very mild conditions to afford magnesium hydride-hydroxide complexes (**3**).[3] By varying the remote ligand bulk, the product (**3**) could be destabilized enough to allow the facile dehydrogenation of the bulkiest example. Alternatively, addition of donor molecules could dehydrogenate complexes **3** to afford **4**. Alternative syntheses for the complexes have been explored, and the oxide system has been used in a proof-of-concept study in the catalytic hydrogenation of 1,1-diphenylethylene at low H_2 pressure. We have studied the oxide hydrogenation to complexes **3** computationally and found it to involve nucleophilic attack of an oxide lone pair at a weakly-bound $H_2\cdots Mg$ complex in an S_N2-like manner that induces a heterolytic dihydrogen cleavage. We have investigated bond activation chemistry of other substrates by low-coordinate magnesium oxide complexes, and related chalcogenides,[4] that further demonstrate their high reactivity.



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[1] Power, P. P. *Nature* **2010**, *463*, 171−177.

[2] Weetman, C.; Inoue, S. *ChemCatChem* **2018**, *10*, 4213−4228.

[3] Thompson, S.; Burnett, S.; Ferns, R.; van Mourik, T.; McKay, A. P.; Slawin, A. M. Z.; Cordes, D. B.; Stasch, A. *J. Am. Chem. Soc.* **2025**, *147*, 5247–5257.

[4] Burnett, S.; Ferns, R.; Cordes, D. B.; Slawin, A. M. Z.; van Mourik, T.; Stasch, A. *Inorg. Chem.* **2023**, *62*, 16443–16450.