

Hydrogen release in magnesium and zinc hydride clusters – a route to low-valent Mg^I and Zn^I clusters?

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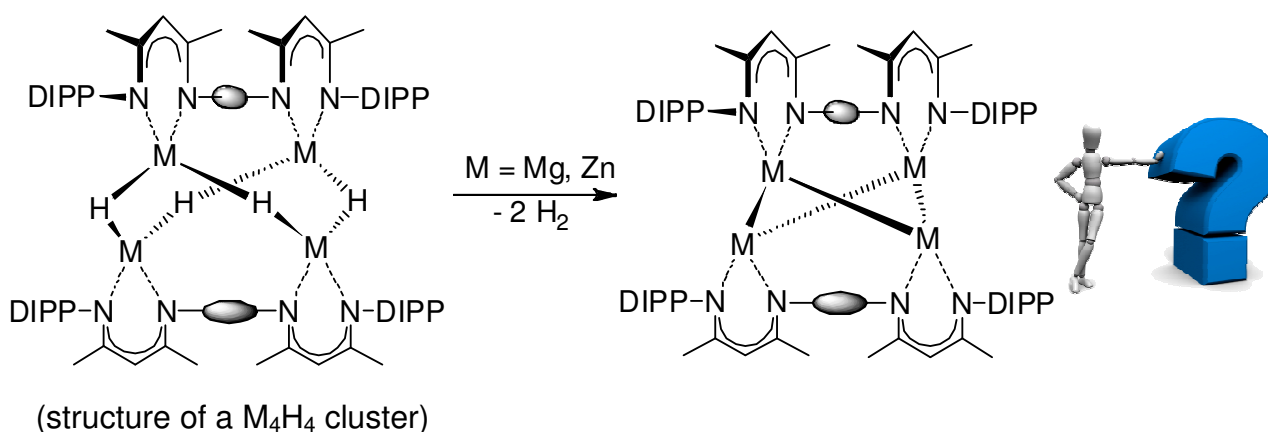
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As the reaction $\text{MgH}_2 \rightleftharpoons \text{Mg}^0 + \text{H}_2$ is reversible, research on magnesium dihydride as a hydrogen storage material is booming.^[1,2] Recent experimental studies and calculations show that small magnesium hydride nano particles are supposed to exhibit much lower dehydrogenation temperatures and faster kinetics.^[3,4] Based on these results, it is our aim to prepare small molecular metal hydride clusters which can function as model systems for hydrogen storage materials.

Using bridged β -diketiminate ligands we were able to obtain several Mg_4H_4 clusters and, depending on the ligand system, in one case a Mg_8H_{10} cluster could be isolated. In these complexes the hydrides occupy different static positions and the first magnetic H,H coupling could be observed by ^1H NMR.

Above 150 °C all magnesium hydride clusters eliminate molecular hydrogen. In addition we were able to study a similar zinc hydride cluster which already releases H_2 at much lower temperatures (< 80 °C).

It is anticipated that hydrogen release results in unique Mg^I and Zn^I clusters. As these multimetallic clusters might be able to take up hydrogen reversibly, their isolation and characterization are an important future goal (see figure).



Literature:

- [1] B. Sakintuna; Lamari-Darkrim, F.; Hirscher, M., *Int. J. Hydrogen Energy* **2007**, *32*, 1121-1140. [2] F. Schüth; Bogdanovic, B.; Felderhoff, M., *Chem.Comm.* **2004**, 2249-2258. [3] L. Pasquini; Callini, E.; Piscopiello, E.; Montone, A.; Antisari, M. V.; Bonetti, E., *Appl. Phys. Lett.* **2009**, *94*. [4] R. W. P. Wagemans; van Lenthe, J. H.; de Jongh, P. E.; van Dillen, A. J.; de Jong, K. P., *J. Am. Chem. Soc.* **2005**, *127*, 16675-16680.