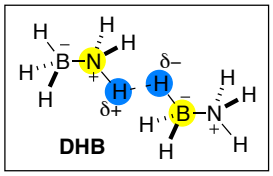
Synthèse et réactivité d'oligomères d'amine-borane

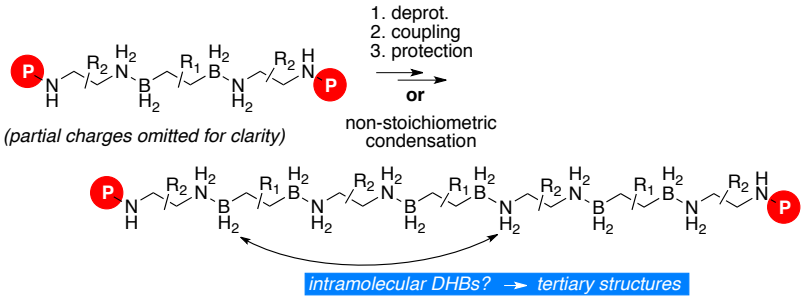
Synthesis and Reactivity of Amine-Borane oligomers

The storage of quickly releasable dihydrogen in dense reservoirs is an important challenge. On a large scale, this would help transition to hydrogen-based clean fuels. On a smaller scale, a portable source of dihydrogen would enable emergency power generation or could be used for chemical reactions. Borazane (NH_3-BH_3) was early on identified as a strong contender for a chemical H_2 reservoir, due to its density and high hydrogen content. However, as a fluffy solid, it is poorly processable; dehydrogenation is not selective in the absence of a catalyst and requires thermal activation at temperature both too high for fuel cells and too low for long-term storage, etc.



The key for the dehydrogenation of amine-boranes in general is the formation of intermolecular dihydrogen-bonds (DHBs). Whenever DHBs are created then dihydrogen can be extruded thermally. Therefore it would be of utmost importance to understand better these interactions. However, contrary to regular H-bonds, DHBs have been overlooked.

The aim of the Ph. D. is to study this weak interaction and to understand how it directs thermal and/or catalytic dehydrogenations through the formation of Boron-based networks. We wish to be able to predict how a specific structure will lead to the release of H_2 that could be used as feedstock, and therefore to optimize the reservoirs.



The Ph. D. candidate will have to prepare a library of short amine-borane oligomers with different spacers (flexible, rigid, chiral, etc.) and study how the molecules self-assemble into structures (including using modeling). Then he•she will have to devise a structure/activity relationship with regard to the dehydrogenation. Beyond, the candidate would have to examine hybrid structures including amino-acids.

The Ph. D. has a focus on synthetic organic chemistry, however at the interface with supramolecular, theoretical, main-group and polymer chemistries. LHCEP is situated on the Lyon-Tech campus, Villeurbanne (69). Potential collaborations with the C2P2 (Villeurbanne, Dr. J. Raynaud) and laboratoire de chimie de l'ENS Lyon (Lyon, Prof. E. Dumont) are foreseen.

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