Carlos Adolfo Castilla Martinez  
Supervisors: Umit Demirci

Synthesis of boranes as potential hydrogen storage materials

One of the alternatives for the increasing energy demand around the world is using hydrogen as an energy carrier, because it is a clean and nontoxic fuel. There are some requirements that a given technology must have to be possibly considered for hydrogen storage, such as high gravimetric/volumetric hydrogen storage capacity, reversibility of storage, stability in use, and cycle life. On this basis, materials (e.g. metal hydrides, carbonaceous porous hosts, metal organic frameworks, and inorganic compounds) have emerged owing to high hydrogen storage capacities. Boron and nitrogen-based compounds have received particular attention as chemical hydrogen storage materials¹.

Hydrazine borane N₂H₄BH₃ (HB) is one boron and nitrogen-based compound that has been studied as hydrogen storage material. Unfortunately, during its decomposition, it releases hazardous and toxic by-products (like N₂H₄ and NH₃). To overcome this problem, derivatives of HB obtained by chemical modification have been developed. Alkali hydrazinidoboranes MN₂H₃BH₃ (MHB) are obtained by substitution of one of the protic Hδ+ of the middle NH₂ of HB by an alkali cation M⁺. Hydrazinidoboranes overcome some issues present in HB thermolysis such as high dehydrogenation temperatures and the formation of the hazardous by-products. To date, some alkaline derivatives of HB have been synthesized (e.g., lithium², sodium³) but some are still missing. It is thus important to obtain them and evaluate their properties.

For the first time, rubidium hydrazinidoborane (RbN₂H₃BH₃) RbHB has been synthesized. This compound is obtained by the reaction of metallic rubidium with HB in THF. The characterizations of this material were done by FTIR, MAS-NMR, XRD and molecular modeling. RbHB presents a crystalline phase and its structure was solved; the evaluation of its dehydrogenation properties and analyses of the solids residues were also carried out.