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Ammonia borane as hydrogen storage material: Study of some of its clusters

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Hydrogen is one of the most promising alternatives as clean fuel. This is because the energy, per unit of fuel mass, released in its reaction with oxygen is higher than that of gasoline, and the chemical product of this combustion is only water. Nevertheless, hydrogen storage methods are still inefficient and expensive. Ammonia borane (AB = H3N-BH3) has emerged as one of the most encouraging hydrogen storage materials due to its relative stability, its versatility, and its capacity of storing high hydrogen densities. However, a series of scientific and technological problems that prevent its use for this purpose remain to be solved. To name one, the methods known today for extracting hydrogen from AB are still insufficient: there is not yet one in which a total hydrogen release from AB is guaranteed at relatively low temperatures. To better address these and others current problems, it would be crucial to know, very precisely, what the structural nature and the intra- and intermolecular interactions involved in AB are. In this work, from a quantum-mechanics point of view, we contribute to this task, revealing important aspects not found by previous studies. A search for stable configurations was performed on the trimers, (AB)3, tetramers, (AB)4 and pentamers, (AB)5, of ammonia borane at high levels of theory. Very rich and complex potential energy surfaces, PESs, are obtained. Cyclic or compact configurations are energetically preferred. Four different types of non-conventional interactions are identified: heteropolar N-H$^{\cdots}$ H-B dihydrogen bonds (the main stabilizing factor), homopolar B-H$^{\cdots}$ H-B dihydrogen bonds, and B$^{\cdots}$H-N and N$^{\cdots}$HB hydrogen bonds. Donor-acceptor charge transfer in heteropolar dihydrogen bonds is the most stabilizing interaction, taking place between a – bonding orbital and a* – anti-bonding one. Despite H$^{\cdots}$H being a priori considered as weak interaction, stabilization energies in ammonia borane clusters are comparable to the interactions responsible for the stabilization of water clusters at the same level to theory.

Biography

Cacier Z Hadad has completed his PhD at the University of Chile. He is the Co-Head of the Theoretical Chemical Physics Group of the University of Antioquia, Colombia. He is author of many relevant papers about theoretical aspects and models of diverse physicochemical phenomena.

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