

Public Abstract

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Chemistry

Sixteen Valence-Electron Species Containing Boron: Structural Diversity Abounds

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[B, C, F, H<sub>2</sub>] and [B, N, O, H<sub>2</sub>] have been investigated via high level *ab initio* calculations. Both cyclic and acyclic connectivities have been examined for the singlet state. Chemical intuition suggests a ketene-like structure for each system, with the general form H<sub>2</sub>XBY, where X = C or N and Y = F or O. The calculations yield a variety of possible structures for these species, including both cyclic and the expected acyclic, hydrogen-bonded and fluorine-bridged. Eight minima have been located for [B, C, F, H<sub>2</sub>] and fifteen minima have been located for [B, N, O, H<sub>2</sub>]. All three possible connectivities for N, B and O have been examined. N-B-O was found to be the most stable connectivity, followed by N-O-B and O-N-B. For both [B, C, F, H<sub>2</sub>] and [B, N, O, H<sub>2</sub>], each isomeric form has at least one unique vibrational frequency of sufficient intensity to be identified through IR. Five transition structures have been located for the [B, C, F, H<sub>2</sub>] system, each connecting two of the minima. Barriers to the rearrangements between isomers have also been evaluated. Each of these systems has been analyzed in terms of the Lewis acidity of BH, and BH affinities have been computed. AIM and NBO analyses have also been carried out to gain an understanding of the bonding in the various isomeric forms of [B, C, F, H<sub>2</sub>] and [B, N, O, H<sub>2</sub>].