SIXTEEN VALENCE-ELECTRON SPECIES CONTAINING BORON: STRUCTURAL DIVERSITY ABOUNDS

Aaron Corum

Dr. Carol A. Deakyne, Advisor

ABSTRACT

[B, C, F, H_2] and [B, N, O, H_2] 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_2XBY, 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_2] at both calculational levels. Fifteen minima have been located for [B, N, O, H_2]. Barriers to the rearrangements between isomers in the [B, C, F, H_2] system have also been evaluated. AIM and NBO analyses have been carried out to gain an understanding of the bonding in the various isomeric forms of [B, C, F, H_2] and [B, N, O, H_2].