Ab initio Calculations of the Nuclear Quadrupole Coupling Constants of $BH_{n=2,4}X^+$ ($X = NH_3, PH_3, H_2O, H_2S$)

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Z. Naturforsch. **60a,** 37 – 40 (2005); received July 31, 2004

The electronic structure and strength of acid-base bonding in the protonated boron-Lewis complexes $BH_{n=2,4}X^+$ ($X = NH_3$, PH_3, H_2O, H_2S) and their neutral parents were studied. The results showed that in the H_2BX^+ monocations the electron releasing from the donor atom in X to BH_3 is significant and more complete than in the other studied complexes. Therefore the bonding between the donor and acceptor in H_2BX^+ is strongest. To obtain these data, the electric field gradient (EFG) at the quadrupolar nuclei in each complex was calculated. The EFG's of the boron atom and other quadrupolar nuclei were calculated by the Gaussian 98 program, using the MP2/6-31G** method.

Key words: Ab initio Calculations; Acid-Base Lewis; Boron; EFG; NQR.