A MICROWAVE STUDY OF PARTIALLY BOUND H_2O-BF_3

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We report the microwave spectrum and structure of the partially bonded donor - acceptor adduct H_2O-BF_3. H_2O and BF_3 react to form two compounds, a monohydrate and a dihydrate, both with well defined stoichiometries and melting points. For the monohydrate, previous X-ray diffraction work[a] indicates a B-O bond distance of 1.532 Å (equal to the sum of covalent radii) and a tetrahedral geometry at the boron. In the gas, however, we find a bond length of 1.90 Å and an out-of-plane distortion of the BF_3 of only 8^o. Thus, while the B-O bond in the solid is an "ordinary" dative linkage, the bond in the gas phase system appears to be only partially developed. The large changes in bond length and bond angle which occur upon crystallization (0.4 Å and 9^o, respectively) will be discussed in comparison with other partially bound systems which have been investigated in our laboratory. Ab initio calculations place the gas phase binding energy at 9.6 kcal/mol, which is a very reasonable value for a partially formed dative bond.

[a] Von D. Mootz and M. Steffen *Z. Anorg. Allg. Chem.* **483**,171,1981.