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A Cluster Beam Study of Boron Oxide Chemistry With HF

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Abstract: Using an improved version of the Cluster Beam technique, we have probed the chemistry of B(x)O(y)H(z)+ clusters with HF as a function of the B:O:H stoichiometry of the cluster reactant. Reactant compositions were varied from pure **boron** to stoichiometric oxide, with and without added hydrogen. **Boron** oxide clusters react with HF at about 50% efficiency and the collision energy dependence suggests that the reaction is sterically hindered, i.e. reaction occurs primarily at certain sites in the oxide network. The principle reaction is attack by the HF on a terminal BO group, followed by loss of fragments such as FBOH and FBO. Addition of a single hydrogen atom has a significant effect on the chemistry. The products of the reaction (and probably the mechanism) are similar to those for the pure oxides, but the reactivity is substantially reduced. We propose that the hydrogen atom blocks a reactive site on the cluster, thereby reducing the reactivity. Pure **boron** clusters react by addition of HF, followed by elimination of fragments such as BF and HBF. For small clusters the reaction is efficient, but we see activation barriers grow in for the larger clusters, suggesting that there may be activation barriers for **boron** surface-HF reactions as well. In contrast to the situation for the oxides, addition of hydrogen to the pure **boron** clusters generally increases the reactivity with HF. (jg)

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