MOLECULAR BEAM INFRARED SPECTRUM OF THE HF STRETCHING FUNDAMENTAL BAND OF THE HF-BF_3 COMPLEX

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The microwave spectrum of the antihydrogen bonded HF-BF_3 complex has recently been reported by Philips et al. [a]. The spectrum reveals a near symmetric F-BF_3 heavy atom frame with the proton slightly off axis, and a small barrier to internal rotation of the H atom against the F atoms. Here, we have investigated the H-F stretching fundamental band of this complex using a molecular beam optothermal spectrometer and a color-center laser. Two subbands are expected: a parallel band with Δ m = 0 selection rules and a perpendicular band with Δ m = ± 1 selection rules. At present, only the perpendicular band has been observed. This band has the appearance of a perpendicular band of a symmetric rotor, but with anomalously strong ^{r}R transitions and weak ^{p}P transitions. Upper state constants are obtained fixing the ground-state constants to the microwave-determined values. The band has a large positive ζ Coriolis constant, from which an estimate of the barrier to internal rotation can be made. A search is presently underway to locate the expected weaker Δ m=0 parallel component.

[a] J. A. Philips, M. Canagaratna, H. Goodfriend, A. Grushow, J. Almlof and K. R. Leopold *J. Am. Chem. Soc.* **117**, 12459 (1995)