ANALYSIS OF THE FIRST HIGH RESOLUTION FTS INFRARED SPECTRA OF $F_2{}^{11}BOH$: THE ν_8, ν_9, $2\nu_9$ AND ν_4 BANDS.

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The reactive F_2BOH molecule was first detected by microwave spectroscopy [a], and very recently observed by matrix IR spectroscopy [b]. We report here the first high resolution infrared study of F_2BOH. F_2BOH has been produced in a slow flow of (^{11}B and natural) BF_3 through a glass tube filled of some specks of quartz (all using stainless stell equipment) on which water had been deposited. The IR spectrum has been recorded from 400 cm^{-1} to 1600 cm^{-1} at high resolution (2-3 x 10^{-3} cm^{-1}) using the Wuppertal Bruker 120 HR interferometer equipped with a cell of 1.2 m path length. In addition, ground state parameters have been determined from recent microwave measurements performed in Lille [c]. Among the recorded infrared bands, two c-type out-of-plane fundamental bands ν_8 (BF_2 bend) and ν_9 (OH torsion) located at 684.16 cm^{-1} and 522.86 cm^{-1}, respectively, were analysed using a simple Watson -type Hamiltonian. The a/b type hybrid $2\nu_9$ and ν_4 bands centered at 1042.87 and 961.49 cm^{-1} were also studied. The analysis of ν_4 (OH bending mode) was complicated by the existence of "classical" vibrational rotational resonances linking the 4^1 energy levels with those of the 7^19^1 dark overtone state. More surprising is the fact that both in the $2\nu_9$ and ν_4 bands, the P- and R-lines exhibit a regular doublets structure (of about 0.005 and 0.003 cm^{-1} respectively) which indicates the existence of large amplitude motions in the F_2BOH molecule.

[a] H. Takeo and R. F. Curl, *J. Chem. Phys.* **56**, 4314 (1972)
[b] M. E. Jacox, K. K. Irikura , and W. E. Thompson, *J. Chem. Phys.***113**, 5705 (2000)
[c] J. Demaison, J.F.D'Eu et al. *private communication*