AN ANALYSIS OF THE FIRST HIGH RESOLUTION FTS INFRARED SPECTRA OF F$_2$BOH: THE $\nu_8$, $\nu_9$, 2$\nu_9$ AND $\nu_4$ BANDS.

A. PERRIN, J.-M. FLAUD, Laboratoire de Photophysique Moléculaire, CNRS, Université Paris Sud, Campus d’Orsay, Bat 350, 91405 Orsay Cedex, France; H. BÜRGER, D.COLLET, Anorganische Chemie, FB 9, Universität-Gesamthochschule, D-42097 Wuppertal, Germany; J.DEMAISON, Laboratoire PhLAM, CNRS, Université de Lille I, Bat. P5, 59655 Villeneuve d’Ascq Cedex, France.

The reactive F$_2$BOH 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$_2$BOH. F$_2$BOH 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 steel 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 $\nu_8$ (BF$_3$ bend) and $\nu_9$ (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 $\nu_4$ bands centered at 1042.87 and 961.49 cm$^{-1}$ were also studied. The analysis of $\nu_4$ (OH bending mode) was complicated by the existence of “classical” vibrational rotational resonances linking the 4$^1$ energy levels with those of the 7$^2$9$^2$ dark overtone state. More surprising is the fact that both in the 2$\nu_9$ and $\nu_4$ 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$_2$BOH molecule.

$^c$J. Demaison, J.F.D’Eu et al. private communication