HIGH RESOLUTION INFRARED STUDY OF THE ν_4 AND $2\nu_9$ BANDS OF $^{11}BF_2OH$ AND $^{10}BF_2OH$: EVIDENCE OF LARGE AMPLITUDE EFFECTS FOR THE OH-TORSION-BENDING MODES IN THE 9^2 AND 4^1 STATES

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High resolution (2-3 x 10^{-3} cm^{-1}) Fourier transform infrared spectra of gas phase ^{11}B and ^{10}B enriched and natural samples of BF_2OH (difluoroboric acid) were recorded at Wuppertal and Richland. Starting from the results of previous studies[a], it has been possible to perform the first rovibrational analysis of the ν_4 (BOH bending) and $2\nu_9$ (first overtone of ν_9, the OH torsional mode) bands located at 961.5 and 1042.9 cm^{-1}) and at 961.7 and 1043.9 cm^{-1}) for the $^{11}BF_2OH$ and $^{10}BF_2OH$ isotopic species respectively. In addition to various "classical" vibration-rotation resonances, large amplitude effects were observed for both the $2\nu_9$ and ν_4 bands. These result in a doubling of levels of about 0.004 and 0.003 cm^{-1}) for the 9^2 and 4^1 states respectively. The energy level calculations account for these large amplitude torsion-bending perturbations using the IAM- type method[b], and for the "classical" vibration -rotation resonances.

[a] A.Perrin, M.Carvajal-Zaera, Z.Dutkiewicz, J.M.Flaud, D.Collet, H.Bürger, J.Demaison, F.Willaert, H.Mader, and N.W.Larsen, Mol. Phys. 102 , 1641 (2004), J.Breidung, J.Demaison, J.F.D'Eu, J.M.Flaud, L.Margulès, D.Collet, E.B.Mkadmi, A.Perrin, and W.Thiel, J. Mol. Spectrosc. 228, 7 (2004).

[b] L.H.Coudert and J.T.Hougen, J. Mol. Spectrosc. 130, 86 (1988)