SEMIEXPERIMENTAL STRUCTURE OF THE NON-RIGID BF_2OH MOLECULE BY COMBINING HIGH RESOLUTION INFRARED SPECTROSCOPY AND AB INITIO CALCULATIONS.

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In BF_2OH, difluoroboric acid, the OH group is the subject of a large amplitude torsion motion which induces a splitting in the rotational spectrum as well as in the high-resolution infrared spectrum. It is interesting to check whether it is still posible to determine a semiexperimental equilibrium structure for such a molecule. For this goal, the rotation-vibration interactions constants have been experimentally determined by analyzing all the fondamental bands. They have also been computed ab initio using two different levels of theory. The results of the analysis as well as the determination of the structure will be reported.