THEORETICAL MODELING OF INFRARED SPECTRA OF ASPIRIN AND ITS DEUTERATED DERIVATIVE

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Theoretical simulation of the ν_s stretching band is presented for aspirin (acetylsalicylic acid) and its OD derivative at 300 and 77 K. The simulation takes into account an adiabatic coupling between the high-frequency O-H(D) stretching and the low-frequency intermolecular O...O stretching modes, linear and quadratic distortions of the potential energy for the low-frequency vibrations in the excited state of the O-H(D) stretching vibration, resonance interaction between two hydrogen bonds in the dimer, and Fermi resonance between the O-H(D) stretching and the overtone of the O-H(D) bending vibrations. The effect of deuteration and the temperature has been successfully reproduced by our model calculations.Infrared, far-infarared, Raman and low-frequency Raman spectra of the polycrystalline aspirin have been measured. The geometry and experimental frequencies is compared with the results of our B3LYP/6-31++G** calculations.