CALCULATED VIBRATIONAL OVERTONE INTENSITIES IN PHENOL AND ITS COMPLEXES WITH WATER, METHANOL AND AMMONIA

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We have calculated fundamental and overtone OH-stretching vibrational band intensities of phenol and hydrogen-bonded complexes of phenol with water, methanol and ammonia. The intensities were determined with a harmonically coupled anharmonic oscillator local mode model, *ab initio* calculated dipole moment functions, and scaled *ab initio* calculated local mode parameters. We compare our calculated intensities for phenol with vapor phase experimental data. The OH bonds involved in hydrogen bonding generally show a strong enhancement of the fundamental intensity and our calculations are in agreement with this. Our calculations for the phenol complexes predict a significant weakening in intensity of the first overtone whereas for intensities of the higher overtone transitions are comparable to those of phenol. We explain this interesting intensity pattern on the basis of the calculated dipole moment function and Morse oscillator matrix elements of the local mode.