Temperature dependence of the ν_s(OH) band shape of ortho-Mannich bases in gas phase and liquid xenon solution.

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Streszczenie

Infrared spectra of the two ortho-Mannich bases 2-(*N*,*N*-dimethylaminomethyl)-4-chlorophenol (**I**) and 2-(*N*,*N*-dimethylaminomethyl)-4,6-dichlorophenol (**II**) with a medium-strong intramolecular hydrogen bond, were measured in a wide frequency (4000-50 cm^{-1}) and temperature (−105°C to +120°C) range in liquid Xe, CCl_4 solutions and gas phase. The temperature studies of the first and second spectral moments of the ν_s(OH) band in liquid Xe within the temperature range from −105 to +30°C allow for the analysis of the ν_s(OH) mode coupled with the low-frequency vibrations (ν_l) of the non-linear hydrogen bond. Transitions located at ca. 150, 250 and 340 cm^{-1} were selected as such ν_l modes. The effective coupling parameter between high-frequency ν_s(OH) and low-frequency ν_l vibrations of the hydrogen bridge was evaluated: $b = \alpha_{ssl}/\omega_l \simeq 0.7$. Model calculations accounting for the hot and combination transitions give satisfactory reproduction of the gas phase ν_s(OH) and ν_s(OD) bands shapes. Both temperature experiments and model calculations predict that even at 0 K the halfwidth of the ν_s(OH) band can be quite large, viz. ca. 200–400 cm^{-1}.

Adres publiczny

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