Temperature dependence studies and model calculations of ν(OH) and ν(OD) band shapes of salicylaldehyde.

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Streszczenie

IR spectra of salicylaldehyde (OH and OD) have been studied over a wide temperature range in teh vapor phase, liquid Xe solution and Ar matrices. Far IR and Raman spectra have been obtained. Ab initio calculations at the 3-21G∗∗ level have been performed in order to establish the geometry of the molecule, normal coordinates and frequencies of vibrations. It has been found that profiles of both ν(OH) and ν(OD) bands are formed by the fundamental transition ν_s, by the weak sum transition $\nu_s + \nu_3$, where $\nu_3 = 264$ cm^{-1} is an in-plane vibration involving deformation of the chelate ring with significant stretching of the intramolecular H-bond, and by a series of hot transitions from levels of ν_3 and other low frequency modes (ν_i) of the chelate ring. The ν(OH) profile is perturbed additionally by several Fermi resonances with overtones and combinations of bending vibrations δ(OH). Anharmonicity constants, which characterize coupling of ν_s with ν_i and δ(OH), have been derived from the temperature dependence of the first spectral moments of the bands, using the results of the 3-21G∗∗ treatment. Model calculations of ν(OH) and ν(OD) band shapes have been performed.

Adres publiczny

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