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Wanted v(CH) band: IR spectra of complex of trifluoroacetic acid and acetone in the gas phase

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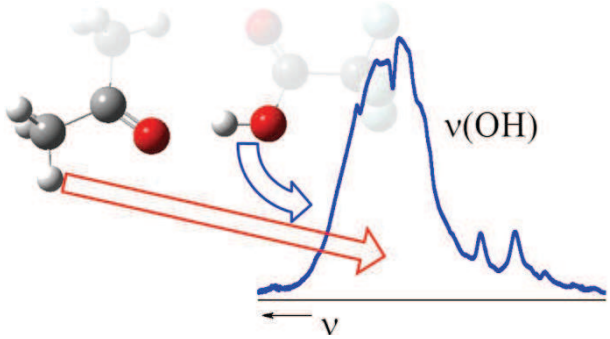
The FTIR spectra of mixtures of trifluoroacetic acid (TFA) and acetone (H6 and D6 isotopologues) were recorded in the gas phase at temperature T = 21 °C. After subtracting the bands of acid and acetone monomers and dimer of TFA, the spectra of TFA···acetone (H6 and D6) were obtained.[1] Additionally, the spectra of complexes between TFA and diethyl ether (H10 and D10) were found in the same way.

All spectra have an intense broad v(OH) band located in the range of 3500 – 2100 cm^{-1}. It was found that in the spectra of TFA···ether the pronounced v(CH) and v(CD) bands are observed against the background of the v(OH) band. These bands are slightly shifted from the corresponded bands in the spectra of ether monomers. In contrast, in the spectra of TFA···acetone complexes there are no explicit v(CH) (v(CD)) bands in the region of these monomer bands. This is the signature of a strong interaction of ν_{OH} and $\nu_{CH(CD)}$ vibrational modes in these complexes. Because the same effect is observed in the spectra of acetic acid dimers,[2] the ν_{OH}–ν_{CH} interaction can be caused by an electronic structure of the (CH_3)–C=O···HO fragment and should be taken into account during a v(OH) band reconstruction of similar complexes.



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[1] R.E. Asfin, *J. Chem. Phys. A,* **2019**, *123*, 3285.
[2] H. T. Flakus, B. Hachuła, *Spectrochim. Acta, Part A*, **2011**, *79*, 1276.