Abstract Submitted
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Ultrafast 2D IR vibrational echo chemical exchange spectroscopy[1] JUNRONG ZHENG, MICHAEL FAYER, Stanford University, Chemistry Department — Ultrafast 2D IR vibrational echo chemical exchange spectroscopy, akin the 2D NMR methods, is applied to the study of dynamics of weakly hydrogen bonded solute-solvent complexes in liquid solutions. The strengths of the solute-solvent hydrogen bonds are adjusted by modifying the chemical structures of the solutes and solvents. For the eight samples studied, the formation enthalpies vary from -0.6 kcal/mol to -2.5 kcal/mol, and the dissociation time constants vary from 3 ps to 32 ps. The dissociation rates of the hydrogen bonds are found to be strongly correlated with their formation enthalpies. The correlation can be described with an equation similar to the Arrhenius equation. As another example of chemical exchange spectroscopy, the rate of carbon-carbon single bond rotational isomerization of an ethane derivative in room temperature liquid solution is measured. Based on the experimental results and density functional theory calculations, the time constant for the ethane internal rotational isomerization under the same conditions is about 12 ps.

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