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Hole-filling spectroscopy of the trans-formanilide-H₂O and tryptamine-H₂O complexes: Solvent shuttling and solvent loss¹ TIMOTHY ZWIER, JASPER CLARKSON, Dept. of Chemistry, Purdue University — Studies of molecular clusters formed and cooled in a supersonic expansion offer unique opportunities to study novel types of dynamical processes under well-defined conditions. This talk will highlight recent studies in our laboratory at Purdue involving water-containing complexes with trans-formanilide (TFA) and tryptamine (TRA). In TFA-H₂O, stimulated emission pumping is used to initiate a unique type of reaction in which a single water molecule is shuttled between remote hydrogen-bonding sites on the same solute molecule. The energy barrier to isomerization is measured for shuttling the molecule in either direction. In TRA-H₂O and TRA(ND₂)-D₂O, infrared excitation is used to dissociate the water molecule from a flexible molecule with well-defined starting geometry. Isomer-specific product quantum yields of the TRA monomer product will be reported as a function of the XH or XD oscillator excited. The interplay between water loss and conformational isomerization of the flexible TRA molecule will be discussed.

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