



## IR spectroscopy of ion-ligand Complexes: Intermolecular potentials, microsolvation processes, and chemical reaction intermediates

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Intermolecular ion-ligand interactions are investigated by high resolution infrared spectroscopy of cation complexes,  $AH^+ \dots L_n$ , in the gas phase and quantum chemical calculations. Spectra at the level of rotational resolution provide detailed information about the interaction potential of dimers and trimers ( $n=1,2$ ), such as structures and reactivity, binding energies, force constants, frequencies of intermolecular and intramolecular modes, anisotropy, transition states for isomerization, tunneling splittings and barriers for internal rotation and inversion, relaxation dynamics and coupling between inter- and intramolecular degrees of freedom. The nature of the interaction can vary from weak induction forces via stronger electrostatic interactions to strong covalent or charge transfer bonds. Size dependent frequency shifts and photofragmentation patterns of larger clusters ( $n=2-15$ ) provide insight into the microsolvation process (structure and stability of isomers, formation of solvation shells) and bridge the gap between the monomer properties and bulk attributes. The investigated systems are prototype systems with relevance for biological binding motifs (hydrogen and pi-bonding), organic reaction mechanisms (e.g., substitution reactions and proton transfer), and ion-molecule reactions (e.g., plasma chemistry).