PROBING INTRA- AND INTER- MOLECULAR INTERACTIONS VIA IRMPD EXPERIMENTS AND COMPUTATIONAL CHEMISTRY

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Experiments carried out at the CLIO Free Electron Facility have been used to probe a range of novel bonding motifs and dissociation dynamics in a variety of chemical systems. Among these are species which exhibit anion-pi interactions in complexes of halide ions with aromatic ring systems with electron withdrawing substituents; charge solvated and zwitterionic clusters of protonated methylamines with phenylalanines; hydrogen bonded dimers of nucleic acid analogues and Pd complexes potentially involving agnostic hydrogen bond interactions. Accompanying DFT computational work is used to assist in identifying the most probable structure(s) present in the IRMPD experiments.