“Probing Non-covalent Interactions Through Vibrational Spectroscopy of Cold Complexes”

A new strategy to probe site-specific non-covalent interactions in peptidic complexes is presented. It exploits the ability of electrospray ionization to inject intact binary structures from solution into the gas phase, and couples it to cryogenic ion infrared spectroscopy. The ions of interest are cooled to 10K and tagged with D_2 in a cryogenic ion trap before being mass-selected and probed by single-photon infrared photodissociation spectroscopy. Although the various transitions recovered with this method are intrinsically sharp (<10 cm^{-1}), the complexity of the congested spectra often preclude structural analysis by direct comparison with calculated patterns. We demonstrate that small molecular variation and single-site isotopic substitution provide a powerful means with which to empirically reveal which transitions, in the dense background, are due to particular functional groups. This is first demonstrated by following the structural changes induced by ion binding in diphenylacetylenes based molecular switches. A similar strategy is also used to unravel the nature of the key intermolecular interactions responsible for the enantioselective activity of a synthetic tripeptide bromination catalyst.

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SPECIAL SEMINAR

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