ISOLATION OF ION-DRIVEN CONFORMATIONS IN DIPHENYLACETYLENE MOLECULAR SWITCHES USING CRYOGENIC INFRARED SPECTROSCOPY

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We report the infrared predissociation spectra of a family of ionic diphenylacetylene molecular switch complexes.[a] The electrosprayed complexes were trapped and cooled in a cryogenic (10K) quadrupole ion trap and tagged with molecular deuterium. The infrared spectra of the vibrationally cold species reveal sharp transitions over a wide energy range (800 - 3800 cm^{-1}), facilitating comparison to harmonic spectra. The evolution of the band pattern upon derivatization of the complexes exposes the signatures of the amide, urea, and carbonyl functionalities, enabling unambiguous identification of the non-covalent interactions that control the secondary structure of the molecule. Complexation with the tetramethylammonium cation reveals a conformation analogous to that of the neutral molecule, while halide ion attachment induces a conformational change similar to that observed earlier in solution. In several cases, both the donor and acceptor groups involved in the multidentate H-bonds are observed, providing a microscopic mechanical picture of the interactions at play.

[a] I. Jones, and A. Hamilton, *Angew. Chem. Intl. Edit.* **50**, 4597 (2011).