VIBRATIONAL CHARACTERIZATION OF SIMPLE PEPTIDES USING CRYOGENIC INFRARED PHOTODISSOCIATION OF H_2-TAGGED, MASS-SELECTED IONS

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We present infrared photodissociation spectra of two protonated peptides that are cooled in a 10 K quadrupole ion trap and tagged with weakly bound H_2 molecules. Spectra are recorded over the range 600 - 4300 cm^{-1} using a table-top laser source, and are shown to result from one-photon absorption events. This arrangement is demonstrated to recover sharp ($\Delta\ \nu$ = 6 cm^{-1}) transitions throughout the fingerprint region, despite the very high density of vibrational states in this energy range. The fundamentals associated with all of the signature N-H and C=O stretching bands are completely resolved. To address the site-specificity of the C=O stretches near 1800 cm^{-1}, we incorporated one ^{13}C into the tripeptide. The labeling affects only one line in the complex spectrum, indicating that each C=O oscillator contributes a single distinct band, effectively reporting its local chemical environment. For both peptides, analysis of the resulting band patterns indicates that only one isomeric form is generated upon cooling the ions initially at room temperature into the H_2 tagging regime.