

VIBRATIONAL SPECTRA OF CRYOGENIC PEPTIDE IONS USING H₂ PREDISSOCIATION SPECTROSCOPY

CHRISTOPHER M. LEAVITT, ARRON B. WOLK, MICHAEL Z. KAMRATH, ETIENNE GARAND, MARK A. JOHNSON , *Sterling Chemistry Laboratory, Yale University, PO Box 208107, New Haven, CT 06520*; and MICHAEL J. VAN STIPDONK, *Department of Chemistry, Wichita State University, 1845 Fairmont Ave, Wichita, KS 67208*.

H₂ predissociation spectroscopy was used to collect the vibrational spectra of the model protonated peptides, GlyGly, GlySar, SarGly and SarSar (Gly=glycine and Sar=sarcosine). H₂ molecules were condensed onto protonated peptide ions in a quadrupole ion trap cooled to approximately 10 K. The resulting spectra yielded clearly resolved vibrational transitions throughout the mid IR region, 600-4200 cm⁻¹, with linewidths of approximately 6 cm⁻¹. Protonation nominally occurred on the amino terminus giving rise to an intramolecular H-bond between the protonated amine and the neighboring amide oxygen. The sarcosine containing peptides incorporate a methyl group onto either the amino group or the amide nitrogen causing the peptide backbone to adopt a different structure, resulting in the shifts in the amide I and II bands and the N-H stretches.