ROTATIONALLY RESOLVED ELECTRONIC SPECTRA OF GAS PHASE AMINO ACIDS[a]

JESSICA A. THOMAS and DAVID W. PRATT, *Department of Chemistry, University of Pittsburgh, Pittsburgh, PA 15260*.

Amino acids contain 10 to 27 atoms, giving rise to a large number of possible conformations in the gas phase.[b,c] Fewer conformations are possible when the amino acids are capped, such as in Ac-Trp-NH_2, to simulate a longer peptide chain. Capped versions of the three amino acid molecules that fluoresce in the UV region have previously been studied using vibrationally resolved UV, as well as UV-UV hole burning and UV-IR hole filling spectroscopic methods.[d] In this study, rotationally resolved UV spectra in combination with ab initio calculations will be compared to these previous results. The preferred conformation of the isolated molecules will be determined, as well as their relative energies, and their dipole moments in the ground and first excited states. Preliminary results on Ac-Trp-NH_2 (NATA) will be reported here.

[a]Work supported by NSF

[b]S.J. Martinez III, J.C. Alfano, and D.H. Levy, J. Mol. Spectros. 156, 421 (1992).

[c]L.C. Snoek, R.T. Kroemer, M.R. Hockridge, and J.P. Simons, Phys. Chem. Chem. Phys., 3, 1819 (2001).

[d]B.C. Dian, A. Longarte, P.R. Winter, T.S. Zwier, J. Chem. Phys., 120, 133 (2004) and references therein.