CONFORMATIONAL INVESTIGATION OF A SERIES OF ISOLATED MODEL DIPEPTIDES

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Model dipeptides based on single amino acids blocked at the amine with an acetyl group and at the carboxylic acid with an N-methylamide group have long served as tractable computational and experimental systems with which to model the relative stabilities of different peptide conformations. Replacing the N-methylamide blocking group with an N-phenylamide allows a very closely related set of compounds to be studied using electronic spectroscopy in supersonic jet expansions. Thus a series of compounds based on amino acids with small side chains, Ac-Gly-NHPh, Ac-Ala-NHPh, and Ac-Pro-NHPh, has been investigated. All evidence, including comparison to the vibronic spectra of the simpler N-phenylamides, formanilide and acetanilide, suggests that the dominant conformer in these model dipeptides adopts a C7 structure. Results from this study are compared to ab initio Hartree-Fock and MP2 calculations as well as to previous condensed phase spectroscopic studies on the N-methylamide-blocked systems.