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Mass spectrometric investigation of the decomposition of canonical structures of α -amino acids

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The decomposition of canonical structures of α -amino acids has been investigated by using charge remote fragmentation. Neutral amino acids in condensed-phase have zwitterionic structures and are non-volatile, which makes gas-phase studies difficult. Previously reported mass spec studies of amino acids generally utilize ionization (protonation, deprotonation, metallation) of the amino acid group. In this work, we describe studies of amino acids where the ionization occurs away from the α -amino acid moiety. Therefore, we report studies of para-substituted phenylalanine derivatives, where the substituents are either a sulfonate (SO_3^-) or trimethylammonium (NMe_3^+) group. For both ions, we find that the main dissociation pathway involves loss of ammonia to form α -lactone. For the sulfonate, loss of ammonia is the only dissociation pathway, whereas loss of CO_2 is also observed for the ammonium derivative, indicating an effect of charge polarity on the dissociation. The dissociation processes of the α -lactones have also been examined, and are also found to be dependent on the charge polarity, which is readily explained in terms of benzylic positive charge character in the decomposition transition state. We have also examined the effect of solvation on the dissociation, and found that while the addition of single water does not change the reaction, dramatic changes are observed upon addition of two solvent molecules, which indicates an interaction between the solvent and the amino acid group.

Biography

Paul G Wenthold received a PhD from Purdue University, and was a Postdoctoral Associate at the University of Colorado. After a short appointment as an Assistant Professor at Texas Tech University, he moved back to Purdue, where he was promoted to Associate Professor in 2004. His work involves the investigation of physical organic chemistry by using mass spectrometry, and is interested in the electronic structures of open-shell intermediates and the reactivity and thermochemical properties of reactive molecules in the gas phase.

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