

4th World Congress on

MASS SPECTROMETRY

June 19-21, 2017 London, UK

Gas-phase dehydration of protonated polyglycines

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Loss of water is a common reaction after collisional activation of protonated polypeptides. We selected polyglycines as prototypical polypeptides for examination of the source of the water loss. Polyglycines labeled with ¹⁸O at specific peptide linkages were custom-synthesized using Wang resin. Protonated tetra-glycine loses water predominantly from its first peptide linkage. Loss of water from the second peptide linkage increases in abundance with increasing peptide length, and becomes the predominant channel in hexaglycine. For tetraglycine, both density functional theory (DFT) calculations and infrared multiple photon dissociation (IRMPD) experiment strongly suggest that the dehydration product is formed by loss of water from the first peptide bond that results in a protonated imidazole-4-one. Preliminary DFT and collision-induced dissociation (CID) results continue to support this structural interpretation for the dehydration products of pentaglycine and hexaglycine that involve loss of water from the first peptide bond. Those results that involve water loss from the second peptide bond suggest a series of rearrangement reactions prior to dissociation. Our results thus indicate multiple pathways of polyglycines dehydration that are competitive.

Biography

K W Michael Siu is a Canadian chemist, currently a Distinguished Research Professor at York University. He is a Fellow of the Royal Society of Canada and Chemical Institute of Canada.

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