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Specific Peptide-Bond Dissociation and Effects of a Phenyl Group of Some Peptide Model Molecules

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Near-edge X-ray absorption fine structure (NEXAFS) spectra at carbon, nitrogen, and oxygen K-edges of some peptide model molecules were measured utilizing an orthogonal acceleration time of flight mass spectrometer and were calculated with time-dependent density functional theory. Excitation source such as soft X-ray photons were from synchrotron radiation at Taiwan Light Source. The intensity and branching ratio (as per cent) as functions of photon energy were obtained for all ionic products. Based on our theoretical calculation, the absorption peaks were assigned as core excitations to various destination virtual orbitals. From the profiles of intensity ratios, the enhancement phenomena resulted from specific dissociation were recognized. To verify what the dissociation paths are, isotopic molecules were utilized to reveal the identities of the enhanced ionic fragments. It is interesting to note that most of the enhanced products were produced via breaking the peptide bond (including hydrogen atom(s) elimination) no matter the initial excited atom was carbon, nitrogen or oxygen. The branching ratios of breaking peptide bonds could be as high as 71% following a specific excitation. Adding a phenyl group on the peptide model, the branching ratios decrease dramatically to about 35%. It is very possible attributed to that the destination molecular orbital is mixed on the amide and phenyl groups.

Summary

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