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## Discovery and mechanistic studies of an unusual remote radical-induced side-chain loss from tyrosine-containing peptide radical cations in the gas phase

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Tyrosine is a constituent amino-acid residue of proteins. Because of the relatively low ionization energy of the aromatic phenol ring in its side chain, tyrosine is prone to be oxidized. The resulting one-electron oxidized tyrosyl radical is an important intermediate in many redox reactions of protein radicals. The intrinsic chemical properties of tyrosyl radical can be revealed from the fragmentations of tyrosine-containing peptide radical cations in the gas phase. The peptide fragment also provides invaluable sequence information that can be applied in mass spectrometry-based protein analyses. Upon ionization in the gas phase, a variety of tyrosyl radical tautomers can be generated and subsequently undergo radical-induced bond cleavages normally in the vicinity of the tyrosine residue. We have recently discovered an unusual radical-induced bond cleavage at the side chain of an amino-acid residue remote from the tyrosine. The plausible reaction mechanisms at the atomic and electronic levels have been examined experimentally using collision-induced dissociation for peptide models and their isotope-labeled and chemical derivatives and theoretically using density functional theory simulations.

### Biography

Chi-Kit Andy Siu completed his PhD in Computational Chemistry at Chinese University of Hong Kong in 2003. After being a Postdoctoral Fellow at TU Munich (2003–2005), supported by Alexander von Humboldt Foundation and York University (2005–2009), he joined City University of Hong Kong in 2009 and has become an Associate Professor since 2015. He is interested in the fundamentals of gas-phase ion chemistry, including structures of ions and their reaction mechanisms, thermodynamics, kinetics and dynamics at the electronic, atomic and molecular levels. He has published over 50 research articles on Gas-Phase Ion Chemistry.

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