Abstract

8-Oxo-2´-deoxygenosine (OG) is a common DNA lesion resulting from oxidatively generated damage. The formation of OG and its secondary reaction with electronically excited singlet oxygen (\(^{1}\text{O}_2\) is a reactive oxygen species generated \textit{in vivo}) are involved in mutagenesis, apoptosis and photodynamic therapy for cancer. This work focuses on reaction of the radical cation of OG with singlet oxygen, aims to provide a molecular-level description for the concurrent ionization radiation damage and singlet oxygen oxidation of DNA nucleobases. The formation of radical cations of 8-Oxo-2´-deoxygenosine (OG*), and their 9-methyl analogues are realized in the gas phase by electrospray ionization (ESI) guided-ion-beam tandem mass spectrometry. Their reactions are examined by the measurement of reaction product ions and cross sections as a function of collision energy (\(E_{\text{col}}\)) from which reaction thermodynamics is measured. One unique feature of this reaction is its multiconfiguration potential energy surface arising from the mixed open- and closed-shell character of the singlet oxygen reactant. Guided by thermodynamics measures in the experiment, this project benchmarks various single- and multi-reference electronic structure theories for tackling this unique reaction system.

All are welcome!