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Dynamics and Potential Energy Surfaces of Singlet Oxygen Oxidation of 8-Oxo-2′-deoxyguanosine and its Methyl Analogue: Elucidated by Guided-Ion-Beam Experiment and Multi-reference Electronic Structure Computation

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Abstract

8-Oxo-2´-deoxyguanosine (OG) is a common DNA lesion resulting from oxidatively generated damage. The formation of OG and its secondary reaction with electronically excited singlet oxygen ($^1O_2$ is a reactive oxygen species generated *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´-deoxyguanosine ($OG^{\bullet+}$), 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_{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!