EXCITED-STATE DYNAMICS IN FOLIC ACID AND 6-CARBOXYPTERIN UPON UVA EXCITATION

HUIJUAN HUANG, R. AARON VOGT and CARLOS E. CRESPO-HERNÁNDEZ, *Department of Chemistry and Center for Chemical Dynamics, Case Western Reserve University, Cleveland, Ohio 44106*.

The excited-state dynamics of folic acid (FA) and 6-carboxypterin (6CP) are poorly understood and work is needed to uncover the relaxation pathways that ultimately lead to their oxidative damage of DNA. In our approach, broad-band transient absorption spectroscopy was used to monitor the evolution of the excited states in FA and 6CP in basic aqueous solution upon excitation at 350 nm. In addition, quantum-chemical calculations were performed to assist in the interpretation of the experimental results and in the postulation of kinetic mechanisms. The combined experimental and computational results support a kinetic model where excitation of FA results in ultrafast charge separation (τ = 0.6 ps), which decays back to the ground state primarily by charge recombination with a lifetime of 2.2 ps. A small fraction of the charge transfer state undergoes intersystem crossing to populate the lowest-energy triplet state with a lifetime of 200 ps. On the other hand, a large fraction of the initially excited singlet state in 6CP decays by fluorescence emission with a lifetime of 100 ps, while intersystem crossing to the triplet state occurs with a lifetime of 4.4 ns. The potential implications of these results to the oxidative damage of DNA by FA and 6CP will be discussed. Funding from the National Science Foundation is gratefully acknowledged (CHE-1255084).