Abstract Submitted
for the SES12 Meeting of
The American Physical Society

Excited state dynamics in imidazole, pyrazole and pyrrole studied by femtosecond time-resolved spectroscopy HUI YU, NICHOLAS EVANS, SUSANNE ULLRICH, University of Georgia — In many biomolecules including nucleic acids and amino acids, ultrafast (<200fs) relaxation from an electronically excited state back to the ground state provides a self-protection mechanism against harmful ultraviolet radiation. The excited state dynamics of gas-phase imidazole, a basic five-membered heterocyclic subunit of the above mentioned biomolecules, is thus investigated experimentally to determine its contribution to the photoprotection. The imidazole photophysics are compared to structurally similar pyrrole and pyrazole that are less common in biological chromophores. Time-resolved photofragment translational spectroscopy and H-atom total kinetic release methods have been applied to follow the deactivation dynamics in real time. All three molecules display two competing pathways that operate on femtosecond timescales: A $\pi\sigma^*$ (N-H dissociation) and a $\pi\pi^*$ (ring deformation) mechanism are identified based on observation of H-atom and larger photoproducts, with an energetic onset specific to the individual molecule.

Hui Yu
University of Georgia

Date submitted: 19 Sep 2012 Electronic form version 1.4