REACTION DYNAMICS OF ANTHRACENE-9,10-ENDOPEROXIDE

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Femtosecond electronic and vibrational spectroscopic studies, steady-state absorption and emission investigations, ^{1}H NMR spectroscopy, and theoretical *ab initio* calculations were combined to obtain a comprehensive picture of the photochemistry of anthracene-9,10-endoperoxide (APO).[1, 2] Femtosecond UV pump excitation at 282 nm triggers the two primary reaction channels: cycloreversion, and homolytic cleavage of the peroxide bridge. The transient evolution of the product absorptions is followed with a white light continuum probe. Control measurements were also performed on two reaction products of APO, i.e., anthracene and anthraquinone. Polarization-resolved femtosecond UV pump/ IR probe, emission excitation studies, and *ab initio* calculations were combined to obtain a consistent assignment of APO electronic states to spectral features. Steady-state absorption spectroscopy and ^{1}H NMR spectroscopy were used to map out both primary and secondary reaction pathways in APO photochemistry. Moreover, the absolute reaction quantum yields for the different photoproducts were extracted for excitation varying from 240 to 450 nm.

1. Corral, I.; Gonzalez, L.; Lauer, A.; Freyer, W.; Fidder, H.; Heyne, K., Identifying the low-lying electronic states of anthracene-9,10-endoperoxide. *Chemical Physics Letters* **2008,** 452, (1-3), 67-71.
2. Fidder, H.; Lauer, A.; Freyer, W.; Koeppe, B.; Heyne, K., Photochemistry of Anthracene-9,10-endoperoxide. *Journal of Physical Chemistry A* **2009,** 113, (22), 6289-6296.