RADICAL INTERMEDIATES IN THE ADDITION OF OH TO PROPENE: PHOTOLYTIC PRECURSORS AND ANGULAR MOMENTUM EFFECTS

MATTHEW D BRYNTESON, CARRIE C WOMACK, RYAN S BOOTH, *Department of Chemistry, The University of Chicago, Chicago, IL, USA*; SHIH -H LEE, *Molecular Science, National Synchrotron Radiation Research Center, Hsinchu, Taiwan*; JIM J LIN, *Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan*; LAURIE BUTLER, *Department of Chemistry, The University of Chicago, Chicago, IL, USA*.

We investigate the photolytic production of two radical intermediates in the reaction of OH with propene, one from addition of the hydroxyl radical to the terminal carbon and the other from addition to the center carbon. In a collision-free environment, we photodissociate a mixture of 1-bromo-2-propanol and 2-bromo-1-propanol at 193 nm to produce these radical intermediates. Using a velocity map imaging apparatus, we measured the speed distribution of the recoiling bromine atoms, yielding the distribution of kinetic energies of the nascent C_3H_6OH radicals + Br. Resolving the velocity distributions of $Br(^2P_{1/2})$ and $Br(^2P_{3/2})$ separately with 2+1 REMPI allows us to determine the total (vibrational + rotational) internal energy distribution in the nascent radicals. Using an impulsive model to estimate the rotational energy imparted to the nascent C_3H_6OH radicals, we predict the percentage of radicals having vibrational energy above and below the lowest dissociation barrier, that to OH + propene; it accurately predicts the measured velocity distribution of the stable C_3H_6OH radicals. In addition, we use photofragment translational spectroscopy to detect several dissociation products of the unstable C_3H_6OH radicals: OH + propene, methyl + acetaldehyde, and ethyl + formaldehyde. We also use the angular momenta of the unstable radicals to estimate the energy partitioned to relative kinetic energy when they dissociate to OH + propene, which agrees very well with the data.