IDENTIFICATION OF PRIMARY AND SECONDARY PHOTOPRODUCTS OF ULTRAVIOLET PHOTODISSOCIATION OF 1,3-BUTADIENE

JAIME A. STEARNS, ALOKE DAS, AND TIMOTHY S. ZWIER, *Department of Chemistry, Purdue University, West Lafayette, IN 47907*.

The recombination of propargyl radicals is thought to be an important route to the formation of benzene both in planetary atmospheres and in flames. 1,3-Butadiene is one likely source of propargyl radical in such environments. We have carried out a study of the primary and secondary products of photodissociation of 1,3-butadiene following excitation near 220 nm in a supersonic expansion. Photoexcitation occurred inside a one-centimeter long reaction tube affixed to the nozzle of the pulsed valve, providing a 20μs window during which primary dissociation products could undergo recombination before expanding. The major primary products in the 118 nm ionization time-of-flight mass spectrum were C_3H_3, C_4H_4, and C_4H_5. The recombination of two C_3H_3 radicals, giving C_6H_6, was shown to be the major secondary reaction channel. Other secondary products were C_5H_8, C_7H_7, and C_7H_8. The primary and secondary products were characterized by resonant two-photon ionization and resonant ion-dip infrared spectroscopies.