

MECHANISM OF THE THERMAL DECOMPOSITION OF BENZALDEHYDE

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We have used a microtubular reactor to study the pyrolysis of benzaldehyde, and furfural. Samples of 1% organic substrate in 1 or 2 atm of a rare gas (He or Ar) are heated in a tubular reactor. The reactor is a 1 mm diam x 3 cm long silicon carbide tube. The walls of the SiC tube are resistively heated to temperatures up to 1700 K for the last 2 cm of the reactor. The residence times of substrates in the heated reactor are about 50 -100 μ sec. Gases emerging from the SiC reactor enter a vacuum chamber with a background pressure of 1×10^{-5} Torr. As the molecules emerge from the SiC tube into the vacuum, the supersonic expansion cools the beam to rotational temperatures of roughly 100 K. We have used computational fluid dynamics to characterize the properties of the gas flow through the hot SiC tubular reactor. Molecular fragments resulting from thermal cracking of the substrates are identified by two independent methods: VUV photoionization mass spectroscopy and infrared absorption. The skimmed molecular beam is intersected by the 9th harmonic of a YAG laser at 118.2 nm (10.487 eV) and ionized. The resultant ions are detected by time-of-flight mass spectroscopy. In addition to PIMS detection, we also capture the molecular beam on a CsI window cooled to 20 K. Molecules trapped in these cryogenic rare-gas matrices are analyzed by infrared absorption spectroscopy. Benzaldehyde and furfural are pyrolysis products that result from sugars. We have observed that heating these heterocyclic aromatic compounds decomposes them to C₆H₆, CH₃CCH, CO, CH₂CCO, and HCCH. propargyl radicals, HCCCH₂. Benzaldehyde decarbonlates to produce benzene and furfural decarbonlates to produce furan.