

Abstract Submitted
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Recombination Reactions in the Thermal Decomposition of Anisole: An Investigation of Benzene and Naphthalene Formation¹

ADAM SCHEER, BARNEY ELLISON, University of Colorado-Boulder, CALVIN MUKARAKATE, DAVID ROBICHAUD, MARK NIMLOS, National Renewable Energy Laboratory — Thermal decompositions of anisole ($C_6H_5OCH_3$) and methyl-deuterated anisole ($C_6H_5OCD_3$) are studied using a hyperthermal tubular reactor and photoionization reflectron time-of-flight mass spectrometer. Gas exiting the reactor is subject to a supersonic expansion after a residence time of 65 μs , allowing detection of highly chemically reactive radical species. Anisole decomposes through loss of a methyl group ($\bullet CH_3$) to form phenoxy radical ($C_6H_5O\bullet$), followed by ejection of a CO to form cyclopentadienyl radical ($c-C_5H_5$; CPDR). Benzene is generated primarily by thermal decomposition of methylcyclopentadiene ($C_5H_5CH_3$; MCPD). The MCPD results from methyl radical recombination with CPDR. The MCPD then undergoes two hydrogen atom losses and a ring expansion resulting in benzene. At $T_{wall} = 1200\text{ }^\circ C - 1300\text{ }^\circ C$ a large amount of propargyl radical (CH_2CCH) is observed. Propargyl radical recombination accounts for a small fraction of the observed benzene. Naphthalene and its precursor intermediates ($C_{10}H_{10}$, $C_{10}H_9$), resulting from CPDR recombination, are also observed. The presence of benzene and naphthalene is confirmed with resonance-enhanced multiphoton ionization (REMPI).

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