

PYROLYSIS OF TROPYL RADICAL (C_7H_7) AND BENZYL RADICAL ($C_6H_5CH_2$) IN A HEATED MICRO-REACTOR

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Benzyl radical ($C_6H_5CH_2$) is a crucial intermediate in the combustion and pyrolysis of substituted aromatic species that are common both in modern gasoline and potential future biofuels. The decomposition of benzyl radical is complicated and has been shown by isotopic labeling to require interesting isomerizations pathways. To better understand these pathways, a set of C_7H_7 radicals has been studied in a heated micro-reactor. Through multiple experiments, it has been shown that benzyl radical and cycloheptatrienyl (tropyl) radical ($c-C_7H_7$) do not interconvert, even at temperatures where both have completely thermally decomposed. To confirm this, tropyl radical has been studied directly and its pyrolysis is quite simple, only cyclopentadienyl radical ($c-C_5H_5$) and acetylene (HCCH) are formed. Cyclopentadienyl radical then decomposes to acetylene and propargyl radical ($HCCCH_2$). These products have all been identified through use of tunable synchrotron radiation by confirming their respective photoionization spectra. Matrix isolation infrared (IR) spectroscopy has also been used to identify these products. A previously unanswered question in benzyl radical decomposition has been addressed by studying the pyrolysis of 2,5-norbornadiene, which indicates benzyl radical may decompose through a norbornadiene-like bicyclic radical intermediate. This pathway successfully predicts the correct isotopically labeled products observed previously during ^{13}C labeled benzyl pyrolysis.