

ABSTRACT

THESIS: Reaction of Hydroxyl Radical with Aromatic Hydrocarbons

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PAGES: 40

Hydroxyl Radical ($\text{HO}\cdot$) is a highly reactive radical species which is an important member of a class of chemical species known as Reactive Oxygen Species (ROS). Hydroxyl radical typically has an extremely short lifetime under most conditions and its highly reactive nature makes it hard to detect by conventional methods used for study of free radical kinetics. In this study we propose and develop an alternative method for relative reactivities and regioselectivities of hydroxyl radical reactions with aromatic compounds in organic solvents. Hydroxyl radical is generated by the thermolysis of a *tert*-butyl azohydroperoxide which dissociates to yield hydroxyl and *tert*-butyl radicals, nitrogen, and acetone. TMIO is used to trap the *tert*-butyl radical, but is less likely to trap hydroxyl radical, which is free to react with the target arene to yield a hydroxycyclohexadienyl species. These species undergo hydrogen abstraction with TMIO to yield phenols, which may be derivatized with an appropriate silylating agent (in this case BTFSA), and analyzed using gas chromatography with detection by flame ionization (GC-FID) and mass spectrometry (GC-MS). The reactivity and selectivity of reaction of hydroxyl radical with various aromatic compounds is determined at different temperatures to obtain relative reaction rates. In this work, the reactivities and selectivities for $\text{HO}\cdot$ reactions with simple arenes, such as toluene and naphthalene are investigated.