

## Experimental and Theoretical Investigation of the OH-initiated Oxidation of Toluene

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Toluene is the most abundant aromatic hydrocarbon in the atmosphere and is emitted primarily from anthropogenic sources. Photochemical oxidation of toluene plays an important role in the formation of tropospheric ozone and secondary organic aerosol (SOA), which profoundly impacts air quality, human health, and climate, but its fundamental chemical mechanism remains largely uncertain. The oxidation of toluene is mainly initiated by the hydroxyl radical OH: the initial OH-toluene reaction results in minor H-abstraction (about 10%) and major OH addition (about 90%). The H-abstraction pathway leads to the formation of benzaldehyde, whose oxidative pathway is well established. The OH addition pathway results in the formation of methylhydroxycyclohexadienyl radicals (the OH-toluene adducts). Under atmospheric conditions, the OH-toluene adducts react with O<sub>2</sub> either by O<sub>2</sub> addition to form primary peroxy radicals, H-abstraction and subsequent O-bridge formation to aromatic oxide/oxepin, or H-abstraction to yield phenolic compounds. In this talk, we will present direct experimental product measurements and quantum chemical and kinetic calculations to elucidate the oxidation mechanism of the OH-initiated reaction with toluene, focusing the preferred pathways between the competing toluene-oxide/methyloxepin, peroxy radicals, and phenolic channels.