STRUCTURAL CHARACTERIZATION OF PHENOXY RADICAL USING A MASS-CORRELATED BROADBAND MICROWAVE SPECTROMETER

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We have combined the high-resolution provided by chirped pulse Fourier transform microwave (CP-FTMW) spectroscopy with a vacuum ultraviolet (VUV) time-of-flight mass spectrometry (TOF-MS) that allows us to find optimal conditions to detect reactive intermediates. This unique setup was used to structurally characterize the phenoxy radical. This is an important intermediate in the oxidation of many aromatic compounds. The decomposition of this radical has as primary product cyclopentadienyl radical, which is an important species in the formation of polynuclear aromatic hydrocarbons. Phenoxy radical was generated through the pyrolysis of anisole and allyl phenyl ether. The work was carried out over a 300-1500 K temperature range, using a high-temperature flash pyrolysis micro-reactor coupled with a supersonic expansion. The 2-18 GHz pure rotational spectrum was obtained concurrently with the mass spectrum and determined the resonant-stabilized radical molecular parameters. For further structural analysis spectra of ¹³C isotopomers were obtained using segmented chirps. The new structural insights and the pyrolysis setup coupled with the CP-FTMW/TOF spectrometer will be discussed.