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Angry Aromatics: Substituted phenyl radical reactions probed with VUV synchrotron photoionization MS

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This presentation will describe our recent results probing the gas-phase radical reaction of various phenyl-radicals using synchrotron VUV photoionization mass spectrometry at the Advanced Light Source synchrotron.

Functionalized aromatic molecules are prevalent in gas-phase reactive environments including combustion, atmospheric chemistry, and extra-terrestrial atmospheres but the precise pathways that initiate PAH and PANH are not well formalized. Using synchrotron VUV photoionization mass spectrometry, the fates of highly-reactive phenyl radicals are probed in the presence of a neutral, closed-shell co-reactant. These phenyl radicals, including substituted variants, are synthesized using laser photolysis and the ensuing chemical reactions are followed. This provides kinetic detail while the VUV photoionization can be tuned to probe reaction products (and transients).

Using this method, our group has been targeting substituted phenyl radicals (ortho, meta) to determine how these additional groups perturb, or indeed dictate, the ensuing chemistry. Recent results with methyl-phenyl radicals reacting with small hydrocarbons (allene, propene, propyne) will be shown and compared to calculations that rationalize the mechanistic pathways and support the product assignments. Several ring-growth pathways are elucidated. These studies also draw on previous results of reactions with O₂.

As might be expected, ortho-substituted phenyl radicals have unique bimolecular reaction pathways (compared to meta variants) due to interactions between the radical adduct site and the adjacent ring-substitute but it is not a simple story...

Summary

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