

Properties of Structural Isomers of Hydronaphthyl Resonance-Stabilized Radicals and Their Role in the Formation of PAHs in Titan's Atmosphere

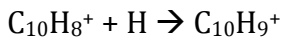
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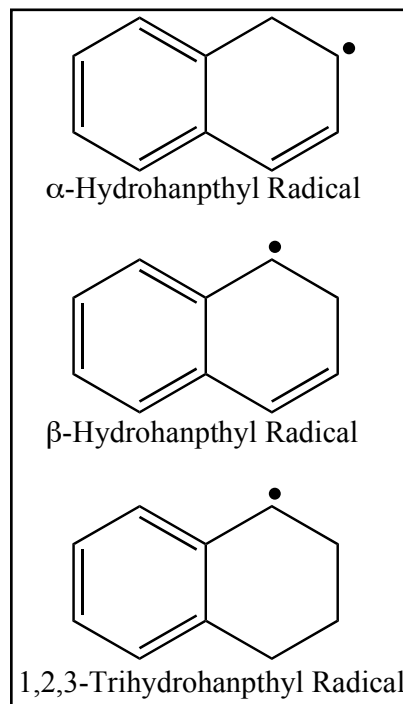
For the past several years, the Cassini mission along with the Huygens probe have been providing compositional data about the atmosphere of Titan's atmosphere in great detail. Recent data has shown the existence of polycyclic aromatic hydrocarbons (PAHs) at higher altitudes than previously expected including naphthalene and anthracene.¹ The formation of naphthalene (C₁₀H₈), the simplest PAH, and its derivatives are of great interest as similar mechanisms may lead to the formation of larger fused-ring systems.

Of specific interest are the resonance-stabilized radicals (RSRs) formed by the hydrogenation of naphthalene. RSRs gain extra stability by delocalizing the unpaired electron through a neighboring conjugated π -system. Because of this extra stability, RSRs are able to build up in concentration allowing for the creation of larger, more complex systems through the recombination of RSRs.

Mass-selected ultraviolet spectra of two monohydrated RSRs, α -hydronaphthyl radical and β -hydronaphthyl radical (C₁₀H₉), and 1,2,3-trihydronaphthyl radical (C₁₀H₁₁) have been collected. Data collected for the C₁₀H₉ species provided an accurate value for the H-atom affinity of naphthalene given by: C₁₀H₈(naphthalene) + H \rightarrow α -naphthyl or β -naphthyl radicals. Since our spectroscopic method includes a determination of the ionization potential for the radicals, alternative thermochemical cycles can also be used to determine the H-atom affinity of naphthalene cation; that is, ΔE for the process:



The possible implications of these measurements for both neutral and ionic pathways to PAH in Titan's atmosphere will also be discussed.



References

- (1) Waite, J. H., Jr.; Young, D. T.; Cravens, T. E.; Coates, A. J.; Crary, F. J.; Magee, B.; Westlake, J. *Science* **2007**, *316*, 870-875.