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Probing Low Temperature Molecular Mass Growth Processes to Polycyclic Aromatic Hydrocarbons (PAHs) via Vacuum Ultraviolet Photoionization Mass Spectrometry –Saturn's Moon Titan as a Case Study

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The detection of benzene in Titan's atmosphere led to the emergence of polycyclic aromatic hydrocarbons as potential nucleation agents triggering the growth of Titan's orange-brownish haze layers. However, the fundamental mechanisms leading to the formation of PAHs in Titan's low temperature atmosphere have remained elusive. We provide persuasive evidence through laboratory experiments exploiting tunable vacuum ultraviolet photoionization mass spectrometry and computations that prototype PAHs like anthracene and phenanthrene ($C_{14}H_{10}$) are synthesized via barrier-less reactions involving naphthyl radicals ($C_{10}H_7^{\bullet}$) with vinylacetylene (CH_2=CHC≡CH) in low-temperature environments. These elementary reactions are rapid, have no entrance barriers, and synthesize anthracene and phenanthrene via van-der-Waals complexes and submerged barriers. This facile route to anthracene and phenanthrene –potential building blocks to complex PAHs and aerosols in Titan - signifies a critical shift in the perception that PAHs can be only formed at high-temperature conditions providing a detailed understanding of the chemistry of Titan's atmosphere through untangling elementary reactions on the most fundamental level. An outlook is also presented on the synthesis of more complex PAHs containing four rings and potential two dimensional nanostructures via complementary hydrogen abstraction –acetylene addition (HACA), hydrogen abstraction –vinylacetylene addition (HAVA), and phenyl addition –cyclization (PAC) reaction mechanisms.

Summary

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