Experimental investigation of naphtalene growth via HACA mechanism

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Polycyclic aromatic hydrocarbons (PAH) and soot are the main pollutants, generated during incomplete combustion of hydrocarbon fuels, and pose a danger to human health and ecology as a whole. Although PAH are harmful to terrestrial beings, they attract a considerable interest in astrochemistry and astrobiology as potential precursors for biorelevant molecules, and therefore, the most primitive lifeforms [1]. One of the possible mechanisms of PAH formation is the mechanism of hydrogen abstraction – acetylene addition (HACA), which consists of consecutive H abstractions and additions of acetylene to the formed radical site [2].

In this work, we present a study of the naphthalene growth via the HACA mechanism by means of molecular beam mass spectrometry. During the experiment, the mixture of nitrosobenzene (precursor of phenyl) and acetylene was fed into a pyrolythic reactor via a piezoelectric pulse valve. In the reactor, the mixture is heated to a certain temperature and then expands into a vacuum chamber, forming a molecular beam. The molecular beam then undergoes soft single photon ionization by a 9^{th} harmonic of an Nd:YAG laser (118 nm), and the ionized molecules are detected via a reflectron time-of-flight mass spectrometer (ReTOF). The experiments were conducted at combustion relevant conditions: pressures 100 – 600 Torr and temperatures 800 – 1200 K. Our results suggest that at lower temperatures and higher pressures naphthalene is predominantly generated via the Bittner-Howard route of the HACA mechanism, while at higher temperatures Frenklach's original pathway dominates.

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References

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