Investigation of polycyclic aromatic hydrocarbons formation during shock wave pyrolysis of benzene and dimethyl ether mixtures

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Polycyclic aromatic hydrocarbons (PAHs) are mainly formed in incomplete combustion processes and generally considered as precursors for soot particles [1]. Precise measuring PAHs formation and growth is significant for better understanding and developing of soot formation kinetics [2]. In this work, laser-induced fluorescence (LIF) was used to detect PAHs formed during shock wave pyrolysis of benzene and dimethyl ether (DME) mixtures. To control the onset of the appearance of the condensed phase, the laser light extinction at 633 nm was registered. It was found, that PAHs LIF spectra shifts toward longer wavelengths with temperature and reaction time increasing. The addition of DME to benzene led to a shift in the PAHs LIF spectra towards shorter wavelengths relative the benzene mixture at the same initial temperature behind the shock wave. The modelling of kinetics of PAHs formation and growth was carried out using OpenSMOKE++ code [3] with a kinetic scheme [4]. The simulations have shown that DME presence leads to the formation of 5-membered aromatic ring (C_5H_5), $C_{10}H_{10}$, $C_{13}H_{10}$ as well as the emerging of alternative formation pathways C_9H_8 and $C_{10}H_8$. This work was supported by the Ministry of Science and Higher Education of the Russian Federation, agreement No. 075-15-2020-806.

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