The formation pathway of soot precursors (PAHs) and its transformation to soot in flame

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Objective

Site effects on PAHs and Soot growth within HACA frame

The growth of PAHs and soot in post flame region (without H atom participating)

Methods

DFT theory       Potential energy surface
TST and RRKM theory       Rate coefficients
0-D reactor simulation       Yield of products
Premixed flame simulation       PAHs concentration

Site effect on PAHs and soot growth

The PAHs with 5-membered Ring is the preferred product in HACA pathway.

Fig. 1 The PES of A_3 to A_4 reaction system.

Fig. 2 Reaction rate coefficients of HACA reactions.

Fig. 3 Yield of products.

The growth of PAHs and soot in post flame region (without H atom participating)

Fig. 4 The PES of PAHs-C_2H_2 reactions.

Fig. 5 The contributions of PAHs-C_2H_2 pathway to soot growth.

Fig. 6 Conceptual mechanism of soot nucleation and surface growth.