

# 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

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Potential energy surface

TST and RRKM theory

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Rate coefficients

0-D reactor simulation

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Yield of products

Premixed flame simulation

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PAHs concentration

## Site effect on PAHs and soot growth

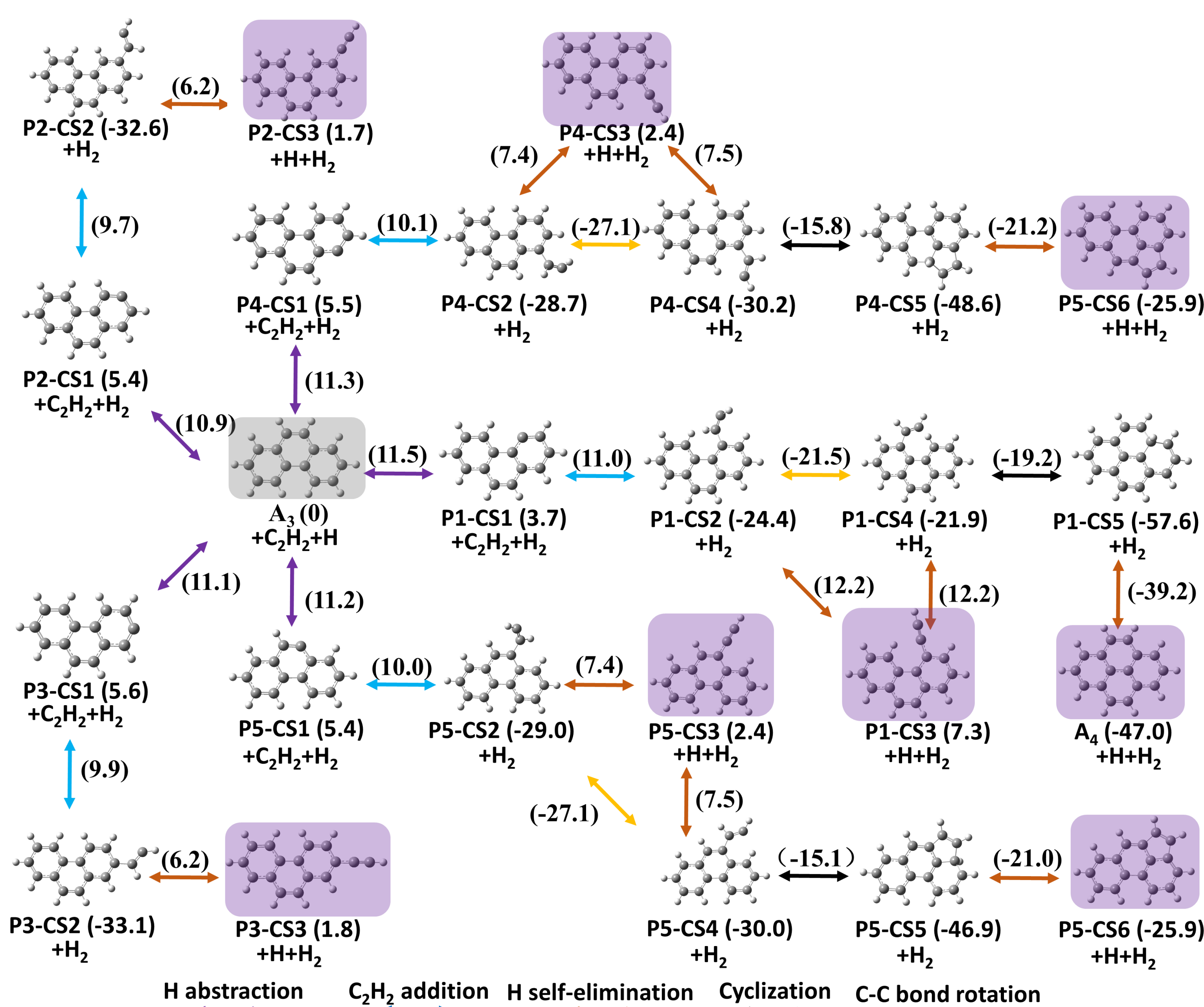


Fig. 1 The PES of  $A_3$  to  $A_4$  reaction system.

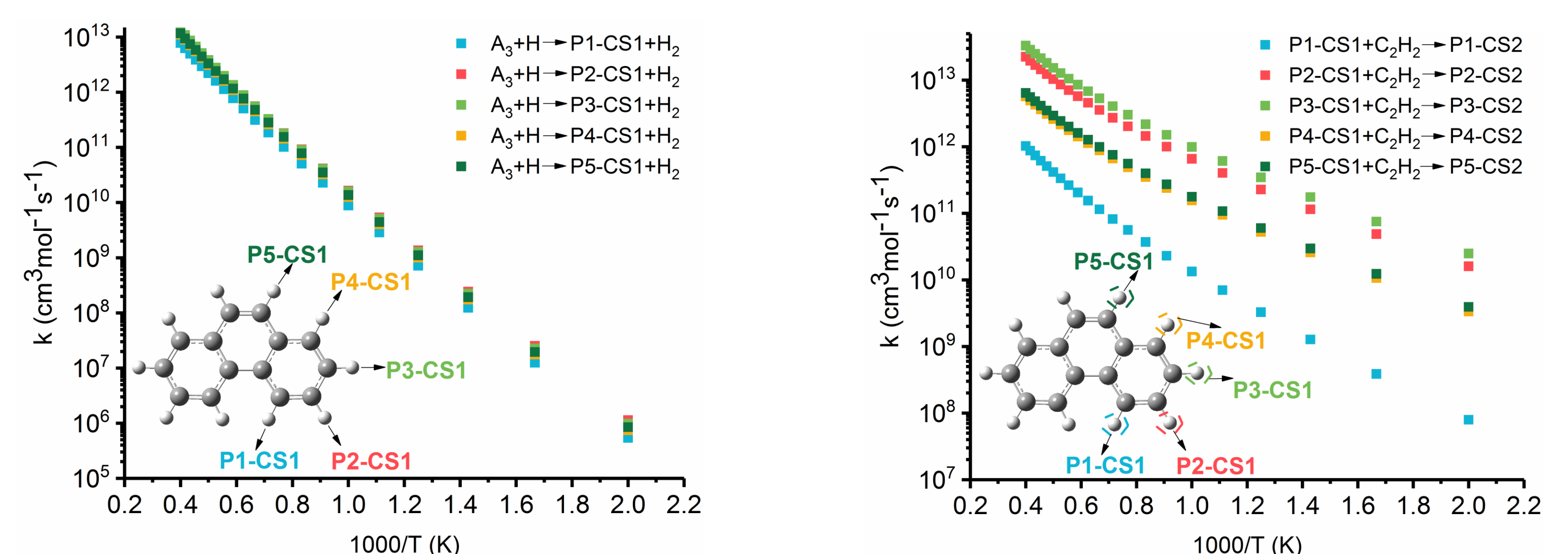


Fig. 2 Reaction rate coefficients of HACA reactions

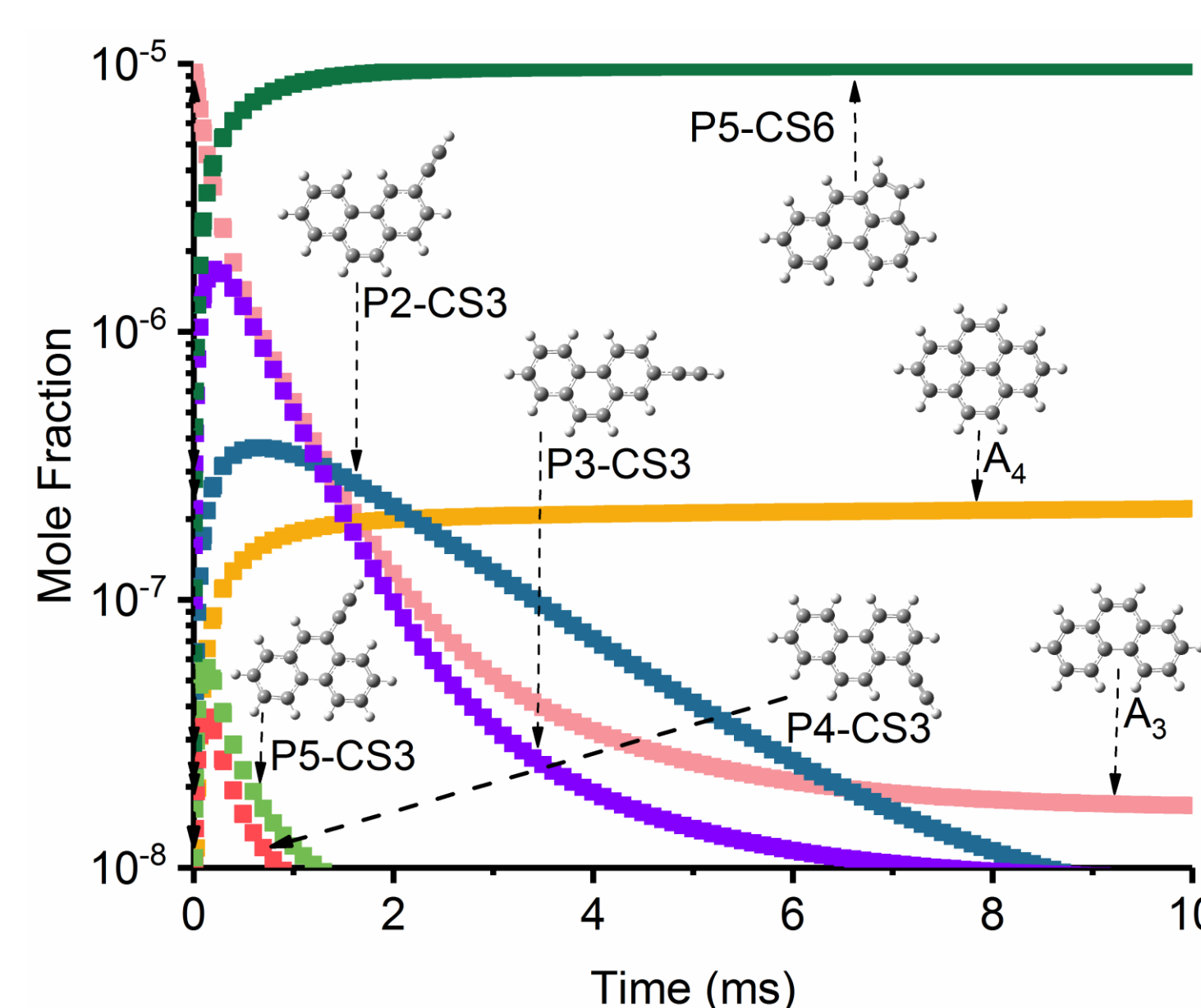


Fig. 3 Yield of products.

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

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

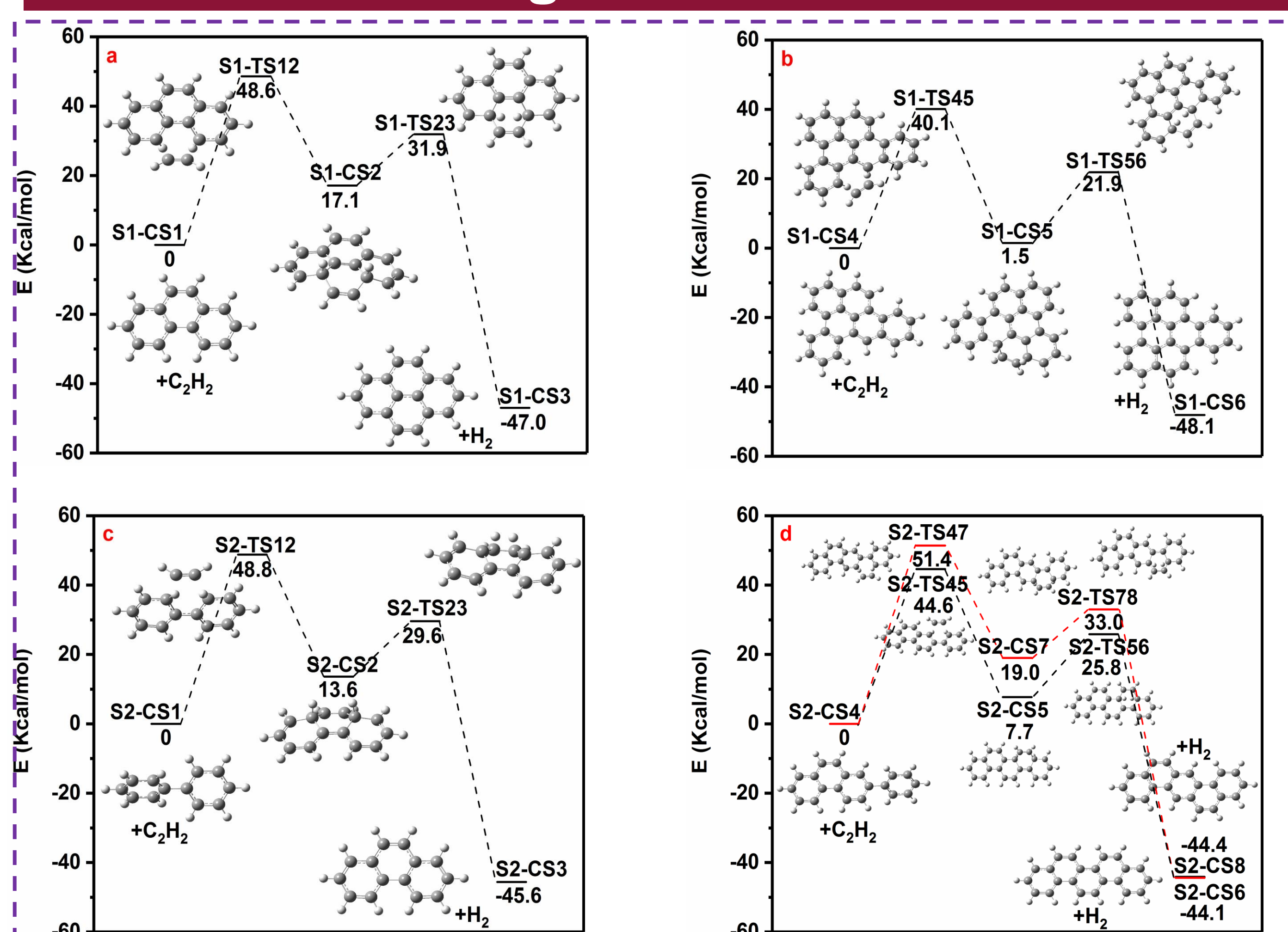


Fig. 4 The PES of PAHs- $C_2H_2$  reactions.

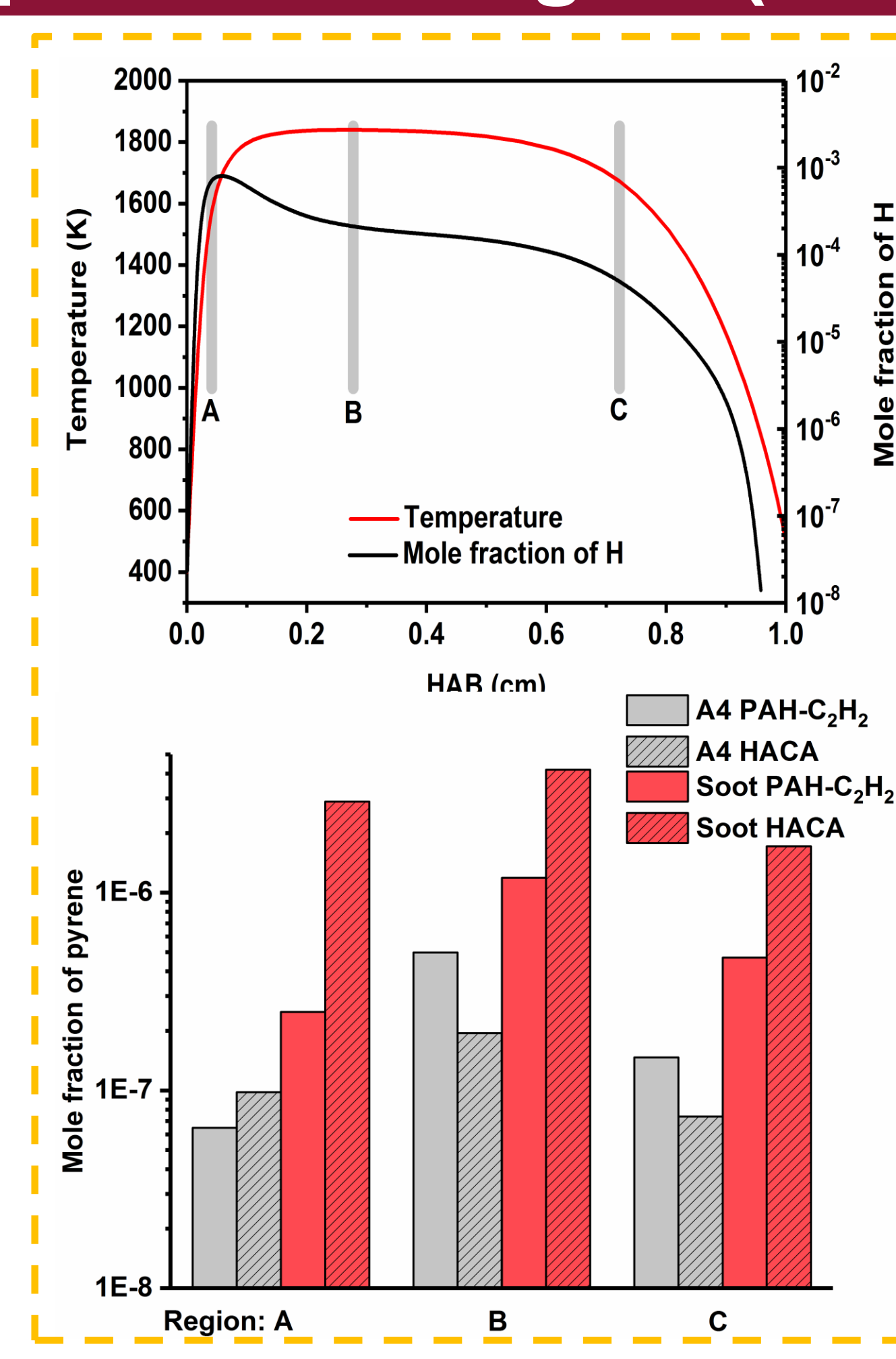


Fig. 5 The contributions of PAHs- $C_2H_2$  pathway to soot growth.

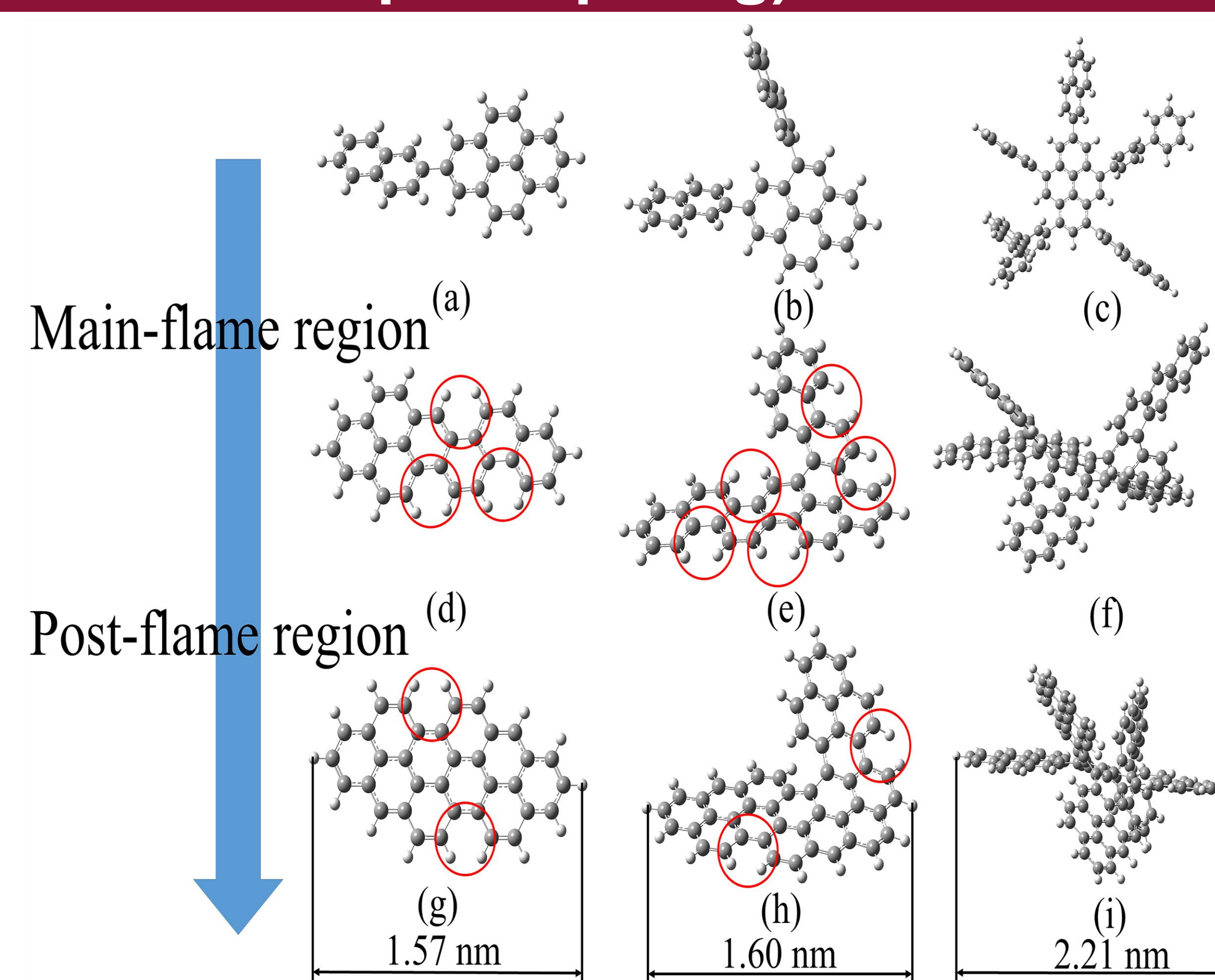


Fig. 6 Conceptual mechanism of soot nucleation and surface growth.