

# Examination of the reaction mechanism of PAHs formation from the pyrolysis of toluene

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A product analysis was carried out for examination of the formation mechanism of the polycyclic aromatic hydrocarbons (PAHs) as a precursor of the particulate matter emitted from an internal combustion engine. The addition of oxygen in toluene pyrolysis system examined by qualitative analysis of the intermediate product inhibition process of PAH formation by oxidation. Heated flow-tube reactor was used and time-of-flight mass spectrometer coupled with single-photon ionization technique was applied for detection of reaction products. Several reaction products such as benzene, styrene, and phenanthrene were found, however, oxygen contained product was not found in this study. Figure 1 shows an estimated reaction mechanism for formation of PAHs.<sup>1,2</sup> Some products such as benzene and styrene decreased in the existence of oxygen. In contrast, naphthalene and acenaphthylene (or biphenyl as a same mass) increased in the same condition. The signal of  $m/z=116$ , which corresponds to indene, also increased in presence of oxygen. However, this point was inconsistent with the decrease of phenanthrene. This result suggests that the signal of  $m/z=116$  includes other products such as 2-methylphenylacetylene or 1-propynyl-benzene. It is also suggested that the routes of acenaphthylene formation should be two possibilities. One is the naphthalene route, and another is acenaphthene or biphenyl as the product of  $m/z=154$ . The addition of 1-butyne as a precursor of small radicals was also performed for examination of hydrogen abstraction- $C_2H_2$  addition (HACA) mechanism. Indeed, naphthalene and acenaphthylene increased in this case. It suggests that HACA reaction is accelerated by the additional  $C_2$  or  $C_3$  radicals generated from 1-butyne.

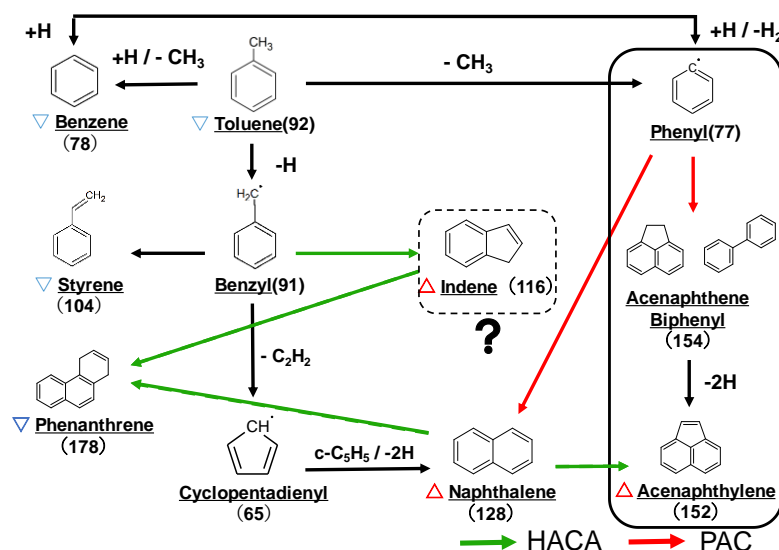


Fig. 1 Estimated reaction mechanism of PAH formation from toluene.

## References

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