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Formation of aromatic hydrocarbons through ion-molecule reactions of C3H4+: J.A.S.M.S.

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Formation of Aromatic Hydrocarbons through ion-molecule reactions of $C_3H_3^+$

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ABSTRACT

Studies involving soot nucleation in flames point to an ionic mechanism, versus a neutral free radical mechanism, driving the formation of aromatic hydrocarbons. Therefore, the small aromatic cation $C_3H_3^+$(m/z 39) has been extensively studied as a precursor ion to the formation of soot in the pyrolysis of fuels and other hydrocarbons. Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR) has been used for the observation of the gas phase reactions of $C_3H_3^+$ with conjugated dienes. Two forms of $C_3H_3^+$ are observed: *i)* The reactive propargyl isomer, which reacts with dienes to produce a phenyl cation, and *ii)* an non-reactive cyclopropenyl isomer. Because the cyclopropenyl form is found in greater than 90% during combustion processes, the reactions of c-$C_3H_3^+$ and associated activation energies are critical to an understanding of soot formation. The activation energy for the endothermic reactions of c-$C_3H_3^+$ with small conjugated dienes has been observed using FT-ICR mass spectrometry and the empirical energy barrier is compared to theoretical calculations.

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