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Formation of Aromatic Hydrocarbons through the Gas-Phase Ion – Molecule Reactions of $C_3H_3^+$

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Tim Burrell, Curtiss D. Hanson; Department of Chemistry, University
of Northern Iowa, Cedar Falls, IA, 50614-0423**

The formation of benzene during the thermal decomposition of hydrocarbons has been attributed to the reactions of $C_3H_3^+$ with low molecular weight hydrocarbons. Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR) permits direct observation of the gas phase reactions of $C_3H_3^+$ with conjugated dienes. Two forms of $C_3H_3^+$ are observed: *i*) The propargyl isomer, which reacts with dienes to produce a phenyl cation, and *ii*) an unreactive cyclopropenyl isomer. Deuterium labeling experiments were utilized to postulate a mechanism for the reaction. An ionic model for the gas phase formation of benzene based on a reactive propargyl cation will be presented.

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