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Single pulse shock tube investigation of the inter-isomerization and decomposition mechanism of quinoline and isoquinoline experimental results and computer simulation

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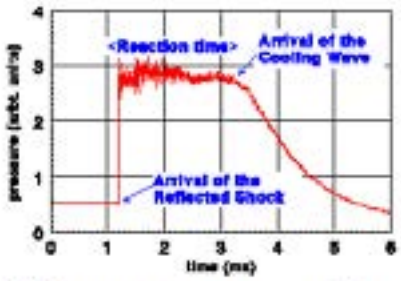
The experimental results on thermal decomposition of quinoline (isoquinoline) were studied behind reflected shock waves in the single pulse shock tube. The distribution of reaction products under various initial conditions and shock temperatures were determined by gas chromatography. Quantum chemical methods were used to determine potential energy surfaces of reaction channels. A detailed kinetics scheme containing 40 elementary steps was constructed. The calculated mole percent of the stable products was compared to the experimental values. The agreement between the experimental and the calculated product distribution was very good. A map of the figures containing the mole-percent of eight stable products in the decomposition vs. temperature is presented. The fast isomerization of o-quinolyl → o-isoquinolyl via the intermediate indene imine radical and the attainment of fast equilibrium between these two radicals is the reason for the identical product distribution regardless whether the reactant radical is quinoline or isoquinoline. Three of the main decomposition products of o-quinolyl radical are those containing the benzene ring, namely, phenyl, benzonitrile and phenylacetylene radicals. They undergo further decomposition mainly at high temperatures via two types of reactions: Opening of the benzene ring in the radicals, followed by splitting into fragments and; dissociative attachment of benzonitrile and phenyl acetylene by hydrogen atoms to form hydrogen cyanide and acetylene. High temperature residence time and cooling wave obtained in the single pulse shock tube.



High temperature residence time and cooling wave obtained in the single pulse shock tube.

Biography

Faina Dubnikov is an established Researcher in Department of Chemistry at Hebrew University. She has been carrying mutual theoretical research in the filed of public safety. Her research efforts are based on theoretical modeling and simulation.

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