

Products of quinoline thermal decomposition and their further reactions. Quantum chemical calculations and kinetic modeling.

Faina Dubnikova¹, Assa Lifshitz²

¹ Institute of Chemistry, Hebrew University of Jerusalem, Israel

Faina.Dubnikov@mail.huji.ac.il

The initiation step in the thermal decomposition of quinoline and isoquinoline is the H-atom ejection from the pyridine ring, where the ortho-position is preferred. In the decomposition process the formation of ortho-quinolyl or ortho-isoquinolyl radicals via H-atom abstraction reactions by hydrogen atom and other radicals plays a very important role.

The product distribution [1] shows that three of the main decomposition products that contain the benzene ring, namely, benzene, benzonitrile and phenyl acetylene undergo further destruction at high temperatures. It is result mainly in two types of the reactions:

- 1) opening of the benzene ring, followed by breaking down into two parts, and
- 2) dissociative attachment of $-C\equiv N$ and $-C\equiv CH$ groups by hydrogen atom.

[1] Laskin, A., Lifshitz, A. *J. Phys. Chem. A*, 102:928-946, 1998.