

Reaction Pathway and Mechanistic Insights into Low-Energy Electron-Induced Conversion of Toluene to Acetylene

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Toluene ($C_6H_5CH_3$) is among one of the most abundant volatile organic compounds (VOC), originating from vehicular emission, industries, fuel combustion and solvent-based processes.[1,2] Electron-induced reaction can prove to be a useful approach to remove (VOC) pollutant like toluene and convert them to value added products like acetylene. Its selective conversion to acetylene is of particular interest because acetylene is a versatile industrial feed-stock.

Electron-induced reactions are studied in condensed phase at cryogenic conditions (14-15 K) in a UHV chamber with base pressure $\sim 10^{-10}$ mbar and monitored using two probes FTIR (Reflection Absorption Infrared) and Mass spectrometry. The energy of electron beam is in range of (100eV to 500eV). 123.6 nm vacuum ultra-violet (VUV) light source was used for photon irradiation.

Here, we demonstrate a previously unrecognized electron induced pathway for the selective conversion of toluene to acetylene. The decomposition of toluene proceeds through selective generation of benzyl radicals ($C_6H_5CH_2^{\bullet}$) as key intermediates, which decompose into cyclopentadienyl radicals ($C_5H_5^{\bullet}$) and acetylene as end product.

Our findings demonstrate that low-energy free electrons drive a low-barrier, benzyl-radical-mediated fragmentation pathway while effectively suppressing competing rearrangements and bi-molecular reactions. This work provides crucial molecular-level insights into electron-driven aromatic volatile organic compound (VOC) degradation, and its potential for pollutant removal and useful chemical production.

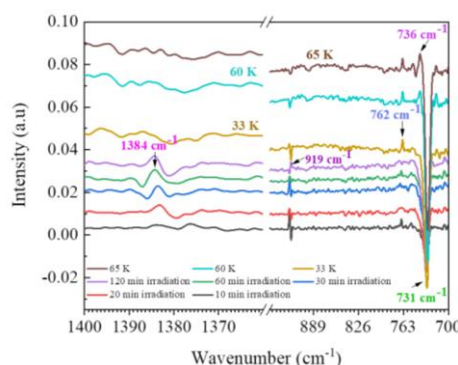


Figure 1. FTIR subtraction spectrum of irradiated and post-irradiation-heated toluene films showing toluene depletion, transient species, and acetylene formation.

Acknowledgements

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References

- [1] R. Atkinson and J. Arey, Chemical Reviews 103, 4605 (2003).
- [2] M. A. Zahed, S. Salehi, M. A. Khoei, P. Esmaeili, and L. Mohajeri, Toxicology in Vitro 98, 105825 (2024).