

Joint CQSE and CASTS Seminar

Weekly Seminar
May 10, 2013 (Friday)

TIME May 10, 14:30 ~ 15:30
TITLE Synthesis of pyridine via the neutral-neutral reaction of ground state cyano radicals, $\text{CN}(X^2\Sigma^+)$, with 1,3-butadiene, $\text{C}_4\text{H}_6(X^1A_g)$
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Abstract

The reaction of ground-state cyano radicals, $\text{CN}(X^2\Sigma^+)$, with the simplest polyene, 1,3-butadiene ($\text{C}_4\text{H}_6(X^1A_g)$), is investigated theoretically to explore probable routes to form pyridine at ultra-low temperature. The isomerization and dissociation channels for each of the six collision complexes are characterized by utilizing the unrestricted B3LYP/cc-pVTZ level of theory and the CCSD(T)/cc-pVTZ calculations. With facilitation of RRKM and variational RRKM rate constants through the web of *ab initio* paths composed of 6 collision complexes, 182 intermediates, and 60 H-, 66 H₂-, and 3 HCN- dissociated products, the most probable paths at collision energies of 0-10 kcal/mo, thus reaction mechanism, are determined. Subsequently the corresponding rate equations are solved that the evolutions of concentrations of collision complexes, intermediates, and products versus time are obtained. As a result, the final products and yields are identified. This study however predicts that six collision complexes, ^bc1-^bc6, would most likely produce a single final product, 1-cyano-1,3-butadiene, $\text{CH}_2\text{CHCHCHCN}$ (^bp1) + H, via the collision complexes ^bc1($\text{CH}_2\text{CHCHCH}_2\text{CN}$) and intermediate ^bi3($\text{CH}_2\text{CHC H}_2\text{CHCN}$). The low-energy routes for the formation of pyridine, though not the most probable product according to RRKM theory, are identified.

