

Pyrolysis of Cyclohexane and 1-Hexene at High Temperatures and Pressures—A Photoionization Mass Spectrometry Study

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Table S1: Photoionization cross sections used in the analysis of mass spectra. A dash indicates either no data are available at that energy or that energy was not used for a particular species.

| Molecule | m/z | IE ^a / eV | Photoionization cross section / Mb | | | | Reference ^b |
|-----------------|-----|----------------------|------------------------------------|----------|---------|---------|------------------------|
| | | | 13.5 eV | 10.75 eV | 10.7 eV | 10.0 eV | |
| Cyclohexane | 84 | 9.88 | - | 30.85 | 29.24 | 3.34 | [31] |
| 1-Hexene | 84 | 9.44 | - | 8.761 | 9.547 | 8.776 | [27] |
| Benzene | 78 | 9.24 | - | 30.32 | 31.49 | 24.28 | [26] |
| 1,3-Pentadiene | 68 | 8.6 | - | 21.872 | 22.064 | 17.235 | [27] |
| Cyclopentadiene | 66 | 8.57 | - | 15.8 | 15.73 | 12.68 | [50] |
| 1-Butene | 56 | 9.55 | - | 10.91 | 11.09 | 8.16 | [51] |
| 1,3-Butadiene | 54 | 9.07 | 39.07 | 18.1 | 17.9 | 14.096 | [27] |
| Vinylacetylene | 52 | 9.58 | - | 37.72 | 38.5 | 25.82 | [26] |
| Diacetylene | 50 | 10.17 | - | 25.17 | 24.14 | 0.04 | [26] |
| Propene | 42 | 9.73 | 33.3 | 12.114 | 11.90 | 7.054 | [36], ([38]) |
| Allyl | 41 | 8.13 | - | 5.5 | 5.6 | 6.227 | [29] |
| Allene | 40 | 9.69 | 45.9 | 19.334 | 18.648 | 7.619 | [27], ([30]) |
| Propyne | 40 | 10.36 | - | 39.61 | 36.27 | 0 | [26] |
| Ethene | 28 | 10.51 | 42.3 | 6.1 | 5.1 | - | [26], ([38]) |
| Acetylene | 26 | 11.4 | 36.13 | - | - | - | ([26]) |
| Methane | 16 | 12.61 | 13.38 | - | - | - | ([35]) |

^a IE = Ionization threshold, all values from [33]. ^b Citations in parentheses are for 13.5 eV. Citation numbers are from the main article and are reproduced below.

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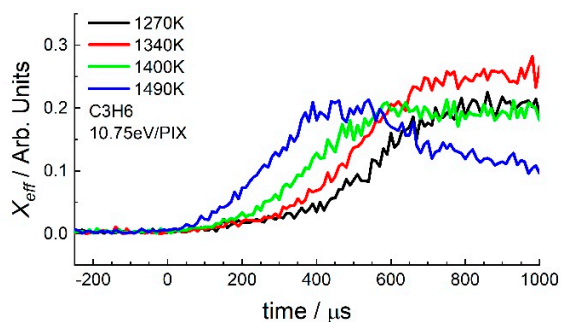


Figure S1: Effective concentrations of propene from the pyrolysis of cyclohexane at various temperatures, ~ 10 bar, 10.75 eV, no MgF_2 . $t=0$ corresponds to formation of the reflected shock wave.

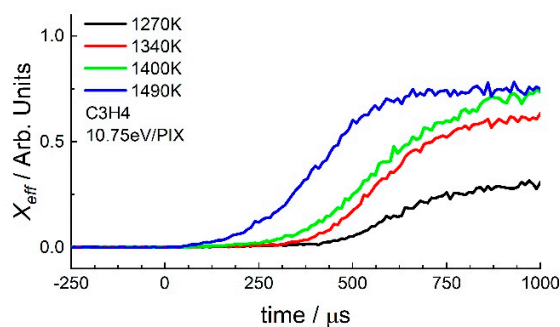


Figure S2: Effective concentrations of allene + propyne from the pyrolysis of cyclohexane at various temperatures, ~ 10 bar, 10.75 eV, no MgF_2 . $t=0$ corresponds to formation of the reflected shock wave.

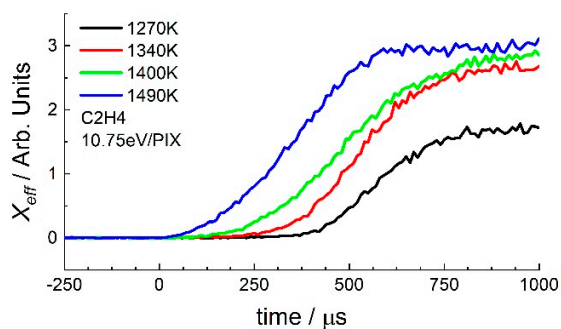


Figure S3: Effective concentrations of ethene from the pyrolysis of cyclohexane at various temperatures, ~ 10 bar, 10.75 eV, no MgF_2 . $t=0$ corresponds to formation of the reflected shock wave.

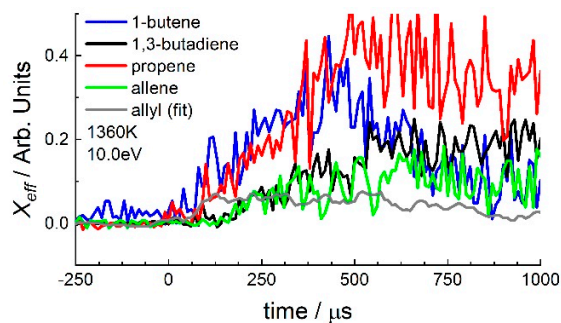


Figure S4: Effective concentration plots at 10.0 eV for several main products from the dissociation of 1-hexene. $T = 1360\text{ K}$ and $P \sim 5\text{ bar}$. $t=0$ corresponds to formation of the reflected shock wave

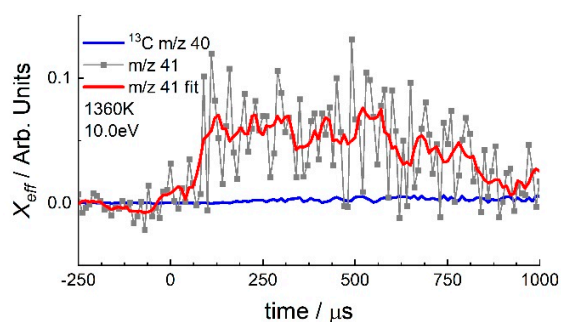


Figure S5: Effective concentration of the allyl radical produced from dissociation of 1-hexene. $T = 1360\text{ K}$ and $P \sim 5\text{ bar}$ $PE = 10.0\text{ eV}$. $m/z\ 41$ is corrected for the ^{13}C isotopologue of $m/z\ 40$. The red line is a best fit to the $m/z\ 41$ signal as a visual aid. $t=0$ corresponds to formation of the reflected shock wave.

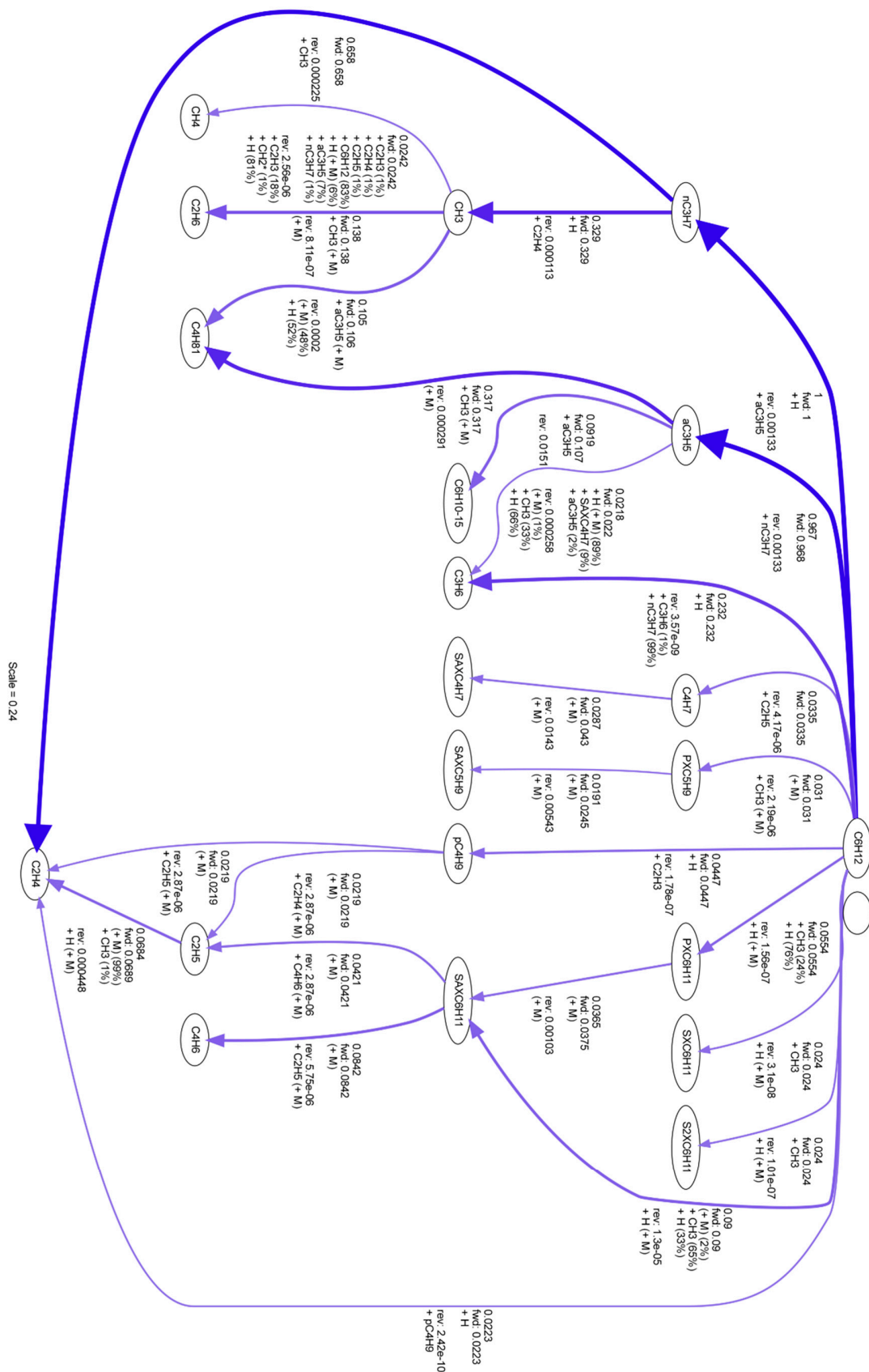


Figure S6: Fan model. Reaction flux diagram for 2% consumption of 1-hexene. 1160 K and 5 bar.

