Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Reactions of Allylic Radicals that Impact Molecular Weight Growth Kinetics

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## Supporting Information

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Table S13: Rate constants at 1 atm and 500- 1800 K for the $C_6H_{11}$ PES, entering the surface from the CC=CC• + $C_2H_4$ channel.

*Table S1: Apparent temperature-and pressure-dependent rate constants for the recombination reactions of two stabilized radicals from 0.001-50 atm and 300-2500 K.*

| Reactions | Forward | | | | Reverse | | | | Note (Pressure in atm) |
|---|---|---|---|---|---|---|---|---|---|
| | A ($cm^3$/mol-s) | n | Ea (kcal/mol) | *k* (1000K) ($cm^3$/mol-s) | A ($s^{-1}$) | n | Ea (kcal/mol) | *k* (1000K) ($s^{-1}$) | |
| | **1.12E+13** | **0** | **-0.31** | 1.31E+13 | 2.37E+15 | 0 | 59.54 | 2.27E+02 | High P limit |
| | **4.99E+52** | **-12.66** | **11.48** | 1.65E+12 | 1.35E+55 | -12.69 | 71.38 | 2.83E+01 | 0.001 |
| | **1.64E+45** | **-10.18** | **9.69** | 3.70E+12 | 3.97E+47 | -10.20 | 69.57 | 6.33E+01 | 0.01 |
| C=CC• + C=CC• ⇄ C=CCCC=C | **7.11E+36** | **-7.47** | **7.39** | 6.75E+12 | 1.49E+39 | -7.47 | 67.24 | 1.15E+02 | 0.1 |
| | **2.23E+28** | **-4.77** | **4.81** | 1.00E+13 | 3.94E+30 | -4.75 | 64.63 | 1.68E+02 | 1 |
| | **7.47E+20** | **-2.42** | **2.39** | 1.21E+13 | 1.18E+23 | -2.39 | 62.17 | 2.00E+02 | 10 |
| | **9.99E+16** | **-1.22** | **1.07** | 1.27E+13 | 1.86E+19 | -1.22 | 60.86 | 2.07E+02 | 50 |
| | **1.12E+13** | **0** | **-0.31** | 1.31E+13 | 5.70E+14 | 0.00 | 59.89 | 4.56E+01 | High P limit |
| | **1.23E+55** | **-13.29** | **12.76** | 2.62E+12 | 8.92E+56 | -13.34 | 73.05 | 9.25E+00 | 0.001 |
| | **1.17E+46** | **-10.37** | **10.31** | 5.16E+12 | 7.07E+47 | -10.39 | 70.56 | 1.80E+01 | 0.01 |
| C=CC• + CC=CC• ⇄ C=CCCC=CC | **1.79E+36** | **-7.24** | **7.38** | 8.25E+12 | 8.87E+37 | -7.24 | 67.59 | 2.86E+01 | 0.1 |
| | **5.63E+26** | **-4.25** | **4.34** | 1.09E+13 | 2.37E+28 | -4.23 | 64.52 | 3.75E+01 | 1 |
| | **1.32E+19** | **-1.88** | **1.79** | 1.24E+13 | 6.12E+20 | -1.87 | 61.96 | 4.15E+01 | 10 |
| | **4.58E+15** | **-0.81** | **0.60** | 1.27E+13 | 3.55E+17 | -0.87 | 60.83 | 4.22E+01 | 50 |
| | **1.12E+13** | **0** | **-0.31** | 1.31E+13 | 2.24E+15 | 0.00 | 61.44 | 8.21E+01 | High P limit |
| | **1.98E+59** | **-14.66** | **13.90** | 1.89E+12 | 5.83E+61 | -14.71 | 75.74 | 1.21E+01 | 0.001 |
| | **5.37E+50** | **-11.86** | **11.68** | 4.02E+12 | 1.34E+53 | -11.88 | 73.49 | 2.53E+01 | 0.01 |
| C=CC• + C=CC•C ⇄ C=CCC(C)C=C | **1.27E+41** | **-8.77** | **8.90** | 6.96E+12 | 2.61E+43 | -8.77 | 70.67 | 4.38E+01 | 0.1 |
| | **1.81E+31** | **-5.66** | **5.82** | 9.90E+12 | 3.07E+33 | -5.64 | 67.55 | 6.15E+01 | 1 |
| | **3.49E+22** | **-2.94** | **2.96** | 1.19E+13 | 5.47E+24 | -2.91 | 64.66 | 7.28E+01 | 10 |
| | **8.84E+17** | **-1.52** | **1.39** | 1.25E+13 | 1.70E+20 | -1.52 | 63.11 | 7.55E+01 | 50 |
| | **1.12E+13** | **0** | **-0.31** | 1.31E+13 | 1.15E+15 | 0 | 59.51 | 1.11E+02 | High P limit |
| | **1.15E+17** | **-1.24** | **1.08** | 1.25E+13 | 1.35E+19 | -1.27 | 60.90 | 1.03E+02 | 50 |
| | **2.09E+21** | **-2.56** | **2.53** | 1.20E+13 | 1.80E+23 | -2.54 | 62.32 | 9.89E+01 | 10 |
| CC=CC• + CC=CC• ⇄ CC=CCCC=CC | **5.68E+29** | **-5.20** | **5.31** | 1.02E+13 | 5.08E+31 | -5.18 | 65.12 | 8.47E+01 | 1 |
| | **3.27E+39** | **-8.28** | **8.37** | 7.19E+12 | 3.52E+41 | -8.28 | 68.22 | 6.07E+01 | 0.1 |
| | **1.37E+49** | **-11.36** | **11.16** | 4.13E+12 | 1.81E+51 | -11.39 | 71.05 | 3.56E+01 | 0.01 |
| | **5.11E+57** | **-14.16** | **13.38** | 1.96E+12 | 7.95E+59 | -14.22 | 73.29 | 1.69E+01 | 0.001 |
| | **1.12E+13** | **0** | **-0.31** | 1.31E+13 | 7.99E+15 | 0.00 | 57.09 | 2.62E+03 | High P limit |
| | **4.76E+23** | **-3.30** | **3.31** | 1.15E+13 | 3.00E+26 | -3.29 | 60.69 | 2.25E+03 | 50 |
| | **7.29E+29** | **-5.24** | **5.32** | 9.87E+12 | 4.88E+32 | -5.23 | 62.72 | 1.95E+03 | 10 |
| C=CC•C + C=CC•C ⇄ C=CC(C)C(C)C=C | **4.02E+39** | **-8.32** | **8.34** | 6.76E+12 | 3.24E+42 | -8.33 | 65.77 | 1.35E+03 | 1 |
| | **1.16E+49** | **-11.36** | **11.03** | 3.78E+12 | 1.14E+52 | -11.40 | 68.51 | 7.62E+02 | 0.1 |
| | **2.18E+57** | **-14.08** | **13.10** | 1.71E+12 | 2.52E+60 | -14.14 | 70.61 | 3.48E+02 | 0.01 |
| | **8.60E+63** | **-16.33** | **14.39** | 6.21E+11 | 1.12E+67 | -16.41 | 71.91 | 1.27E+02 | 0.001 |

Note: The forward rate constants are based on literature measurements as discussed in the text; the reverse rate constants are calculated using the principle of microscopic reversibility, using thermochemical parameters for each reactant.

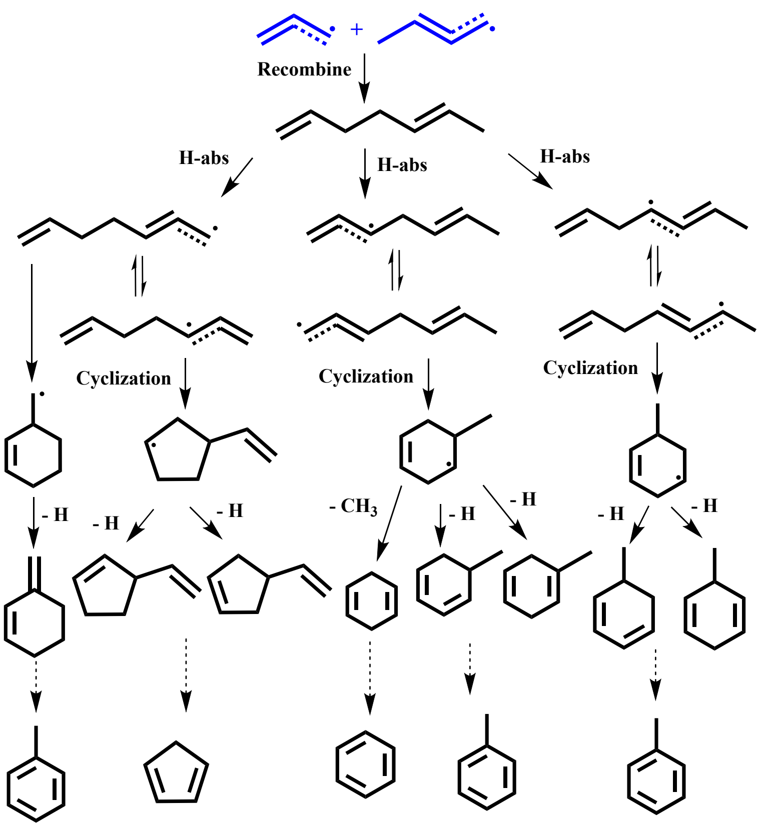


*Figure S1: Pathways leading to formation of aromatic species after recombination of methyl-allyl and allyl radicals.*

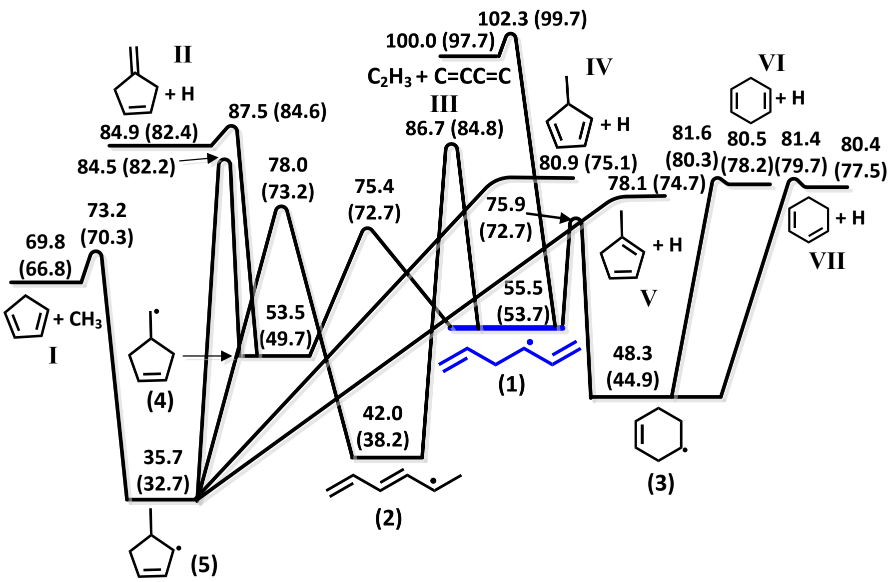


*Figure S2: Simplified $C_6H_9$ PES depicting the energetics of the reaction sequence after hydrogen abstraction from the initially-formed linear adduct in the recombination of two allyl radicals. (The numbers are enthalpies (kcal/mol) at 298K based on CBS-QB3 calculations; the numbers in parenthesis are based on rate rule estimates).*

*Table S2: High pressure limit rate constants for reactions shown in the $C_6H_9$ PES in Figure S2 and Figure 5 in text (based on CBS-QB3 calculations).*

| Reactions | Forward | | | Reverse | | |
|---|---|---|---|---|---|---|
| | A ($s^{-1}$) | Ea (kcal/mol) | *k* (1000K) ($s^{-1}$) | A ($s^{-1}$ or $cm^3$/mol-s) | Ea (kcal/mol) | *k* (1000K) ($s^{-1}$ or $cm^3$/mol-s) |
| C=CCC•C=C <=> 2 | 1.84E+12 | 31.3 | 2.68E+05 | 1.32E+13 | 44.8 | 2.12E+03 |
| C=CCC•C=C <=> 3 | 1.10E+11 | 21.1 | 2.67E+06 | 5.03E+13 | 28.8 | 2.60E+07 |
| C=CCC•C=C <=> 4 | 4.29E+11 | 20.9 | 1.14E+07 | 4.68E+13 | 23.4 | 3.52E+08 |
| C=CCC•C=C <=> III | 1.71E+15 | 45.1 | 2.35E+05 | 1.38E+13 | 2.31 | 4.30E+12 |
| 2 <=> 5 | 2.45E+12 | 36.6 | 2.40E+04 | 5.30E+13 | 43.2 | 1.88E+04 |
| 3 <=> VI | 2.01E+14 | 35.0 | 4.40E+06 | 4.15E+14 | 3.71 | 6.41E+13 |
| 3 <=> VII | 8.94E+13 | 34.6 | 2.44E+06 | 1.32E+14 | 3.33 | 2.47E+13 |
| 4 <=> 5 | 5.84E+12 | 30.5 | 1.24E+06 | 8.28E+12 | 48.1 | 2.47E+02 |
| 4 <=> II | 2.85E+13 | 35.9 | 4.01E+05 | 2.47E+13 | 4.94 | 2.05E+12 |
| 5 <=> I | 9.89E+14 | 38.9 | 3.11E+06 | 1.50E+13 | 6.83 | 4.82E+11 |
| 5 <=> IV | 4.95E+12 | 46.4 | 3.57E+02 | 2.60E+13 | 2.16 | 8.76E+12 |
| 3 <=> V | 1.54E+13 | 43.0 | 5.98E+03 | 2.60E+13 | 2.16 | 8.76E+12 |

*Table S3: Rate constants at 1 atm for the reactions shown in the $C_6H_9$ PES in Figure S2 and Figure 5 in text for the temperature range 300- 2500 K.*

| Reactions | | | A ($s^{-1}$) | n | E (kcal/mol) | k (1000K) ($s^{-1}$) | Reactions | | | A ($s^{-1}$) | n | E (kcal/mol) | k (1000K) ($s^{-1}$) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| C=CCC•C=C | <=> | III | 2.13E+37 | -7.08 | 51.56 | 6.65E+04 | 3 | <=> | III | 8.11E+48 | -10.32 | 65.18 | 4.88E+03 |
| C=CCC•C=C | <=> | 3 | 3.90E+41 | -9.86 | 29.57 | 3.46E+05 | 3 | <=> | VI | 8.03E+35 | -7.18 | 40.16 | 3.86E+05 |
| C=CCC•C=C | <=> | VI | 2.90E+41 | -9.04 | 41.53 | 1.82E+05 | 3 | <=> | VII | 8.58E+35 | -7.28 | 39.95 | 2.24E+05 |
| C=CCC•C=C | <=> | VII | 1.70E+41 | -9.06 | 41.32 | 1.00E+05 | 3 | <=> | 4 | 1.08E+57 | -13.93 | 48.56 | 4.28E+04 |
| C=CCC•C=C | <=> | 4 | 5.84E+39 | -9.31 | 27.77 | 6.02E+05 | 3 | <=> | II | 1.38E+52 | -12.09 | 59.40 | 7.43E+02 |
| C=CCC•C=C | <=> | II | 3.99E+36 | -7.78 | 42.68 | 8.25E+03 | 3 | <=> | 5 | 5.29E+61 | -15.54 | 57.95 | 2.70E+02 |
| C=CCC•C=C | <=> | 2 | 2.94E+36 | -7.63 | 38.84 | 1.24E+05 | 3 | <=> | I | 8.14E+55 | -12.90 | 62.29 | 3.77E+03 |
| C=CCC•C=C | <=> | 5 | 1.57E+45 | -11.02 | 39.86 | 2.66E+03 | 3 | <=> | V | 1.24E+51 | -12.15 | 62.29 | 1.03E+01 |
| C=CCC•C=C | <=> | I | 2.12E+39 | -8.29 | 45.03 | 4.09E+04 | 3 | <=> | IV | 1.45E+48 | -11.54 | 62.40 | 7.76E-01 |
| C=CCC•C=C | <=> | V | 6.95E+34 | -7.62 | 45.35 | 1.15E+02 | 4 | <=> | III | 2.41E+43 | -8.75 | 58.26 | 2.45E+04 |
| C=CCC•C=C | <=> | IV | 1.97E+32 | -7.11 | 45.80 | 8.84E+00 | 4 | <=> | VI | 4.92E+51 | -11.86 | 51.23 | 8.04E+04 |
| 2 | <=> | III | 1.88E+43 | -8.47 | 73.41 | 6.47E+01 | 4 | <=> | VII | 4.19E+51 | -11.93 | 51.14 | 4.45E+04 |
| 2 | <=> | 3 | 1.48E+49 | -11.64 | 60.42 | 1.10E+01 | 4 | <=> | II | 3.67E+25 | -4.50 | 36.91 | 9.86E+03 |
| 2 | <=> | VI | 9.97E+49 | -11.10 | 68.66 | 4.94E+01 | 4 | <=> | 5 | 4.29E+46 | -11.49 | 37.64 | 8.60E+03 |
| 2 | <=> | VII | 7.28E+49 | -11.15 | 68.59 | 2.65E+01 | 4 | <=> | I | 1.36E+33 | -6.58 | 40.17 | 4.15E+04 |
| 2 | <=> | 4 | 2.07E+43 | -9.87 | 57.36 | 1.45E+01 | 4 | <=> | V | 5.57E+27 | -5.64 | 40.36 | 1.01E+02 |
| 2 | <=> | II | 1.24E+43 | -9.27 | 67.63 | 3.21E+00 | 4 | <=> | IV | 5.17E+24 | -4.98 | 40.89 | 6.97E+00 |
| 2 | <=> | 5 | 1.21E+43 | -9.98 | 44.90 | 2.14E+03 | 5 | <=> | III | 3.89E+41 | -8.44 | 77.70 | 1.96E-01 |
| 2 | <=> | I | 8.69E+32 | -5.99 | 49.91 | 1.13E+04 | 5 | <=> | VI | 5.44E+54 | -12.92 | 75.35 | 3.20E-01 |
| 2 | <=> | V | 4.88E+28 | -5.38 | 50.83 | 2.81E+01 | 5 | <=> | VII | 5.22E+54 | -13.00 | 75.32 | 1.74E-01 |
| 2 | <=> | IV | 4.98E+26 | -5.01 | 52.02 | 1.99E+00 | 5 | <=> | II | 7.53E+32 | -6.90 | 62.65 | 3.06E-02 |
| | | | | | | | 5 | <=> | I | 6.50E+42 | -8.96 | 46.77 | 5.03E+05 |
| | | | | | | | 5 | <=> | V | 7.82E+39 | -8.70 | 50.15 | 6.53E+02 |
| | | | | | | | 5 | <=> | IV | 1.24E+38 | -8.37 | 52.70 | 2.79E+01 |

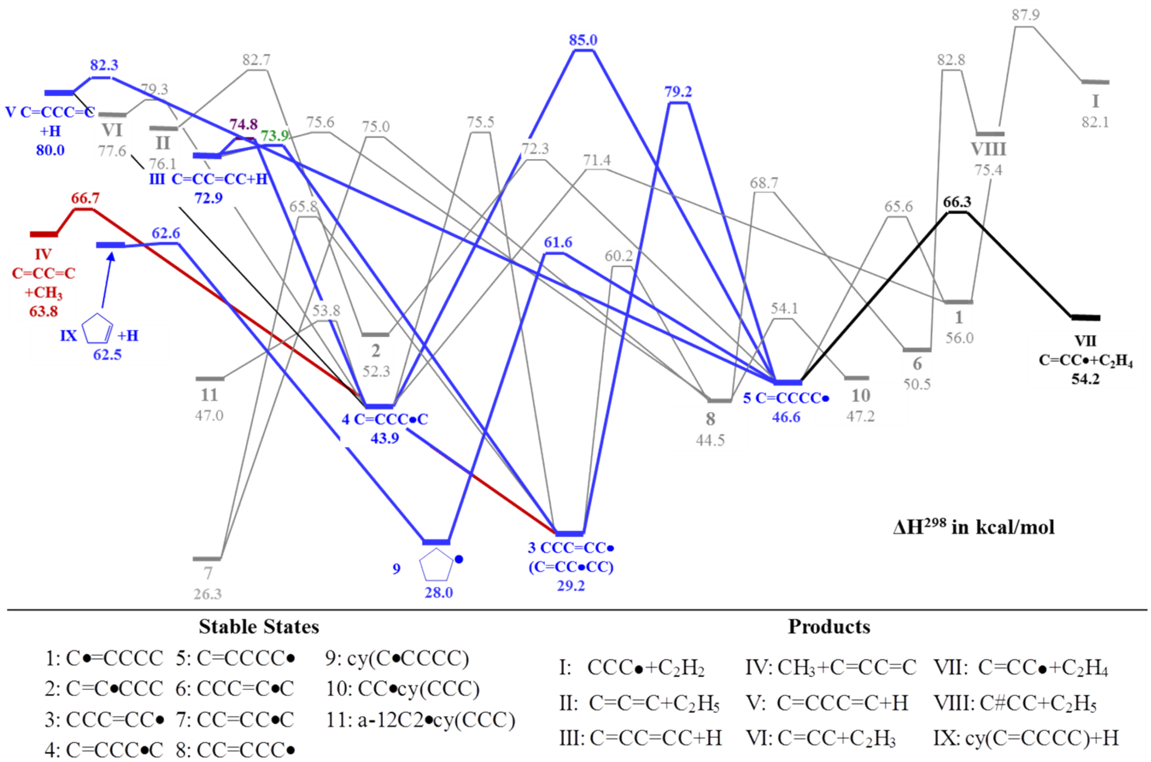


*Figure S3: A more complete $C_5H_9$ PES by CBS-QB3.*

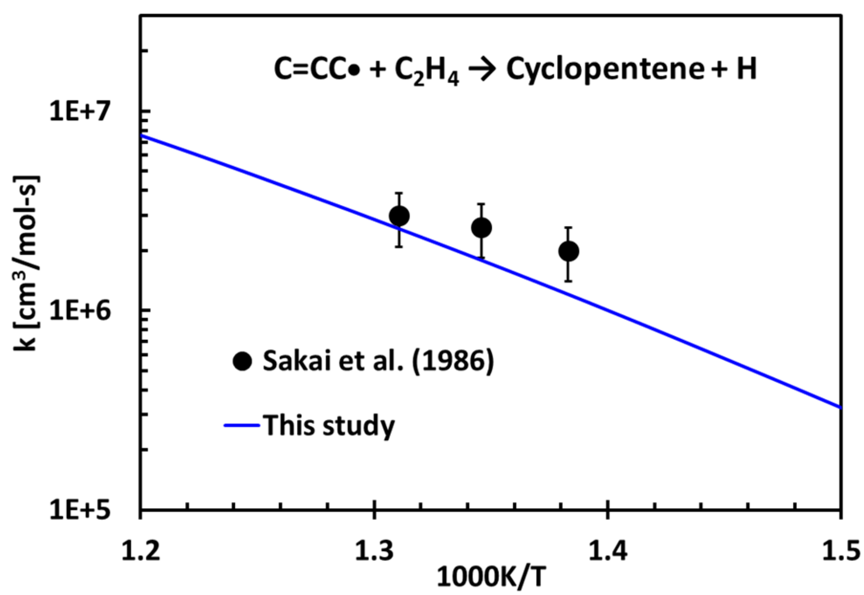


*Figure S4: Comparison of the rate constant for formation of cyclopentene + H from the reaction allyl + ethylene calculated in this study with literature values at 1 atm.*

*Table S4: High pressure limit rate constants for reactions shown in the $C_5H_9$ PES in Figure 7 in text (CBS-QB3 calculations vs. rate rule estimates).*

| | **Forward reaction** | | | **Reverse reaction** | | | | **Note** |
|---|---|---|---|---|---|---|---|---|
| | **Rate constants from CBS-QB3 calculation** | | | | | | | |
| Reactions | A ($s^{-1}$ or $cm^3$/mol-s) | Ea (kcal/mol) | k(1000K) ($s^{-1}$ $cm^3$/mol-s) | A ($s^{-1}$ or $cm^3$/mol-s) | n | Ea (kcal/mol) | k(1000K) ($s^{-1}$ $cm^3$/mol-s) | |
| I ⇄ 1 | 2.13E+12 | 14.7 | 1.28E+09 | 1.48E+13 | 0 | 20.7 | 4.44E+08 | |
| 1 ⇄ II | 1.44E+13 | 36.9 | 1.22E+05 | 9.74E+13 | 0 | 3.66 | 1.54E+13 | |
| 1 ⇄ 4 | 7.67E+10 | 16.4 | 1.99E+07 | 3.28E+13 | 0 | 14.3 | 2.46E+10 | |
| 4 ⇄ VI | 3.00E+14 | 38.7 | 1.03E+06 | 1.30E+13 | 0 | 1.6 | 5.93E+12 | |
| 1 ⇄ 5 | 7.69E+10 | 15.4 | 3.30E+07 | 1.70E+14 | 0 | 34.5 | 4.80E+06 | |
| 5 ⇄ IV | 4.41E+14 | 36.1 | 5.71E+06 | 1.78E+14 | 0 | 2.18 | 5.93E+13 | All rate constants are based on CBS-QB3 calculation |
| 1 ⇄ 3 | 1.62E+12 | 32.2 | 1.50E+05 | 1.27E+13 | 0 | 49.6 | 1.84E+02 | |
| 3 ⇄ III | 1.62E+14 | 46.6 | 1.03E+04 | 1.02E+14 | 0 | 3.02 | 2.23E+13 | |
| 3 ⇄ V | 6.16E+14 | 38.0 | 2.95E+06 | 5.82E+12 | 0 | 5.44 | 3.76E+11 | |
| 1 ⇄ 2 | 9.01E+12 | 38.1 | 4.26E+04 | 1.10E+13 | 0 | 41.3 | 1.01E+04 | |
| 2 ⇄ II | 2.38E+13 | 39.2 | 6.52E+04 | 2.60E+13 | 0 | 1.56 | 1.19E+13 | |
| 2 III | 1.45E+13 | 33.9 | 5.72E+05 | 5.84E+13 | 0 | 4.39 | 6.39E+12 | |
| | **Rate constants based on estimation techniques** | | | | | | | |
| I ⇄ 1 | **2.00E+12** | **13.1** | 2.80E+09 | 1.09E+13 | 0 | 20.3 | 3.90E+08 | Estimated A-factor, Ea from CBS-QB3 calculation of Saeys et al. (2004) |
| 1 ⇄ II | 1.95E+12 | 36.7 | 1.80E+04 | **1.26E+12** | **0.29** | **2.77** | 2.36E+12 | Rate rules for H + larger olefin |
| 1 ⇄ 4 | **4.21E+10** | **12.9** | 6.35E+07 | 8.52E+12 | 0.00 | 8.98 | 9.26E+10 | 4-member ring, Estrain=5, Eaddion analogy to $C_2H_5$+$C_3H_6$_CCC(C)C. at 1000 K |
| 4 VI | 3.71E+13 | 35.1 | 7.73E+05 | **1.26E+12** | **0.29** | **2.77** | 2.36E+12 | Rate rules for H + larger olefin |
| 1 ⇄ 5 | **4.21E+10** | **15.0** | 2.21E+07 | 3.37E+14 | 0 | 33.4 | 1.65E+07 | 5-member ring, $E_{strain}$=6, $E_{addion}$ analogy to $C_2H_5$+$C_3H_6$_2-$C_5H_{11}$ at 1000 K |
| 5 IV | 1.26E+14 | 36.5 | 1.31E+06 | **1.26E+12** | **0.29** | **2.77** | 2.36E+12 | Rate rules for H + larger olefin |
| 1 ⇄ 3 | **2.99E+11** | **32.9** | 1.91E+04 | 3.37E+14 | 0 | 48.4 | 8.99E+03 | 1,3-H transfer, $E_{strain}$=22.8, $E_{abs}$ analogy to $C_2H_5$+$C_3H_6$_$C_2H_6$+a$C_3H_5$ at 1000 K |
| 3 ⇄ III | 9.70E+13 | 45.0 | 1.42E+04 | **1.26E+12** | **0.29** | **2.77** | 2.36E+12 | Rate rules for H + larger olefin |
| 3 V | 1.25E+15 | 36.8 | 1.14E+07 | **5.71E+12** | **0** | **5.49** | 3.61E+11 | From CBS-QB3 calculation (Saeys at el.) |
| 1 ⇄ 2 | **1.96E+13** | **38.7** | 6.74E+04 | 1.95E+13 | 0 | 41.8 | 1.41E+04 | 1,2-H transfer, $E_{strain}$=24.4, $E_{abs}$ analogy to $C_2H_5$+$C_3H_8$_$C_2H_6$+i$C_3H_7$ at 1000 K |
| 2 ⇄ II | 4.01E+12 | 39.6 | 8.57E+03 | **2.52E+12** | **0.29** | **2.77** | 4.72E+12 | Rate rules for H + larger olefin |
| 2 III | 2.56E+12 | 32.6 | 1.92E+05 | **1.26E+12** | **0.29** | **2.77** | 2.36E+12 | Rate rules for H + larger olefin |

Note: The bold blue are the initially estimated numbers; the reverse rate constants are calculated from the thermodynamic data.

*Table S5: Rate constants at 1 atm for 500- 1800 K for the $C_5H_9$ PES, entering from the C=CC• + $C_2H_4$.*

| Reactions | | | A ($s^{-1}$ or $cm^3$/mol-s) | n | Ea (kcal/mol) | *k* (1000K) ($s^{-1}$ or $cm^3$/mol-s) |
|---|---|---|---|---|---|---|
| I | <=> | (3) | 1.41E+48 | -11.83 | 37.87 | 2.37E+04 |
| I | <=> | III | 4.23E+28 | -4.89 | 38.25 | 3.91E+05 |
| I | <=> | IV | 6.90E+19 | -2.68 | 38.02 | 3.09E+03 |
| I | <=> | (1) | 5.30E+26 | -5.02 | 16.49 | 1.13E+08 |
| I | <=> | V | 6.41E+16 | -1.31 | 33.58 | 3.44E+05 |
| I | <=> | (2) | 9.45E+42 | -9.61 | 43.74 | 3.89E+04 |
| I | <=> | IV | 1.89E+37 | -7.09 | 51.61 | 5.30E+04 |
| I | <=> | V | 1.40E+34 | -6.23 | 52.37 | 1.02E+04 |
| I | <=> | (5) | 8.31E+66 | -17.33 | 36.70 | 8.19E+06 |
| I | <=> | II | 1.13E+42 | -9.01 | 34.21 | 3.61E+07 |
| I | <=> | (4) | 6.65E+24 | -5.29 | 17.97 | 1.03E+05 |
| I | <=> | VI | 4.14E+12 | -0.55 | 34.50 | 2.71E+03 |
| (3) | <=> | III | 2.32E+56 | -12.97 | 53.12 | 6.92E+05 |
| (3) | <=> | IV | 2.20E+50 | -11.61 | 57.46 | 8.73E+02 |
| (3) | <=> | (1) | 8.00E+41 | -10.23 | 52.66 | 4.92E-01 |
| (3) | <=> | V | 2.75E+29 | -6.31 | 59.82 | 2.75E-03 |
| (3) | <=> | (2) | 5.99E+50 | -13.09 | 68.21 | 3.94E-04 |
| (3) | <=> | IV | 6.44E+42 | -10.06 | 73.56 | 3.53E-04 |
| (3) | <=> | V | 6.57E+37 | -8.68 | 73.13 | 5.93E-05 |
| (3) | <=> | (5) | 1.01E+68 | -18.50 | 64.12 | 3.04E-02 |
| (3) | <=> | II | 6.54E+58 | -14.92 | 66.65 | 3.03E-01 |
| (3) | <=> | (4) | 1.46E+39 | -10.31 | 52.79 | 5.04E-04 |
| (3) | <=> | VI | 3.94E+22 | -4.81 | 58.95 | 1.92E-05 |
| (1) | <=> | III | 6.90E+22 | -3.90 | 35.53 | 2.35E+03 |
| (1) | <=> | IV | 6.11E+11 | -1.07 | 34.28 | 1.20E+01 |
| (1) | <=> | V | 6.57E+07 | 0.57 | 29.14 | 1.44E+03 |
| (1) | <=> | (2) | 2.61E+29 | -6.22 | 38.40 | 2.29E+02 |
| (1) | <=> | IV | 4.50E+23 | -3.82 | 45.92 | 1.40E+02 |
| (1) | <=> | V | 6.21E+19 | -2.77 | 46.37 | 2.19E+01 |
| (1) | <=> | (5) | 3.83E+60 | -15.73 | 31.93 | 2.51E+06 |
| (1) | <=> | II | 1.47E+46 | -10.81 | 34.50 | 1.56E+06 |
| (1) | <=> | (4) | 6.82E+28 | -7.01 | 15.17 | 3.00E+04 |
| (1) | <=> | VI | 8.41E+02 | 1.53 | 29.93 | 9.09E+00 |
| (2) | <=> | III | 6.09E+38 | -8.66 | 56.63 | 2.64E+00 |
| (2) | <=> | IV | 2.28E+30 | -6.62 | 55.42 | 2.42E-02 |
| (2) | <=> | V | 1.17E+30 | -6.01 | 53.07 | 2.69E+00 |
| (2) | <=> | IV | 2.49E+40 | -8.41 | 44.35 | 3.00E+05 |
| (2) | <=> | V | 3.41E+41 | -8.77 | 49.43 | 2.56E+04 |
| (2) | <=> | (5) | 4.88E+50 | -13.14 | 49.95 | 2.19E+00 |
| (2) | <=> | II | 1.29E+48 | -11.34 | 55.72 | 8.18E+01 |
| (2) | <=> | (4) | 3.93E+26 | -6.20 | 41.93 | 6.69E-02 |
| (2) | <=> | VI | 7.57E+24 | -5.00 | 52.80 | 2.21E-02 |

| | | | | | | |
|---|---|---|---|---|---|---|
| (5) | <=> | III | 1.08E+59 | -14.24 | 69.72 | 1.21E+01 |
| (5) | <=> | IV | 8.89E+45 | -10.87 | 67.08 | 4.71E-02 |
| (5) | <=> | V | 8.96E+41 | -9.21 | 61.93 | 5.91E+00 |
| (5) | <=> | IV | 2.26E+52 | -12.04 | 76.05 | 4.10E-01 |
| (5) | <=> | V | 6.14E+47 | -10.80 | 76.09 | 5.59E-02 |
| (5) | <=> | II | 6.88E+56 | -13.26 | 50.66 | 9.34E+05 |
| (5) | <=> | (4) | 2.15E+68 | -17.82 | 56.85 | 2.79E+02 |
| (5) | <=> | VI | 4.92E+35 | -7.89 | 61.87 | 3.19E-02 |
| (4) | <=> | III | 1.50E+26 | -4.89 | 36.84 | 2.89E+03 |
| (4) | <=> | IV | 1.34E+15 | -2.05 | 35.63 | 1.54E+01 |
| (4) | <=> | V | 1.75E+11 | -0.43 | 30.53 | 1.84E+03 |
| (4) | <=> | IV | 4.38E+27 | -4.99 | 47.54 | 1.86E+02 |
| (4) | <=> | V | 5.59E+23 | -3.93 | 47.99 | 2.97E+01 |
| (4) | <=> | II | 3.05E+50 | -12.10 | 36.39 | 1.74E+06 |
| (4) | <=> | VI | 1.33E+02 | 2.31 | 29.09 | 4.78E+02 |

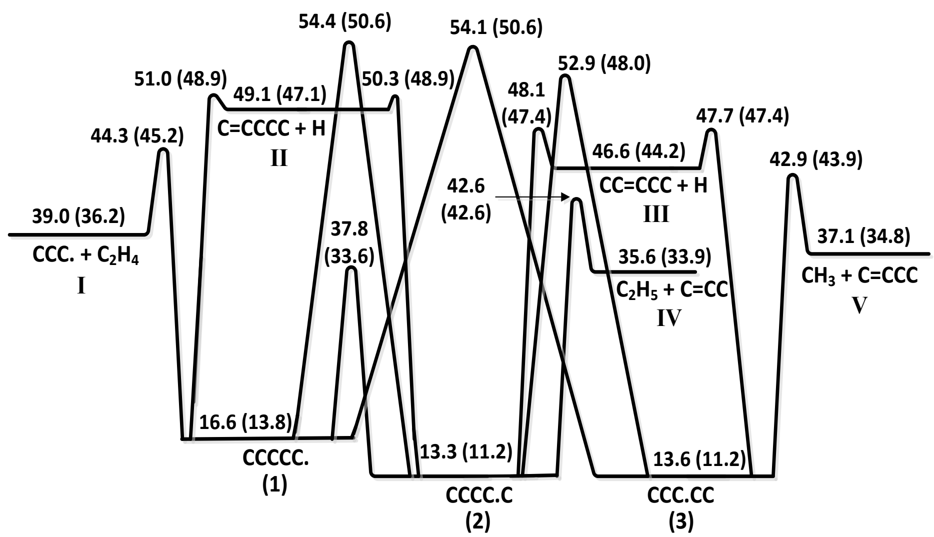


*Figure S5: Simplified $C_5H_{11}$ potential energy surface calculated at the CBS-QB3 level of theory, showing enthalpies in kcal/mol at 298 K. Numbers in parenthesis are based on rate rule estimates.*

*Table S6: High pressure limit rate constants for reactions shown in the $C_5H_{11}$ PES in Figure S5 and Figure 10 in text (CBS-QB3 calculations vs. rate rule estimates). The solid lines are obtained from the CBS-QB3 high pressure rate constants, while the dashed lines are obtained from the estimated high pressure rate constants.*

| Reactions | Forward reaction | | | Reverse reaction | | | Note |
|---|---|---|---|---|---|---|---|
| | Rate constants by CBS-QB3 calculation | | | | | | |
| | A ($s^{-1}$ or $cm^3$/mol-s) | Ea (kcal/mol) | *k* (1000K) ($s^{-1}$ or $cm^3$/mol-s) | A ($s^{-1}$ or $cm^3$/mol-s) | Ea (kcal/mol) | *k* (1000K) ($s^{-1}$ or $cm^3$/mol-s) | |
| I ⇄ 1 | 1.32E+12 | 8.52 | 1.81E+10 | 1.96E+13 | 28.5 | 1.13E+07 | CBS-QB3 calculation |
| 1 ⇄ II | 2.03E+13 | 36.1 | 2.57E+05 | 1.20E+14 | 4.35 | 1.34E+13 | |
| 1 ⇄ 2 (Duplicate reaction) | 3.27E+10 | 20.8 | 9.22E+05 | 1.68E+11 | 24.6 | 6.87E+05 | |
| 1 ⇄ 2 (Duplicate reaction) | 1.79E+12 | 37.3 | 1.25E+04 | 9.21E+12 | 41.1 | 9.36E+03 | |
| 1 ⇄ 3 | 4.77E+11 | 36.7 | 4.40E+03 | 1.84E+12 | 40.3 | 2.85E+03 | |
| 2 ⇄ IV | 4.82E+13 | 28.9 | 2.28E+07 | 4.74E+12 | 8.27 | 7.39E+10 | |
| 2 ⇄ II | 1.56E+14 | 38.6 | 5.78E+05 | 1.80E+14 | 2.96 | 4.05E+13 | |
| 2 ⇄ III | 4.29E+13 | 36.8 | 3.89E+05 | 8.80E+13 | 3.86 | 1.26E+13 | |
| 2 ⇄ 3 | 5.50E+12 | 39.2 | 1.45E+04 | 4.14E+12 | 39.0 | 1.26E+04 | |
| 3 ⇄ III | 4.06E+13 | 36.2 | 4.93E+05 | 1.10E+14 | 3.56 | 1.83E+13 | |
| 3 ⇄ V | 1.43E+14 | 30.9 | 2.46E+07 | 6.08E+12 | 8.99 | 6.57E+10 | |
| | Rate constants from estimation | | | | | | |
| I ⇄ 1 | **2.11E+12** | **8.99** | 2.29E+10 | **2.12E+13** | **28.6** | 1.18E+07 | From CBS-QB3 calculation |
| 1 ⇄ II | 1.58E+13 | 36.0 | 2.11E+05 | **1.16E+13** | **3.23** | 2.28E+12 | H inner addition to C=CC by Curran 2006 |
| 1 ⇄ 2 (Duplicate reaction) | **2.99E+11** | **19.1** | 1.99E+07 | 2.86E+11 | 22.1 | 4.17E+06 | 1,4-H transfer, $E_{strain}$=5.8, $E_{abs}$ analogy to $CH_3$+$C_2H_6$_$CH_4$+$C_2H_5$ at 1000 K |
| 1 ⇄ 2 (Duplicate reaction) | **1.96E+13** | **37.7** | 1.12E+05 | 1.87E+13 | 40.7 | 2.33E+04 | 1,2-H transfer, $E_{strain}$=24.4, $E_{abs}$ analogy to $CH_3$+$C_2H_6$_$CH_4$+$C_2H_5$ at 1000 K |
| 1 ⇄ 3 | **2.42E+12** | **36.1** | 3.09E+04 | 4.60E+12 | 39.1 | 1.28E+04 | 1,3-H transfer, $E_{strain}$=22.8, $E_{abs}$ analogy to $CH_3$+$C_2H_6$_$CH_4$+$C_2H_5$ at 1000 K |
| 2 ⇄ IV | 5.33E+13 | 29.0 | 2.39E+07 | **7.38E+12** | **8.71** | 9.20E+10 | From CBS-QB3 calculation |
| 2 ⇄ II | 2.55E+13 | 37.6 | 1.50E+05 | **1.96E+13** | **1.84** | 7.77E+12 | H inner addition to C=CC by Curran 2006 |
| 2 ⇄ III | 1.51E+13 | 39.0 | 4.40E+04 | **1.16E+13** | **3.23** | 2.28E+12 | H inner addition to C=CC by Curran 2006 |
| 2 ⇄ 3 | **1.96E+13** | **37.7** | 1.12E+05 | 3.91E+13 | 37.7 | 2.23E+05 | 1,2-H transfer, $E_{strain}$=24.4, $E_{abs}$ analogy to $CH_3$+$C_2H_6$_$CH_4$+$C_2H_5$ at 1000 K |
| 3 ⇄ III | 3.01E+13 | 39.0 | 8.78E+04 | **1.16E+13** | **3.23** | 2.28E+12 | H inner addition to C=CC by Curran 2006 |
| 3 ⇄ V | 1.79E+14 | 30.8 | 3.24E+07 | **4.95E+12** | **8.56** | 6.64E+10 | From CBS-QB3 calculation |

Note: The bold blue are the initially estimated numbers; reverse rate constants are calculated from the thermodynamic data.

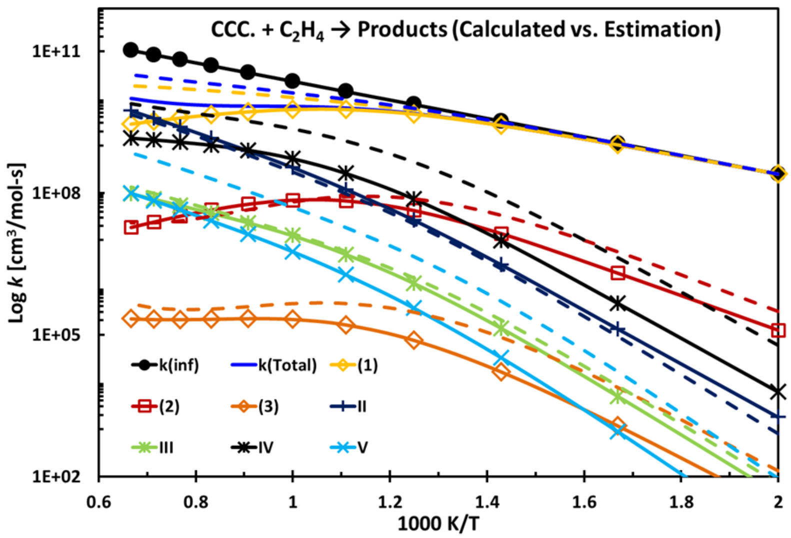


*Figure S6: Predicted apparent rate constants at 1 atm for the $C_5H_{11}$ PES, entering from the CCC• + $C_2H_4$ channel.*

*Table S7: Rate constants at 1 atm and 500- 1800 K for the $C_5H_{11}$ PES, from the CCC• + $C_2H_4$ channel.*

| Reactions | | | A ($s^{-1}$ or $cm^3$/mol-s) | *n* | Ea (kcal/mol) | *k* (1000K) ($s^{-1}$ or $cm^3$/mol-s) | Note |
|---|---|---|---|---|---|---|---|
| I | <=> | 1 | 2.69E+24 | -4.36 | 9.48 | 1.92E+09 | |
| I | <=> | II | 4.82E+20 | -2.41 | 25.3 | 8.50E+07 | Duplicate reaction |
| I | <=> | 2 | 7.10E+54 | -13.2 | 27.7 | 1.78E+09 | Duplicate reaction |
| I | <=> | II | 8.77E+39 | -7.94 | 34.2 | 4.42E+08 | Duplicate reaction |
| I | <=> | III | 4.77E+41 | -8.58 | 34.3 | 2.79E+08 | Duplicate reaction |
| I | <=> | IV | 1.31E+52 | -11.4 | 35.5 | 1.11E+10 | Duplicate reaction |
| I | <=> | 2 | 1.13E+32 | -7.12 | 25.3 | 1.42E+05 | Duplicate reaction |
| I | <=> | II | 2.85E+22 | -3.24 | 33.4 | 2.78E+05 | Duplicate reaction |
| I | <=> | III | 3.91E+23 | -3.70 | 33.4 | 1.57E+05 | Duplicate reaction |
| I | <=> | IV | 3.14E+31 | -5.83 | 33.9 | 3.83E+06 | Duplicate reaction |
| I | <=> | 3 | 1.79E+54 | -13.6 | 35.6 | 5.50E+05 | Duplicate reaction |
| I | <=> | III | 3.80E+36 | -7.55 | 38.2 | 3.78E+05 | Duplicate reaction |
| I | <=> | V | 1.69E+44 | -9.51 | 39.5 | 1.20E+07 | |
| 1 | <=> | II | 1.10E+17 | -1.95 | 32.4 | 1.28E+04 | Duplicate reaction |
| 1 | <=> | 2 | 9.63E+52 | -12.8 | 34.1 | 1.11E+07 | Duplicate reaction |
| 1 | <=> | II | 4.23E+41 | -8.92 | 45.2 | 9.87E+04 | Duplicate reaction |
| 1 | <=> | III | 1.43E+44 | -9.77 | 45.5 | 7.70E+04 | Duplicate reaction |
| 1 | <=> | IV | 2.95E+56 | -13.1 | 46.9 | 7.46E+06 | Duplicate reaction |
| 1 | <=> | 2 | 2.17E+34 | -8.13 | 37.3 | 6.44E+01 | Duplicate reaction |
| 1 | <=> | II | 2.84E+17 | -2.36 | 41.7 | 1.74E+01 | Duplicate reaction |
| 1 | <=> | III | 1.46E+19 | -2.99 | 41.9 | 1.11E+01 | Duplicate reaction |
| 1 | <=> | IV | 3.60E+29 | -5.80 | 43.4 | 4.51E+02 | Duplicate reaction |
| 1 | <=> | 3 | 1.55E+58 | -14.9 | 49.6 | 4.01E+02 | Duplicate reaction |
| 1 | <=> | III | 2.19E+38 | -8.57 | 50.3 | 4.32E+01 | Duplicate reaction |
| 1 | <=> | V | 6.84E+47 | -11.0 | 52.6 | 2.00E+03 | Duplicate reaction |
| 2 | <=> | II | 6.53E+41 | -9.60 | 50.8 | 8.25E+01 | Duplicate reaction |
| 2 | <=> | II | 8.70E+33 | -6.68 | 42.2 | 4.74E+04 | Duplicate reaction |
| 2 | <=> | III | 2.74E+35 | -7.25 | 41.6 | 3.89E+04 | Duplicate reaction |
| 2 | <=> | IV | 1.94E+42 | -9.07 | 38.2 | 5.08E+06 | Duplicate reaction |
| 2 | <=> | 2 | 3.14E+53 | -14.0 | 53.6 | 5.25E-01 | Duplicate reaction |
| 2 | <=> | II | 6.64E+33 | -7.60 | 54.9 | 1.06E-01 | Duplicate reaction |
| 2 | <=> | III | 1.34E+36 | -8.38 | 55.5 | 6.98E-02 | Duplicate reaction |
| 2 | <=> | IV | 2.20E+48 | -11.7 | 58.4 | 3.13E+00 | Duplicate reaction |
| 2 | <=> | 3 | 4.09E+54 | -13.8 | 49.2 | 2.18E+02 | Duplicate reaction |
| 2 | <=> | III | 4.74E+37 | -8.35 | 52.2 | 1.69E+01 | Duplicate reaction |
| 2 | <=> | V | 4.73E+46 | -10.6 | 54.0 | 8.31E+02 | Duplicate reaction |
| 2 | <=> | II | 2.07E+24 | -4.47 | 48.7 | 1.77E+00 | Duplicate reaction |
| 2 | <=> | II | 1.56E+42 | -9.57 | 57.0 | 1.05E+01 | Duplicate reaction |
| 2 | <=> | III | 3.85E+44 | -10.4 | 57.7 | 7.05E+00 | Duplicate reaction |
| 2 | <=> | IV | 1.01E+57 | -13.7 | 60.7 | 3.37E+02 | Duplicate reaction |
| 2 | <=> | II | 7.64E+36 | -7.59 | 43.3 | 4.50E+04 | Duplicate reaction |
| 2 | <=> | III | 2.27E+38 | -8.15 | 42.8 | 3.69E+04 | Duplicate reaction |
| 2 | <=> | IV | 1.06E+45 | -9.92 | 39.3 | 4.85E+06 | Duplicate reaction |
| 2 | <=> | 3 | 1.63E+57 | -14.6 | 50.2 | 2.09E+02 | Duplicate reaction |
| 2 | <=> | III | 4.80E+40 | -9.27 | 53.3 | 1.60E+01 | Duplicate reaction |
| 2 | <=> | V | 4.36E+49 | -11.6 | 55.1 | 7.92E+02 | Duplicate reaction |
| 3 | <=> | II | 3.84E+28 | -5.98 | 50.1 | 5.05E-01 | Duplicate reaction |
| 3 | <=> | II | 3.52E+40 | -9.16 | 53.8 | 2.00E+01 | Duplicate reaction |
| 3 | <=> | III | 8.53E+42 | -9.97 | 54.3 | 1.38E+01 | Duplicate reaction |
| 3 | <=> | IV | 2.01E+55 | -13.3 | 57.0 | 7.57E+02 | Duplicate reaction |
| 3 | <=> | II | 9.43E+39 | -9.02 | 53.5 | 1.72E+01 | Duplicate reaction |
| 3 | <=> | III | 2.38E+42 | -9.83 | 54.0 | 1.18E+01 | Duplicate reaction |
| 3 | <=> | IV | 6.99E+54 | -13.2 | 56.7 | 6.57E+02 | Duplicate reaction |
| 3 | <=> | III | 6.32E+43 | -9.79 | 44.6 | 4.84E+04 | Duplicate reaction |
| 3 | <=> | V | 1.18E+49 | -11.1 | 42.5 | 4.32E+06 | |

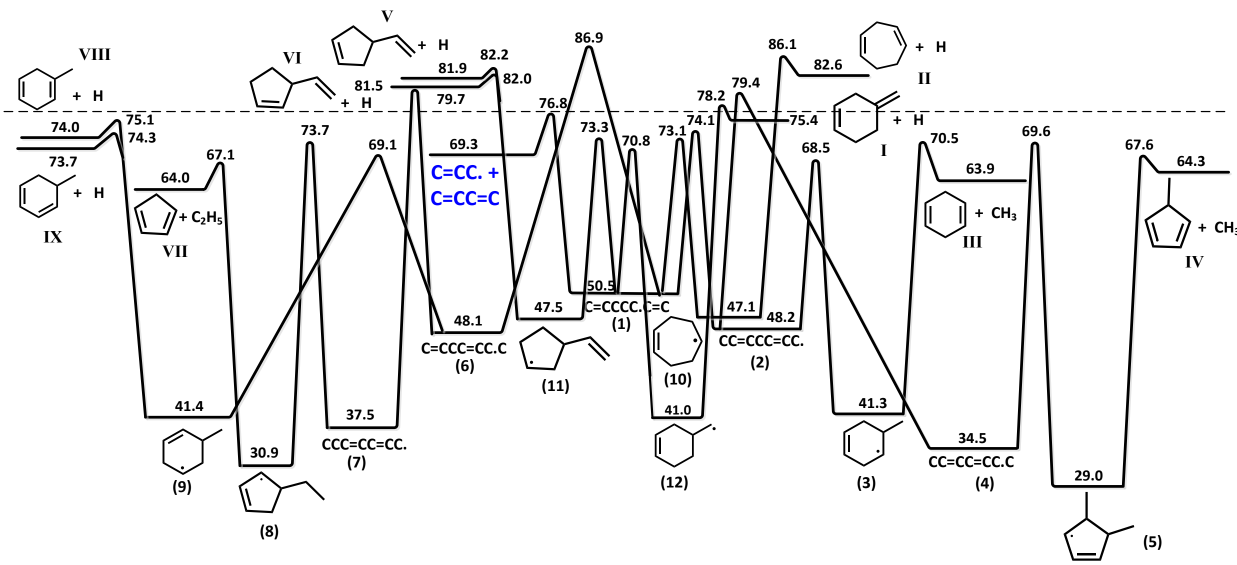


*Figure S7: Simplified $C_7H_{11}$ potential energy surface calculated at the CBS-QB3 level of theory, showing the enthalpies in kcal/mol at 298 K. (Note that this is the same as Figure 12 in the text, however the numbering of the product channels differs. This numbering corresponds to Tables S8 and S9 below.)*

*Table S8: High pressure limit rate constants for reactions shown in the $C_7H_{11}$ PES in Figure S7 (CBS-QB3 calculations).*

| Reactions | Forward | | | Reverse | | |
|---|---|---|---|---|---|---|
| | **A ($s^{-1}$ or $cm^3$/mol-s)** | **Ea (kcal/mol)** | ***k* (1000K) ($s^{-1}$ or $cm^3$/mol-s)** | **A ($s^{-1}$ or $cm^3$/mol-s)** | **Ea (kcal/mol)** | ***k* (1000K) ($s^{-1}$ or $cm^3$/mol-s)** |
| C=CC• + C=CC=C <=> 1 | 1.76E+12 | 11.06 | 6.71E+09 | 2.74E+13 | 28.11 | 1.95E+07 |
| 1 <=> 2 | 5.41E+11 | 24.01 | 3.03E+06 | 1.13E+12 | 26.40 | 1.91E+06 |
| 2 <=> 3 | 1.04E+11 | 21.25 | 2.34E+06 | 7.54E+13 | 28.46 | 4.51E+07 |
| 3 <=> III | 5.44E+14 | 30.25 | 1.32E+08 | 1.32E+13 | 9.89 | 9.08E+10 |
| 2 <=> 4 | 1.77E+12 | 31.15 | 2.73E+05 | 1.41E+13 | 44.97 | 2.07E+03 |
| 4 <=> 5 | 1.78E+12 | 35.63 | 2.88E+04 | 5.08E+13 | 41.10 | 5.23E+04 |
| 5 <=> IV | 1.95E+15 | 40.00 | 3.49E+06 | 1.52E+13 | 6.68 | 5.25E+11 |
| 1 <=> 6 | 3.77E+12 | 35.95 | 5.18E+04 | 1.34E+13 | 38.71 | 4.60E+04 |
| 6 <=> 7 | 5.25E+12 | 31.69 | 6.17E+05 | 1.38E+13 | 41.91 | 9.45E+03 |
| 7 <=> 8 | 2.33E+12 | 36.95 | 1.94E+04 | 5.64E+13 | 43.81 | 1.48E+04 |
| 8 <=> VII | 3.02E+14 | 36.99 | 2.46E+06 | 2.15E+13 | 6.78 | 7.07E+11 |
| 6 <=> 9 | 1.33E+11 | 22.06 | 2.00E+06 | 5.49E+13 | 28.72 | 2.88E+07 |
| 9 <=> VIII | 8.11E+13 | 34.83 | 1.96E+06 | 4.34E+13 | 3.12 | 9.04E+12 |
| 9 <=> IX | 8.14E+13 | 34.79 | 2.01E+06 | 6.90E+13 | 3.28 | 1.32E+13 |
| 1 <=> 10 | 7.75E+09 | 23.17 | 6.65E+04 | 1.68E+13 | 27.12 | 1.98E+07 |
| 10 <=> II | 2.44E+14 | 38.23 | 1.06E+06 | 8.00E+13 | 3.50 | 1.37E+13 |
| 1 <=> 11 | 4.94E+10 | 23.49 | 3.61E+05 | 1.92E+13 | 26.72 | 2.75E+07 |
| 11 <=> V | 2.51E+14 | 36.80 | 2.25E+06 | 1.25E+14 | 3.42 | 2.23E+13 |
| 11 <=> VI | 4.10E+14 | 36.60 | 4.07E+06 | 1.57E+14 | 2.90 | 3.65E+13 |
| 1 <=> 12 | 1.22E+11 | 20.32 | 4.39E+06 | 1.67E+14 | 32.59 | 1.25E+07 |
| 12 <=> I | 1.72E+14 | 39.96 | 3.16E+05 | 2.06E+14 | 3.92 | 2.85E+13 |

*Table S9: Rate constants from 500- 1800 K at 1 atm for the $C_7H_{11}$ PES (Figure S7), from allyl + C=CC=C.*

| Reactions | | | A ($s^{-1}$ or $cm^3$/mol-s) | n | Ea (kcal/mol) | *k* (1000K) ($s^{-1}$ or $cm^3$/mol-s) |
|---|---|---|---|---|---|---|
| C=CC• + C=CC=C | <=> | 1 | 1.47E+31 | -6.00 | 17.26 | 2.51E+09 |
| C=CC• + C=CC=C | <=> | 2 | 1.80E+52 | -11.94 | 36.63 | 2.70E+08 |
| C=CC• + C=CC=C | <=> | 6 | 2.23E+44 | -9.59 | 39.77 | 7.51E+06 |
| C=CC• + C=CC=C | <=> | 10 | 1.51E+57 | -14.34 | 36.56 | 1.51E+06 |
| C=CC• + C=CC=C | <=> | II | 3.04E+54 | -12.68 | 48.27 | 7.86E+05 |
| C=CC• + C=CC=C | <=> | 11 | 2.64E+60 | -15.13 | 37.48 | 7.03E+06 |
| C=CC• + C=CC=C | <=> | VI | 5.01E+59 | -13.99 | 49.38 | 8.37E+06 |
| C=CC• + C=CC=C | <=> | V | 1.69E+59 | -13.92 | 49.36 | 4.66E+06 |
| C=CC• + C=CC=C | <=> | 12 | 1.08E+63 | -15.83 | 36.03 | 4.62E+07 |
| C=CC• + C=CC=C | <=> | I | 3.76E+57 | -13.39 | 46.23 | 2.00E+07 |
| C=CC• + C=CC=C | <=> | 3 | 1.42E+74 | -19.52 | 46.69 | 2.36E+05 |
| C=CC• + C=CC=C | <=> | III | 4.93E+69 | -16.77 | 53.16 | 5.82E+07 |
| C=CC• + C=CC=C | <=> | 4 | 4.80E+69 | -16.82 | 55.12 | 1.47E+07 |
| C=CC• + C=CC=C | <=> | 5 | 1.07E+82 | -21.16 | 63.83 | 3.88E+04 |
| C=CC• + C=CC=C | <=> | IV | 6.25E+81 | -19.81 | 72.57 | 3.12E+06 |
| C=CC• + C=CC=C | <=> | 7 | 9.41E+66 | -15.90 | 58.89 | 2.47E+06 |
| C=CC• + C=CC=C | <=> | 9 | 1.39E+59 | -14.58 | 47.74 | 9.26E+04 |
| C=CC• + C=CC=C | <=> | IX | 1.91E+64 | -15.20 | 59.53 | 4.56E+05 |
| C=CC• + C=CC=C | <=> | VIII | 1.71E+64 | -15.19 | 59.53 | 4.48E+05 |
| C=CC• + C=CC=C | <=> | 8 | 1.07E+73 | -18.23 | 65.71 | 9.45E+03 |
| C=CC• + C=CC=C | <=> | VII | 2.23E+79 | -18.95 | 76.82 | 5.12E+05 |
| 1 | <=> | 2 | 1.27E+37 | -7.93 | 33.09 | 1.17E+06 |
| 1 | <=> | 6 | 1.09E+34 | -6.97 | 41.90 | 9.42E+03 |
| 1 | <=> | 10 | 1.59E+44 | -10.82 | 34.78 | 1.36E+04 |
| 1 | <=> | II | 5.42E+49 | -11.69 | 53.68 | 8.32E+02 |
| 1 | <=> | 11 | 1.92E+47 | -11.53 | 35.98 | 6.92E+04 |
| 1 | <=> | VI | 1.63E+55 | -13.05 | 55.11 | 1.02E+04 |
| 1 | <=> | V | 5.56E+54 | -12.98 | 55.11 | 5.57E+03 |
| 1 | <=> | 12 | 1.26E+52 | -12.87 | 34.61 | 8.14E+05 |
| 1 | <=> | I | 3.38E+52 | -12.31 | 50.57 | 3.42E+04 |
| 1 | <=> | 3 | 5.29E+66 | -17.68 | 48.69 | 1.06E+03 |
| 1 | <=> | III | 1.48E+62 | -15.00 | 55.92 | 8.82E+04 |
| 1 | <=> | 4 | 2.65E+56 | -13.32 | 56.16 | 1.49E+04 |
| 1 | <=> | 5 | 1.15E+74 | -19.13 | 68.97 | 3.80E+01 |
| 1 | <=> | IV | 3.41E+72 | -17.52 | 77.27 | 1.20E+03 |
| 1 | <=> | 7 | 9.07E+52 | -12.19 | 60.87 | 1.24E+03 |
| 1 | <=> | 9 | 4.54E+53 | -13.27 | 53.55 | 1.34E+02 |
| 1 | <=> | IX | 7.87E+56 | -13.48 | 64.58 | 2.17E+02 |
| 1 | <=> | VIII | 6.97E+56 | -13.47 | 64.57 | 2.13E+02 |
| 1 | <=> | 8 | 1.61E+62 | -15.41 | 70.35 | 3.97E+00 |
| 1 | <=> | VII | 2.05E+67 | -15.86 | 80.91 | 1.07E+02 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 2 | <=> | 6 | 7.74E+51 | -11.96 | 59.69 | 8.92E+02 |
| 2 | <=> | 10 | 3.80E+64 | -16.54 | 56.66 | 3.67E+02 |
| 2 | <=> | II | 3.16E+64 | -15.81 | 69.32 | 8.44E+01 |
| 2 | <=> | 11 | 3.50E+67 | -17.24 | 57.56 | 1.77E+03 |
| 2 | <=> | VI | 6.70E+69 | -17.13 | 70.63 | 9.71E+02 |
| 2 | <=> | V | 2.20E+69 | -17.06 | 70.60 | 5.37E+02 |
| 2 | <=> | 12 | 3.54E+71 | -18.34 | 56.68 | 1.35E+04 |
| 2 | <=> | I | 2.38E+68 | -16.72 | 67.69 | 2.64E+03 |
| 2 | <=> | 3 | 1.74E+50 | -12.89 | 31.03 | 5.96E+04 |
| 2 | <=> | III | 1.46E+37 | -7.66 | 36.76 | 1.41E+06 |
| 2 | <=> | 4 | 4.12E+28 | -5.11 | 37.07 | 1.54E+05 |
| 2 | <=> | 5 | 3.49E+53 | -12.95 | 55.55 | 3.54E+02 |
| 2 | <=> | IV | 8.14E+53 | -11.83 | 66.26 | 8.72E+03 |
| 2 | <=> | 7 | 6.03E+70 | -17.21 | 77.10 | 1.90E+02 |
| 2 | <=> | 9 | 3.31E+67 | -17.16 | 68.46 | 1.20E+01 |
| 2 | <=> | IX | 7.15E+71 | -17.67 | 79.26 | 3.27E+01 |
| 2 | <=> | VIII | 6.38E+71 | -17.66 | 79.25 | 3.21E+01 |
| 2 | <=> | 8 | 1.00E+77 | -19.59 | 84.19 | 6.60E-01 |
| 2 | <=> | VII | 7.77E+81 | -19.99 | 94.11 | 2.25E+01 |
| 3 | <=> | 1 | 4.81E+73 | -18.54 | 63.88 | 1.22E+04 |
| 3 | <=> | 2 | 1.87E+62 | -15.33 | 44.41 | 3.79E+06 |
| 3 | <=> | 6 | 2.09E+75 | -18.96 | 80.92 | 5.60E+00 |
| 3 | <=> | 10 | 4.68E+92 | -24.80 | 80.65 | 4.42E+00 |
| 3 | <=> | II | 1.29E+89 | -23.16 | 91.20 | 5.01E-01 |
| 3 | <=> | 11 | 1.84E+95 | -25.37 | 81.45 | 2.20E+01 |
| 3 | <=> | VI | 3.46E+94 | -24.50 | 92.65 | 6.09E+00 |
| 3 | <=> | V | 1.07E+94 | -24.42 | 92.61 | 3.35E+00 |
| 3 | <=> | I | 1.24E+94 | -24.38 | 90.08 | 1.86E+01 |
| 3 | <=> | III | 2.61E+57 | -13.67 | 43.27 | 8.86E+06 |
| 3 | <=> | 4 | 1.37E+59 | -14.15 | 61.69 | 1.56E+03 |
| 3 | <=> | 5 | 2.38E+80 | -20.91 | 78.48 | 3.08E+00 |
| 3 | <=> | IV | 7.97E+76 | -18.74 | 86.99 | 4.43E+01 |
| 3 | <=> | 7 | 3.05E+91 | -23.43 | 97.22 | 8.41E-01 |
| 3 | <=> | 9 | 4.20E+91 | -24.33 | 90.31 | 7.87E-02 |
| 3 | <=> | IX | 5.52E+94 | -24.54 | 100.38 | 1.44E-01 |
| 3 | <=> | VIII | 4.90E+94 | -24.53 | 100.37 | 1.42E-01 |
| 3 | <=> | 8 | 1.57E+98 | -25.94 | 104.85 | 2.75E-03 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 4 | <=> | 1 | 2.12E+57 | -13.22 | 72.41 | 7.05E+01 |
| 4 | <=> | 2 | 2.48E+29 | -5.06 | 50.91 | 1.20E+03 |
| 4 | <=> | 6 | 1.35E+69 | -16.58 | 90.24 | 4.45E-01 |
| 4 | <=> | 10 | 3.04E+77 | -19.94 | 86.58 | 5.29E-02 |
| 4 | <=> | II | 4.20E+79 | -19.81 | 98.39 | 4.66E-02 |
| 4 | <=> | 11 | 5.01E+79 | -20.44 | 86.94 | 2.31E-01 |
| 4 | <=> | VI | 2.45E+83 | -20.70 | 98.83 | 4.85E-01 |
| 4 | <=> | V | 9.03E+82 | -20.64 | 98.81 | 2.72E-01 |
| 4 | <=> | 12 | 7.21E+80 | -20.71 | 85.19 | 1.30E+00 |
| 4 | <=> | I | 1.17E+82 | -20.30 | 96.57 | 1.10E+00 |
| 4 | <=> | 3 | 1.75E+55 | -13.76 | 63.75 | 1.08E+00 |
| 4 | <=> | III | 1.06E+54 | -11.96 | 72.74 | 1.79E+02 |
| 4 | <=> | 5 | 1.96E+52 | -12.52 | 49.87 | 6.52E+03 |
| 4 | <=> | IV | 2.99E+52 | -11.44 | 63.78 | 1.65E+04 |
| 4 | <=> | 7 | 1.47E+92 | -23.07 | 108.53 | 1.71E-01 |
| 4 | <=> | 9 | 2.33E+80 | -20.54 | 96.12 | 5.24E-03 |
| 4 | <=> | IX | 1.65E+91 | -22.91 | 109.75 | 2.98E-02 |
| 4 | <=> | VIII | 1.52E+91 | -22.91 | 109.75 | 2.93E-02 |
| 4 | <=> | 8 | 8.33E+98 | -25.61 | 115.53 | 6.72E-04 |
| 5 | <=> | 1 | 6.93E+77 | -19.41 | 92.11 | 3.02E-01 |
| 5 | <=> | 2 | 1.88E+57 | -13.31 | 76.31 | 4.69E+00 |
| 5 | <=> | 6 | 1.68E+81 | -20.42 | 103.78 | 1.92E-03 |
| 5 | <=> | 10 | 1.39E+93 | -24.76 | 102.88 | 2.28E-04 |
| 5 | <=> | II | 2.05E+90 | -23.25 | 110.96 | 1.99E-04 |
| 5 | <=> | 11 | 1.54E+95 | -25.21 | 103.18 | 9.92E-04 |
| 5 | <=> | VI | 1.15E+94 | -24.13 | 111.43 | 2.05E-03 |
| 5 | <=> | V | 3.79E+93 | -24.05 | 111.37 | 1.15E-03 |
| 5 | <=> | 12 | 1.29E+97 | -25.69 | 102.06 | 5.46E-03 |
| 5 | <=> | I | 1.26E+94 | -24.12 | 110.10 | 4.67E-03 |
| 5 | <=> | 3 | 1.34E+79 | -20.87 | 86.43 | 4.17E-03 |
| 5 | <=> | III | 2.11E+75 | -18.38 | 92.83 | 7.66E-01 |
| 5 | <=> | 4 | 5.00E+54 | -12.79 | 55.91 | 1.27E+04 |
| 5 | <=> | IV | 2.86E+54 | -12.21 | 54.20 | 9.29E+05 |
| 5 | <=> | 7 | 7.25E+99 | -25.66 | 119.05 | 7.21E-04 |
| 5 | <=> | 9 | 1.08E+91 | -23.97 | 108.77 | 2.24E-05 |
| 5 | <=> | IX | 3.12E+98 | -25.39 | 119.97 | 1.24E-04 |
| 5 | <=> | VIII | 2.83E+98 | -25.38 | 119.96 | 1.22E-04 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 6 | <=> | 10 | 1.56E+54 | -13.51 | 58.84 | 6.48E+00 |
| 6 | <=> | II | 3.98E+53 | -12.57 | 69.61 | 4.53E+00 |
| 6 | <=> | 11 | 3.28E+56 | -14.03 | 59.28 | 2.88E+01 |
| 6 | <=> | VI | 9.15E+57 | -13.63 | 70.34 | 4.77E+01 |
| 6 | <=> | V | 3.16E+57 | -13.57 | 70.30 | 2.68E+01 |
| 6 | <=> | 12 | 1.77E+58 | -14.46 | 57.76 | 1.68E+02 |
| 6 | <=> | I | 6.16E+56 | -13.29 | 68.05 | 1.12E+02 |
| 6 | <=> | 3 | 2.70E+72 | -19.08 | 69.11 | 1.17E+00 |
| 6 | <=> | III | 6.02E+69 | -16.92 | 75.53 | 3.30E+02 |
| 6 | <=> | 4 | 1.77E+68 | -16.53 | 76.41 | 8.91E+01 |
| 6 | <=> | 5 | 5.05E+78 | -20.33 | 83.83 | 2.36E-01 |
| 6 | <=> | IV | 2.33E+81 | -19.88 | 93.56 | 1.86E+01 |
| 6 | <=> | 7 | 1.52E+30 | -5.38 | 38.52 | 4.22E+05 |
| 6 | <=> | 9 | 1.88E+40 | -9.23 | 31.65 | 4.55E+05 |
| 6 | <=> | IX | 3.82E+46 | -10.26 | 49.77 | 8.17E+04 |
| 6 | <=> | VIII | 3.49E+46 | -10.25 | 49.78 | 7.97E+04 |
| 6 | <=> | 8 | 2.40E+51 | -11.91 | 58.06 | 9.05E+02 |
| 6 | <=> | VII | 7.80E+58 | -13.06 | 71.46 | 1.22E+04 |
| 7 | <=> | 1 | 1.18E+56 | -12.78 | 75.37 | 1.73E+01 |
| 7 | <=> | 2 | 4.08E+74 | -18.12 | 89.72 | 4.39E+00 |
| 7 | <=> | 6 | 4.65E+30 | -5.40 | 48.72 | 6.35E+03 |
| 7 | <=> | 10 | 1.66E+72 | -18.41 | 86.10 | 1.41E-02 |
| 7 | <=> | II | 5.94E+76 | -18.96 | 98.11 | 2.82E-02 |
| 7 | <=> | 11 | 2.46E+73 | -18.62 | 85.89 | 5.64E-02 |
| 7 | <=> | VI | 5.03E+79 | -19.60 | 98.13 | 2.71E-01 |
| 7 | <=> | V | 1.89E+79 | -19.55 | 98.11 | 1.52E-01 |
| 7 | <=> | 12 | 8.23E+73 | -18.68 | 84.18 | 2.85E-01 |
| 7 | <=> | I | 3.95E+78 | -19.26 | 96.31 | 5.63E-01 |
| 7 | <=> | 3 | 7.97E+92 | -24.67 | 97.49 | 3.66E-03 |
| 7 | <=> | III | 2.35E+93 | -23.40 | 104.79 | 1.78E+00 |
| 7 | <=> | 4 | 7.48E+92 | -23.36 | 105.51 | 5.46E-01 |
| 7 | <=> | 9 | 3.53E+57 | -13.75 | 65.60 | 8.78E+01 |
| 7 | <=> | IX | 5.72E+68 | -16.21 | 82.18 | 1.41E+02 |
| 7 | <=> | VIII | 5.32E+68 | -16.20 | 82.19 | 1.38E+02 |
| 7 | <=> | 8 | 6.03E+44 | -10.23 | 47.85 | 4.35E+03 |
| 7 | <=> | VII | 1.03E+50 | -10.73 | 62.95 | 1.11E+04 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 8 | <=> | 1 | 1.38E+66 | -15.82 | 91.90 | 3.83E-02 |
| 8 | <=> | 2 | 3.70E+81 | -20.28 | 103.85 | 1.03E-02 |
| 8 | <=> | 6 | 1.07E+54 | -12.13 | 76.08 | 9.79E+00 |
| 8 | <=> | 10 | 1.03E+79 | -20.53 | 100.30 | 3.09E-05 |
| 8 | <=> | II | 3.77E+80 | -20.23 | 109.87 | 7.32E-05 |
| 8 | <=> | 11 | 9.62E+79 | -20.68 | 100.02 | 1.20E-04 |
| 8 | <=> | VI | 3.84E+83 | -20.90 | 109.99 | 6.89E-04 |
| 8 | <=> | V | 1.36E+83 | -20.84 | 109.94 | 3.86E-04 |
| 8 | <=> | 12 | 1.79E+81 | -20.95 | 98.91 | 6.01E-04 |
| 8 | <=> | I | 1.85E+83 | -20.78 | 108.75 | 1.41E-03 |
| 8 | <=> | 3 | 3.39E+99 | -26.75 | 111.41 | 8.55E-06 |
| 8 | <=> | III | 2.63E+98 | -25.03 | 117.42 | 4.49E-03 |
| 8 | <=> | 4 | 9.06E+96 | -24.72 | 117.34 | 1.40E-03 |
| 8 | <=> | 7 | 1.61E+47 | -10.51 | 55.35 | 3.64E+03 |
| 8 | <=> | 9 | 6.24E+72 | -18.21 | 87.07 | 1.35E-01 |
| 8 | <=> | IX | 2.96E+80 | -19.71 | 99.96 | 3.14E-01 |
| 8 | <=> | VIII | 2.68E+80 | -19.69 | 99.96 | 3.07E-01 |
| 8 | <=> | VII | 8.63E+45 | -9.78 | 48.60 | 9.38E+05 |
| 9 | <=> | 1 | 9.15E+59 | -14.12 | 65.58 | 1.79E+03 |
| 9 | <=> | 2 | 2.78E+74 | -18.29 | 78.58 | 2.52E+02 |
| 9 | <=> | 6 | 1.06E+44 | -9.56 | 38.89 | 6.93E+06 |
| 9 | <=> | 10 | 6.46E+75 | -19.61 | 77.13 | 1.26E+00 |
| 9 | <=> | II | 1.25E+71 | -17.57 | 84.72 | 7.27E-01 |
| 9 | <=> | 11 | 9.44E+77 | -20.09 | 77.53 | 5.71E+00 |
| 9 | <=> | VI | 3.24E+75 | -18.64 | 85.51 | 7.83E+00 |
| 9 | <=> | V | 9.95E+74 | -18.56 | 85.45 | 4.35E+00 |
| 9 | <=> | 12 | 3.62E+80 | -20.76 | 76.60 | 3.37E+01 |
| 9 | <=> | I | 5.20E+75 | -18.68 | 84.12 | 1.89E+01 |
| 9 | <=> | 3 | 3.13E+93 | -25.06 | 86.84 | 2.19E-01 |
| 9 | <=> | III | 9.91E+88 | -22.39 | 91.78 | 5.57E+01 |
| 9 | <=> | 4 | 1.88E+85 | -21.38 | 91.39 | 1.45E+01 |
| 9 | <=> | 5 | 8.57E+93 | -24.66 | 97.70 | 3.78E-02 |
| 9 | <=> | IV | 9.51E+92 | -23.21 | 104.92 | 2.56E+00 |
| 9 | <=> | 7 | 4.03E+61 | -14.26 | 63.59 | 8.20E+04 |
| 9 | <=> | IX | 7.32E+35 | -7.17 | 40.51 | 3.19E+05 |
| 9 | <=> | VIII | 6.64E+35 | -7.16 | 40.53 | 3.10E+05 |
| 9 | <=> | 8 | 2.49E+75 | -18.71 | 77.81 | 1.73E+02 |
| 9 | <=> | VII | 6.07E+78 | -18.73 | 88.19 | 2.01E+03 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 10 | <=> | 1 | 4.48E+49 | -11.38 | 40.17 | 5.19E+06 |
| 10 | <=> | 2 | 2.09E+69 | -16.98 | 60.11 | 1.73E+05 |
| 10 | <=> | 6 | 5.81E+58 | -13.98 | 62.17 | 1.71E+03 |
| 10 | <=> | II | 1.15E+33 | -6.17 | 42.59 | 1.69E+05 |
| 10 | <=> | 11 | 6.06E+76 | -19.77 | 61.83 | 8.72E+03 |
| 10 | <=> | VI | 1.98E+78 | -19.61 | 74.09 | 1.88E+03 |
| 10 | <=> | V | 5.92E+77 | -19.52 | 74.04 | 1.03E+03 |
| 10 | <=> | 12 | 1.11E+83 | -21.51 | 62.13 | 8.38E+04 |
| 10 | <=> | I | 1.49E+78 | -19.57 | 71.69 | 6.03E+03 |
| 10 | <=> | 3 | 1.14E+93 | -25.07 | 71.61 | 1.55E+02 |
| 10 | <=> | III | 2.48E+88 | -22.43 | 77.38 | 1.55E+04 |
| 10 | <=> | 4 | 1.68E+81 | -20.37 | 76.27 | 2.81E+03 |
| 10 | <=> | 5 | 5.08E+94 | -25.00 | 86.20 | 7.11E+00 |
| 10 | <=> | IV | 3.28E+91 | -22.97 | 92.74 | 2.13E+02 |
| 10 | <=> | 7 | 3.17E+73 | -18.05 | 77.65 | 2.28E+02 |
| 10 | <=> | 9 | 1.62E+75 | -19.38 | 71.72 | 2.46E+01 |
| 10 | <=> | IX | 1.55E+77 | -19.30 | 81.00 | 3.91E+01 |
| 10 | <=> | VIII | 1.37E+77 | -19.28 | 80.99 | 3.86E+01 |
| 10 | <=> | 8 | 4.14E+79 | -20.39 | 84.96 | 7.19E-01 |
| 10 | <=> | VII | 1.82E+83 | -20.47 | 94.19 | 1.77E+01 |
| 11 | <=> | 1 | 8.28E+50 | -11.79 | 40.00 | 6.19E+06 |
| 11 | <=> | 2 | 1.76E+72 | -17.90 | 60.43 | 2.22E+05 |
| 11 | <=> | 6 | 4.62E+60 | -14.62 | 61.58 | 2.15E+03 |
| 11 | <=> | 10 | 3.36E+76 | -19.94 | 61.08 | 2.24E+03 |
| 11 | <=> | II | 5.37E+74 | -18.91 | 71.92 | 1.88E+02 |
| 11 | <=> | VI | 7.80E+35 | -7.01 | 41.76 | 5.44E+05 |
| 11 | <=> | V | 3.21E+35 | -6.96 | 41.86 | 2.95E+05 |
| 11 | <=> | 12 | 5.83E+84 | -22.06 | 62.01 | 1.06E+05 |
| 11 | <=> | I | 2.42E+80 | -20.30 | 71.30 | 7.68E+03 |
| 11 | <=> | 3 | 2.70E+95 | -25.83 | 71.56 | 2.02E+02 |
| 11 | <=> | III | 6.33E+90 | -23.22 | 77.08 | 1.96E+04 |
| 11 | <=> | 4 | 9.71E+82 | -20.97 | 75.58 | 3.45E+03 |
| 11 | <=> | 5 | 8.43E+95 | -25.45 | 85.19 | 8.74E+00 |
| 11 | <=> | IV | 3.07E+92 | -23.37 | 91.48 | 2.45E+02 |
| 11 | <=> | 7 | 2.55E+74 | -18.43 | 76.41 | 2.65E+02 |
| 11 | <=> | 9 | 3.85E+76 | -19.87 | 70.84 | 3.10E+01 |
| 11 | <=> | IX | 2.81E+78 | -19.77 | 79.89 | 4.57E+01 |
| 11 | <=> | VIII | 2.46E+78 | -19.76 | 79.88 | 4.46E+01 |
| 11 | <=> | 8 | 1.74E+80 | -20.68 | 83.56 | 8.24E-01 |
| 11 | <=> | VII | 3.10E+83 | -20.66 | 92.53 | 1.88E+01 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 12 | <=> | 1 | 1.98E+54 | -12.54 | 46.85 | 2.80E+06 |
| 12 | <=> | 2 | 7.23E+76 | -18.98 | 69.26 | 6.15E+04 |
| 12 | <=> | 6 | 2.18E+65 | -15.71 | 71.02 | 4.64E+02 |
| 12 | <=> | 10 | 6.30E+81 | -21.19 | 70.39 | 7.11E+02 |
| 12 | <=> | II | 8.54E+79 | -20.15 | 81.74 | 4.01E+01 |
| 12 | <=> | 11 | 9.68E+83 | -21.63 | 71.10 | 3.65E+03 |
| 12 | <=> | VI | 1.80E+85 | -21.45 | 83.22 | 5.06E+02 |
| 12 | <=> | V | 4.99E+84 | -21.36 | 83.15 | 2.76E+02 |
| 12 | <=> | I | 7.04E+39 | -8.30 | 47.03 | 4.64E+04 |
| 12 | <=> | III | 1.22E+96 | -24.49 | 86.73 | 4.41E+03 |
| 12 | <=> | 4 | 1.59E+87 | -21.93 | 84.82 | 7.09E+02 |
| 12 | <=> | IV | 2.26E+96 | -24.22 | 100.91 | 4.32E+01 |
| 12 | <=> | 7 | 5.93E+77 | -19.13 | 85.46 | 4.82E+01 |
| 12 | <=> | 9 | 9.94E+81 | -21.17 | 80.83 | 6.73E+00 |
| 12 | <=> | IX | 3.23E+82 | -20.68 | 89.32 | 8.42E+00 |
| 12 | <=> | VIII | 2.81E+82 | -20.67 | 89.30 | 8.19E+00 |
| 12 | <=> | 8 | 1.06E+84 | -21.51 | 93.04 | 1.44E-01 |
| 12 | <=> | VII | 3.36E+87 | -21.55 | 102.32 | 3.13E+00 |

*Table S10: Rate constants for abstraction by resonant radicals from $CH_4$ and comparison between TST rate constants and the rate estimation rules.*

| Category | Reactions | Modified Arrhenius parameters[a] | | | | Arrhenius parameters[a] | | $\Delta_R H^{298K}$ | *k* (TST, | *k* (rate rule)[b] / *k* (TST) | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | $n_H$ | $A_H$ | *n* | E | $A'_H$ | Ea | (kcal/mol) | 1000K)/# $n_H$ [a] | 500 K | 1000 K | 1500 K |
| Primary | trans-CC=CC• + $CH_4$ trans-CC=CC + $CH_3$ | 6 | 82.5 | 3.19 | 26.1 | 1.27E+12 | 32.4 | 18.2 | 6.32E+05 | 1.57 | 1.67 | 1.61 |
| | cis-CC=CC• + $CH_4$ cis-CC=CC + $CH_3$ | 6 | 181.7 | 3.04 | 26.9 | 8.14E+11 | 32.9 | 19.9 | 3.18E+05 | 4.08 | 3.31 | 2.99 |
| | CCC=CC• + $CH_4$ CC=CCC + $CH_3$ | 3 | 188.0 | 3.18 | 26.0 | 5.18E+12 | 32.3 | 18.7 | 1.34E+06 | 0.71 | 0.79 | 0.77 |
| | C=CC• + $CH_4$ C=CC + $CH_3$ | 3 | 626.7 | 3.10 | 25.7 | 9.03E+12 | 31.9 | 18.2 | 2.96E+06 | 0.26 | 0.36 | 0.38 |
| | C=C(C•)CC + $CH_4$ C=C(C)CC + $CH_3$ | 3 | 436.7 | 3.13 | 24.7 | 8.17E+12 | 30.9 | 17.1 | 4.30E+06 | 0.11 | 0.25 | 0.30 |
| | $C=CC_2$• + $CH_4$ $C=CC_2$ + $CH_3$ | 6 | 106.7 | 3.24 | 24.4 | 2.27E+12 | 30.8 | 17.0 | 2.53E+06 | 0.17 | 0.42 | 0.52 |
| | trans-$CC=CC_2$• + $CH_4$ $CC=CC_2$ + $CH_3$ | 3 | 185.7 | 3.16 | 25.5 | 4.37E+12 | 31.8 | 18.3 | 1.47E+06 | 0.50 | 0.72 | 0.76 |
| | cis-$CC=CC_2$• + $CH_4$ $CC=CC_2$ + $CH_3$ | 3 | 50.5 | 3.32 | 25.2 | 4.28E+12 | 31.8 | 18.3 | 7.37E+05 | 0.93 | 1.43 | 1.53 |
| | C•$C=CC_2$ + $CH_4$ $CC=CC_2$ + $CH_3$ | 3 | 119.7 | 3.22 | 26.8 | 4.35E+12 | 33.2 | 20.0 | 7.30E+05 | 2.00 | 1.44 | 1.21 |
| | **Average** | | | | | **4.42E+12** | **32.0** | | **1.67E+06** | | | |
| | **Standard deviation** | | | | | **2.82E+12** | **0.80** | | **1.33E+06** | | | |
| Secondary | C=CC•CC=C + $CH_4$ C=CCCC=C + $CH_3$ | 4 | 75.3 | 3.30 | 26.5 | 2.19E+17 | 33.1 | 20.8 | 1.28E+10 | 0.46 | 1.12 | 1.43 |
| | CC=CC•C + $CH_4$ CC=CCC + $CH_3$ | 2 | 202.5 | 3.31 | 27.6 | 3.45E+17 | 34.1 | 21.6 | 1.20E+10 | 0.45 | 0.64 | 0.69 |
| | C=CC•C + $CH_4$ C=CCC + $CH_3$ | 2 | 402.5 | 3.20 | 27.5 | 2.49E+17 | 33.8 | 21.4 | 1.01E+10 | 0.42 | 0.67 | 0.76 |
| | C=CC•CC + $CH_4$ C=CCCC + $CH_3$ | 2 | 133.5 | 3.24 | 27.2 | 2.25E+17 | 33.6 | 21.1 | 1.02E+10 | 0.70 | 1.28 | 1.51 |
| | C=C(C)C•C + $CH_4$ C=C(C)CC + $CH_3$ | 2 | 77.5 | 3.42 | 26.0 | 1.50E+17 | 32.8 | 19.6 | 1.03E+10 | 0.86 | 1.32 | 1.45 |
| | **Average** | | | | | **2.38E+17** | **33.5** | | **1.11E+10** | | | |
| | **Standard deviation** | | | | | **7.03E+16** | **0.55** | | **1.25E+09** | | | |
| Tertiary | C=CC•$C_2$ + $CH_4$ $C=CCC_2$ + $CH_3$ | 1 | 58.4 | 3.40 | 28.0 | 7.90E+17 | 34.7 | 23.4 | 2.04E+10 | 0.83 | 0.88 | 0.84 |
| | C=CC•(C)CC + $CH_4$ C=CC(C)CC + $CH_3$ | 1 | 92.7 | 3.30 | 28.2 | 5.82E+17 | 34.8 | 22.9 | 1.44E+10 | 1.27 | 1.21 | 1.13 |
| | **Average** | | | | | **6.86E+17** | **34.8** | | **1.74E+10** | | | |
| | **Standard deviation** | | | | | **1.47E+17** | **0.06** | | | | | |
| Secondary (Cyclics) | CYPE3• + $CH_4$ $CYC_5H_8$ + $CH_3$ | 4 | 232.3 | 3.11 | 26.9 | 3.69E+17 | 33.1 | 21.6 | 2.13E+10 | 1.00 | 1.00 | 1.00 |
| | $CYC_6H_9A$ + $CH_4$ $CYC_6H_{10}$ + $CH_3$ | 4 | 225.5 | 3.12 | 27.1 | 3.51E+17 | 33.3 | 21.8 | 1.88E+10 | 1.10 | 1.02 | 0.99 |
| | **Average** | | | | | **3.60E+17** | **33.2** | | **2.01E+10** | | | |
| | **Standard deviation** | | | | | **1.26E+16** | **0.11** | | | | | |
| Tertiary (Cyclics) | MeCYPE3• + $CH_4$ $MeCYC_5H_8$ + $CH_3$ | 1 | 37.9 | 3.29 | 27.8 | 1.25E+18 | 34.3 | 23.8 | 4.02E+10 | 1.30 | 1.26 | 1.19 |
| | $MeCYC_6H_9A$ + $CH_4$ $MeCYC_6H_{10}$ + $CH_3$ | 1 | 43.4 | 3.31 | 27.6 | 1.54E+18 | 34.2 | 24.0 | 5.16E+10 | 0.85 | 0.87 | 0.84 |
| | **Average** | | | | | **1.40E+18** | **34.2** | | **4.59E+10** | | | |
| | **Standard deviation** | | | | | **2.08E+17** | **0.05** | | | | | |
| Extended resonance | C=CC•C=C + $CH_4$ C=CCC=C + $CH_3$ | 2 | 2.51E+04 | 2.84 | 36.1 | 1.77E+19 | 41.7 | 31.7 | 1.34E+10 | | | |
| | C=CC=CC• + $CH_4$ C=CC=CC + $CH_3$ | 3 | 513.3 | 3.14 | 30.5 | 5.57E+17 | 36.7 | 24.5 | 5.30E+09 | 0.57 | 0.51 | 0.47 |
| | C=CC(C)=CC• + $CH_4$ C=CC(C)=CC + $CH_3$ | 3 | 136.3 | 3.30 | 29.8 | 4.48E+17 | 36.3 | 23.8 | 5.12E+09 | 0.39 | 0.43 | 0.41 |
| | $C=CC=CC_2$• + $CH_4$ $C=CC=CC_2$ + $CH_3$ | 6 | 59.0 | 3.22 | 30.0 | 3.49E+17 | 36.4 | 24.3 | 3.88E+09 | 1.72 | 1.87 | 1.79 |
| | **Average** | | | | | **4.76E+18** | **37.8** | | **6.91E+09** | | | |
| | **Standard deviation** | | | | | **8.61E+18** | **2.63** | | **4.34E+09** | | | |
| Extended resonance (Cyclics) | $CYC_6H_7$ + $CH_4$ CHD14 + $CH_3$ | 4 | 272.5 | 3.11 | 34.6 | 4.66E+19 | 40.8 | 31.1 | 5.75E+10 | 1.40 | 1.18 | 1.07 |
| | $CYC_6H_7$ + $CH_4$ CHD13 + $CH_3$ | 4 | 277.5 | 3.15 | 35.7 | 4.36E+19 | 42.0 | 31.0 | 2.93E+10 | 3.48 | 1.61 | 1.18 |
| | MeCY13PD5• + $CH_4$ MeCY13PD + $CH_3$ | 1 | 26.8 | 3.36 | 30.5 | 8.65E+18 | 37.1 | 27.2 | 6.62E+10 | 0.05 | 0.26 | 0.42 |
| | CY13PD5• + $CH_4$ CY13PD + $CH_3$ | 2 | 32.5 | 3.05 | 27.7 | 5.50E+17 | 33.7 | 22.7 | 2.35E+10 | 0.02 | 0.48 | 1.41 |
| | **Average** | | | | | **2.49E+19** | **38.4** | | **4.41E+10** | | | |
| | **Standard deviation** | | | | | **2.37E+19** | **3.73** | | **2.09E+10** | | | |
| Aromatics | Phenyl + $CH_3$ Benzene + $CH_4$ | 6 | 63.7 | 3.24 | 5.97 | 1.54E+11 | 12.4 | -10.1 | 2.98E+08 | | | |
| | Benzyl + $CH_3$ Toulene + $CH_4$ | 3 | 723.3 | 3.09 | 23.5 | 4.28E+15 | 29.6 | 14.5 | 1.42E+09 | | | |

Note: [a] The units for $A_H$, $A'_H$, and *k*(TST,1000 K) are $cm^3$/mol-s, and are kcal/mol for $\Delta_R H^{(298)}$, E and $E_a$; [b] The rate constant *k*(rate rule) has been calculated using the bold estimate rate rule listed at the bottom of the each subset. The rows of estimate rate rule list refitted parameters with the averaged values of rate constants of each group in the temperature range of 300 - 2500 K. Molecule structures are presented in abbreviated form as these in Table 1 in the text, with CYC5H8—cyclopentene, CYC6H10—cyclohexene, MeCYC5H8—methyl-cyclopentene, MeCYC6H10—methyl-cyclohexene, CHD13—1,3-cyclohexadiene, CHD14—1,4-cyclohexadiene, CY13PD—1,3-cyclopentadiene, MeCY13PD—methy-1,3-cyclopentadiene.

*Table S11: Reaction rate constants for abstraction by resonant radicals from propene and comparison between TST rate constants and the rate estimation rules.*

| Category | Reactions | Modified Arrhenius parameters[a] | | | | Arrhenius parameters[a] | | $\Delta_R H^{(298K)}$ | *k* (TST, | *k* (rate rule)[b]/*k* (TST) | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | $n_H$ | $A_H$ | n | E | $A'_H$ | Ea | (kcal/mol) | 1000K)/$n_H$[a] | 500 K | 1000 K | 1500 K |
| Primary | C=C(C)C• + C=CC   C=C(C)C + C=CC• | 6 | 0.99 | 3.70 | 14.2 | 5.05E+12 | 21.5 | -1.21 | 9.93E+07 | 0.21 | 0.39 | 0.45 |
| | C=CC• + C=CC   C=CC + C=CC• | 3 | 4.20 | 3.62 | 16.0 | 1.12E+13 | 23.2 | 0 | 9.57E+07 | 0.50 | 0.40 | 0.35 |
| | CC=CC• + CC=CC   CC=CC + CC=CC• | 6 | 2.25 | 3.63 | 15.3 | 6.54E+12 | 22.5 | 0 | 7.97E+07 | 0.42 | 0.48 | 0.48 |
| | trans-CC=C(C)C• + C=CC   CC=C(C)C + C=CC• | 3 | 0.73 | 3.71 | 14.0 | 3.94E+12 | 21.4 | 0.05 | 8.20E+07 | 0.24 | 0.47 | 0.55 |
| | CCC=CC• + C=CC   CCC=CC + C=CC• | 3 | 0.20 | 3.69 | 15.1 | 9.29E+11 | 22.5 | 0.43 | 1.14E+07 | 2.88 | 3.37 | 3.38 |
| | trans-CC=CC• + C=CC   trans-CC=CC + C=CC• | 6 | 0.46 | 3.64 | 15.3 | 1.47E+12 | 22.6 | 0.49 | 1.72E+07 | 2.03 | 2.24 | 2.18 |
| | C•C=C(C)C + C=CC   CC=C(C)C + C=CC• | 3 | 0.71 | 3.71 | 15.7 | 3.79E+12 | 23.1 | 1.76 | 3.40E+07 | 1.33 | 1.13 | 1.01 |
| | Average (restricted fits) | | | | | **4.70E+12** | **22.4** | | **5.99E+07** | | | |
| | Standard deviation | | | | | **3.45E+12** | **0.69** | | **3.78E+07** | | | |
| Secondary | C=CC•CC=C + C=CC   C=CCCC=C + C=CC• | 4 | 0.17 | 3.85 | 15.8 | 2.93E+12 | 23.4 | 2.60 | 2.21E+07 | 0.83 | 0.88 | 0.81 |
| | C=CC•C + CC=CC   C=CCC + CC=CC | 2 | 2.59 | 3.64 | 16.2 | 1.62E+13 | 23.4 | 2.70 | 1.23E+08 | 0.31 | 0.32 | 0.30 |
| | C=CC•CC + C=CC   C=CCCC + C=CC• | 2 | 0.12 | 3.77 | 15.9 | 3.29E+12 | 23.4 | 2.92 | 2.51E+07 | 1.46 | 1.56 | 1.45 |
| | C=CC•C + C=CC   C=CCC + C=CC• | 2 | 0.98 | 3.70 | 16.6 | 4.91E+12 | 24.0 | 3.21 | 2.84E+07 | 1.76 | 1.38 | 1.16 |
| | CC=CC•C + C=CC   CC=CCC + C=CC• | 2 | 0.84 | 3.80 | 16.5 | 9.24E+12 | 24.0 | 3.33 | 5.20E+07 | 0.97 | 0.75 | 0.63 |
| | Average (restricted fits) | | | | | **7.32E+12** | **23.6** | | **5.01E+07** | | | |
| | Standard deviation | | | | | **5.58E+12** | **0.31** | | **4.24E+07** | | | |
| Tertiary | C=CC•(C)CC + C=CC   C=CC(C)CC + C=CC• | 1 | 0.27 | 3.83 | 16.3 | 3.72E+12 | 23.9 | 4.64 | 2.24E+07 | 1.49 | 1.36 | 1.23 |
| | C=CC(C)C• + C=CC   C=CC(C)C + C=CC• | 1 | 0.27 | 3.87 | 16.3 | 5.55E+12 | 24.0 | 5.18 | 3.21E+07 | 1.01 | 0.95 | 0.85 |
| | Average (restricted fits) | | | | | **4.64E+12** | **23.9** | | **2.73E+07** | | | |
| Secondary (Cyclics) | CYPE3• + C=CC   $CYC_5H_8$ + C=CC• | 4 | 0.52 | 3.59 | 15.9 | 1.07E+12 | 23.0 | 3.39 | 1.00E+07 | 1.46 | 1.24 | 1.10 |
| | $CYC_6H_9A$ + C=CC   $CYC_6H_{10}$ + C=CC• | 4 | 0.49 | 3.60 | 15.8 | 1.15E+12 | 22.9 | 3.61 | 1.11E+07 | 1.29 | 1.12 | 1.00 |
| | Average (restricted fits) | | | | | **1.11E+12** | **23.0** | | **1.06E+07** | | | |
| Tertiary (Cyclics) | MeCYPE3• + C=CC   $MeCYC_5H_8$ + C=CC• | 1 | 0.11 | 3.72 | 15.9 | 6.65E+11 | 23.3 | 5.62 | 5.44E+06 | 1.52 | 1.28 | 1.15 |
| | $MeCYC_6H_9A$ + C=CC   $MeCYC_6H_{10}$ + C=CC• | 1 | 74.9 | 3.12 | 10.2 | 2.77E+10 | 16.4 | 5.79 | 7.23E+06 | 0.98 | 0.96 | 0.91 |
| | Average (restricted fits) | | | | | **3.46E+11** | **19.8** | | **6.34E+06** | | | |
| Extended resonance | C=CC•C=C + C=CC   C=CCC=C + C=CC• | 2 | 3.63 | 3.60 | 23.1 | 8.46E+12 | 30.3 | 13.5 | 2.03E+06 | | | |
| | C=CC=C(C)C• + C=CC   C=CC=C(C)C + C=CC• | 6 | 0.32 | 3.66 | 18.8 | 1.21E+12 | 26.1 | 6.03 | 2.37E+06 | 2.16 | 2.30 | 2.26 |
| | C=CC=CC• + C=CC   C=CC=CC + C=CC• | 3 | 0.06 | 4.08 | 19.1 | 6.12E+12 | 27.2 | 6.28 | 7.05E+06 | 1.13 | 0.77 | 0.61 |
| | C=CC(C)=CC• + C=CC   C=CC(C)=CC + C=CC• | 3 | 0.11 | 4.10 | 19.2 | 1.32E+13 | 27.4 | 7.41 | 1.38E+07 | 0.64 | 0.39 | 0.30 |
| | Average (restricted fits) | | | | | **6.86E+12** | **26.9** | | **7.74E+06** | | | |
| | Standard deviation | | | | | **6.05E+12** | **0.67** | | **5.75E+06** | | | |
| Extended resonance (cyclics) | CY13PD5• + C=CC   CY13PD + C=CC | 2 | 0.2 | 3.46 | 15.6 | 1.15E+11 | 22.4 | 4.46 | 1.44E+06 | 0.03 | 0.47 | 1.22 |
| | MeCY13PD5• + C=CC   MeCY13PD + C=CC• | 1 | 0.2 | 3.71 | 17.7 | 8.34E+11 | 25.0 | 9.01 | 2.80E+06 | 0.05 | 0.24 | 0.40 |
| | $CYC_6H_7$• + C=CC   CHD13 + C=CC• | 4 | 0.3 | 3.58 | 22.3 | 6.78E+11 | 29.5 | 12.8 | 2.45E+05 | 5.33 | 2.78 | 2.18 |
| | $CYC_6H_7$• + C=CC   CHD14 + C=CC• | 4 | 1.2 | 3.51 | 22.1 | 1.29E+12 | 29.0 | 12.9 | 5.80E+05 | 1.84 | 1.18 | 1.00 |
| | Average (restricted fits) | | | | | **7.28E+11** | **26.5** | | **1.27E+06** | | | |
| | Standard deviation | | | | | **4.84E+11** | **3.36** | | **1.14E+06** | | | |

Note: [a] The units for $A_H$, $A'_H$, and *k*(TST,1000 K) are $cm^3$/mol-s, and $\Delta_R H^{(298)}$, E and Ea are kcal/mol; [b] The rate constant *k*(rate rule) has been calculated using the values of estimate rate rule listed at the bottom of the table. The rows of estimate rate rule list refitted parameters with the averaged values of rate constants of each group in the temperature range of 300 - 2500 K. The ratio uses the original *k*(TST) value. Molecule structures are presented in abbreviated form as these in Table 1 in the text, with CYC5H8—cyclopentene, CYC6H10—cyclohexene, MeCYC5H8—methyl-cyclopentene, MeCYC6H10—methyl-cyclohexene, CHD13—1,3-cyclohexadiene, CHD14—1,4-cyclohexadiene, CY13PD—1,3-cyclopentadiene, MeCY13PD—methy-1,3- cyclopentadiene.

*Table S12: High pressure limit rate constants for the reactions shown in the $C_6H_{11}$ PES in Figure 19 in the text.*

| Reactions | Forward | | | Reverse | | | Note |
|---|---|---|---|---|---|---|---|
| | A ($s^{-1}$ or $cm^3$/mol-s) | Ea (kcal/mol) | *k* (1000K) ($s^{-1}$ or $cm^3$/mol-s) | A ($s^{-1}$ or $cm^3$/mol-s) | Ea (kcal/mol) | *k* (1000K) ($s^{-1}$ or $cm^3$/mol-s) | |
| I <=> 1 | **4.55E+11** | **15.0** | 2.37E+08 | 4.15E+12 | 19.0 | 2.89E+08 | From CBS-QB3 calculation |
| II <=> 7 | **5.35E+11** | **15.0** | 2.79E+08 | 4.39E+12 | 21.2 | 1.01E+08 | From CBS-QB3 calculation |
| 1 <=> IX | 3.78E+12 | 36.7 | 3.57E+04 | **1.16E+13** | **3.2** | 2.28E+12 | Rate rules for H + larger olefin* |
| 1 <=> 6 | **4.21E+10** | **15.9** | 1.40E+07 | 2.41E+14 | 33.7 | 1.02E+07 | 5-member ring, $E_{strain}$=6, $E_{addion}$ analogy to $CH_3$+$C_3H_6$_2-$C_4H_9$* |
| 1 <=> 2 | **5.55E+10** | **15.8** | 1.90E+07 | 5.13E+11 | 31.5 | 6.48E+04 | 1,6-H thift, Estrain=2.3, Ebi analogy to CCC.+2-$C_4H_8$_CCC+CC=CC.* |
| 6 <=> IV | 1.94E+14 | 36.0 | 2.64E+06 | **1.16E+13** | **3.2** | 2.28E+12 | Rate rules for H + larger olefin* |
| 6 <=> V | 3.32E+14 | 34.5 | 9.36E+06 | **1.16E+13** | **3.2** | 2.28E+12 | Rate rules for H + larger olefin* |
| 6 <=> VI | 5.28E+15 | 30.2 | 1.28E+09 | **4.44E+12** | **9.1** | 4.59E+10 | Rate rules for $CH_3$ + larger olefin* |
| 6 <=> 7 | 4.79E+14 | 31.9 | 5.16E+07 | **4.21E+10** | **15.2** | 2.05E+07 | 5-member ring, Estrain=6, Eaddion analogy to $C_2H_5$+$C_3H_6$_CCCC.C* |
| 2 <=> VIII | 4.12E+15 | 34.8 | 9.94E+07 | **7.43E+13** | **5.8** | 3.93E+12 | From CBS-QB3 calculation |
| 2 <=> 3 | 2.12E+14 | 29.7 | 6.69E+07 | **3.70E+10** | **18.2** | 3.88E+06 | 1,4-H thift, Estrain=5.8, Ebi analogy to CCC.+1-C4H8_CCC+C=CC.C* |
| 3 <=> 4 | **5.10E+09** | **8.3** | 7.81E+07 | 1.04E+14 | 27.9 | 8.36E+07 | 6-member ring, $E_{strain}$=8, $E_{addion}$ analogy to $CH_3$+$C_3H_6$_2-$C_4H_9$* |
| 4 <=> IV | 7.96E+13 | 33.9 | 3.09E+06 | **2.32E+13** | **3.2** | 4.57E+12 | Rate rules for H + larger olefin* |
| 3 <=> 5 | **4.21E+10** | **8.8** | 5.01E+08 | 5.54E+14 | 25.7 | 1.32E+09 | 5-member ring, $E_{strain}$=6, $E_{addion}$ analogy to $CH_3$+$C_3H_6$_2-$C_4H_9$* |
| 5 <=> VII | 3.53E+13 | 35.1 | 7.48E+05 | **2.32E+13** | **3.2** | 4.57E+12 | Rate rules for H + larger olefin* |

*Table S13: Rate constants at 1 atm for 500- 1800 K* for the $C_6H_{11}$ PES, from *CC=CC• + $C_2H_4$.*

| Reactions | | | A ($cm^3$/mol-s or $s^{-1}$) | n | Ea (kcal/mol) | *k* (1000K) ($cm^3$/mol-s or $s^{-1}$) |
|---|---|---|---|---|---|---|
| I | <=> | (1) | 3.33E+20 | -2.96 | 17.0 | 8.65E+07 |
| I | <=> | IX | 9.84E+34 | -6.88 | 45.4 | 2.53E+04 |
| I | <=> | (6) | 1.90E+36 | -8.96 | 23.2 | 2.16E+04 |
| I | <=> | III | 1.63E+48 | -11.01 | 38.1 | 7.26E+06 |
| I | <=> | V | 2.83E+41 | -9.57 | 38.4 | 2.23E+04 |
| I | <=> | VI | 9.44E+42 | -9.92 | 38.3 | 7.20E+04 |
| I | <=> | (2) | 1.71E+59 | -15.91 | 33.3 | 1.74E+04 |
| I | <=> | VIII | 9.80E+50 | -11.88 | 40.5 | 3.06E+06 |
| I | <=> | (3) | 8.05E+54 | -13.46 | 40.7 | 4.29E+05 |
| I | <=> | (4) | 3.66E+84 | -23.36 | 49.8 | 4.10E+03 |
| I | <=> | IV | 5.26E+72 | -18.71 | 53.2 | 9.28E+04 |
| I | <=> | (5) | 7.98E+66 | -18.20 | 41.8 | 1.43E+03 |
| I | <=> | VII | 1.14E+60 | -15.20 | 48.8 | 5.98E+03 |
| I | <=> | (7) | 7.56E+51 | -12.69 | 39.5 | 1.50E+05 |
| I | <=> | II | 1.17E+63 | -15.54 | 51.4 | 1.65E+05 |
| (1) | <=> | IX | 1.10E+13 | -0.67 | 33.8 | 4.33E+03 |
| (1) | <=> | (6) | 3.41E+34 | -8.60 | 17.2 | 9.36E+04 |
| (1) | <=> | III | 5.82E+38 | -8.50 | 29.6 | 6.20E+06 |
| (1) | <=> | V | 5.51E+29 | -6.40 | 29.4 | 1.33E+04 |
| (1) | <=> | VI | 7.09E+31 | -6.92 | 29.3 | 4.71E+04 |
| (1) | <=> | (2) | 2.41E+56 | -15.18 | 27.3 | 7.30E+04 |
| (1) | <=> | VIII | 3.93E+42 | -9.66 | 33.1 | 2.41E+06 |
| (1) | <=> | (3) | 3.45E+48 | -11.80 | 34.1 | 4.96E+05 |
| (1) | <=> | (4) | 5.06E+83 | -23.19 | 46.6 | 8.67E+03 |
| (1) | <=> | IV | 1.18E+67 | -17.26 | 47.8 | 7.13E+04 |
| (1) | <=> | (5) | 8.04E+62 | -17.18 | 36.4 | 2.64E+03 |
| (1) | <=> | VII | 5.92E+49 | -12.44 | 40.8 | 3.46E+03 |
| (1) | <=> | (7) | 2.30E+43 | -10.36 | 32.2 | 1.72E+05 |
| (1) | <=> | II | 3.40E+49 | -11.78 | 42.9 | 6.63E+04 |
| (6) | <=> | IX | 6.21E+22 | -3.83 | 53.9 | 3.38E-01 |
| (6) | <=> | III | 1.82E+48 | -10.81 | 37.7 | 3.96E+07 |
| (6) | <=> | V | 1.15E+34 | -7.19 | 36.6 | 3.20E+04 |
| (6) | <=> | VI | 5.39E+37 | -8.17 | 36.9 | 1.45E+05 |
| (6) | <=> | (2) | 4.48E+83 | -23.10 | 58.4 | 3.81E+01 |
| (6) | <=> | VIII | 1.07E+63 | -15.83 | 58.5 | 5.48E+02 |
| (6) | <=> | (3) | 4.14E+70 | -18.40 | 60.7 | 1.40E+02 |
| (6) | <=> | (4) | 1.91+103 | -28.96 | 72.7 | |
| (6) | <=> | IV | 1.34E+86 | -23.03 | 72.5 | 1.57E+01 |
| (6) | <=> | (5) | 9.37E+84 | -23.70 | 63.6 | 9.38E-01 |
| (6) | <=> | VII | 4.01E+68 | -18.18 | 65.2 | 6.48E-01 |
| (6) | <=> | (7) | 3.70E+48 | -11.30 | 39.4 | 1.12E+06 |
| (6) | <=> | II | 1.16E+43 | -9.32 | 47.6 | 4.75E+04 |

| | | | | | | |
|---|---|---|---|---|---|---|
| (2) | <=> | IX | 2.69E+33 | -7.89 | 60.1 | 4.23E-04 |
| (2) | <=> | III | 1.18E+86 | -23.27 | 70.1 | 8.13E+00 |
| (2) | <=> | V | 7.24E+72 | -20.04 | 67.3 | 1.03E-02 |
| (2) | <=> | VI | 1.53E+76 | -20.90 | 68.0 | 4.22E-02 |
| (2) | <=> | VIII | 4.41E+60 | -14.38 | 48.9 | 6.50E+06 |
| (2) | <=> | (3) | 6.15E+60 | -14.73 | 45.9 | 3.79E+06 |
| (2) | <=> | (4) | 6.87E+94 | -25.38 | 61.4 | 1.96E+05 |
| (2) | <=> | IV | 8.09E+89 | -23.31 | 67.7 | 1.54E+05 |
| (2) | <=> | (5) | 2.92E+75 | -19.96 | 49.4 | 6.38E+04 |
| (2) | <=> | VII | 4.75E+68 | -17.49 | 57.6 | 3.92E+03 |
| (2) | <=> | (7) | 6.83E+84 | -23.34 | 70.5 | 2.54E-01 |
| (2) | <=> | II | 2.72E+81 | -22.21 | 75.2 | 2.26E-02 |
| (3) | <=> | IX | 1.46E+35 | -8.43 | 58.7 | 1.10E-03 |
| (3) | <=> | III | 9.49E+70 | -18.98 | 61.9 | 3.33E+00 |
| (3) | <=> | V | 2.29E+60 | -16.47 | 60.2 | 6.37E-03 |
| (3) | <=> | VI | 8.58E+62 | -17.11 | 60.6 | 2.34E-02 |
| (3) | <=> | VIII | 2.10E+46 | -10.28 | 43.2 | 1.09E+06 |
| (3) | <=> | (4) | 3.68E+47 | -11.87 | 21.7 | 1.58E+07 |
| (3) | <=> | IV | 3.97E+40 | -8.82 | 32.7 | 9.63E+06 |
| (3) | <=> | (5) | 6.23E+44 | -11.39 | 16.6 | 1.04E+07 |
| (3) | <=> | VII | 1.88E+18 | -2.62 | 22.7 | 2.82E+05 |
| (3) | <=> | (7) | 9.94E+71 | -19.75 | 62.9 | 9.89E-02 |
| (3) | <=> | II | 3.52E+74 | -20.26 | 70.2 | 2.64E-02 |
| (4) | <=> | IX | 1.48E+61 | -15.92 | 88.7 | 1.03E-06 |
| (4) | <=> | III | 6.44+107 | -29.52 | 97.5 | |
| (4) | <=> | V | 3.71E+95 | -26.57 | 94.8 | 1.31E-05 |
| (4) | <=> | VI | 4.17E+98 | -27.35 | 95.5 | 5.02E-05 |
| (4) | <=> | VIII | 7.01E+88 | -22.45 | 81.9 | 3.83E+03 |
| (4) | <=> | IV | 2.42E+53 | -12.34 | 48.1 | 7.26E+05 |
| (4) | <=> | (5) | 4.03E+86 | -22.83 | 59.9 | 1.02E+05 |
| (4) | <=> | VII | 2.19E+70 | -17.55 | 66.7 | 1.33E+03 |
| (4) | <=> | (7) | 1.39+107 | -29.77 | 97.9 | |
| (4) | <=> | II | 5.58+105 | -29.22 | 102.8 | |
| (5) | <=> | IX | 3.47E+47 | -11.97 | 77.1 | 5.97E-06 |
| (5) | <=> | III | 5.07E+89 | -24.33 | 83.0 | 3.87E-02 |
| (5) | <=> | V | 1.04E+78 | -21.52 | 80.7 | 6.30E-05 |
| (5) | <=> | VI | 7.90E+80 | -22.25 | 81.3 | 2.40E-04 |
| (5) | <=> | VIII | 4.55E+66 | -16.11 | 64.5 | 1.70E+04 |
| (5) | <=> | IV | 9.91E+68 | -16.99 | 57.5 | 2.88E+05 |
| (5) | <=> | IV | 1.19E+30 | -6.09 | 35.5 | 1.10E+04 |
| (5) | <=> | (7) | 4.84E+89 | -24.77 | 83.7 | 1.19E-03 |
| (5) | <=> | II | 9.55E+89 | -24.67 | 89.9 | 2.03E-04 |

| | | | | | | |
|---|---|---|---|---|---|---|
| (7) | <=> | IX | 2.33E+31 | -6.85 | 47.0 | 3.44E+00 |
| (7) | <=> | III | 6.93E+40 | -8.98 | 31.0 | 1.30E+07 |
| (7) | <=> | V | 6.90E+32 | -7.17 | 31.4 | 2.82E+04 |
| (7) | <=> | VI | 4.50E+34 | -7.61 | 31.2 | 9.99E+04 |
| (7) | <=> | VIII | 3.16E+62 | -16.18 | 49.9 | 1.11E+03 |
| (7) | <=> | IV | 2.84E+83 | -22.78 | 62.2 | 3.30E+01 |
| (7) | <=> | IV | 5.22E+69 | -18.99 | 57.1 | 1.84E+00 |
| (7) | <=> | II | 1.15E+22 | -3.04 | 24.0 | 5.10E+07 |