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Abstract

The reaction between vinyl radical, C_2H_3, and 1,3-butadiene, $1,3-C_4H_6$, has long been recognized as a potential route to benzene, particularly in 1,3-butadiene flames, but the lack of reliable rate coefficients has hindered assessments of its true contribution. Using laser flash photolysis and visible laser absorbance ($\lambda = 423.2$ nm) we measured the overall rate coefficient for $C_2H_3 + 1,3-C_4H_6$, k_1, at 297 K $\leq$ T $\leq$ 494 K and 4 $\leq$ P $\leq$ 100 Torr. k_1 was in the high pressure limit in this range and could be fit by the simple Arrhenius expression below.

$$k_1 = (1.1 \pm 0.2) \times 10^{-12}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1} \times \exp\left(-\frac{9.9 \pm 0.6\ \text{kJ mol}^{-1}}{\text{RT}}\right)$$

Using photoionization time-of-flight mass spectrometry (PI TOF-MS) we also investigated the products formed. At T $\leq$ 494 K and P = 25 Torr we found only C_6H_9 adduct species, while at 494 K $\leq$ T $\leq$ 700 K and P = 4 Torr, we observed $\leq \sim 10\%$ branching to cyclohexadiene in addition to C_6H_9. Quantum chemistry master-equation calculations using the modified strong collision model indicate that $n-C_6H_9$ is the dominant product at low T, consistent with our experimental results, and predict the rate and branching ratios at higher T where chemically activated channels become important. Predictions of k_1 are in close agreement with our experimental results, allowing us to recommend the following modified Arrhenius expression in the high pressure limit from 300-2000 K:

$$k_1 = 6.5 \times 10^{-20}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1} \times T^{2.40} \exp\left(-\frac{1.76\ \text{kJ mol}^{-1}}{\text{RT}}\right)$$

Keywords: Soot, PAH, vinyl radical, 1,3-butadiene, flash photolysis, laser absorbance, mass spectrometry, kinetic modeling, combustion modeling, master equation modeling

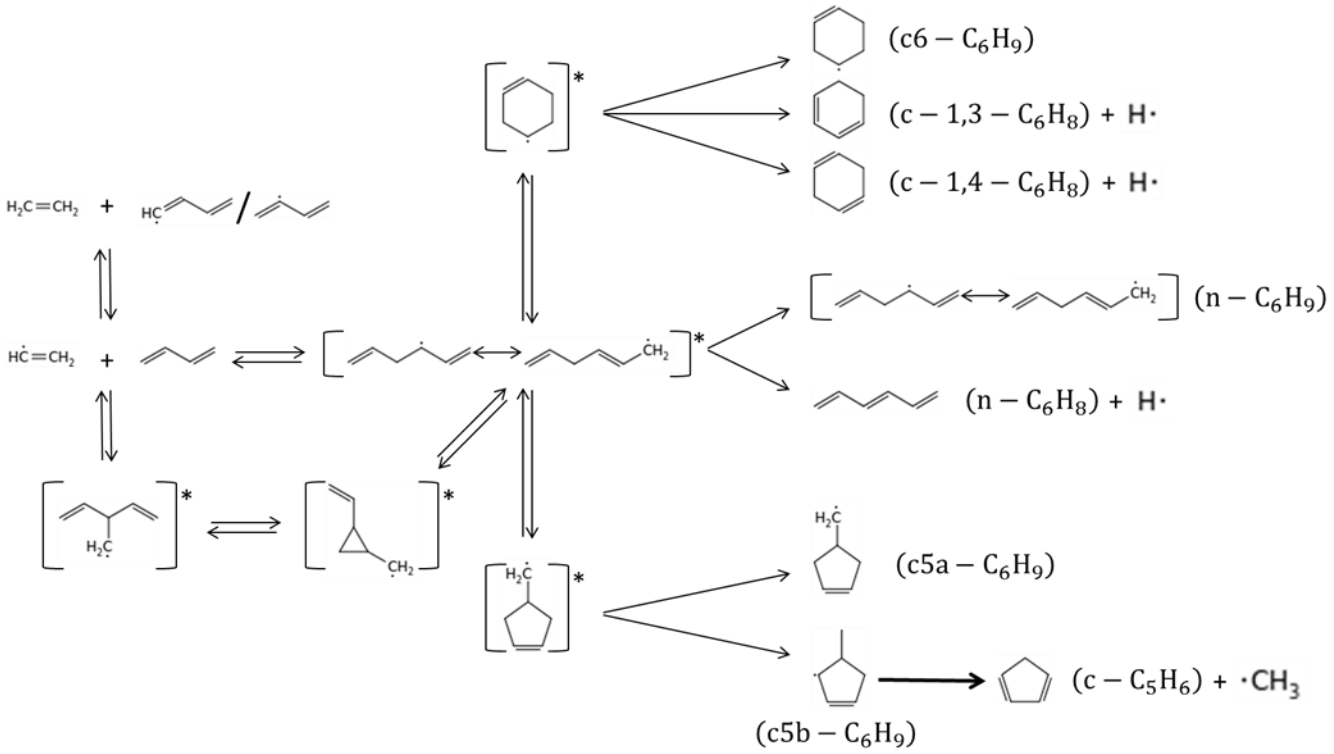
INTRODUCTION

Soot is an undesirable by-product of hydrocarbon combustion that is primarily composed of polycyclic aromatic hydrocarbons (PAH).[1] Besides being deleterious to human health[2] and the environment,[3, 4, 5] soot formation also represents an inefficient use of hydrocarbon fuel. For all of these reasons, it is important to understand the physical and chemical processes leading to soot formation so that these pathways can be minimized.

As described in detail in the reviews of Richter and Howard,[1] McEnally et al.[6] and Wang,[7] formation of the first aromatic ring is a crucial step in the path to PAH and eventually soot. For many flames it is thought to be the rate limiting step.[8, 9, 10] Benzene is the prototypical first aromatic ring, although others such as toluene, styrene, phenylacetylene, indene and naphthalene are certainly possible and have been considered in the literature. Several reactions that have received special attention over the last 30 years as potential sources of benzene in various flames are the following: 1. $\mathrm{n-C_4H_3/n-C_4H_5 + C_2H_2}$,[11, 12, 13, 14, 15] 2. $\mathrm{C_2H_3 + 1{,}3-C_4H_6}$ [11, 16, 17, 12, 18, 19, 20, 21, 22, 23] and 3. $\mathrm{C_3H_3 + C_3H_3}$.[13, 24, 25, 26] Chemistry of five carbon rings (i.e., cyclopentadienyl, cyclopentadiene and fulvene) is also thought to lead to larger aromatic rings.[27, 24, 28] With the exception of propargyl radical recombination, $\mathrm{C_3H_3 + C_3H_3}$, there is a dearth of direct experimental measurements of the reactions listed above.

Scheme 1 summarizes the currently accepted pathways for the reaction of vinyl radical with 1,3-butadiene, $\mathrm{C_2H_3 + 1{,}3-C_4H_6}$. There are several pathways leading to cyclic species that could conceivably undergo subsequent reactions to form benzene or other aromatics. Specifically, the cyclohexadiene isomers ($\mathrm{c-C_6H_8}$) could lose two hydrogen atoms, either by $\mathrm{H_2}$ elimination or H-abstraction followed by spontaneous H emission, to form benzene.[29, 30, 31, 32, 33, 34, 35] Cavallotti

et al. computed the pathway to cyclopentadiene $(c - C_5H_6)$ that could also lead to aromatic ring formation.[20]



Scheme 1: Proposed reaction network for $\mathbf{C_2H_3 + 1,3 - C_4H_6}$ (modified from Cavallotti et al.[20]), with nomenclature used in this paper. Asterisks denote ro-vibrationally excited isomers.

As early as 1984, Cole et al. considered the role of $C_2H_3 + 1,3 - C_4H_6$ in a 1,3-butadiene flame, but they concluded that this reaction did not produce sufficient cyclohexadiene to explain the amount of benzene formed.[11] Weissman and Benson reached a similar conclusion when studying methyl chloride pyrolysis.[17] However, others have concluded that $C_2H_3 + 1,3 - C_4H_6$ is a significant pathway to benzene formation in 1,3-butadiene flames,[12, 18, 19] hexane pyrolysis[16], a 1,3-butadiene doped methane flame[22] and ethane pyrolysis.[23]

Of course, whether a certain reaction is important in a given system depends on a host of system variables, which are myriad for something as complex as a flame. For example, temperature, pressure, equivalence ratio and chemical identity of the fuel are all sensitive variables. So the

lack of consensus in the literature with respect to the importance of $C_2H_3 + 1,3-C_4H_6$ to benzene formation in different environments is not surprising. What is concerning, however, is the large disagreement in the literature with respect to the overall rate coefficient for the title reaction. In particular, the overall rate coefficient predictions of Westmoreland et al.[12], Cavallotti et al.[20] and Xu et al.[23] disagree by more than two orders of magnitude at some conditions and display strikingly different temperature and pressure dependence. While they differ on the rate, all three predictions agree that at atmospheric pressure and below ~ 1000 K the dominant product is the linear adduct ($n-C_6H_9$). Above this temperature, however, Westmoreland et al. predict the linear C_6H_8 isomer ($n-C_6H_8$) to dominate, whereas Cavallotti et al. and Xu et al. predict cyclic species ($c-C_6H_8$ or $c-C_5H_6$) to eventually dominate. In at least one recent case, this disagreement has prevented the inclusion of the $C_2H_3 + 1,3-C_4H_6$ reaction in a model of a 1,3-butadiene flame.[36]

Despite these clear discrepancies for a reaction that is of known importance, to our knowledge there has not yet been any direct experimental measurement of either the overall rate of $C_2H_3 + 1,3-C_4H_6$, nor the product branching. In this work, we report the first such experiment over a relatively limited temperature and pressure range of $297-700$ K and $4-100$ Torr. Coupled with theoretical predictions, however, these results can be extrapolated to combustion temperatures for direct use in modeling. Discrepancies between our results and the literature are discussed, along with possible implications for soot formation.

EXPERIMENTAL METHODS

All experiments were conducted on a modified version of the MIT laser-photolysis/Herriott multiple-pass laser-absorption apparatus described by Ismail et al.[37] This apparatus was modified

to incorporate a photoionization time-of-flight mass spectrometer (PI TOF-MS) with supersonic molecular beam sampling from the center of the reactor. A detailed description of this apparatus has been given previously[38] and only the essential details are included here. The reactor is 86 cm long, 6 cm in diameter, constructed of stainless steel and resistively heated by four heaters wrapped along the length of the reactor to create a uniform temperature profile (standard deviation $\pm 2\%$) through the overlap region of the absorption laser. The heaters enable the gas mixture to be heated up to 700 K. The internal pressure of the reactor was monitored by a capacitance manometer and controlled *via* an automated butterfly valve. For some control experiments the inside of the reactor was coated with polydimethylsiloxane (PDMS), which has previously been used to minimize wall reactions in both a stainless steel[39] and Pyrex reactor[40] up to 750 K. The fourth harmonic output of a Nd:YAG laser (266 nm) operated at a repetition rate of 0.91, 2 or 5 Hz was used to photolyze vinyl iodide, C_2H_3I, and produce C_2H_3 + I. Unless noted otherwise, the repetition rate of the photolysis laser was such that the contents of the reaction cell were completely refreshed between photolysis flashes (Flashes per Refresh, FPR, < 1). The frequency-doubled output of a Ti:Sapphire laser (80 MHz pulsed laser with 1.2 ps full width at half maximum, FWHM, pulses) was used to generate the visible probe beam. The fundamental wavelength was measured before each experiment using a recently calibrated Ocean Optics HR2000+ spectrometer. The wavelength, λ, of the probe beam was 423.2 nm for all experiments reported here due to the strong absorption of C_2H_3 at this wavelength as we have previously observed[37, 41, 42, 43] and the lack of interference by other absorbing species (i.e., allylic species) at least at low temperatures ($T < 400$ K). The path length of the multiple-pass visible probe laser was around 20 m, allowing sensitive detection of C_2H_3 at concentrations as low as $\sim 10^{12}$ molecules cm^{-3} as used here. Absorbance traces were averaged over 500 flashes.

A small amount of the reactive gas was continuously sampled *via* a small pinhole at the tip of a cone that juts slightly into the photolysis beam at the center of the reaction cell. The sampled gas was supersonically expanded, and the center of the resultant free jet passed through a Beam Dynamics skimmer to form a collimated molecular beam. The gas in the molecular beam was effectively "frozen" in composition by cooling while in transit to the ionization region of the PI TOF-MS, where it was photoionized using 118.2 nm (10.487 eV) light. The 118.2 nm light was generated by focusing the third harmonic (355 nm) output of a pulsed Nd:YAG laser (<12 ns FWHM pulses, repetition rate set to match the photolysis laser) in a 1:10 Xe:Ar gas cell at a total pressure of 90-100 Torr. The relative abundance of ions at different mass-to-charge ratios $\left(\frac{m}{z}\right)$ were analyzed using a Kore TOF-MS and detected using the Kore supplied discrete dynode electron multiplier detector and analog pre-amplifier. Mass spectra were also averaged over 500 acquisitions. The correspondence between time-of-flight and $\frac{m}{z}$ was determined by calibration with a mixture of stable species.

Helium was used as the bath gas in all of the experiments reported here. C_2H_3I was purchased from Oakwood Chemicals at $\geq 95\%$ purity and was further purified by successive freeze-pump-thaw cycles. Helium (Airgas, 99.999%) and 1,3-butadiene (Sigma-Aldrich, $\geq 99\%$) were used directly without further purification. Although the purchased 1,3-butadiene contains p-tert-butylcatechol as an inhibitor, PI TOF-MS analysis revealed no signal at the parent mass of this species or its fragment ($\frac{m}{z} = 166$ and 151 amu, respectively). The largest observable impurity in the 1,3-butadiene was its dimer (4-vinylcyclohexene), which from Gas Chromatography analysis is only ~0.1%. PDMS ($\text{MW} = 70{,}000 - 80{,}000$) was purchased from Spectrum Chemical.

COMPUTATIONAL METHODS

Electronic energies of all species studied in this work were determined at the CCSD(T)-F12a/cc-pVTZ-F12[44, 45, 46, 47] level of theory using Molpro[48]. Molecular geometries and force constants for species and saddle points were determined at the M08SO/MG3S[49, 50] level of theory, utilizing QChem 4.1,[51] and are shown in Figure 1 below. A computational grid with 75 radial points and 434 angular points per radial point was used in the calculations for all species. Frequencies were scaled by the recommended value of 0.983[52]. Loose internal degrees of freedom for relevant adducts and transition states (i.e., hindered rotors) were treated separately by performing relaxed potential energy scans about the bond defining the internal rotor; these calculations were performed in Gaussian 03[53] at the BMK/6-311+G(d,p) level of theory[54]. Reduced internal moments of inertia for all internal rotors were estimated at the $I^{(2,3)}$ level as defined by East and Radom.[55] Cantherm[56] was used for all TST and RRKM/Master Equation calculations, which were performed in the regions of 300-2000 K, and $1\ \text{Torr} - 7.6 \times 10^4\ \text{Torr}$ (or 100 atm) in both Helium and Nitrogen bath gases. The master equation for energy transfer was solved using the modified strong collision (MSC) method, which is documented elsewhere.[57, 58] Eckart[59] tunneling corrections were applied to all relevant reactions. All information pertaining to the calculations in this work can be found in the supporting information, including rate coefficients suitable for combustion modeling (in CHEBYSHEV format).

The exponential down model for collisional energy transfer was adopted in this work. A temperature dependent formulation was used for the average downward energy transferred per collision,

$$\langle \Delta E_d \rangle = \langle \Delta E_d \rangle_{300} \left(\frac{T}{300\ \text{K}} \right)^n\ \text{cm}^{-1} \quad (1)$$

With $\langle \Delta E_d \rangle_{300} = 175.5$ and 400 cm^{-1}, and n = 0.95 and 0.7 for He and N_2 respectively. Values for Nitrogen were adopted based on toluene energy collision parameters,[25, 15] while those for Helium were adopted from recent calculations of Jasper and Miller,[60] with $\langle \Delta E_d \rangle_{300}$ increased by 50%. Lennard Jones collision diameters and well depths were estimated via the Joback[61] method, which is based on the critical temperature and pressure of parent compounds. The method of corresponding states was subsequently used to estimate the LJ parameters[62] and is described in the context of RMG elsewhere.[63]

RESULTS AND DISCUSSION

Potential Energy Surface for C_2H_3 + 1,3-C_4H_6

Regarding the terminal addition of vinyl to 1,3-butadiene, a Gaussian 03 IRC calculation at the CBS-QB3 level of theory followed by single point electronic calculations at the CCSD(T)-F12a/cc-pVTZ-F12 indicated the presence of a van der Waals complex stabilized by -1.0 kcal/mol relative to the reactants, and a 0 K barrier height of 0.14 kcal/mol (not including ZPE, 0.3 with ZPE). A stable transition state could not be located for the entrance channel at the M08SO/MG3S level of theory; transition state searches repeatedly resulted in multiple imaginary frequencies. Thus, CBS-QB3 (B3LYP/CBSB7) geometries and frequencies were used for computing the high pressure limit rate of the entrance channel.

We note that the uncertainty in the present addition barrier height (1 kcal/mol for CCSD(T)-F12a/cc-pVTZ-F12) exceeds the barrier height itself. Thus, a high level variational TST or variable reaction coordinate approach would be more appropriate for this reaction, and is recommended as future work. However, because the predicted entrance channel rate is in good agreement with the experimental values obtained in this work, a higher level rate theory

calculation for the entrance channel was not conducted. The potential energy surface relevant to the ME/RRKM calculations discussed below is illustrated in Figure 1. A sensitivity analysis of the predicted entrance channel rate constant to a ± 1.0 kcal mol^{-1} change in entrance barrier height demonstrates that the contributions to overall rate uncertainties at 300, 500, and 1000 K are a factor of 5.4, 2.7, and 1.7, respectively. The overall estimated uncertainty in the high pressure limit entrance channel rate is further discussed below.

In this work, vinyl addition to the secondary carbon of 1,3-butadiene, forming 2-methylene-3-butenyl, was not considered in the ME/RRKM simulations because this slower channel does not contribute significantly to the overall rate of vinyl + 1,3-butadiene under the conditions of this study. This was confirmed through a calculation at the CCSD(T)-F12a/cc-pVTZ-F12 level of theory, with a computed barrier of 4.9 kcal/mol (at 0 K, including ZPE). Thus, the corresponding high-pressure limit rate relative to the preferred terminal addition reaction is negligible (less than 0.02% at 300 K, rising to 2% at 1000 K, and 5% at 2000 K). Similarly, the two possible H-abstraction channels were also not included in the ME simulations because the barriers for H-abstraction from the 1- and 2- sites of 1,3-butadiene were calculated to be 11.5 and 9.4 kcal/mol, respectively (at 0 K, including ZPE). Thus, they are not competitive with the addition reactions under the conditions of this work. Nevertheless, the rate coefficients were calculated using TST and are included in the Supporting Information, in modified Arrhenius form.

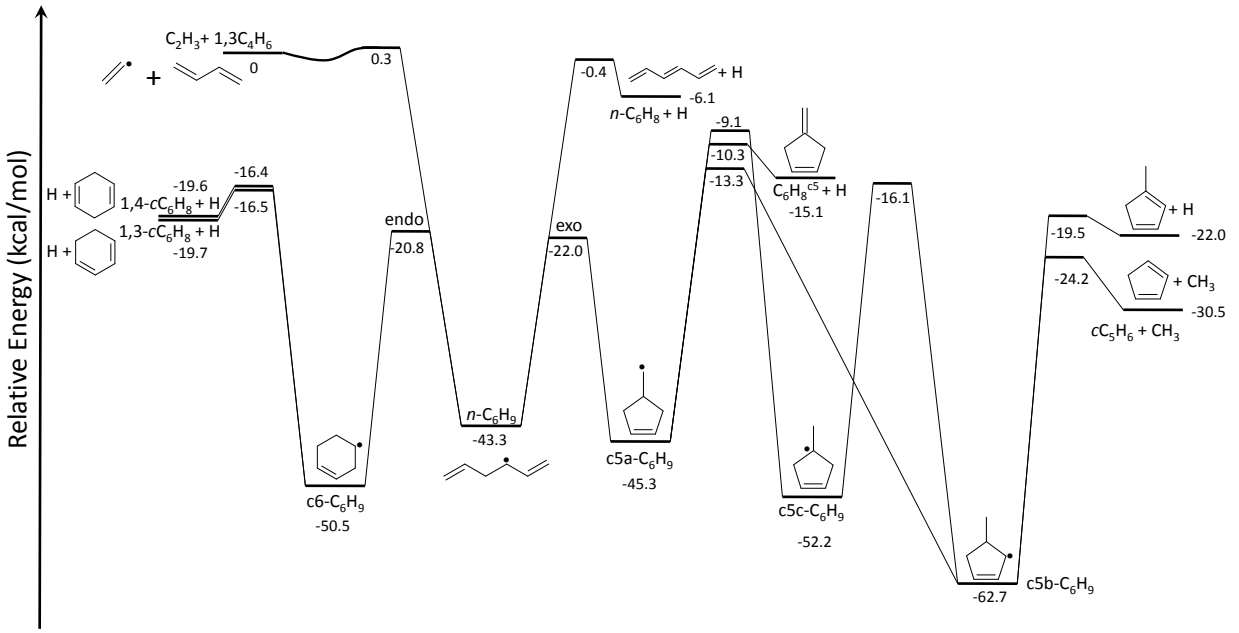


Figure 1: Zero Kelvin relative energy diagram (ZPE included) for the reaction of vinyl + 1,3-butadiene, with selected channels shown. All energies other than the entrance barrier height calculated at the CCSD(T)-F12a/cc-pVTZ-F12 level of theory. See text for discussion.

Overall Rate of C_2H_3 + 1,3-C_4H_6

In order to measure the overall reaction rate of $\mathrm{C_2H_3 + 1{,}3 - C_4H_6}$, k_1, several kinetic models described below and in the Supporting Information were developed and fit to the absorbance data. k_1 can be apportioned into the fraction, α, that forms the linear adduct isomer, $\mathrm{n - C_6H_9}$, and the remaining fraction, $1 - \alpha_{n-C_6H_9}$, that forms all of the other products.

$$\mathrm{C_2H_3 + 1{,}3 - C_4H_6} \xrightarrow{\alpha_{n-C_6H_9} k_1} \mathrm{n - C_6H_9} \qquad \text{(R1a)}$$

$$\mathrm{C_2H_3 + 1{,}3 - C_4H_6} \xrightarrow{(1-\alpha_{n-C_6H_9}) k_1} \mathit{Other\ Products} \qquad \text{(R1b)}$$

The reason for this distinction will become clear in coming paragraphs. In addition to undergoing bimolecular reaction with $\mathrm{1{,}3 - C_4H_6}$, $\mathrm{C_2H_3}$ can also undergo a number of other first-order and pseudo-first-order processes such as diffusion out of the probe beam, unimolecular decay and reaction with the $\mathrm{C_2H_3I}$ precursor. The total first-order rate of all of these processes, k_2, should

be constant for a given experiment where temperature (T), pressure (P), $[C_2H_3I]$ and the laser alignment are kept fixed, as was done here. Therefore, all of these processes may be adequately captured by a single pseudo-reaction in our models.

$$C_2H_3 \xrightarrow{k_2} Products \quad \text{(R2)}$$

C_2H_3 can also undergo self-reaction with rate coefficient k_{self}. However, we have found that including k_{self} decreases k_2 from $\sim 250\ s^{-1}$ to $\sim 150\ s^{-1}$ with no impact on k_1 (Figure S4 and Figure S5). For the sake of simplicity and because the goal of this work is to measure k_1, the model presented here neglects k_{self}. This approximation is most convincingly justified by the observation that in the absence of $1,3-C_4H_6$ the decay of C_2H_3 is fit well by a single-exponential decay with rate k_2, as shown for representative traces in Figure 2 and Figure 3.

A major challenge to measuring k_1 using laser flash photolysis is the well-known ultraviolet photodissociation of $1,3-C_4H_6$.[64] The major products of this process are thought to be propargyl and methyl radicals $(C_3H_3 + CH_3)$ with measurable contributions of ethylene + acetylene $(C_2H_4 + C_2H_2)$ and vinylacetylene + H_2 $(C_4H_4 + H_2)$ as well. This complicating side-phenomenon is likely a major reason why there is currently no direct measurement of $C_2H_3 + 1,3-C_4H_6$. Recently, while measuring the branching fractions of ethynyl radical, C_2H, reacting with $1,3-C_4H_6$, Lockyear et al. found that using 248 nm photolysis there is a noticeable amount of C_3H_3 and C_4H_4 formed from $1,3-C_4H_6$ photodissociation.[65] We indeed observe transient absorbance of our visible probe laser light if a sufficiently high concentration of $1,3-C_4H_6$ is photolyzed at 266 nm, which we attribute to C_3H_3. Although, to our knowledge, the visible absorption spectrum of C_3H_3 has not yet been measured, given the chemical similarity between C_3H_3 and the allyl radical, C_3H_5, which is known to absorb visible light,[66] it is

reasonable to assume that C_3H_3 can also absorb substantially around 400 nm. Photodissociation of $1,3-C_4H_6$ is therefore undesirable for our experiment for two reasons: 1. Visible absorbance of C_3H_3 will convolute the interpretation of our transient absorbance results, and 2. The additional radicals formed, i.e. C_3H_3 and CH_3, can react with C_2H_3 from C_2H_3I photolysis and make it difficult to extract the actual rate coefficient of interest, k_1. For both of these reasons, in all experiments reported here $[1,3-C_4H_6]$ and the 266 nm photolysis energy were kept sufficiently low ($< 5\times10^{16}$ molecules cm^{-3} and <30 mJ/pulse, respectively) such that no transient absorbance was detectable at $\lambda = 423.2$ nm when only $1,3-C_4H_6$ was photolyzed (Figure S1). At these conditions CH_3 is also not observed using PI TOF-MS and we can therefore estimate $[CH_3]_0 < 0.3\times10^{12}$ molecules cm^{-3} based on the sensitivity of the TOF-MS. Only at 700 K is a measurable amount of CH_3 detected. While this constraint resolves the first issue mentioned above, it doesn't guarantee that side reactions involving C_3H_3 and CH_3 are not occurring. To address this concern we conducted control experiments to measure k_1 at different photolysis energies. If $1,3-C_4H_6$ photodissociation is affecting the measured kinetics *via* C_3H_3, CH_3 or some other channel, then by doubling the photolysis power the measured k_1 should also change substantially. As shown later, this is not what was observed and we therefore conclude that at our experimental conditions $1,3-C_4H_6$ photodissociation does not affect the main results presented here.

Table 1 summarizes the experimental conditions of this work. At each T, P, Photolysis Energy and $[C_2H_3I]$ condition, $\lambda = 423.2$ nm absorbance traces were recorded at 6-9 different $[1,3-C_4H_6]$ values ranging from $0-5\times10^{16}$ molecules cm^{-3}**,** in evenly spaced intervals. Note that in all but two experiments the photolysis energy was kept relatively low at 15 mJ/pulse to minimize $1,3-C_4H_6$ photodissociation. For the two experiments where the energy was doubled,

$[C_2H_3I]$ was also halved in order to maintain close to the same $[C_2H_3]$ and therefore keep the effects of C_2H_3 self-reaction negligible on the obtained values of k_1. Attempts were also made to measure k_1 at 599 and 700 K, but unfortunately at these elevated temperatures $1,3-C_4H_6$ photodissociation significantly interfered with the measurements.

Table 1: Summary of experimental conditions for $\boldsymbol{\lambda = 423.2\ nm}$ absorbance experiments. In all cases the number of Flashes per Refresh (FPR) was less than one and $[\boldsymbol{1,3-C_4H_6}]$ was varied from $\boldsymbol{0-5\times10^{16}\ molecules\ cm^{-3}}$ for each experiment.

T (K)	P (Torr)	Photolysis Energy (mJ/pulse)	$[C_2H_3I]$ (10^{14} molecule/ cm^3)	$[C_2H_3]_0$ (10^{12} molecule/ cm^3)	A_0 (10^{-4})	Number of traces	Model Used
297	4	15	2.4	1.5 ± 0.5	9	9	Low-T
297	25	15	2.4	1.8 ± 0.9	10	9	
297	25	30	1.2	1.6 ± 0.8	9	6	
297	50	15	2.4	1.5 ± 0.8	10	9	
297	100	15	2.4	1.0 ± 0.6	10	9	
340	25	15	2.4	2.0 ± 1.1	11	9	Low-T
390	25	15	2.4	2.1 ± 1.2	11	9	High-T
444	25	15	2.4	1.7 ± 1.0	8	9	High-T
494	4	15	2.4	1.7 ± 0.9	7	8	High T
494	25	15	2.4	1.9 ± 1.1	8	9	
494	25	30	1.2	1.9 ± 1.1	8	6	
494	100	15	2.4	1.7 ± 1.1	10	9	

In these experiments, $[C_2H_3]_0$ was determined from the initial absorbance of the visible probe laser, A_0, its pathlength, $l_{probe}(=2000\pm600$ cm), and the measured cross section of vinyl as a function of temperature and pressure at the probe wavelength, $\sigma_{C_2H_3}(\lambda = 423.2\ nm)$, according the following equation.

$$[C_2H_3]_0 = \frac{A_0}{\sigma_{C_2H_3}(\lambda=423.2\ nm)l_{probe}} \quad (2)$$

Using the values of A_0 in Table 1 and of $\sigma_{C_2H_3}(\lambda = 423.2\ nm)$ in Table S3, it is straightforward to see how the values of $[C_2H_3]_0$ were calculated. Note that the measured fraction of C_2H_3I that photodissociates to C_2H_3 is ~0.7% (~1.4%), consistent with $\sigma_{C_2H_3I}(\lambda = 266$ nm$) \approx 5\times$

10^{-19} cm^2 molecule^{-1} reported in the literature,[67] and our photolysis diameter and energy of 1.2 cm and 15 mJ (30 mJ).

As shown in Table 1 a distinction is made between "Low-T" ($T < 390$ K) and "High-T" ($T \geq 390$ K) data. For the Low-T data, only reactions R1 and R2 are necessary to completely describe the transient absorbance traces. This Low-T model emerges as the well-known pseudo-first-order model.

$$\frac{[C_2H_3](t)}{[C_2H_3]_0} = e^{-(k_1' + k_2)t} \quad (3)$$

$$\frac{A(t)}{A_0} = (1 + a)\frac{[C_2H_3](t)}{[C_2H_3]_0} - a \quad (4)$$

$$a = \frac{(k_1' + k_2)}{RC - (k_1' + k_2)} \quad (5)$$

$[C_2H_3]_0$ is the initial concentration of C_2H_3, $k_1' = k_1[1,3-C_4H_6]$, A(t) is the time-dependent absorbance and RC is the time constant for our electronic data collection circuit that acts as a high-bandpass filter on the recorded decays ($= 65$ ms as we have shown previously[68]). Each Low-T experiment was fit to this model, where k_1 and k_2 are both global fit parameters (a single value of each was fit for all 6-9 traces of a given experiment). A more conventional pseudo-first-order analysis was also employed where a local k' value ($= k_1' + k_2$) was fit to each trace and k_1 was extracted from the slope of k' versus $[1,3-C_4H_6]$ (Fig. S3). As shown in Fig. S4 and S5, the values of k_1 and k_2 obtained are the same in either case (global or local fit), but the uncertainty bounds are smaller when global values of k_1 and k_2 are fit to the whole body of data by virtue of parameter reduction. For this reason, we prefer the global model. For the chemical decays of this work that occur on timescales ≤ 10 ms, the effect of the RC electronics is

adequately captured by including a without distorting the measured decay time constant (k_1 and k_2 in this case). Values of a are $\leq \sim 0.05$. Figure 2 shows representative fits of the Low-T model to 300 K absorbance traces. Considering that only 2 parameters are used to fit 6-8 decays, the fits are in good agreement.

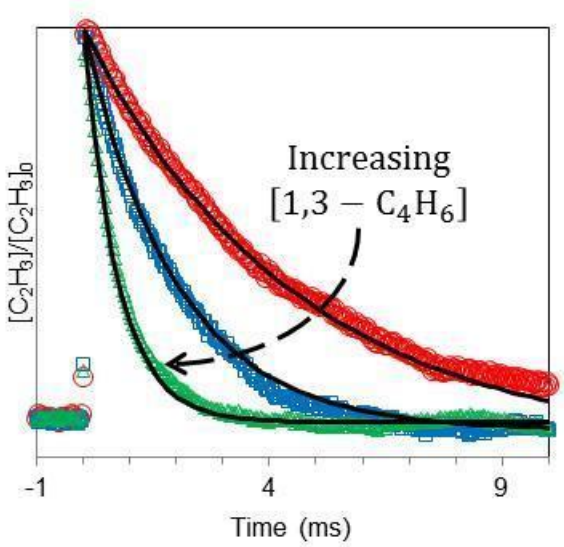


Figure 2: Representative measured decays of $\mathbf{C_2H_3}$ using $\boldsymbol{\lambda = 423.2\ nm}$ absorbance at relatively low-T (297 K, 100 Torr) and at the following $\mathbf{1,3-C_4H_6}$ concentrations (units of $\mathbf{molecules\ cm^{-3}}$): $\mathbf{0}$ (red circles), $\mathbf{1.2 \times 10^{16}}$ (blue squares) and $\mathbf{5 \times 10^{16}}$ (green triangles). The experimental decays have been smoothed using a 200 point moving average. Solid black lines are fits of the low-T model (single-exponential).

Implicit in the Low-T model is the assumption that C_2H_3 is the sole contributor to the 423.2 nm absorbance. This assumption is justified for T $<$ 390 K by the good fits of the single-exponential model to the data, but for T $\geq$ 390 K this assumption breaks down because at these higher temperatures the allylic products of the title reaction also contribute to the absorbance. Two of the expected C_6H_9 products are allylic radicals so it is expected that like allyl, they also absorb visible light relatively strongly. However, from earlier predictions of the product branching,[12, 20, 23] as well as our predictions shown later, we can assume that at our experimental conditions only the $n-C_6H_9$ allylic radical was produced at concentrations sufficient to affect the measured

absorbance. As mentioned earlier, $\lambda = 423.2$ nm was specifically chosen to avoid competing absorbance by allylic radicals. This approach was successful for $T < 390\ K$, where the vibronic bands we are probing are defined relatively sharply.[66, 69] At higher temperatures, however, the bands broaden and merge due to population of higher vibrational states at the ground electronic energy. This makes it much more difficult, if not impossible, to find a wavelength to probe one species selectively in a mixture. Here, we have taken the approach of modelling the contributions of both C_2H_3 and $n-C_6H_9$ to the overall 423.2 nm absorbance. R1 and R2 serve as the basis for this model, which only needs to be expanded on by the addition of one reaction of the allylic product.

$$n-C_6H_9 \xrightarrow{k_3} Products \qquad \text{(R3)}$$

R3 is analogous to R2 already considered for C_2H_3. Initially, we also included a fourth reaction of $n-C_6H_9 + 1{,}3-C_4H_6$, but found that this reaction was too slow for us to detect. Again we have neglected possible radical-radical reactions, i.e. self-reaction or cross reaction of $C_2H_3 + n-C_6H_9$, on the basis of low experimental radical concentrations; if these reactions were important exponentials would not fit the data. A straightforward analytical solution exists for this High-T model represented by R1-3. The solution for $[C_2H_3](t)$ is the same exponential decay function as in Eq. 3, whereas $[n-C_6H_9](t)$ is a biexponential function.

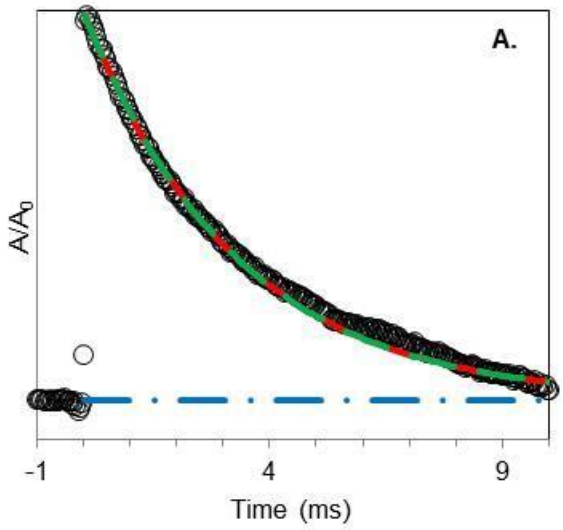
$$[n-C_6H_9](t) = \frac{\alpha_{n-C_6H_9} k_1'[C_2H_3]_0}{k_1'+k_2-k_3}\left[1-e^{-(k_1'+k_2-k_3)t}\right]e^{-k_3 t} \qquad (6)$$

The expression for the overall $A(t)$ can then be determined by weighting the contributions of $[C_2H_3](t)$ and $[n-C_6H_9](t)$ by their respective absorption cross sections, $\sigma(423.2\ \text{nm})$. The normalized solution is shown below.

$$\frac{\mathrm{A(t)}}{\mathrm{A_0}} = \mathrm{e}^{-(k_1'+k_2)t} + \frac{bk_1'}{k_1'+k_2-k_3}\left[1 - \mathrm{e}^{-(k_1'+k_2-k_3)t}\right]\mathrm{e}^{-k_3 t} \quad (7)$$

$$b = \frac{\alpha_{n-C_6H_9}\sigma_{n-C_6H_9}(423.2\ \mathrm{nm})}{\sigma_{C_2H_3}(423.2\ \mathrm{nm})} \quad (8)$$

Equations 7 and 8 constitute the High-T model. k_1, k_2, k_3 and b are all global fit parameters. There is no a parameter as in the Low-T model because it is a small correction (typically <5% of the full scale as mentioned earlier) and Eqs. 4 and 5 were derived for the case of a simple exponential chemical decay. A benefit of this model is that there are a reasonable number of fit parameters (4 parameters to fit the entire transient behavior of 6-9 absorbance decays) each of which can be ascribed to an observable physical process. Furthermore, values of $[\mathrm{C_2H_3}]_0$, $\sigma_{C_2H_3}$, $\sigma_{n-C_6H_9}$, $\alpha_{n-C_6H_9}$ and the probe laser pathlength don't need to be known in order to obtain accurate values of k_1, the quantity of interest. Note that if $b = 0$ (no contribution of $\mathrm{n-C_6H_9}$ either because it is not being produced, $\alpha_{n-C_6H_9} = 0$, or its cross sections is small compared to that of $\mathrm{C_2H_3}$) the pseudo-first-order model of Eq. 3 is recovered. Representative fits of 494 K absorbance traces to the high-T model are shown in Figure 3. Clearly the decays are not single exponential, this is most evident for high $[1,3-\mathrm{C_4H_6}]$. As shown, the High-T biexponential model describes this behavior very well, especially considering the use of only four fit parameters.


A.
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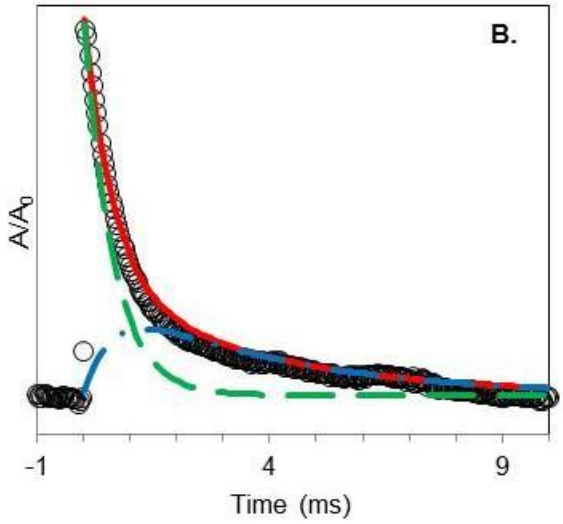
Time (ms)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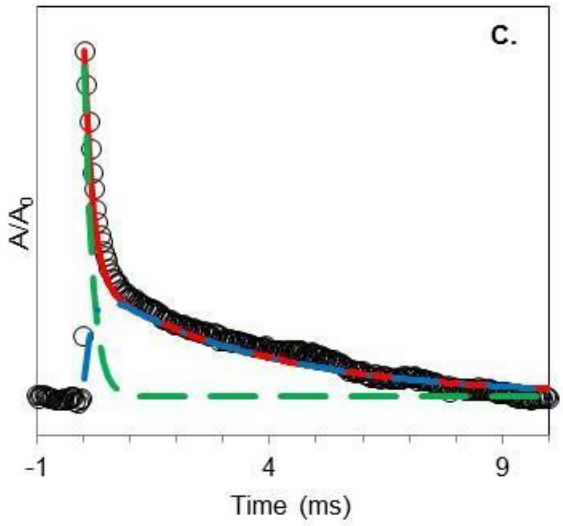
C.
A/A0
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9
Time (ms)

Figure 3: Representative measured absorbance decays using $\boldsymbol{\lambda = 423.2\ nm}$ at relatively high-T (494 K, 100 Torr) and at the following $\boldsymbol{1,3-C_4H_6}$ concentrations (units of $\boldsymbol{molecules\ cm^{-3}}$): $\mathbf{0}$ (*Panel A*), $\boldsymbol{1.2 \times 10^{16}}$ (*Panel B*) and $\boldsymbol{5 \times 10^{16}}$ (*Panel C*). The experimental decays have been smoothed using a 200 point moving average. Green dashed lines are the modeled C_2H_3 decay, blue dashed-dotted lines are the modeled n-C_6H_9 growth and decay and the solid red lines are the fits of the overall high-T model.

A table of all the fit parameter values for the High-T model is included in Table S2. It is worth mentioning here that the fit values of b vary from $\sim 0.25 - 0.40$ and increase as a function of increasing T and decreasing P. Assuming that $\alpha_{n-C_6H_9} \approx 1$, which is predicted at our conditions as shown in the next section, these values of b simply represent the ratio of $n-C_6H_9$ to C_2H_3 cross sections. We have previously measured T- and P-dependent values of $\sigma_{C_2H_3}(\lambda)$ using the approach of Ismail et al.,[41] but currently we cannot measure $\sigma_{n-C_6H_9}(\lambda)$ without available $n-C_6H_9I$ or $n-C_6H_9Br$ precursors nor, to our knowledge, have these values been measured in the literature. Nonetheless, we have measured the T- and P-dependent cross section of the allyl radical, C_3H_5, which we expect to be similar to $\sigma_{n-C_6H_9}(\lambda)$. As shown in Fig. S2, our measured $\frac{\sigma_{C_3H_5}}{\sigma_{C_2H_3}}(423.2\ \text{nm})$ values are in excellent agreement with the fit b values mentioned above, lending credibility to our model, and supporting the conclusion made later that $n-C_6H_9$ is the dominant product at our conditions $\left(\alpha_{n-C_6H_9} \approx 1\right)$.

Figure 4 is an Arrhenius plot that summarizes our measured temperature dependence of k_1 with comparisons to literature. The error bars on individual k_1 measurements in Figure 4 and Figure 5 include fitting uncertainty as well as systematic uncertainty due to 10% uncertainty in $[1,3-C_4H_6]$ as discussed previously.[70] Our experimental results are fit well by the simple Arrhenius expression $(1.1 \pm 0.2) \times 10^{-12}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1} \times \exp\left(-\frac{9.9 \pm 0.6\ \text{kJ mol}^{-1}}{\text{RT}}\right)$, as shown by the dotted-dashed black line. The fact that k_1 values obtained from both the Low- and High-T

models all lie along the same Arrhenius fit provides confidence in our interpretation of the absorbance results. The calculations of the total rate of vinyl + 1,3-butadiene performed in this work at 25 Torr He and 760 Torr N_2 are also shown in Figure 4 and are in good agreement with the current experimental data. From these predictions, k_1 in the high pressure limit can be expressed in modified Arrhenius form as 6.5×10^{-20} cm^3 molecule^{-1} s^{-1} $\times T^{2.40}$ exp $\left(-\frac{1.76 \text{ kJ mol}^{-1}}{\text{RT}}\right)$ from 300 to 2000 K. The slope of our measurements and predictions also agree well with the TST predictions of Cavallotti et al.[20, 21] However, the absolute values of our measurements and predictions are significantly different from any of the predictions mentioned above (one order of magnitude lower than the value reported in Ref. 20). Most strikingly, our results disagree both quantitatively and qualitatively with the pressure dependent predictions of Cavallotti et al and Xu et al.[23] These differences are discussed in more detail in the following section on product branching.

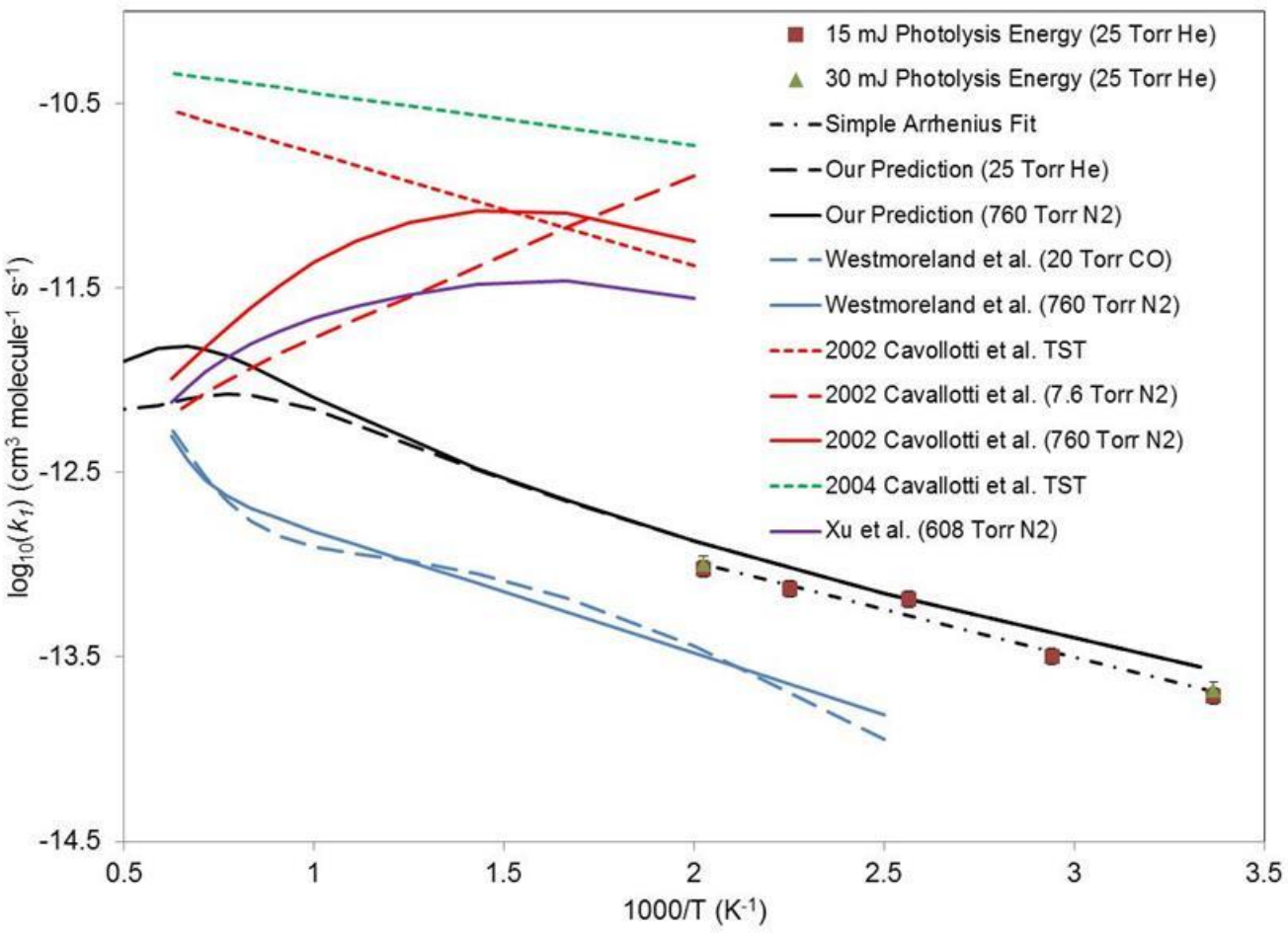

Figure 4: Arrhenius plot of our measured overall rate constant for $\mathbf{C_2H_3 + 1,3 - C_4H_6}$ at 25 Torr (red squares and green triangles) with a simple Arrhenius fit (dotted-dashed black line) and comparison to literature predictions: Westmoreland et al.[12] (blue lines), 2002 Cavallotti et al.[20] (red lines), 2004 Cavallotti et al.[21] (green line) and Xu et al.[23] (purple line). Also shown are the theoretical predictions of this work (black lines).

At the two temperature extremes of our experiments (297 and 494 K) we measured k_1 at both 15 and 30 mJ pulse^{-1} of photolysis energy and found the values to be within their error bars. These results justify our assumption that $1,3 - C_4H_6$ photodissociation is not affecting the measured kinetics as discussed earlier. The 494 K result is particularly convincing given that photodissociation is more likely to occur at higher temperature.

Figure 5 shows the measured pressure dependence of k_1 again at the temperature extremes of 297 and 494 K. Although some of the measurements at the same T are outside of the error bars

of others, no consistent trend is discernible from these results. The outlying data points are suggestive not that there is any pressure dependence at our conditions, but that our error bars are underestimated perhaps by a factor of two. The measured lack of pressure dependence is consistent with both our own predictions and those of Westmoreland et al.[12] (Figure 4) showing that even at the relative low P of this work (≤ 100 Torr) we are already near the high-P limit (k_∞).

It is informative to compare our measured k_1 for vinyl radical addition to 1,3-butadiene with other radical additions to 1,3-butadiene. Phenyl + 1,3-butadiene provides a good comparison because its overall rate coefficient has been measured in an experimental study quite similar to this work.[71] Phenyl decay was measured by cavity ringdown spectrometry (CRDS) at $\lambda = 504.8$ nm from $298 - 450$ K at 40 Torr. At these conditions the authors also concluded they were already in the high-pressure limit and the dominant product was expected to be the radical adduct. The Arrhenius pre-exponential factor that they measured is around an order of magnitude higher than what we measured for vinyl + 1,3-butadiene in the same T,P-range, while the E_A values are nearly identical. A similar difference between vinyl and phenyl radical addition to the same unsaturated C-C bond has also been observed for vinyl/phenyl radical addition to acetylene.[14, 72] This comparison provides greater confidence in our measurement. Refer to Figure S6 for Arrhenius comparison plots of vinyl/phenyl + 1,3-butadiene/acetylene.

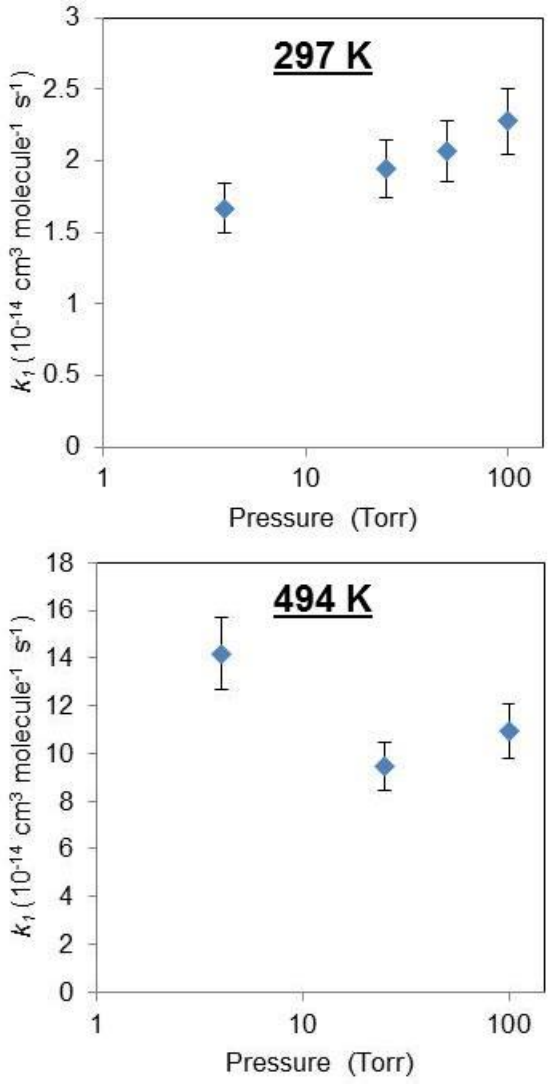

Figure 5: Measured pressure dependence of overall $\mathbf{C_2H_3 + 1,3 - C_4H_6}$ rate constant at $\mathbf{297\ K}$ (upper panel) and $\mathbf{494\ K}$ (lower panel).

Product Branching of C_2H_3 + 1,3-C_4H_6

Experiments were conducted at both 4 and 25 Torr over a range of temperatures using PI TOF-MS in order to measure the products of $C_2H_3 + 1,3 - C_4H_6$, as summarized in Table 2. For the 4 Torr experiments, we were able to obtain useful results for $T \geq 494$ K despite significant $1,3 - C_4H_6$ photodissociation that prevented absorbance measurements at 599 and 700 K. At

each T and P there is a "Base Case" experiment, and several control experiments to aid in interpreting the results.

Table 2: Summary of experimental conditions for PI TOF-MS experiments.

Experiment Title	T (K)	P (Torr)	PDMS coated?	Photolysis Energy (mJ/pulse)	Photolysis Diameter (cm)	$[C_2H_3I]$ (10^{14} molecule/ cm^3)	$[1,3\text{-}C_4H_6]$ (10^{16} molecule/ cm^3)	FPR[1]
Base Case	297	25	No	50	1.2	2.5	1.2	0.94
C_2H_3 Only Control	297	25	No	50	1.2	2.5	0	0.94
1,3-C_4H_6 Control	297	25	No	50	1.2	0	1.2	0.94
Base Case	494	25	No	30	1.2	1.2	1.2	0.92
C_2H_3 Only Control	494	25	No	30	1.2	1.2	0	0.92
1,3-C_4H_6 Only Control	494	25	No	30	1.2	0	1.2	0.92
2x$[C_2H_3I]$ Control	494	25	No	30	1.2	2.4	1.2	0.92
2x Photolysis Control	494	25	No	50	1.2	1.2	1.2	0.92
2x FPR Control	494	25	No	30	1.2	1.2	1.2	2.30
Base Case	494	4	No	30	1.2	1.2	1.2	0.92
1,3-C_4H_6 Only Control	494	4	No	30	1.2	0	1.2	0.92
No Cal Mix Control	494	4	No	30	1.2	1.2	1.2	0.92
PDMS Coated Control	494	4	Yes	30	1.2	1.2	1.2	0.92
1.5 cm Photolysis Diameter Control	494	4	Yes	30	1.5	1.2	1.2	0.92
Maximum Photolysis Power Control	494	4	Yes	80	1.2	1.2	1.2	0.92
Base Case	599	4	No	30	1.2	1.2	1.2	0.93
1,3-C_4H_6 Only Control	599	4	No	30	1.2	0	1.2	0.93
No Cal Mix Control	599	4	No	30	1.2	1.2	1.2	0.93
C_2H_3 Only Control	599	4	No	30	1.2	1.2	0	0.93
Base Case	700	4	No	30	1.2	1.2	1.2	0.93
1,3-C_4H_6 Only Control	700	4	No	30	1.2	0	1.2	0.93
No Cal Mix Control	700	4	No	30	1.2	1.2	1.2	0.93
Half 1,3-C_4H_6 Control	700	4	No	30	1.2	1.2	0.6	0.93

[1]FPR = Flashes per Refresh

Figure 6 shows a section of our measured transient mass spectra at both 25 and 4 Torr (494 K and 599 K, respectively) under conditions where $C_2H_3 + 1{,}3 - C_4H_6$ occurs. Other than the I Atom signal at 127 amu, transient behavior was not observed in any other region of the spectrum (due to significant dissociative ionization of C_2H_3I to C_2H_3, the transient behavior of C_2H_3 could not be discerned even after background subtraction). At both pressures, there is clearly growth occurring at $\frac{m}{z} = 81$ amu, which we tentatively assign to some mixture of C_6H_9 isomers

produced by the title reaction (Scheme 1 and Figure 1). This assignment was confirmed by control experiments showing that the 81 amu species requires the simultaneous presence of C_2H_3 and $1,3-C_4H_6$ to form. The mass spectra obtained at 297 K and 25 Torr exhibits identical behavior as at 494 K and 25 Torr (Supporting Information), although the signal-to-noise was lower due to the slower $C_2H_3 + 1,3-C_4H_6$ reaction rate at this temperature, resulting in a lower product concentration.

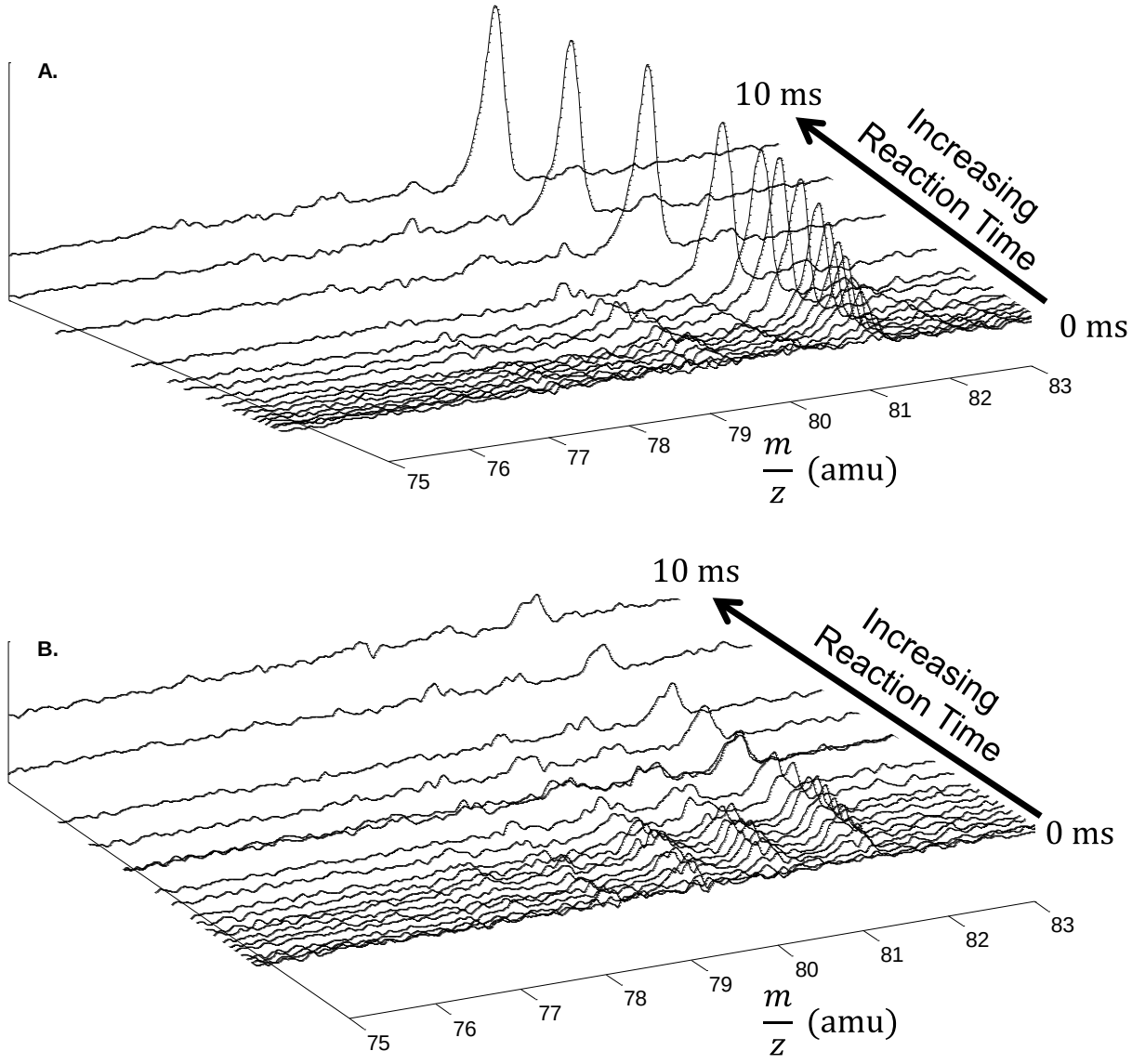

Figure 6: Transient mass spectra obtained under conditions where $\mathbf{C_2H_3 + 1,3 - C_4H_6}$ can occur for A. 494 K and 25 Torr, and B. 599 K and 4 Torr. In both cases $\mathbf{[C_2H_3I] = 1.2 \times}$

$\mathbf{10^{14}}$ and $[\mathbf{1,3-C_4H_6}] = \mathbf{1.2 \times 10^{16}\ molecules\ cm^{-3}}$. The spectrum acquired at a reaction time of $\mathbf{-0.20\ ms}$ was subtracted from all subsequent spectra so that only transient changes are observed. The spectra were also smoothed and baseline corrected.

At 4 Torr, there is also a transient peak at 80 amu, which control experiments confirm as another product of $C_2H_3 + 1,3-C_4H_6$. This species was not observable in any of the 25 Torr experiments. We assign this species to a mixture of 1,3- and 1,4-cyclohexadiene isomers ($c-C_6H_8$), based on our predictions of the product branching shown in Figure 9 below.

There is one final peak at 79 amu that is present at both pressures and that does not correspond to an expected product of $C_2H_3 + 1,3-C_4H_6$. In the Supporting Information we discuss control experiments aimed at identifying this species and ultimately conclude that it is likely not a product of $C_2H_3 + 1,3-C_4H_6$. At 700 K there were also several other transient species besides 79, 80 and 81 amu, (e.g., 15 and 78 amu) but none of these species required the presence of C_2H_3 and are therefore attributed to $1,3-C_4H_6$ photodissociation and subsequent reactions. Despite these complications, the transient signals at 80 and 81 amu were found to be the only species clearly attributable only to $C_2H_3 + 1,3-C_4H_6$ at all of the T and P conditions of Table 2.

Unfortunately, we cannot discern among C_6H_9 isomers using our PI TOF-MS with fixed ionization energy. Neither can we provide an estimate of the quantitative branching fraction to this channel because the photoionization cross sections of the C_6H_9 isomers have not yet been measured. Nonetheless, our theoretical predictions below provide strong evidence that the 81 amu signal is solely due to $n-C_6H_9$ $\left(\alpha_{n-C_6H_9} \approx 1\right)$, which is also consistent with our interpretation of the fit b parameters in the previous section.

Similarly, we can't distinguish between 1,3- and 1,4-cyclohexadiene. However, the photoionization cross sections of both isomers are known at our ionization energy (10.5 eV).[73, 74]

Therefore we were able to quantify the total branching to both cyclohexadiene isomers at 4 Torr and relatively high temperature conditions (494, 599 and 700 K) where they become significant products (see Supporting Information for details of quantification). Control experiments conducted after coating the inside of the stainless steel reactor with PDMS gave the same quantitative cyclohexadiene branching fractions as experiments without the coating. PDMS has previously been used in similar kinetic studies to render reactor walls inert up to 750 K.[39, 40] Therefore, we conclude that wall reactions do not consume a significant portion of the vinyl radical pool, possibly due to the unique geometry of our apparatus.

Figure 7 compares our measurement of this branching with our predictions. In both cases, the branching fraction of total C_6H_8 + H products increases with higher temperature, as expected for a chemically activated channel. However, the model greatly overpredicts the branching. The large error bars on the experimental measurements are from propagation of uncertainty (see Supporting Information for an account of the various contributors).

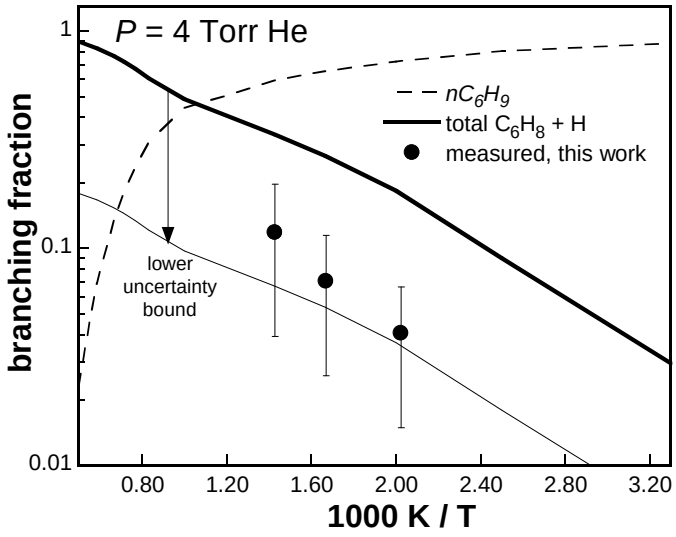

Figure 7: Branching fractions for major bimolecular product species (minor contributions not shown) of the reaction of vinyl + 1,3-butadiene at 4 Torr He. Predicted branching fractions of

$\mathbf{n-C_6H_9}$ (dashed line) and total $\mathbf{C_6H_8+H}$ (thick solid line), are compared with measured branching fractions (filled circles). Also depicted is an estimated uncertainty bound in the calculations of a factor of 5; see text for discussion.

Sensitivity analyses of the predicted total branching fraction for the C_6H_8 isomers [+ H] were performed with respect to several input parameters: relevant barrier heights, the average downward energy transferred upon collision with the He bath gas, and the influence of 1,3-butadiene as a colliding partner. The lower bound illustrated in Figure 7 represents a combined ±1 kcal/mol barrier uncertainty with a factor of two increase in $\langle \Delta E_d \rangle_{300}$ for Helium. Additional uncertainties arise from the use of Eckart tunneling corrections, the MSC solution to the master equation, and A-factors for reactions where hindered internal motions are important. Last, uncertainties also arise from the fact that gas mixtures for 4 Torr experiments contained up to 22% 1,3-butadiene (see Table S5 for details), which was not considered in the branching fractions predicted in Figure 7. The average downward energy transferred upon collision for 1-butene (a suitable analog to 1,3-butadiene) is a factor of eight larger than that for Helium in observations of excited toluene stabilization.[75] Simulations performed using weighted averages of energy transfer properties where the bath gas consists of 20% 1,3-butadiene and 80% Helium suggest branching to total C_6H_8 + H is twice as low between 500-700 K and at 4 Torr. Although the current branching fractions are uncertain by at least a downward factor of five, it is expected that future high-accuracy rate calculations may reconcile predicted branching fractions with those observed in this work at 4 Torr in Helium. We also note that while uncertainties in predicted branching are high for simulations at low pressure and with Helium as a bath gas, the simulations in N_2 at and above 1 atm – combustion relevant conditions – are more reliable due to the larger $\langle \Delta E_d \rangle_{300}$ of N_2.

The product branching calculations performed here and shown in Figure 9 support the observation that the dominant product species at and above 25 Torr is $n-C_6H_9$, of mass 81 amu. Thus, at 1 atmosphere, the formation of $c-C_5H_6+CH_3$ is negligible, in contrast to previous predictions by Cavallotti et al.[20, 21] As noted in previous works and also illustrated in Figure 4, there remains a great deal of disparity between theoretical predictions of the total rate of vinyl + 1,3-butadiene. The two sets of computed results by Cavallotti et al.[20-21] and predictions of recent work by Xu et al.[23] are more than an order of magnitude faster than those predicted here and earlier by Westmoreland et al.[12]. We note that the rate constant for the entrance channel computed by Cavallotti (private communications) used a 2-dimensional treatment of the hindered rotor that not only accounts for the rotation of the two moieties about the axis defining the forming bond, but also one of the rocking motions in the transition state. Cavallotti et al. employed the Unimol code originally developed by Gilbert and Smith[76]. Use of this code to treat a 2D internal rotor resulted in a factor of 400 increase in the pre-exponential factor compared with treating all internal degrees of freedom as harmonic oscillators. It was further noted by Cavallotti that this approach, as implemented in the Unimol code, can lead to substantial errors, thus explaining the large discrepancy between computed high pressure limit rate coefficients presented in this work and those of Cavallotti et al. (private communications).

The discrepancy between the high-pressure limit entrance channel rate computed in this work and that reported by Xu et al.[23] is primarily due to differences in predicted barrier heights (0.3 kcal/mol via the F12 method and -0.6 via CBSQB3) and in choice of rate parametrization (strict vs modified Arrhenius). Gaussian output files used for the TST calculation by Xu et al along with their corresponding TST-derived rates for the high pressure limit rate of the entrance channel were provided by means of personal communication. One can see that the RRHO rates

computed using the Xu et al. geometry and frequencies (blue line of Figure 8), and the RRHO rate computed using the geometry and frequencies computed here using a different DFT functional and basis set, are very similar after compensating for the 1 kcal/mole difference in computed barrier height (black dashed line), differing by less than a factor of 3 over the full T range. The strict Arrhenius fit used by Xu et al. (red line of Figure 8) differs significantly from the computed k(T) at some temperatures, since it does not allow for the strong curvature of k(T) on the Arrhenius plot. Considering all the calculations and the experimental data, it appears that the computed rates are all uncertain by a factor of 3 or more; the rates computed here are (perhaps fortuitously) close to the low temperature experimental measurements giving us a little more confidence in the predictions at higher temperatures. Thus, an overall factor of 3 uncertainty is recommended for the predicted high-pressure limit rate coefficient for the reaction of vinyl + 1,3-butadiene.

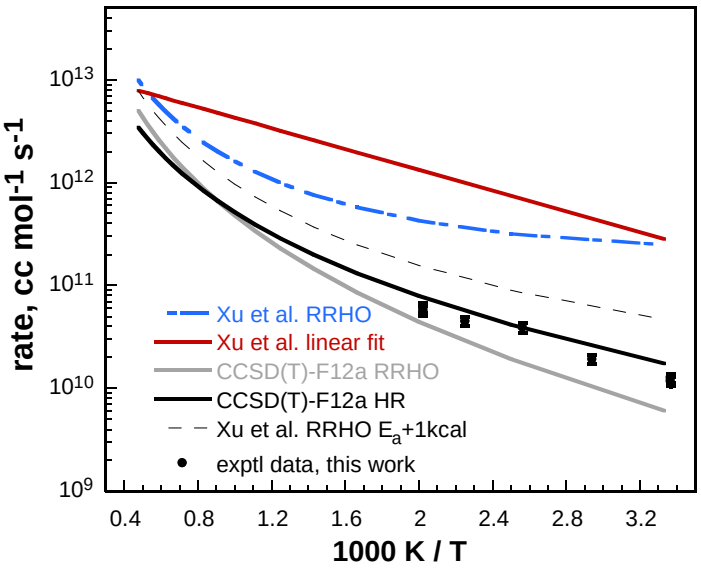

Figure 8. Comparisons of computed high pressure limit rates for the reaction of vinyl + 1,3-butadiene between experimental and computed values of this work, as well as those of Xu et al.[23]

In comparing predicted rates of individual product channels between this work and previous studies, the 25 Torr rates shown in Figure 9 are in good qualitative agreement with the corresponding lower pressure estimates of Westmoreland et al.,[12] albeit their simulations were performed in a CO bath gas. However, the aforementioned authors predict the formation of $n-C_6H_8+H$ to dominate around 1250 K, while the current calculations suggest this channel to dominate at considerably higher temperatures.

A general observation made in this work and supported both by present experiments and computation is the negligible chemically activated well skipping to bimolecular product channels at temperatures below 500 K and pressures above 25 Torr. Clearly evident from Figure 9 is that $n-C_6H_9$ is the dominant product not just at 25 Torr, but also at 760 Torr. At 25 Torr and 300 K, 94% of the product is predicted to be the linear adduct, while at 1000 K, 71% of the product is $n-C_6H_9$, with the two $c-C_6H_8$ species representing the remaining product distribution. At 1000 K and 760 Torr, only 2% of the product species are predicted to be the two $c-C_6H_8$ species + H. This is in contrast to the recent work by Xu et al.,[23] who predict these channels to contribute more equally to the total product distribution at 0.8 atm and at 1000 K and above. Because the PES used here and the Master Equation solution method, MSC, are both similar to that employed by Xu et al., it is unclear why these differences exist. Higher level collisional energy transfer models may increase the total predicted branching to bimolecular products, further increasing the discrepancy in predicted and measured branching shown in Figure 7. Nonetheless, recommended future work entails a rate theory calculation more reliable than the MSC method.

The overall dominance of the $n-C_6H_9$ adduct suggests this species could persist long enough to undergo bimolecular reactions with other gas phase species at low enough temperatures, and of

course where there is sufficient vinyl and 1,3-butadiene. If this is the case, and if the rates provided in the SI are to be used for combustion modeling, care should be taken to ensure that the fate of $n-C_6H_9$ is properly accounted for. Compared to some previous kinetic models which use rates that predict a larger proportion of bimolecular *c5*- and *c6*-ring products, inclusion of the present rates in kinetic models may in fact decrease overall predicted benzene concentrations for relevant conditions.

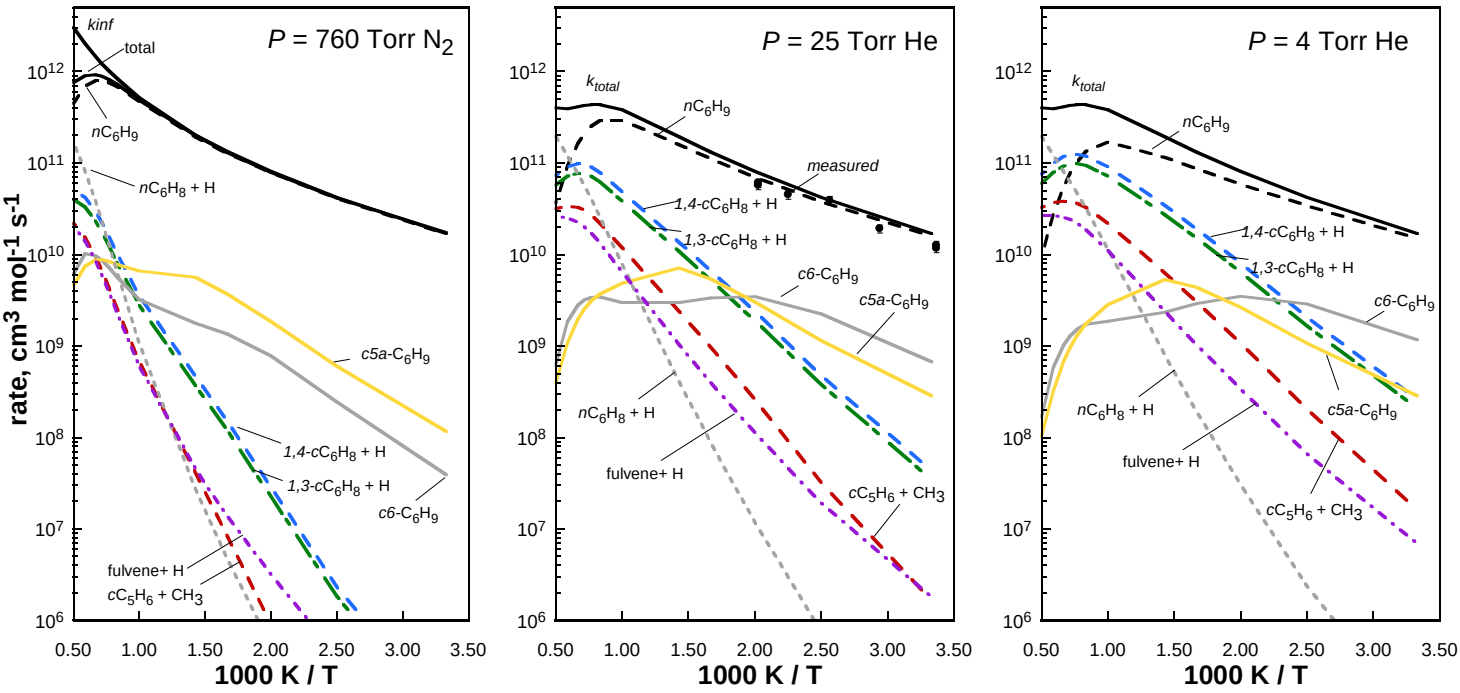

Figure 9: Predicted rates of major channels for the reaction of vinyl + 1,3-butadiene for 760 Torr N_2 (left), 25 Torr He (middle) and 4 Torr He (right). Measurements of the overall rate at 25 Torr He, are shown as black circles, and accompanied by an Arrhenius fit.

Implications for Soot Formation

The impact of our newly measured rate coefficient on pre-existing pyrolysis or combustion models will depend on the conditions of the system. For example, if $C_2H_3 + 1,3-C_4H_6$ is already the dominant route for benzene production, then a larger k_1 will increase the predicted benzene formation if the addition step is rate-limiting. If, however, another route involving vinyl

radicals dominates benzene formation, such as $C_2H_3 \xrightarrow{C_2H_2} n-C_4H_5 \xrightarrow{C_2H_2} C_6H_6 + H$ as suggested by Miller et al.,[14] it is conceivable that increasing k_1 will actually decrease benzene formation by converting reactive C_2H_3 to stable, resonantly-stabilized $n-C_6H_9$, acting effectively as a trap for vinyl radicals. Regardless of the overall effect, we recommend that future models incorporate the rates reported here (Supporting Information) to improve the accuracy of predictions and to assess the true role of $C_2H_3 + 1,3-C_4H_6$.

CONCLUSIONS

We report the first direct rate coefficient measurement of $C_2H_3 + 1,3-C_4H_6$, k_1, using laser flash-photolysis with visible probe absorbance. Photodissociation of $1,3-C_4H_6$ is kept at an acceptable level by using relatively low $[1,3-C_4H_6]$ and photolysis energy, as well as maintaining $297\ \text{K} \leq T \leq 494\ \text{K}$ for all absorbance experiments reported here. For $T < 390\ K$ the decay of C_2H_3 could be monitored selectively using $\lambda = 423.2$ nm as the probe wavelength, enabling a straightforward pseudo-first-order analysis of the results. For $T \geq 390$ K, however, the major allylic product, $n-C_6H_9$, makes a non-negligible contribution to the absorbance and a model that accounts for this behavior is used. Our interpretation of the absorbance traces at different temperatures is validated by the good fits of the model to the data, as well as the fact that a simple Arrhenius fit is able to capture the resulting temperature dependent k_1 measurements, shown below.

$$k_1 = (1.1 \pm 0.2) \times 10^{-12}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1} \times \exp\left(-\frac{9.9 \pm 0.6\ \text{kJ mol}^{-1}}{RT}\right)$$

k_1 is pressure-independent at the conditions of our experiment $(4-100\ \text{Torr}, \text{T} \leq 494\ \text{K})$, leading us to conclude that we are already in the high-pressure limit, consistent with our predictions and others in literature.[12]

Analysis of the reaction products at $\text{T} \leq 494$ K and $\text{P} = 25$ Torr using photoionization time-of-flight mass spectrometry (PI TOF-MS) reveals only species with $\frac{m}{z} = 81$ amu, consistent with the molecular formula C_6H_9. Predictions of the product branching using quantum chemistry and pressure dependent rate calculations show the dominant product at almost all combustion relevant T and P (including our experimental conditions) to be the linear allylic species $\text{n}-\text{C}_6\text{H}_9$. This prediction is consistent both with the PI TOF-MS results cited above, and with the measured contribution of $\text{n}-\text{C}_6\text{H}_9$ to the absorbance traces at $\text{T} \geq 390$ K. Furthermore, the measured overall rate of $\text{C}_2\text{H}_3 + 1{,}3-\text{C}_4\text{H}_6$ is in excellent agreement with the predictions. However, for $494 \leq \text{T} \leq 700$ K and $\text{P} = 4$ Torr we experimentally measured ~10% or less branching to the sum of 1,3- and 1,4-cyclohexadiene isomers, which was a factor of five lower than the predicted branching. We attribute this discrepancy to uncertainty in $\langle \Delta E_d \rangle_{300}$ and the computed barrier heights.

The predicted temperature and pressure dependent product branching rates are presented in a form that can be easily incorporated into combustion and pyrolysis models for $300 \leq \text{T} \leq 2000$ K and $\text{P} \geq 1$ Torr. We recommend that these rates be used in future detailed kinetic models so that the role of $\text{C}_2\text{H}_3 + 1{,}3-\text{C}_4\text{H}_6$ in the formation of the first aromatic ring can finally be elucidated.

ASSOCIATED CONTENT

Details of the absorbance and PI TOF-MS experiments (tables of fit parameters for the Low- and High-T absorbance models; representative absorbance trace following $1,3-C_4H_6$ photolysis; interpretation of the physical meaning of the b fit parameter in the High-T model; results from fitting alternative absorbance models; summary of the PI TOF-MS experiments; explanation of how the cyclohexadiene channel was quantified) as well as computational details (M08SO/MG3S computed geometries, energies, vibrational frequencies; raw k(T,P) Cantherm outputs and example input file; CHEBYSHEV fitted rate coefficients for both N_2 and He bath gases; high-pressure limit rate coefficients for all channels, including the H-abstraction channels from 1,3-butadiene + vinyl) are included in the Supporting Information. This material is available free of charge via the Internet at http://pubs.acs.org.

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Notes
The authors declare no competing financial interests.

ACKNOWLEDGMENTS

This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences under the Energy Frontier Research Center for Combustion Science (Grant No. DE-SC0001198). This research used resources of the National Energy Research Scientific Computing Center, a DOE Office of Science User Facility supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. G.L. is supported by China Scholarship Council (No. 201308120042) and Program for New Century Excellent Talents of MOE, China (NCET-13-0408). R.M.I.E. gratefully acknowledges financial support from the Fulbright

Commission and Alexandria University. The authors would like to thank Joshua Middaugh and Mickaël Matrat for their foundational experiments and analysis on reactions of vinyl with alkenes that enabled the current work, J.A. Miller for providing the flame model of Ref. 36 and Vadim Knyazev for many helpful suggestions.

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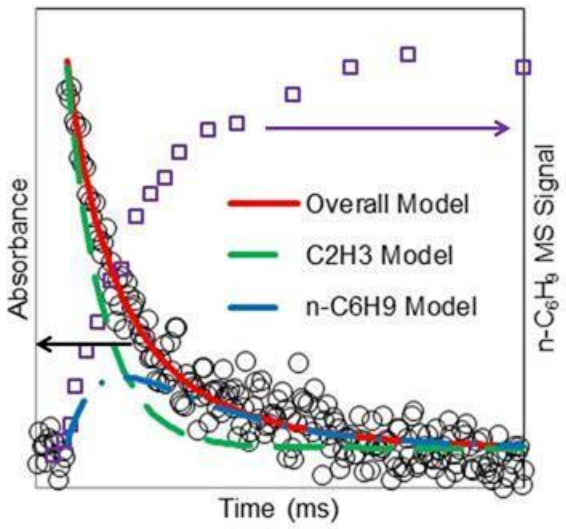
TOC Figure


Absorbance
Overall Model
C2H3 Model
n-C6H9 Model
n-C6H9 MS Signal
Time (ms)

Supporting Information

Kinetics and Products of Vinyl + 1,3-Butadiene, a Potential Route to Benzene

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Experimental Details

1. Photolysis of 1,3-Butadiene

During each absorbance experiment, a trace was recorded at the maximum $[1{,}3-C_4H_6]$ ($= 5 \times 10^{16}$ molecules cm^{-3}) without C_2H_3I present (and hence no C_2H_3 either). The purpose of these traces was to photolyze $1{,}3-C_4H_6$ by itself and check for any photoproducts that absorb at $\lambda = 423.2$ nm. Figure S1 shows one such representative trace, with the corresponding trace recorded in the presence of C_2H_3 also shown for comparison. As described in the main text, if $[1{,}3-C_4H_6]$, the photolysis power and temperature are all high enough, we have observed absorbance at 423.2 nm which we attribute to propargyl radical, C_3H_3 produced by $1{,}3-C_4H_6$ photodissociation.[1] In all of the absorbance experiments reported here, however, even at the maximum $[1{,}3-C_4H_6]$, photolysis power and temperature there is no 423.2 nm absorbance discernible from the noise when $1{,}3-C_4H_6$ is photolyzed by itself, just as shown in Figure S1.

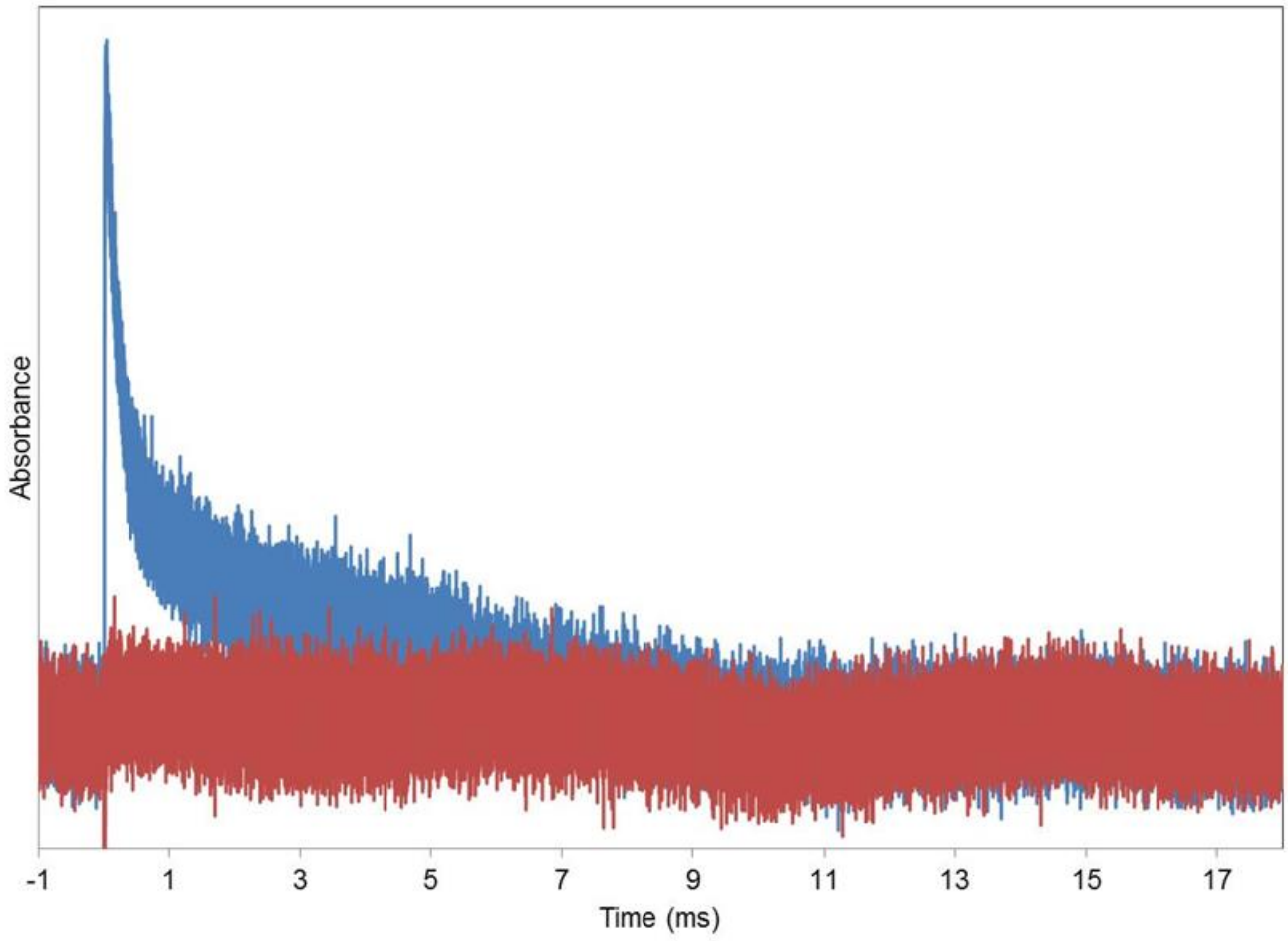

Figure S1: Comparison of 423.2 nm absorbance traces at identical conditions (494 K, 100 Torr, $\mathbf{15\ mJ\ pulse^{-1}}$ photolysis energy and $\mathbf{1,3-[C_4H_6]=5\times10^{16}\ molecules\ cm^{-3}}$) except for the presence (blue) or absence (red) of $\mathbf{C_2H_3I}$ ($\mathbf{[C_2H_3I]=2.4\times10^{14}\ molecules\ cm^{-3}}$).

2. *Summary of Fit Parameters to Absorbance Data*

Table S1 and Table S2 summarize all of the fit parameters obtained for both the Low- and High-T models. Quoted error bars include both fitting uncertainty, which is quite small due to the high density of points in an absorbance trace, and systematic uncertainty due to the $\sim 10\%$ uncertainty in $[1{,}3-C_4H_6]$ as described in our previous work.[2] The fit values of b deserve special attention and are discussed in the next section.

Table S1: Summary of fit parameters for Low-T absorbance experiments.

T (K)	P (Torr)	Photolysis Energy (mJ/pulse)	$[C_2H_3I]$ (10^{14} molecule/ cm^3)	Number of traces	k_1 (10^{-14} cm^3 $molecule^{-1}s^{-1}$)	k_2 (s^{-1})
297	4	15	2.4	9	1.7 ± 0.17	297 ± 0.5
297	25	15	2.4	9	1.9 ± 0.20	243 ± 0.4
297	25	30	1.2	6	2.1 ± 0.22	245 ± 0.4
297	50	15	2.4	9	2.1 ± 0.21	251 ± 0.4
297	100	15	2.4	9	2.3 ± 0.23	220 ± 0.3
340	25	15	2.4	9	3.2 ± 0.32	222 ± 0.3

Table S2: Summary of fit parameters for High-T absorbance experiments.

T (K)	P (Torr)	Photolysis Energy (mJ/pulse)	$[C_2H_3I]$ (10^{14} molecule/ cm^3)	Number of traces	k_1 (10^{-14} cm^3 $molecule^{-1}s^{-1}$)	k_2 (s^{-1})	k_3 (s^{-1})	b
390	25	15	2.4	9	6.5 ± 0.69	294 ± 0.4	461 ± 4.1	0.257 ± 0.002
444	25	15	2.4	9	7.4 ± 0.79	255 ± 0.4	408 ± 3.7	0.268 ± 0.002
494	4	15	2.4	8	14.2 ± 1.5	381 ± 0.8	360 ± 2.1	0.403 ± 0.001
494	25	15	2.4	9	9.5 ± 1.0	255 ± 0.4	239 ± 1.3	0.336 ± 0.001
494	25	30	1.2	6	10.0 ± 1.1	260 ± 0.4	203 ± 1.1	0.359 ± 0.001
494	100	15	2.4	9	10.9 ± 1.1	306 ± 0.4	277 ± 1.3	0.299 ± 0.001

3. *Interpretation of "b" Fit Parameter*

As shown in the main text, b is a lumped fit parameter that has the following definition.

$$b = \frac{\alpha_{n-C_6H_9}\sigma_{n-C_6H_9}(423.2\text{ nm})}{\sigma_{C_2H_3}(423.2\text{ nm})}$$

For the conditions of our absorbance experiments $\alpha_{n-C_6H_9} \approx 1$ (the title reaction proceeds entirely to $\mathrm{n-C_6H_9}$). Therefore the following should be true.

$$b = \frac{\sigma_{n-C_6H_9}}{\sigma_{C_2H_3}}(423.2\text{ nm})$$

Unfortunately, $\sigma_{n-C_6H_9}(423.2\text{ nm})$ is not known, so we cannot exactly verify the equality above. We can make the approximation, however, that the absolute absorption cross section of the allylic product, $n-\mathrm{C_6H_9}$, is similar to that of allyl radical, $\mathrm{C_3H_5}$.

$$b \approx \frac{\sigma_{C_3H_5}}{\sigma_{C_2H_3}}(423.2\text{ nm})$$

We have measured the cross sections of both vinyl and allyl radical at 423.2 nm as a function of temperature and pressure using the same approach as Ismail et al.[3] The only difference between our approaches is that we measured the path length of the Iodine Atom laser more accurately as described previously.[4] Because only the ratio of cross sections is of interest, there is a large cancellation of errors (i.e., uncertainties in path lengths and the cross section of the Iodine Atom $F = 3\ {}^2\mathrm{P}_{1/2} \leftarrow F = 4\ {}^2\mathrm{P}_{3/2}$ transition cancel out), and the uncertainty of the ratio is very small. Figure S2 compares fit b values at 25 Torr and 15 mJ pulse^{-1} photolysis energy to $\frac{\sigma_{C_3H_5}}{\sigma_{C_2H_3}}(423.2\text{ nm})$ as a function of temperature. Given the coarseness of our approximation

$\left(\sigma_{n-C_6H_9} \approx \sigma_{C_3H_5}\right)$, the agreement between the two quantities is remarkable. This agreement gives credibility to both our High-T model, as well as the conclusion that $\alpha_{n-C_6H_9} \approx 1$.

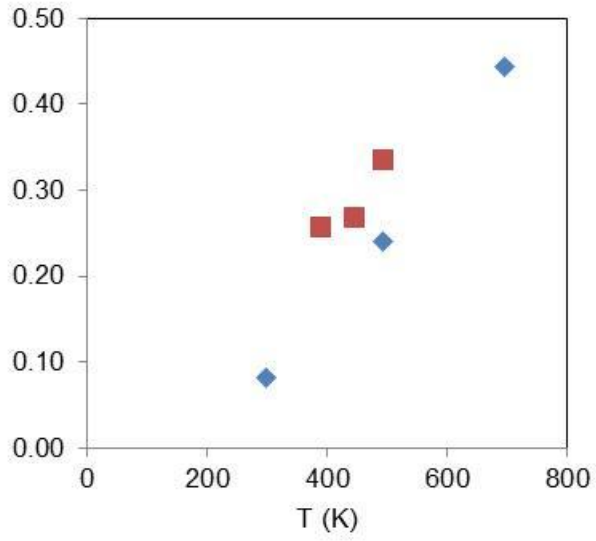

Figure S2: Comparison of fit $\boldsymbol{b}$ parameters from High-T model (red squares) and measured ratio of allyl to vinyl radical cross sections at $\boldsymbol{\lambda = 423.2\ nm}$, $\frac{\sigma_{C_3H_5}}{\sigma_{C_2H_3}}$ (blue diamonds). $\mathbf{P = 25\ Torr}$ for all measurements and all $\boldsymbol{b}$ values were obtained at a $\mathbf{15\ mJ\ pulse^{-1}}$ photolysis energy.

4. Alternative Absorbance Models

In addition to the Low-T model presented in the main text (hereafter referred to as the "Global 1st Order Model") we considered two other models, described below, to fit the absorbance decays obtained at $T < 390$ K.

a. Global 1st Order + Self-Reaction Model

The only difference between this model and the Global 1st Order Model is the inclusion of vinyl radical self-reaction:

$$2C_2H_3 \xrightarrow{k_{self}} \text{Products} \qquad \text{(R4)}$$

The time-dependent behavior of vinyl radical is then described by the following equation.

$$\frac{[\mathrm{C_2H_3}](t)}{[\mathrm{C_2H_3}]_0} = \frac{k_1[1,3-\mathrm{C_4H_6}]+k_2}{(k_1[1,3-\mathrm{C_4H_6}]+k_2+2k_{self}[\mathrm{C_2H_3}]_0)\mathrm{e}^{(k_1[1,3-\mathrm{C_4H_6}]+k_2)t}-2k_{self}[\mathrm{C_2H_3}]_0} \quad \text{(S1)}$$

The measured absorbance is related to the equation above through Eqs. 3 and 4 of the main text.

In this model, just as in the Global 1st Order Model, k_1 and k_2 are the only fit parameters. Values of k_{self} $\left(= 1.2 \times 10^{-11}\mathrm{e}^{\frac{400}{T}}\ \mathrm{cm^3\ molecule^{-1}\ s^{-1}}\right)$ are taken from the 300-700 K and 20 Torr measurements of Ismail et al.[3] $[\mathrm{C_2H_3}]_0$ was determined for each experiment using the absorbance of 423.2 nm at $t = 0$ (time of photolysis flash), A_0, the pathlength of the visible probe laser, $l_{probe}(= 2000 \pm 600\ \mathrm{cm})$, and the temperature/pressure dependent absorption cross section of the vinyl radical at this wavelength, $\sigma_{C_2H_3}(\lambda = 423.2\ nm)$ (Table S3).

$$[\mathrm{C_2H_3}]_0 = \frac{A_0}{\sigma_{C_2H_3}(\lambda=423.2\ nm)l_{probe}} \quad \text{(S2)}$$

$\sigma_{C_2H_3}(\lambda = 423.2\ nm)$ was quantified in a separate set of experiments using the same method as Ismail[3] (i.e., $[\mathrm{C_2H_3}]_0$ was initially quantified by probing the $F = 3\ ^2P_{1/2} \leftarrow F = 2\ ^2P_{3/2}$ transition of photolytically co-produced I Atom and assuming $[\mathrm{C_2H_3}]_0 = [\mathrm{I}]_0$) with the exception that the pathlength of the I Atom laser, l_I, was determined in a more precise manner.[4] Despite this difference our measurement at 297 K and 25 Torr $(0.29 \pm 0.12\ \mathrm{cm^2\ molecule^{-1}})$ and Ismail's at 293 K and 20 Torr $(0.18 \pm 0.04\ \mathrm{cm^2\ molecule^{-1}})$ have overlapping uncertainties. The major contributors to our large uncertainty are the laser pathlengths, l_{probe} and l_I, and the cross section of I atom, σ_I.

Table S3: Temperature and pressure dependent vinyl radical absorption cross section at 423.2 nm. Units are $\mathbf{10^{-18}\ cm^2\ molecule^{-1}}$.

	Temperature (K):		
Pressure (Torr):	*297*	*390*	*494*
4	0.30 ± 0.15	-	0.21 ± 0.08
25	0.29 ± 0.12	0.25 ± 0.11	0.21 ± 0.09
50	0.35 ± 0.16	-	-
100	0.52 ± 0.24	-	0.28 ± 0.15

The values of $[C_2H_3]_0$ obtained using this approach are given in Table 1 of the main text and are $\sim 1-2\times10^{12}$ molecules cm^{-3}.

Including vinyl radical self-reaction in the Global 1st Order Model had no effect on the quality of the fits to the absorbance data. Fit values of k_1 and k_2 obtained for all experiments at $T < 390$ K using this model are summarized in Figure S4 and Figure S5, respectively, and compared against the other two models considered. k_1 is unaffected by the inclusion of self-reaction in the model, while k_2 decreased from $\sim 250\ s^{-1}$ to $\sim 150\ s^{-1}$. Clearly self-reaction is a non-negligible sink of vinyl radicals in the absence of 1,3-butadiene, but because the goal of this work is to measure k_1 we chose not to include self-reaction in the Global 1st Order Model described in the main text for the sake of simplicity. We did not consider the impact of self-reaction at $T \geq 390$ K (High-T) because the negative temperature dependence of k_{self} will render this reaction even less important at higher temperatures.

b. Local 1st Order Model

In this model, absorbance traces were fit to the same first order equations as the Global 1st Order Model, but rather than fitting single "Global" values of k_1 and k_2 to all 6-9 traces at different $[1,3-C_4H_9]$, a "Local" value of $k'(=k_1[1,3-C_4H_6]+k_2)$ was fit to each decay individually. k_1 and k_2 were then extracted from the slope and intercept, respectively, of k' versus $[1,3-$

C_4H_6] (Figure S3). The resulting k_1 and k_2 values are shown in Figure S4 and Figure S5. Within the uncertainty, k_1 is the same whether a Global or Local fit is used and k_2 is also the same in almost every case. We prefer the Global fit, however, by virtue of a reduced number of fit parameters (2 as compared to x, where x is the number of traces recorded at different [1,3 − C_4H_6]), which translates into a noticeably reduced uncertainty in both k_1 and k_2.

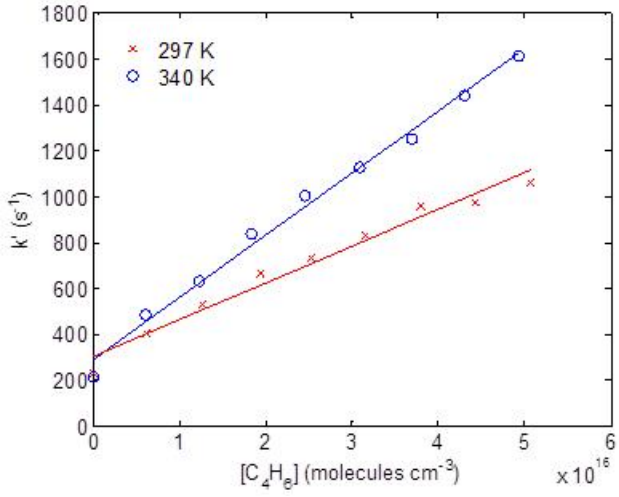

Figure S3: Representative linear dependence of local pseudo-first-order rate constants, $\boldsymbol{k'}$, on $\boldsymbol{[1,3-C_4H_6]}$.

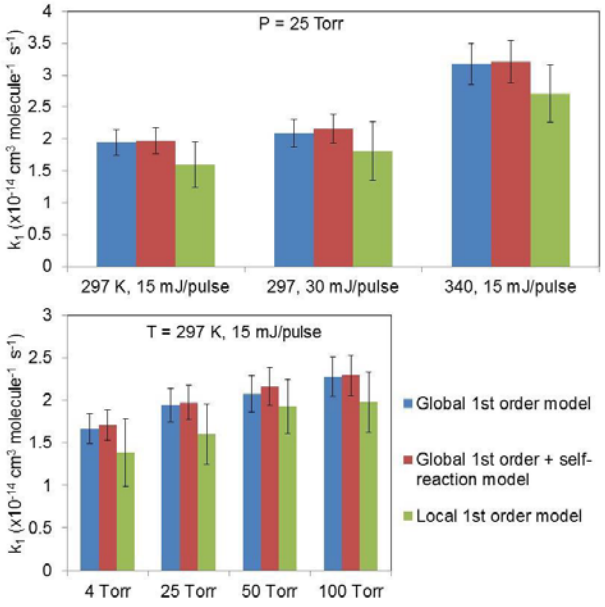

Figure S4: Comparison of fit k_1 values obtained using different models.

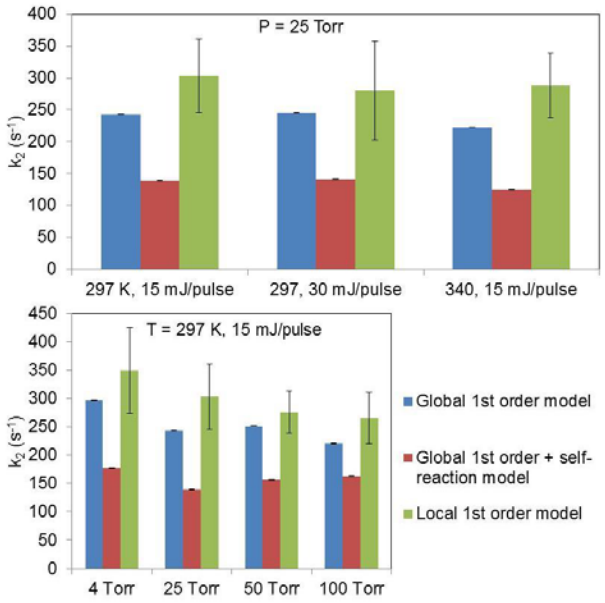

Figure S5: Comparison of fit k_2 values obtained using different models.

5. Comparison of Vinyl/Phenyl + 1,3-Butadiene/Acetylene Addition Rates

Figure S6 compares the measured temperature dependence of the vinyl + 1,3-butadiene addition rate coefficient from 297 to 494 K obtained in this work to the analogous radical addition rate

coefficients for phenyl + 1,3-butadiene, vinyl + acetylene and phenyl + acetylene over the same temperature range (all rate coefficients are in the high-pressure limit) from Ismail et al.,[5] Miller et al.[6] and Tokmakov et al.,[7] respectively. All three literature *k*'s were obtained from experiments conducted in this temperature range (or in the case of Miller et al., theoretical predictions were scaled to match experimental measurements) so this is a fair comparison without any extrapolation.

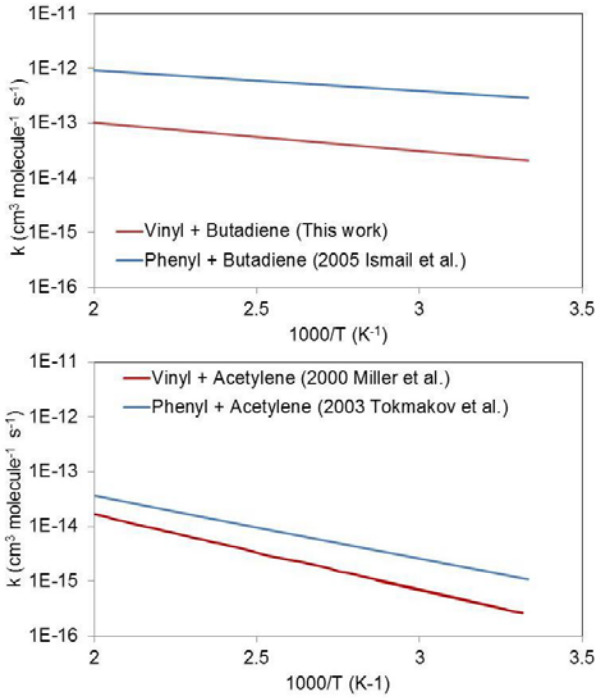

Figure S6: Arrhenius plots of vinyl + 1,3-butadiene (this work), phenyl + 1,3-butadiene,[5] vinyl + acetylene[6] and phenyl + acetylene[7] from 300 to 500 K.

6. *Summary of Photoionization Time-of-Flight Mass Spectrometry (PI TOF-MS) Experiments*

Figure S7 is representative of the full mass spectrum obtained in the presence of 1,3-C_4H_6 and C_2H_3I (helium bath gas) without photolysis (stable species only). The spectrum has been smoothed and baseline corrected. Some of the large peaks have been truncated due to signal saturation. Although relatively "soft" 10.5 eV photoionization was employed in this work, there is still significant fragmentation of species present in high concentration (i.e., 1,3-C_4H_6 and C_2H_3I). Unfortunately, large daughter ion signal at $\frac{m}{z} = 27$ amu from both 1,3-C_4H_6 and C_2H_3I obscure any small transient behavior due to vinyl radical, C_2H_3. Similarly, fragmentation of 1,3-C_4H_6 at 39 amu blocks any small propargyl radical signal from 1,3-butadiene photodissociation. The spectrum is relatively clean, however, in the range of 60-150 amu, which encompasses the observed products of C_2H_3 + 1,3-C_4H_6 (80 and 81 amu), some of the species in a calibration mixture used as an internal standard (84 and 100 amu) and I atom (127 amu). The only significant stable signals in that range are from the 1,3-butadiene dimer and its daughter ions, impurities in the vinyl iodide (THF and vinyl bromide), small fragment signals of vinyl iodide at 127 and 128 amu, and an unidentified impurity in the 1,3-butadiene at 142 amu. The presence of a small helium signal suggests other ionization sources besides 10.5 eV photoionization, but by careful alignment of the photoionization laser before every TOF-MS experiment this effect can be minimized to the acceptably low level shown in Figure S7.

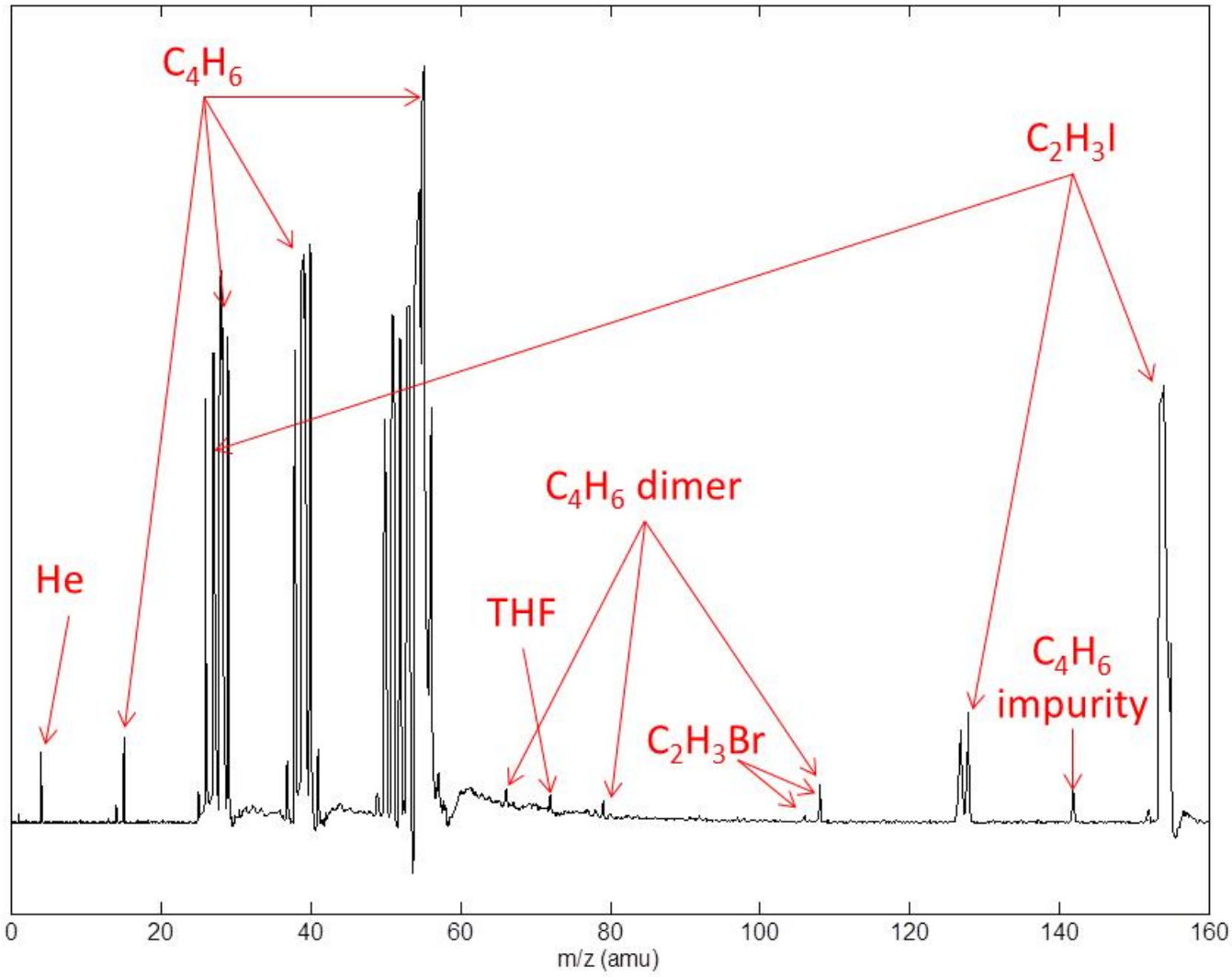

Figure S7: Representative mass spectrum of C_2H_3I and 1,3-C_4H_6 without photolysis.

Table 2 of the main text summarizes all of the PI TOF-MS experiments conducted for this work. At each T and P condition there is one "Base Case" experiment and then several "Control" experiments. The control experiments with C_2H_3 only and $1,3-C_4H_6$ only are particularly important as they displayed no transient behavior at $\frac{m}{z} = 79, 80$ or 81 amu, allowing us to identify these species as possible products of $C_2H_3 + 1,3-C_4H_6$. Figure S8 shows the transient mass spectra obtained in the 25 Torr and 297 K "Base Case" experiment. As mentioned in the main text, the signal to noise at this temperature is lower than at 500 K (Figure 6 of main text)

because of the lower production rate, and hence overall concentration, of 81 amu product. This lower signal to noise is also the reason why both a larger $[C_2H_3I]$ and photolysis power were needed at 297 K, as shown in Table 2.

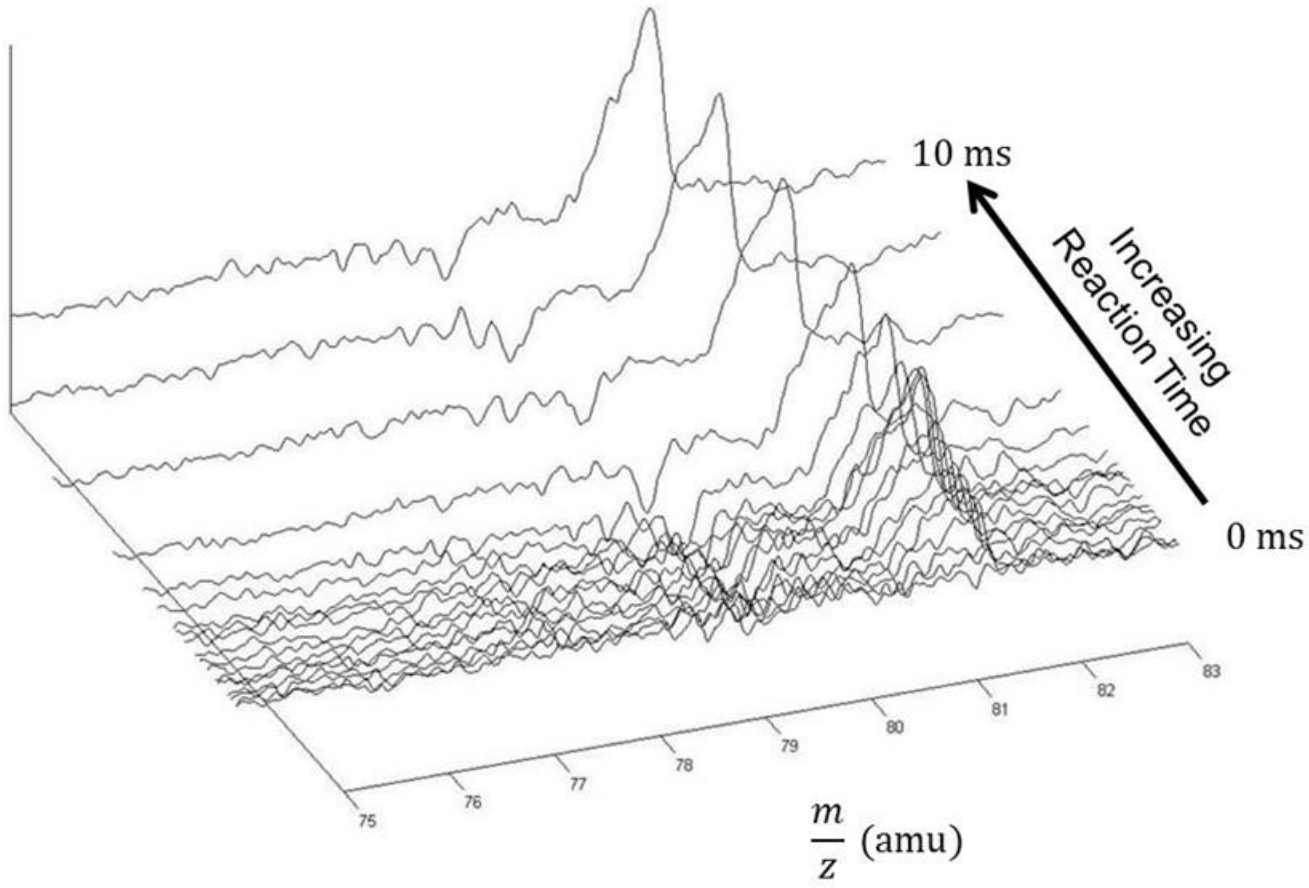

Figure S8: Transient mass spectra obtained under conditions where $\mathbf{C_2H_3 + 1,3 - C_4H_6}$ can occur (297 K, 25 Torr, $\mathbf{[C_2H_3I] = 2.5 \times 10^{14}}$ and $\mathbf{[1,3 - C_4H_6] = 1.2 \times 10^{16}\ molecules\ cm^{-3}}$, 297 K "Base Case" experiment). The spectrum acquired at a reaction time of $\mathbf{-0.20\ ms}$ was subtracted from all subsequent spectra so that only transient changes are observed. Other than the I Atom signal at $\frac{m}{z} = \mathbf{127}$ no other section of the mass spectrum displayed time-dependent behavior. The spectra were also smoothed and baseline corrected.

The purpose of the remaining control experiments at 25 Torr and 494 K was to determine if both the 79 and 81 amu species were products of the title reaction. For example, if 81 amu is a product of $C_2H_3 + 1,3 - C_4H_6$ as expected, and secondary chemistry is producing something at

79 amu, then by more than doubling the Flashes per Refresh (FPR), which has the effect of enhancing secondary chemistry, the ratio of 79 to 81 amu PI TOF-MS signal should increase noticeably. This is not what was observed, however, for any of the control experiments, as shown in Figure S9.

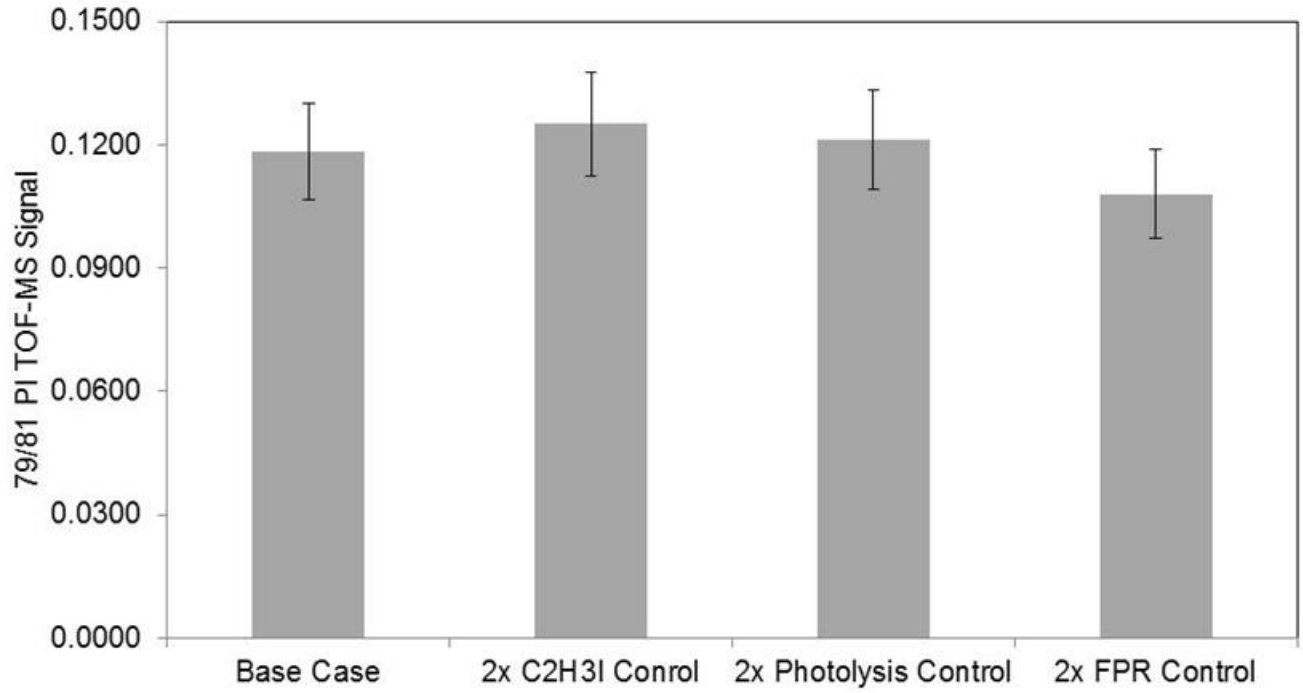

Figure S9: Ratio of steady state $\frac{m}{z} = \mathbf{79}$ to 81 amu PI TOF-MS signals (integrated peak areas) at 494 K and 25 Torr for various control experiments.

However, we did notice one significant difference between the 79 and 81 amu signals, which is that they display noticeably different time-dependence (Figure S10). This same result was obtained for all four of the 25 Torr and 494 K experiments where $C_2H_3 + 1,3 - C_4H_6$ occurs. Therefore, 79 is not from dissociative ionization of 81. From previous literature measurements, we know it is also not a daughter ion of either cyclohexadiene isomer.[8, 9] One conceivable reaction that could produce a species with a 79 amu mass is H-abstraction from cyclohexadiene.

However, the low concentration of cyclohexadiene produced from $C_2H_3 + 1{,}3 - C_4H_6$ compared to the abundance of 1,3-butadiene present makes this pathway seem unlikely.

Reaction between C_2H_3 with vinylacetylene, C_4H_4, would also produce an adduct with formula C_6H_7 and mass 79 amu. Vinylacetylene is not a large impurity in the purchased butadiene (≤ 10 ppm from Gas Chromatographic, GC, analysis), therefore it might be produced in the reactor by photodissociation of 1,3-butadiene (along with H_2 as a coproduct), as observed by Lockyear et al. and others at shorter wavelengths.[10, 11, 12] Unfortunately, we cannot discern if there is an increase in the TOF-MS signal at $\frac{m}{z} = 52$ amu (C_4H_4) following photolysis because of significant dissociative ionization of the large 1,3-butadiene signal at that $\frac{m}{z}$ value. If C_4H_4 is being formed photolytically from $1{,}3 - C_4H_6$, then based on the insensitivity of our measured k_1 to photolysis power, we can conclude that our measurement of the overall rate is unaffected by this phenomenon. Furthermore, it is not possible for $C_2H_3 + C_4H_4$ to produce species with masses 80 and 81 amu (other than ^{13}C isomers, which will have negligibly small concentrations). Therefore, our TOF-MS measurements of $\frac{m}{z} = 80$ and 81 amu would be unaffected by $C_2H_3 + C_4H_4$.

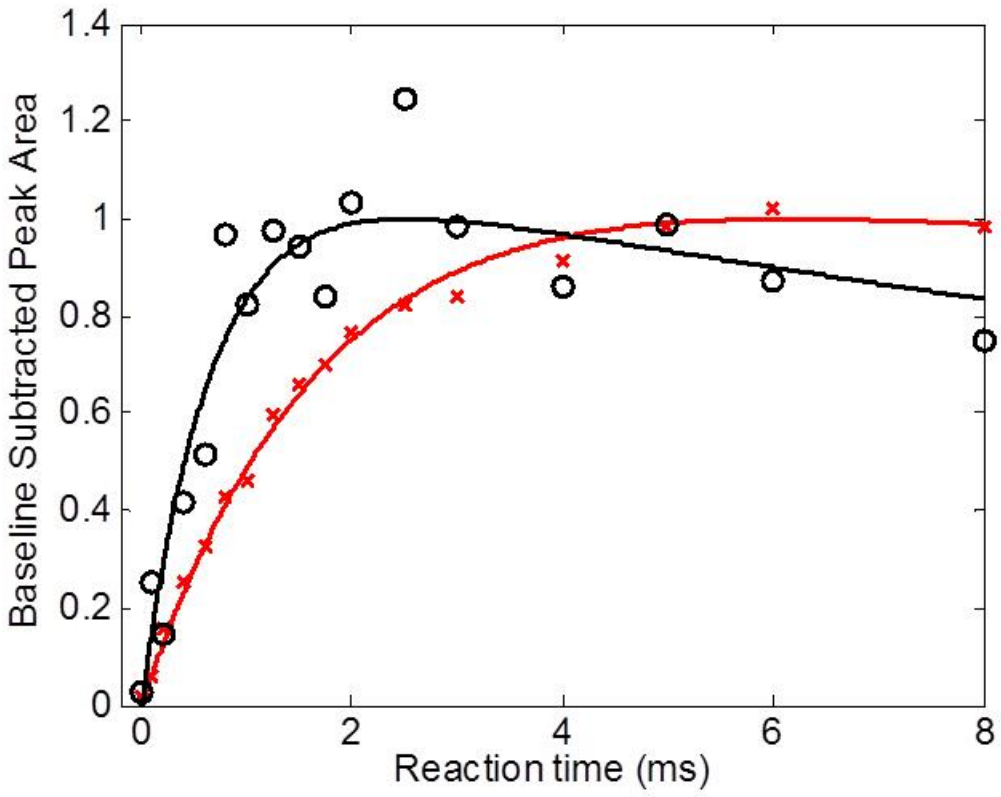

Figure S10: Comparison of time-dependent behavior for normalized $\frac{m}{z} = \mathbf{79}$ (black circles) and 81 amu (red crosses) PI TOF-MS signals in 25 Torr and 494 K "Base Case" experiment. Solid lines are biexponential fits to the data.

Further complicating our interpretation of the 79 amu species is the fact that 79 amu is a daughter ion of the butadiene dimer. Although the dimer is only ~0.1% of the purchased butadiene as confirmed by GC analysis, this low concentration of dimer in the reactor ($\sim 10^{13}$ molecules cm^{-3}) is comparable to the concentrations of radicals and products that are of interest to us ($\sim 10^{12}$ molecules cm^{-3}). Therefore, fluctuations in the dimer concentrations, as measured by the parent ion signal at 108 amu, are correlated with fluctuations in the daughter ion signal at 79 amu that are of the same magnitude as the changes in signal we are trying to observe. We attempted to minimize such fluctuations in dimer concentration by keeping the butadiene cylinder in an ice bath during experiments and verifying with TOF-MS that the 108 amu signal is stable as a function of time before beginning experiments.

We are unable to definitively identify the origin of the 79 amu species at this time. Perhaps PI TOF-MS experiments using tunable ionization energy could provide critical insight. Nonetheless, whatever side reaction is responsible for producing the species at 79 amu, will not impact the three main experimental results presented in this work:

1. Measured values of k_1.
2. Observation that at 25 Torr the dominant product of $C_2H_3 + 1,3-C_4H_6$ is $n-C_6H_9$.
3. Quantification of branching fraction to cyclohexadiene isomers at 4 Torr, assuming that 80 amu signal of cyclohexadiene is not being diverted to 79 amu either by dissociative ionization or reaction. Both of these assumptions are justified above.

The TOF-MS experiments at 700 K deserve special attention. Besides the increased propargyl absorbance, the TOF-MS data also provides evidence for enhanced 1,3-butadiene photodissociation at this elevated temperature. Table S4 summarizes the nine transient species observed in the 700 K, 4 Torr Base Case experiment. Of these nine species, only 79, 80 and 81 amu disappear when vinyl iodide is removed. The other six are present in the same amount when only $1,3-C_4H_6$ is photolyzed, suggesting that they are products of $1,3-C_4H_6$ photodissociation and subsequent reactions of the propargyl and methyl radicals. For example, the signal at 15 amu is clearly attributable to methyl radical, while that at 78 amu is likely from propargyl radical recombination. The purpose of the "No Cal Mix" control experiments will be explained in the next section.

Table S4: Summary of observations from control experiments at 700 K.

Transient Species Observed (amu):									
	15	66	69	77	78	79	80	81	91
C_2H_3 Required?	No	No	No	No	No	**Yes**	**Yes**	**Yes**	No
Cal Mix Required?	No	No	No	No	No	No	No	No	No

7. *Quantifying* $\boldsymbol{\alpha_{c-C_6H_8}}$

As discussed in the previous section, the species at $\frac{m}{z} = 80$ and 81 amu are the only clear products of $\mathrm{C_2H_3} + 1{,}3 - \mathrm{C_4H_6}$ that we observed using PI TOF-MS. Based on our predictions of the product branching, Fig. 9, we assumed that at all of the conditions of our experiment the transient 80 and 81 amu TOF-MS signals were entirely attributable to the 1,3-/1,4-cyclohexadiene isomers, $\mathrm{c-C_6H_8}$, and the linear, allylic adduct, $\mathrm{n-C_6H_9}$, respectively. Because the photoionization cross section, $\sigma_{PI}(E = 10.5\ \mathrm{eV})$, is not known for $\mathrm{n-C_6H_9}$, we cannot currently quantify the branching to this channel, which we expect to be dominant at our conditions. However, $\sigma_{PI}(E = 10.5\ \mathrm{eV})$ is known for both cyclohexadiene isomers (27.63 ± 5.5 for 1,3-[8] and 25 ± 6.3 MB for 1,4-[9]), allowing us to quantify the summed branching fraction to these channels, $\alpha_{c-C_6H_8}$. TOF-MS signal at 80 amu was only observed for experiments conducted at 4 Torr ($\mathrm{T} = 494, 599$ and 700 K), so we limit our discussion here to those experiments. This section explains the steps in experimentally quantifying $\alpha_{c-C_6H_8}$.

Reactions R1, R2 and R4 are reproduced below for convenience, with the addition of an explicit channel for $\mathrm{c-C_6H_8 + H}$ that wasn't included in the main text.

$$\mathrm{C_2H_3} + 1{,}3 - \mathrm{C_4H_6} \xrightarrow{\alpha_{n-C_6H_9} k_1} \mathrm{n-C_6H_9} \qquad \text{(R1a)}$$

$$\mathrm{C_2H_3} + 1{,}3 - \mathrm{C_4H_6} \xrightarrow{\alpha_{c-C_6H_8} k_1} \mathrm{c-C_6H_8 + H} \qquad \text{(R1b)}$$

$$\mathrm{C_2H_3} + 1{,}3 - \mathrm{C_4H_6} \xrightarrow{(1-\alpha_{n-C_6H_9}-\alpha_{c-C_6H_8})k_1} Other\ Products \quad \text{(R1c)}$$

$$\mathrm{C_2H_3} \xrightarrow{k_2} Products \quad \text{(R2)}$$

$$2\mathrm{C_2H_3} \xrightarrow{k_{self}} \mathrm{Products} \quad \text{(R4)}$$

This model includes vinyl self-reaction but ignores all other possible radical-radical reactions (i.e. cross radical reactions), which is justified by the low radical concentrations used in all experiments ($[\mathrm{C_2H_3}]_0 = 1 - 2 \times 10^{12}$ molecules $\mathrm{cm^{-3}}$ for all experiments at 4 Torr with one exception). This model also ignores $\mathrm{C_2H_3} + \mathrm{C_4H_4}$, where $\mathrm{C_4H_4}$ is derived from 1,3-butadiene photodissociation as discussed in the previous section, because $[\mathrm{C_4H_4}] \ll [\mathrm{C_4H_6}]$, at least by two orders of magnitude based on the cross section of $1{,}3 - \mathrm{C_4H_6}$ near 266 nm alone.[13] The analytical solution for the maximum amount of cyclohexadine, $[\mathrm{c} - \mathrm{C_6H_8}]_{max}$, approached as $t \to \infty$ is shown below.

$$[\mathrm{c} - \mathrm{C_6H_8}]_{max} = \frac{\alpha_{c-C_6H_8} k_1 [1{,}3-\mathrm{C_4H_6}]}{2k_{self}} \ln\left(\frac{k_1[1{,}3-\mathrm{C_4H_6}]+k_2+2k_{self}[\mathrm{C_2H_3}]_0}{k_1[1{,}3-\mathrm{C_4H_6}]+k_2}\right) \quad \text{(S2)}$$

The above can then be rearranged for the quantity of interest.

$$\alpha_{c-C_6H_8} = \frac{\frac{2k_{self}[\mathrm{c-C_6H_8}]_{max}}{k_1[1{,}3-\mathrm{C_4H_6}]}}{\ln\left(\frac{k_1[1{,}3-\mathrm{C_4H_6}]+k_2+2k_{self}[\mathrm{C_2H_3}]_0}{k_1[1{,}3-\mathrm{C_4H_6}]+k_2}\right)} \quad \text{(S3)}$$

Each term in the above equation is known experimentally. Values of k_1 are known from our experimental Arrhenius fit (Fig. 4). Based on our predictions of the overall rate, it should be possible to accurately extrapolate this simple fit to 599 and 700 K where measurements of k_1 could not be conducted due to 1,3-butadiene photodissociation. k_{self} values are taken from Ismail et al.[3] k_2 values were obtained by fits of Eq. S1 to 423.2 nm absorbance measurements of

$[C_2H_3](t)$ in the absence of $1,3-C_4H_6$. $[1,3-C_4H_6]$ is known to within 10% uncertainty from the T and P of the reactor, as well as the relative flow rates of the mass flow controllers (MFC's). $[C_2H_3]_0$ was measured by simultaneously probing the $F=3\ {}^2P_{1/2} \leftarrow F=4\ {}^2P_{3/2}$ atomic transition of I atom following the same method described by Ismail et al.[3] However, we use a different method than Ismail et al. to quantify the pathlength of the continuous wave I atom laser, l_I, as described in an earlier work.[4] Furthermore, 1,3-butadiene was used as the quenching gas to bring excited I atom back to the ground state as opposed to oxygen or ethylene. I atom is a photolytic co-product of vinyl iodide, C_2H_3I, photodissociation along with vinyl radical. Therefore, by measuring $[I]_0$ and assuming $[C_2H_3]_0 = [I]_0$ we can determine $[C_2H_3]_0 \pm 50\%$. This large error bound is primarily due to uncertainty in the pathlength of the continuous wave I atom laser, l_I, $(\pm 30\%)$ and the absolute Doppler and collision-broadened I atom cross section, σ_I $(\pm 20\%)$.[14] The only remaining quantity needed to determine $\alpha_{c-C_6H_8}$ is $[c-C_6H_8]_{max}$, which can be obtained from the TOF-MS data as explained below.

For some species i, its TOF-MS signal, S_i, is proportional to its concentration, $[i]$, as shown below.

$$S_i = FR_i\sigma_{PI,i}(E)[i] \tag{S4}$$

The proportionality constant includes the instrument response factor, F, the mass discrimination factor, R_i and the photoionization cross section of species i at ionization energy E, $\sigma_{PI,i}(E)$. In our case, a calibration gas containing nine species (propene, methylamine, 1,3-butadiene, propanol, furan, benzene, cyclohexane, toluene and heptane) was simultaneously present in the reactor during TOF-MS experiments when $C_2H_3 + 1,3-C_4H_6$ was occurring. The concentration of each calibration gas species was very small $(1.8 \pm 0.2 \times 10^{11}\ \text{molecules cm}^{-3})$ to prevent

any interference with the chemistry. Of these nine species, only two of them were suitable internal standards for this reaction because their masses did not overlap with any other large, stable signals: cyclohexane and heptane. As shown in Table 2 and Table S4, control experiments were conducted in the absence of the calibration gas mixture (referred to hereafter as "cal mix") as confirmation of two assumptions: 1.) The cal mix does not affect the measured amounts of transient species, i.e. 80 and 81 amu, and 2.) In the absence of cal mix, there is no signal at the masses of the internal standards cyclohexane (84 amu) or heptane (100 amu). The ratio between the maximum $\mathrm{c-C_6H_8}$ signal, $S_{c-C_6H_8,max}$, and the average signal for cal mix species i, $\bar{S}_{calmix,i}$, is shown below.

$$\frac{S_{c-C_6H_8,max}}{\bar{S}_{calmix,i}} = \left(\frac{FR_{c-C_6H_8}}{FR_{calmix,i}}\right)\left(\frac{\sigma_{PI,c-C_6H_8}(E=10.5\text{ eV})}{\sigma_{PI,calmix,i}(E=10.5\text{ eV})}\right)\left(\frac{[\mathrm{c-C_6H_8}]_{max}}{[\mathrm{calmix,I}]}\right) \quad \text{(S5)}$$

In this equation, F is a constant and cancels out of the ratio. Furthermore, for this apparatus we have observed the mass discrimination factor to have negligible mass dependence in our range.[15] Therefore R also cancels out and the ratio simplifies to the following.

$$\frac{S_{c-C_6H_8,max}}{\bar{S}_{calmix,i}} = \left(\frac{\sigma_{PI,c-C_6H_8}(E=10.5\text{ eV})}{\sigma_{PI,calmix,i}(E=10.5\text{ eV})}\right)\left(\frac{[\mathrm{c-C_6H_8}]_{max}}{[\mathrm{calmix,i}]}\right) \quad \text{(S6)}$$

This equation is rearranged for the quantity of interest.

$$[\mathrm{c-C_6H_8}]_{max} = [\mathrm{calmix,i}]\left(\frac{S_{c-C_6H_8,max}}{\bar{S}_{calmix,i}}\right)\left(\frac{\sigma_{PI,calmix,i}(E=10.5\text{ eV})}{\sigma_{PI,c-C_6H_8}(E=10.5\text{ eV})}\right) \quad \text{(S7)}$$

All of the terms in Eq. S7 are known experimentally. $[\mathrm{calmix,i}]$ is known from the reactor conditions. The photoionization cross sections for the internal standards cyclohexane and heptane at the relevant ionization energy are known from literature (21.3[16] and 9.9 MB[17], respectively, both with $\pm 20\%$ uncertainty). $\sigma_{PI,c-C_6H_8}(E = 10.5\text{ eV})$ is also known for both

cyclohexadiene isomers from literature, as mentioned earlier. $S_{c-C_6H_8,max}$ and $\bar{S}_{calmix,i}$ are obtained from the TOF-MS data as shown in Figure S11. $S_{c-C_6H_8,max}$ is taken as the maximum of a biexponential fit to the integrated $\frac{m}{z} = 80$ peak area as a function of reaction time and $\bar{S}_{calmix,i}$ is simply the average of the integrated cal mix species i peak area over the same reaction time. Clearly, the 80 amu signal is not at steady state because it continues to decrease after it reaches a maximum. However, the difference in time scales between the growth of 80 amu and its decay are sufficiently separated to allow us to approximate the maximum value as what the steady state value would be in the absence of any decay phenomenon. The error due to this approximation is certainly within the large error bars of our measurement reported later. We attribute this decay of what should be a chemically stable species (cyclohexadiene) to fast diffusion out of the TOF-MS sampling volume at the low pressure conditions of these experiments (4 Torr). For comparison, the growth and decay of C_6H_9 at 81 amu during the same experiment is also shown in Figure S11. From the biexponential fits to the TOF-MS signals both species have a characteristic decay rate of $40 \pm 20\ s^{-1}$ (error bounds are 95% confidence intervals of fit). The fact that both species decay at the same rate is indicative of the chemical stability of the C_6H_9 isomer (likely it is the resonantly stabilized $n - C_6H_9$ isomer), which apparently diffuses faster than it reacts at these conditions.

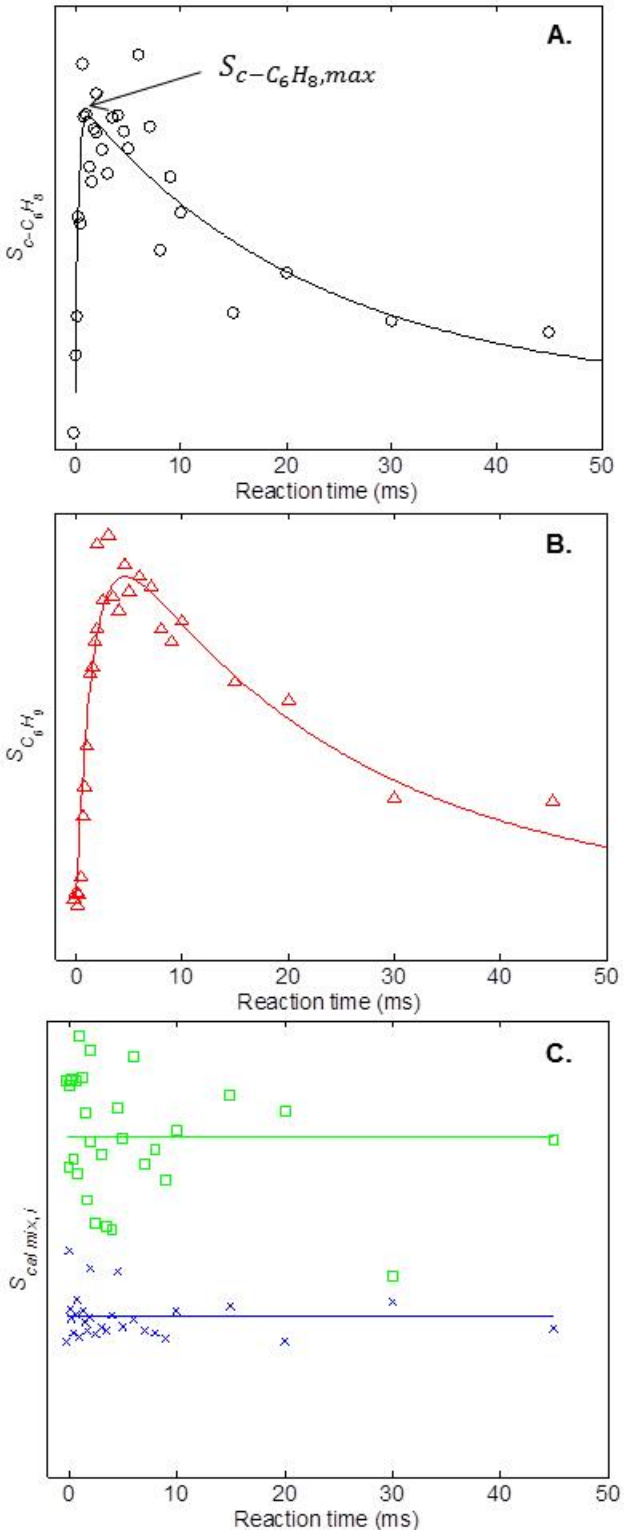

Figure S11: Simultaneously measured TOF-MS signals at 494 K and 4 Torr for A. $\frac{m}{z} = \mathbf{80\ amu}$ $(\mathbf{c-C_6H_8})$, B. $\frac{m}{z} = \mathbf{81\ amu}$ $(\mathbf{c-C_6H_9})$ and C. cyclohexane (green squares) and heptane (blue

crosses). The lines in A. and B. are biexponential fits to the data, while the lines in C. are average values, $\overline{\boldsymbol{S}}_{\boldsymbol{calmix,i}}$.

The initial concentrations of I atom and methyl radical, $[\mathrm{I}]_0$ and $[\mathrm{CH_3}]_0$, can also be quantified from their respective TOF-MS signals using an analogous form of Eq. S7 and the recently measured values of $\sigma_{PI,i}(E = 10.5\ eV)$ for both species (74^{+33}_{-23}[18] and 5.7 ± 0.67[19] MB). Their initial TOF-MS signals, $S_{I,0}$ and $S_{CH_3,0}$, were obtained by fitting an exponential decay and back-extrapolating to $t = 0$, as shown in Figure S12 and Figure S13. Back-extrapolation is necessary due to the finite rise times of both I atom and CH_3 (species that are produced essentially instantaneously by photolysis) caused by molecular beam sampling effects that have been discussed extensively elsewhere.[20, 21, 22] Transient signal at 15 amu was only observed at 700 K, where 1,3-butadiene photodissociation is more favorable compared to lower temperatures. Therefore, at all other temperatures only a conservative upper bound estimate of $[\mathrm{CH_3}]_0 < 0.3 \times 10^{12}$ molecules $\mathrm{cm^{-3}}$ could be asserted based on the sensitivity of the TOF-MS and the relatively small photoionization cross section of CH_3.

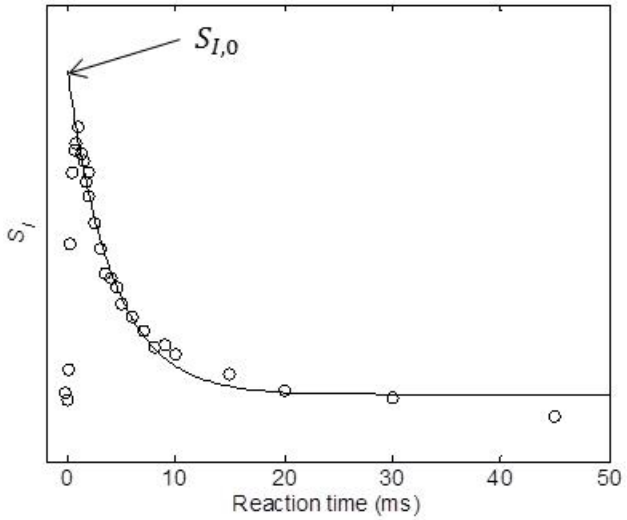

Figure S12: TOF-MS signals at 494 K and 4 Torr for $\frac{\boldsymbol{m}}{\boldsymbol{z}} = \mathbf{127\ amu}$ (I Atom). The line is an exponential fit to the decay portion of the data.

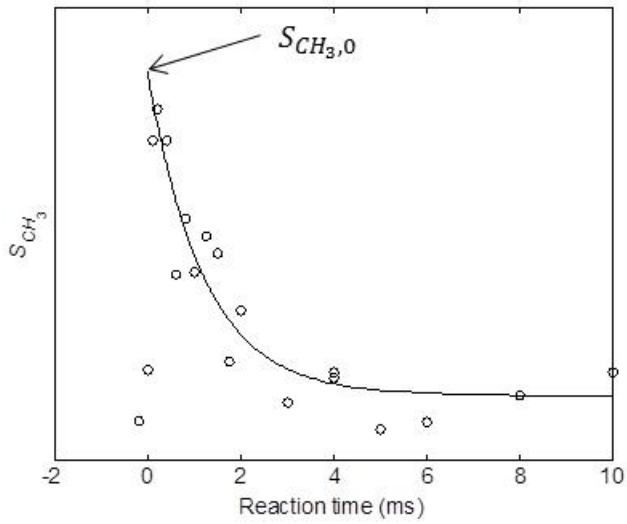

Figure S13: TOF-MS signals at 700 K and 4 Torr for $\frac{m}{z} = \mathbf{15\ amu}$ (CH_3 radical). The line is an exponential fit to the decay portion of the data.

Once $[\mathrm{c-C_6H_8}]_{max}$ is known for a given experiment, $\alpha_{c-C_6H_8}$ can be computed using Eq. S3. Table S5 summarizes the inputs to Eq. S3 (along with uncertainties) for all of the experiments to measure $\alpha_{c-C_6H_8}$ reported here, as well as the final values of $\alpha_{c-C_6H_8}$, which are plotted in Fig. 7. The final quoted error bars on $\alpha_{c-C_6H_8}$ are based on propagation of uncertainty and include the range of possible values if either the 1,3- or the 1,4-isomer is 100% dominant (because the cross sections of the two isomers are so close, this contribution to the uncertainty is very small).

Table S5: Summary of $\alpha_{c-C_6H_8}$ calculation at 4 Torr.

T (K)	PDMS coated?	[1,3-C_4H_6][1] (10^{16} molecule/ cm^3)	$x_{1,3-C_4H_6}$[2]	Photolysis Energy (mJ/pulse)	Photolysis diameter (cm)	k_1 (10^{-14} cm^3 $molecule^{-1}s^{-1}$)	k_2 (s^{-1})	$[I]_0$[3] (10^{12} molecule/ cm^3)	$[I]_0$[4] (10^{12} molecule/ cm^3)	$[CH_3]_0$[4] (10^{12} molecule/cm^3)	$[c-C_6H_8]_{max}$[4] (10^{12} molecule/ cm^3)	$\alpha_{c-C_6H_8}$
494	No	1.2	0.156	30	1.2	10.1 ± 0.2	$0-210$	1.6 ± 0.6	0.45 ± 0.2	< 0.3	0.05 ± 0.02	0.04 ± 0.02
494	Yes	1.2	0.156	30	1.2	10.1 ± 0.2	$0-194$	1.6 ± 0.8	1.3 ± 0.7	< 0.3	0.06 ± 0.03	0.04 ± 0.03
494	Yes	1.2	0.156	30	1.5	10.1 ± 0.2	$0-113$	1.2 ± 0.7	1.0 ± 0.5	< 0.3	0.04 ± 0.02	0.04 ± 0.03
494	Yes	1.2	0.156	80	1.2	10.1 ± 0.2	$0-229$	3.6 ± 1.6	3.5 ± 2.0	< 0.3	0.14 ± 0.06	0.05 ± 0.03
599	No	1.2	0.19	30	1.2	15.3 ± 0.3	$0-236$	1.9 ± 0.8	0.6 ± 0.3	< 0.3	0.12 ± 0.04	0.07 ± 0.04
700	No	1.2	0.222	30	1.2	20.4 ± 0.4	$0-530$	1.4 ± 0.7	0.4 ± 0.2	1.0 ± 0.5	0.14 ± 0.05	0.12 ± 0.08
700	No	0.6	0.111	30	1.2	20.4 ± 0.4	$0-530$	1.4 ± 0.7	0.6 ± 0.3	0.5 ± 0.3	0.09 ± 0.04	0.09 ± 0.06

[1]Uncertainty in [1,3-C_4H_6] is 10% due to uncertainty in MFC calibration

[2]Mole fraction of $1,3-C_4H_6$

[3]Obtained from simultaneous measurements of I Atom absorbance. This value of $[I]_0$ was assumed to equal $[C_2H_3]_0$ in analysis.

[4]Obtained from TOF-MS as detailed in the text

A range of k_2 values is given where the upper limit represents the value measured by the multiple-pass absorbance. This is because a large component, if not most, of the k_2 value measured using absorbance is due to diffusion of vinyl out of the probe beam area. The time scale of this diffusion will depend on the geometry of the Herriott multiple-pass alignment, which is totally unrelated to the time scale of diffusion out of the sampling region for the TOF-MS. We therefore estimate that the "real" k_2 for the TOF-MS measurement is somewhere between $0\ s^{-1}$ and the k_2 value measured by absorbance. This assumption is validated by the time scale of decay observed for transient TOF-MS signals such as $\frac{m}{z} = 80$ and 81 amu shown in Figure S11, which have decay time constants of $40\ s^{-1}$.

As expected, the branching to the chemically activated cyclohexadiene channel increases as a function of temperature. The agreement between $\alpha_{c-C_6H_8}$ values measured at 700 K and different $[1{,}3-C_4H_6]$ provides further confidence in our results and analysis. As discussed in the main text, these measurements are within the large uncertainty of the predictions. One important contributor to the prediction uncertainty is the value of $\langle \Delta E_d \rangle_{300}$, which our results suggest needs to be increased from the value recommended by Jasper et al. for methane in helium bath gas.[23] This might be partially explained by the experimental presence of a significant mole fraction of $1{,}3-C_4H_6$ (as much as 0.22) for the 4 Torr experiments, as shown in Table S5. Unfortunately, this concentration of $1{,}3-C_4H_6$ is needed to produce enough cyclohexadiene for TOF-MS detection.

To allay concerns regarding unaccounted loss of vinyl radical to the stainless steel wall of the reactor (which would cause a systematic deviation in our measured values of $\alpha_{c-C_6H_8}$) additional experiments were conducted at 500 K and 4 Torr after coating the inside of the

reactor with polydimethylsiloxane (PDMS). As shown in Table S5, coating the reactor clearly had an effect on $[I]_0$ measured using TOF-MS, bringing those values into much closer agreement with $[I]_0$ measured by I Atom absorbance. This point is most clearly illustrated by the parity plot of Figure S14. This result suggests that prior to coating the reactor, I atom was being lost to the walls. Coating with PDMS appears to have eliminated this issue.

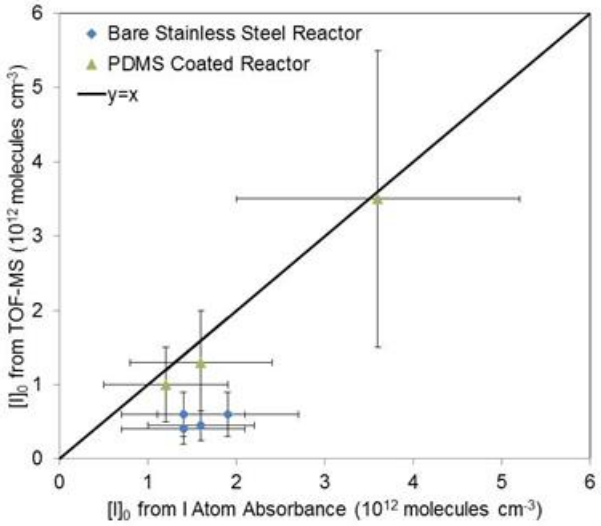

Figure S14: Parity plot of $[\mathbf{I}]_\mathbf{0}$ measured using I Atom Absorbance and TOF-MS.

Despite the dramatic increase in $[I]_0$ measured using TOF-MS, coating had no effect on the quantification of $\alpha_{c-C_6H_8}$. Furthermore, we also enlarged the photolysis beam diameter from 1.2 to 1.5 cm in order to submerge more of the TOF-MS sampling cone in the photolyzed region and to also shorten the distance between the edge of the photolyzed region and the reactor walls. Enlargement of the photolysis beam also induced no change in $\alpha_{c-C_6H_8}$. All of this suggests wall reactions are not consuming a significant portion of the vinyl radical pool, even when the reactor surface is bare stainless steel. This could be due to the unique geometry of our apparatus, where only the small tip of the sampling cone is in direct contact with the

photolyzed region, or perhaps because loss to the walls is already captured by our large range of k_2 values.

Computational Details

1. *Cantherm output showing CCSD(T)-F12a/cc-pVTZ-F12 relative energies, frequencies, and geometries of all species, as well as tables of predicted k(T,P)'s for N_2 as the bath gas*

Rate units: cm, mol, s

```
# Coordinates for C6H9 (angstroms):
#   C    0.0000    0.0000    0.0000
#   C    1.3042    0.1811    0.1858
#   H    1.8971   -0.5112    0.7793
#   H    1.8242    1.0325   -0.2539
#   C   -0.8876    0.9306   -0.7985
#   H   -0.2808    1.7530   -1.1992
#   H   -1.3085    0.3864   -1.6587
#   C   -2.0018    1.4654    0.0585
#   H   -1.8355    2.4114    0.5715
#   C   -3.1912    0.7752    0.2880
#   C   -3.5105   -0.4534   -0.2492
#   H   -2.8284   -0.9851   -0.9103
#   H   -4.4595   -0.9329   -0.0273
#   H   -3.9198    1.2452    0.9502
#   H   -0.5040   -0.8535    0.4603
conformer(
    label = 'C6H9',
    E0 = (218.314, 'kJ/mol'),
    modes = [
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        NonlinearRotor(
            inertia = ([58.9946, 268.602, 294.916], 'amu*angstrom^2'),
            symmetry = 1,
        ),
        HarmonicOscillator(
            frequencies = ([202.568, 263.498, 366.565, 414.96, 531.756, 543.896, 635.352, 719.167, 812.382, 853.211, 916.612,
943.162, 962.215, 982.275, 1002.03, 1016.07, 1090.2, 1145.17, 1167.81, 1210.74, 1263.72, 1281.06, 1379.44, 1403.56, 1408.86,
1445, 1491.17, 1677.33, 2923.07, 2977.66, 3036.53, 3045.23, 3049.53, 3060.82, 3090.01, 3124, 3151.16], 'cm^-1'),
        ),
        HinderedRotor(
            inertia = (14.5379, 'amu*angstrom^2'),
            symmetry = 1,
            fourier = (
                [
                    [-1.64932, -3.79037, -0.695719, 0.134551, 0.668662],
                    [5.96998, 0.122248, -1.21609, -0.83645, 0.0416769],
                ],
                'kJ/mol',
            ),
        ),
        HinderedRotor(
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            symmetry = 1,
            fourier = (
```

```
            [
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                [0.836835, -1.53911, 1.40528, -0.621016, -0.0196738],
            ],
            'kJ/mol',
        ),
    ),
],
spinMultiplicity = 2,
opticalIsomers = 2,
)

# Coordinates for C2H3 (angstroms):
#   C    0.0000    0.0000    0.0000
#   H    0.9087    0.5894   -0.0000
#   C   -1.2940    0.1702    0.0000
#   H   -1.9868   -0.6734   -0.0000
#   H   -1.7421    1.1707   -0.0000
conformer(
    label = 'C2H3',
    E0 = (291.328, 'kJ/mol'),
    modes = [
        IdealGasTranslation(mass=(27.0235, 'amu')),
        NonlinearRotor(
            inertia = ([2.13743, 15.509, 17.6464], 'amu*angstrom^2'),
            symmetry = 1,
        ),
        HarmonicOscillator(
            frequencies = ([678.291, 813.039, 913.725, 1009.14, 1352.92, 1634.06, 2971.51, 3059.2, 3193.55], 'cm^-1'),
        ),
    ],
    spinMultiplicity = 2,
    opticalIsomers = 1,
)

# Coordinates for C4H6 (angstroms):
#   C    0.0000    0.0000    0.0000
#   H   -0.1360    1.0836    0.0000
#   C    1.2311   -0.5167    0.0000
#   H    1.3870   -1.5952    0.0000
#   H    2.1161    0.1143    0.0000
#   C   -1.2195   -0.8107    0.0000
#   H   -1.0835   -1.8944    0.0000
#   C   -2.4506   -0.2941    0.0000
#   H   -2.6065    0.7845    0.0000
#   H   -3.3356   -0.9250    0.0000
conformer(
    label = 'C4H6',
    E0 = (106.849, 'kJ/mol'),
    modes = [
        IdealGasTranslation(mass=(54.047, 'amu')),
        NonlinearRotor(
            inertia = ([12.1052, 113.723, 125.828], 'amu*angstrom^2'),
            symmetry = 2,
        ),
        HarmonicOscillator(
            frequencies = ([278.484, 496.591, 524.584, 767.985, 875.172, 943.512, 948.137, 969.888, 993.746, 1034.58, 1191.37,
1275.58, 1276.14, 1377.53, 1430.46, 1630.83, 1690.89, 3038.9, 3042.89, 3047.46, 3051.83, 3133.21, 3133.26], 'cm^-1'),
        ),
        HinderedRotor(
            inertia = (3.39076, 'amu*angstrom^2'),
            symmetry = 1,
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            fourier = (
                [
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                    [0.00246769, 0.00106732, -0.00387952, -0.00734169, -0.00381081],
                ],
                'kJ/mol',
            ),
        ),
    ],
    spinMultiplicity = 1,
    opticalIsomers = 1,
)

# Coordinates for C6H8 (angstroms):
#   C    0.0000    0.0000    0.0000
#   C    1.1968    0.5961    0.0009
#   H    2.1206    0.0235    0.0012
#   H    1.2825    1.6823    0.0015
#   C   -1.2662    0.7240   -0.0000
#   C   -2.4694    0.1259   -0.0001
#   H   -2.5233   -0.9660   -0.0003
#   C   -3.7356    0.8500   -0.0000
#   C   -4.9324    0.2539    0.0009
#   H   -5.0181   -0.8324    0.0016
#   H   -5.8562    0.8264    0.0013
#   H   -3.6729    1.9403   -0.0006
#   H   -0.0626   -1.0903   -0.0005
#   H   -1.2123    1.8160   -0.0001
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    label = 'C6H8',
    E0 = (159.385, 'kJ/mol'),
    modes = [
        IdealGasTranslation(mass=(80.0626, 'amu')),
        NonlinearRotor(
            inertia = ([19.2207, 377.317, 396.537], 'amu*angstrom^2'),
            symmetry = 1,
        ),
        HarmonicOscillator(
            frequencies = ([101.012, 138.146, 219.379, 255.844, 332.359, 430.12, 518.819, 606.061, 701.044, 904.683, 916.405,
935.76, 945.58, 949.875, 963.419, 1008.28, 1033.55, 1124.72, 1183.28, 1235.87, 1278.26, 1286.08, 1287.06, 1396.2, 1422.19,
1621.08, 1669.61, 1690.08, 3030.52, 3032.15, 3039.26, 3040.68, 3045.72, 3046, 3132.33, 3132.35], 'cm^-1'),
        ),
    ],
    spinMultiplicity = 1,
    opticalIsomers = 2,
)

# Coordinates for H (angstroms):
conformer(
    label = 'H',
    E0 = (211.794, 'kJ/mol'),
    modes = [],
    spinMultiplicity = 2,
    opticalIsomers = 1,
)

# Coordinates for c6-C6H9 (angstroms):
#   C    0.0000    0.0000    0.0000
#   C   -1.3709    0.3102   -0.5036
#   H   -2.0873   -0.4669   -0.2108
#   H   -1.3631    0.3349   -1.6111
#   C    1.0811    1.0108   -0.2026
```

```
#   H    1.8185    0.9586    0.6148
#   H    1.6631    0.7869   -1.1199
#   C    0.5440    2.4192   -0.2997
#   H    1.2747    3.2156   -0.4445
#   C   -0.7491    2.7263   -0.1940
#   C   -1.8365    1.6945   -0.0140
#   H   -2.1220    1.6403    1.0484
#   H   -2.7380    2.0036   -0.5612
#   H   -1.0510    3.7734   -0.2380
#   H    0.2538   -0.9969    0.3528
conformer(
    label = 'c6-C6H9',
    E0 = (184.028, 'kJ/mol'),
    modes = [
        IdealGasTranslation(mass=(81.0705, 'amu')),
        NonlinearRotor(
            inertia = ([102.15, 109.428, 196.141], 'amu*angstrom^2'),
            symmetry = 1,
        ),
        HarmonicOscillator(
            frequencies = ([120.584, 197.207, 363.081, 381.559, 476.356, 515.066, 653.616, 728.417, 830.887, 877.773, 891.445,
910.79, 954.721, 986.665, 1020.86, 1029.1, 1089.5, 1135.57, 1147.6, 1172.1, 1237.95, 1298.59, 1311.62, 1344.29, 1368.24,
1387.94, 1417.23, 1430.27, 1443.37, 1696.07, 2847.41, 2864.28, 2927.86, 2928.61, 2969.51, 2982.65, 3045.47, 3067.23,
3130.56], 'cm^-1'),
        ),
    ],
    spinMultiplicity = 2,
    opticalIsomers = 2,
)

# Coordinates for c5-C6H9 (angstroms):
#   C    0.0000    0.0000    0.0000
#   C   -1.3854   -0.0024   -0.5438
#   H   -1.9593    0.9197   -0.6081
#   H   -1.8983   -0.9360   -0.7651
#   C    0.8583   -1.2295   -0.3984
#   H    0.7320   -2.0685    0.2983
#   H    0.5779   -1.5966   -1.3996
#   C    2.2628   -0.6671   -0.4159
#   H    3.1536   -1.2894   -0.4662
#   C    2.2628    0.6659   -0.4218
#   C    0.8585    1.2292   -0.4094
#   H    0.7318    2.0733    0.2809
#   H    0.5780    1.5882   -1.4133
#   H    3.1537    1.2877   -0.4780
#   H   -0.0380    0.0083    1.1071
conformer(
    label = 'c5-C6H9',
    E0 = (210.261, 'kJ/mol'),
    modes = [
        IdealGasTranslation(mass=(81.0705, 'amu')),
        NonlinearRotor(
            inertia = ([73.3366, 150.962, 209.167], 'amu*angstrom^2'),
            symmetry = 2,
        ),
        HarmonicOscillator(
            frequencies = ([108.914, 301.973, 391.232, 398.795, 552.417, 560.834, 698.574, 758.164, 828.953, 861.67, 900.823,
958.675, 966.278, 970.944, 1001.39, 1087.32, 1098.66, 1119.29, 1135.35, 1162.17, 1248.35, 1258.89, 1278.45, 1328.87,
1341.29, 1422.89, 1445.27, 1452.94, 1658, 2860.9, 2913.46, 2915.75, 2979.8, 2982.19, 3077.7, 3078.48, 3101.28, 3180.04],
'cm^-1'),
        ),
        HinderedRotor(
```

```
            inertia = (1.72227, 'amu*angstrom^2'),
            symmetry = 2,
            fourier = (
                [
                    [-0.124781, -1.12284, 0.0492952, -0.0230086, 0.0390837],
                    [0.0214983, 0.607288, -0.0754072, 0.00396834, -0.166761],
                ],
                'kJ/mol',
            ),
        ),
    ],
    spinMultiplicity = 2,
    opticalIsomers = 2,
)

# Coordinates for c5-C6H9-3 (angstroms):
#   C    0.0000    0.0000    0.0000
#   C   -1.4866    0.0006   -0.0657
#   H   -1.9109   -0.9110    0.3771
#   H   -1.9141    0.8650    0.4620
#   C    0.8525    1.2369   -0.0492
#   H    0.6554    1.8555   -0.9459
#   H    0.6802    1.9073    0.8131
#   C    2.2567    0.6698   -0.0603
#   H    3.1475    1.2934   -0.0706
#   C    2.2585   -0.6637   -0.0602
#   C    0.8559   -1.2346   -0.0493
#   H    0.6610   -1.8538   -0.9461
#   H    0.6855   -1.9055    0.8130
#   H    3.1510   -1.2848   -0.0705
#   H   -1.8568    0.0516   -1.1067
conformer(
    label = 'c5-C6H9-3',
    E0 = (181.952, 'kJ/mol'),
    modes = [
        IdealGasTranslation(mass=(81.0705, 'amu')),
        NonlinearRotor(
            inertia = ([71.2504, 159.084, 220.876], 'amu*angstrom^2'),
            symmetry = 1,
        ),
        HarmonicOscillator(
            frequencies = ([104.252, 214.056, 288.604, 385.624, 564.458, 674.448, 775.637, 799.521, 882.322, 903.789, 911.516,
957.591, 959.801, 971.508, 994.108, 1097, 1105.07, 1115.87, 1190.14, 1237.92, 1274.55, 1346.01, 1357.16, 1382.21, 1425.71,
1430.27, 1439.54, 1447.11, 1657.25, 2862.36, 2864.74, 2874.4, 2885.13, 2886.33, 2946.68, 2988.96, 3086.96, 3110.31], 'cm^-
1'),
        ),
    ],
    spinMultiplicity = 2,
    opticalIsomers = 2,
)

# Coordinates for c5-C6H9-2 (angstroms):
#   C    0.0000    0.0000    0.0000
#   C   -0.9188    1.2313   -0.2643
#   H   -1.0834    1.8204    0.6514
#   H   -0.4664    1.9191   -0.9961
#   C   -2.2097    0.6339   -0.7623
#   H   -3.0616    1.2177   -1.0990
#   C   -2.1550   -0.7519   -0.6940
#   C   -0.9214   -1.1767   -0.2215
#   H   -0.6184   -2.2104   -0.0755
#   H   -2.9703   -1.4143   -0.9744
```

```
#   H    0.3799    0.0106    1.0331
#   C    1.2025   -0.0378   -0.9585
#   H    1.8559    0.8307   -0.8020
#   H    1.7989   -0.9477   -0.8155
#   H    0.8491   -0.0215   -1.9987
conformer(
    label = 'c5-C6H9-2',
    E0 = (136.544, 'kJ/mol'),
    modes = [
        IdealGasTranslation(mass=(81.0705, 'amu')),
        NonlinearRotor(
            inertia = ([79.0879, 145.757, 193.705], 'amu*angstrom^2'),
            symmetry = 1,
        ),
        HarmonicOscillator(
            frequencies = ([56.74, 298.954, 358.792, 485.631, 626.559, 672.741, 695.653, 784.501, 813.435, 875.728, 894.193,
946.46, 972.427, 1001.94, 1021.89, 1049.26, 1077.76, 1093.4, 1172.47, 1253.48, 1266.22, 1276.16, 1292.51, 1348.56, 1361.97,
1434.5, 1451.14, 1453.46, 1465.77, 2914.99, 2925.59, 2929.14, 2947.75, 3000.79, 3008.54, 3095.24, 3117.86, 3128.91], 'cm^-
1'),
        ),
        HinderedRotor(
            inertia = (2.86432, 'amu*angstrom^2'),
            symmetry = 3,
            barrier = (15.49, 'kJ/mol'),
        ),
    ],
    spinMultiplicity = 2,
    opticalIsomers = 2,
)

# Coordinates for c5-C6H8 (angstroms):
#   C    0.0000    0.0000    0.0000
#   C   -1.3288   -0.0279    0.0000
#   H   -1.8971   -0.0401    0.9289
#   H   -1.8971   -0.0401   -0.9289
#   C    0.8874    0.0121   -1.2421
#   H    0.6839   -0.8495   -1.8946
#   H    0.7197    0.9137   -1.8504
#   C    2.2850   -0.0243   -0.6662
#   H    3.1777   -0.0432   -1.2868
#   C    2.2850   -0.0243    0.6662
#   C    0.8874    0.0121    1.2421
#   H    0.6839   -0.8495    1.8946
#   H    0.7197    0.9137    1.8504
#   H    3.1777   -0.0432    1.2868
conformer(
    label = 'c5-C6H8',
    E0 = (121.346, 'kJ/mol'),
    modes = [
        IdealGasTranslation(mass=(80.0626, 'amu')),
        NonlinearRotor(
            inertia = ([70.0597, 144.406, 208.134], 'amu*angstrom^2'),
            symmetry = 2,
        ),
        HarmonicOscillator(
            frequencies = ([44.8963, 345.459, 369.651, 428.337, 602.613, 676.725, 685.609, 775.638, 811.305, 904.427, 918.611,
922.984, 963.882, 967.575, 979.711, 983.591, 1098.23, 1132.33, 1157.88, 1230.29, 1268.1, 1269, 1347.86, 1406.9, 1429.55,
1435.05, 1662.74, 1712.06, 2928.07, 2929.85, 2955.35, 2955.61, 3039.45, 3086.93, 3109.93, 3116.33], 'cm^-1'),
        ),
    ],
    spinMultiplicity = 1,
    opticalIsomers = 2,
```

```
)

# Coordinates for C6H8-c6-13 (angstroms):
#   C    0.0000    0.0000    0.0000
#   C    0.3374    0.7040   -1.2944
#   H   -0.0501    0.1462   -2.1557
#   H    1.4369    0.7297   -1.4016
#   C   -0.0568    0.6935    1.1439
#   H   -0.2582    0.1927    2.0894
#   C    0.1847    2.1462    1.1439
#   H    0.3861    2.6470    2.0894
#   C    0.1279    2.8397    0.0000
#   C   -0.2095    2.1357   -1.2944
#   H   -1.3090    2.1100   -1.4016
#   H    0.1780    2.6935   -2.1557
#   H    0.2682    3.9199   -0.0019
#   H   -0.1402   -1.0802   -0.0019
conformer(
    label = 'C6H8-c6-13',
    E0 = (102.293, 'kJ/mol'),
    modes = [
        IdealGasTranslation(mass=(80.0626, 'amu')),
        NonlinearRotor(
            inertia = ([99.5651, 99.569, 186.411], 'amu*angstrom^2'),
            symmetry = 4,
        ),
        HarmonicOscillator(
            frequencies = ([193.858, 286.783, 452.056, 510.151, 545.936, 669.672, 731.471, 772.043, 853.571, 926.136, 948.269,
965.714, 983.877, 994.505, 1025.7, 1053.19, 1136.52, 1155.93, 1167.26, 1234.41, 1317.07, 1332.06, 1370.19, 1404.26, 1424.45,
1436.28, 1625.5, 1679.58, 2892.46, 2904.02, 2982.89, 2982.91, 3054.45, 3063.69, 3079.89, 3084.78], 'cm^-1'),
        ),
    ],
    spinMultiplicity = 1,
    opticalIsomers = 1,
)

# Coordinates for C6H8-c6-14 (angstroms):
#   C    0.0000    0.0000    0.0000
#   C   -0.8351    1.2531    0.0000
#   C   -2.1662    1.2531    0.0000
#   C   -3.0014   -0.0000    0.0000
#   C   -2.1662   -1.2531    0.0000
#   C   -0.8351   -1.2531    0.0000
#   H   -0.3006   -2.2037    0.0001
#   H   -2.7008   -2.2037    0.0001
#   H   -3.6733   -0.0000   -0.8742
#   H   -3.6734   -0.0000    0.8741
#   H   -2.7008    2.2037    0.0001
#   H   -0.3006    2.2037    0.0001
#   H    0.6720    0.0000   -0.8742
#   H    0.6720    0.0000    0.8741
conformer(
    label = 'C6H8-c6-14',
    E0 = (102.683, 'kJ/mol'),
    modes = [
        IdealGasTranslation(mass=(80.0626, 'amu')),
        NonlinearRotor(
            inertia = ([98.0355, 103.226, 195.101], 'amu*angstrom^2'),
            symmetry = 4,
        ),
        HarmonicOscillator(
```

```
        frequencies = ([114.999, 379.619, 402.156, 521.351, 557.392, 625.308, 722.123, 854.458, 888.312, 939.119, 939.316, 945.167, 967.487, 1005.46, 1026.04, 1026.87, 1146.57, 1191.66, 1193.34, 1195.38, 1330.75, 1359.61, 1388.4, 1406.21, 1432.43, 1434.98, 1689.89, 1734.87, 2901.89, 2903.59, 2918.01, 2919.48, 3039.27, 3039.31, 3060.17, 3061.9], 'cm^-1'),
      ),
   ],
   spinMultiplicity = 1,
   opticalIsomers = 1,
)

# Coordinates for C5H6 (angstroms):
#   C    0.0000    0.0000    0.0000
#   C   -0.4419    1.2705   -0.0000
#   C    0.7366    2.2075    0.0000
#   H    0.7364    2.8672    0.8822
#   C    1.9155    1.2711   -0.0000
#   C    1.4743    0.0004   -0.0000
#   H    2.0934   -0.8919   -0.0000
#   H    2.9508    1.5969   -0.0000
#   H   -1.4773    1.5957   -0.0000
#   H   -0.6187   -0.8926   -0.0000
#   H    0.7364    2.8672   -0.8822
conformer(
   label = 'C5H6',
   E0 = (130.741, 'kJ/mol'),
   modes = [
      IdealGasTranslation(mass=(66.047, 'amu')),
      NonlinearRotor(
         inertia = ([59.7268, 61.5412, 118.131], 'amu*angstrom^2'),
         symmetry = 2,
      ),
      HarmonicOscillator(
         frequencies = ([334.545, 511.107, 668.027, 718.183, 793.191, 794.422, 896.774, 916.345, 955.775, 956.346, 962.749, 993.205, 1080.76, 1100.37, 1101.16, 1242.36, 1294.55, 1366.18, 1382.65, 1537.43, 1615.67, 2927.35, 2957.2, 3104.56, 3114.58, 3133.3, 3139.05], 'cm^-1'),
      ),
   ],
   spinMultiplicity = 1,
   opticalIsomers = 1,
)

# Coordinates for CH3 (angstroms):
#   C    0.0000    0.0000    0.0000
#   H    0.2003    1.0653    0.0000
#   H   -1.0229   -0.3591    0.0000
#   H    0.8224   -0.7061    0.0000
conformer(
   label = 'CH3',
   E0 = (137.353, 'kJ/mol'),
   modes = [
      IdealGasTranslation(mass=(15.0235, 'amu')),
      NonlinearRotor(
         inertia = ([1.77622, 1.77649, 3.55271], 'amu*angstrom^2'),
         symmetry = 3,
      ),
      HarmonicOscillator(
         frequencies = ([529.26, 1359.43, 1360.54, 3059.73, 3235.37, 3246.29], 'cm^-1'),
      ),
   ],
   spinMultiplicity = 2,
   opticalIsomers = 1,
)
```

```
# Coordinates for TSadd (angstroms):
#   C    0.0000    0.0000    0.0000
#   C   -0.0185    0.0343    1.3489
#   C    2.4542   -0.1537    2.1191
#   C    3.3362    0.1352    1.1986
#   C    0.1454    1.1697   -0.8409
#   H   -0.0702   -0.9598   -0.5071
#   H   -0.1862   -0.8612    1.9328
#   H    2.4963   -0.4232    3.1663
#   H    4.4091    0.1448    1.4067
#   H    3.0430    0.3808    0.1799
#   H   -0.0061    0.9747    1.8880
#   C    0.1835    1.1438   -2.1816
#   H    0.2261    2.1260   -0.3275
#   H    0.2904    2.0501   -2.7652
#   H    0.1056    0.2114   -2.7319
conformer(
    label = 'TSadd',
    E0 = (402.694, 'kJ/mol'),
        NonlinearRotor(
            inertia = ([91.9824, 259.161, 316.375], 'amu*angstrom^2'),
            symmetry = 1,
        ),
        HarmonicOscillator(
            frequencies = ([15.4123, 49.7073, 74.4916, 150.606, 180.792, 245.955, 347.565, 372.375, 420.45, 472.866, 517.094,
624.504, 710.35, 782.072, 888.67, 937.872, 963.463, 997.731, 1065.93, 1159.21, 1212.03, 1295.23, 1429.82, 1589.89, 1708.16,
1780.84, 1952.33, 2221.53, 2297.54, 2970.37, 3086.52, 3266.93, 4016.72, 4460.25, 4681.37, 4891.36, 5507.75], 'cm^-1'),
        ),
        HinderedRotor(
            inertia = (13.1946, 'amu*angstrom^2'),
            symmetry = 1,
            fourier = (
                [
                    [-1.0687, -1.57283, -0.607636, -0.162672, -0.0106181],
                    [0.0826985, 0.275347, 0.0798759, -0.0541432, -0.105683],
                ],
                'kJ/mol',
            ),
        ),
    ],
    spinMultiplicity = 2,
    opticalIsomers = 2,
    frequency = (-175.254, 'cm^-1'),
)

# Coordinates for TS_C6H8_H-l (angstroms):
#   C    0.0000    0.0000    0.0000
#   C    1.3988    0.4142    0.1472
#   C    2.4376   -0.3879   -0.0966
#   H    3.4624   -0.0429    0.0128
#   H    2.2888   -1.4205   -0.4111
#   H    1.5684    1.4435    0.4690
#   H   -0.2422   -0.8864    1.6980
#   C   -1.0389    0.8738    0.0752
#   H   -0.8193    1.9172    0.3087
#   C   -2.4407    0.5031   -0.0898
#   C   -2.9182   -0.7374    0.0760
#   H   -2.2706   -1.5588    0.3825
#   H   -3.9720   -0.9615   -0.0675
#   H   -3.1343    1.3086   -0.3340
#   H   -0.1772   -1.0062   -0.3867
conformer(
```

```
    label = 'TS_C6H8_H-l',
    E0 = (394.735, 'kJ/mol'),
    modes = [
        IdealGasTranslation(mass=(81.0705, 'amu')),
        NonlinearRotor(
            inertia = ([41.0824, 323.008, 355.491], 'amu*angstrom^2'),
            symmetry = 1,
        ),
        HarmonicOscillator(
            frequencies = ([120.249, 142.923, 146.558, 238.094, 312.363, 361.909, 413.099, 463.177, 562.268, 621.939, 681.6,
881.536, 922.374, 936.114, 942.034, 967.408, 983.68, 1004.82, 1023.81, 1047.47, 1164.52, 1239.97, 1259.18, 1285.58, 1301.48,
1406.24, 1413.44, 1577.46, 1636.41, 1670.17, 3033.69, 3037.75, 3038.73, 3044.63, 3048.24, 3061.08, 3124.51, 3130.71], 'cm^-
1'),
        ),
    ],
    spinMultiplicity = 2,
    opticalIsomers = 2,
    frequency = (-1102.45, 'cm^-1'),
)

# Coordinates for TSendo (angstroms):
#   C    0.0000    0.0000    0.0000
#   C   -0.6537    0.9438    0.7405
#   H   -0.3799    1.9932    0.6429
#   H   -1.1882    0.6685    1.6477
#   C   -0.4067   -1.4539    0.0254
#   H   -0.1889   -1.9065   -0.9551
#   H    0.2057   -2.0186    0.7476
#   C   -1.8663   -1.6557    0.3752
#   H   -2.1405   -2.6259    0.7881
#   C   -2.8179   -0.7093    0.2632
#   C   -2.6060    0.6383   -0.2516
#   H   -2.1971    0.7794   -1.2488
#   H   -3.2995    1.4190    0.0657
#   H   -3.8094   -0.9387    0.6610
#   H    0.6893    0.3217   -0.7807
conformer(
    label = 'TSendo',
    E0 = (308.261, 'kJ/mol'),
    modes = [
        IdealGasTranslation(mass=(81.0705, 'amu')),
        NonlinearRotor(
            inertia = ([106.776, 121.502, 198.713], 'amu*angstrom^2'),
            symmetry = 1,
        ),
        HarmonicOscillator(
            frequencies = ([108.508, 288.113, 348.808, 403.998, 453.011, 592.871, 620.117, 669.101, 745.093, 793.989, 861.52,
909.51, 937.818, 941.985, 948.673, 976.539, 999.154, 1059.48, 1075.14, 1181.01, 1204.01, 1249.07, 1313.36, 1365.7, 1388.75,
1423.59, 1444.06, 1527.62, 1610.56, 2914.76, 2942.23, 3027.35, 3041.61, 3044.22, 3071.61, 3072.59, 3125.71, 3132.49], 'cm^-
1'),
        ),
    ],
    spinMultiplicity = 2,
    opticalIsomers = 2,
    frequency = (-664.284, 'cm^-1'),
)

# Coordinates for TSexo (angstroms):
#   C    0.0000    0.0000    0.0000
#   C   -1.2147    0.3025   -0.5405
#   H   -1.9080    0.9749   -0.0409
#   H   -1.4968   -0.0664   -1.5262
```

```
#   C    0.8811   -1.1175   -0.5341
#   H    0.6935   -2.0366    0.0405
#   H    0.6007   -1.3421   -1.5768
#   C    2.3336   -0.7179   -0.4342
#   H    3.1141   -1.4742   -0.3708
#   C    2.6002    0.5902   -0.4126
#   C    1.4794    1.5332   -0.5758
#   H    1.3755    2.3726    0.1130
#   H    1.1116    1.7254   -1.5836
#   H    3.6193    0.9608   -0.2770
#   H    0.1847    0.2674    1.0436
conformer(
    label = 'TSexo',
    E0 = (303.489, 'kJ/mol'),
    modes = [
        IdealGasTranslation(mass=(81.0705, 'amu')),
        NonlinearRotor(
            inertia = ([82.0832, 162.673, 225.771], 'amu*angstrom^2'),
            symmetry = 1,
        ),
        HarmonicOscillator(
            frequencies = ([74.1508, 243.827, 342.957, 363.101, 429.273, 530.068, 544.774, 660.896, 713.958, 786.227, 841.387, 873.271, 893.237, 946.693, 973.554, 978.381, 1009.42, 1043.04, 1087.25, 1142.95, 1184.94, 1235.02, 1286.67, 1349.07, 1393.61, 1422.47, 1432.85, 1529.75, 1651.39, 2917.44, 2953.77, 3017.41, 3024.77, 3037.44, 3043.78, 3077.53, 3120.99, 3134.98], 'cm^-1'),
        ),
    ],
    spinMultiplicity = 2,
    opticalIsomers = 2,
    frequency = (-649.864, 'cm^-1'),
)

# Coordinates for TS_C6H8_H (angstroms):
#   C    0.0000    0.0000    0.0000
#   C   -0.8867    1.2403    0.1406
#   C   -2.2350    1.2403    0.1015
#   H   -2.7998    2.1707    0.1137
#   H   -2.7998    0.3100    0.1137
#   C   -0.0000    2.4807   -0.0001
#   C    1.3920    1.9071    0.1491
#   C    1.3920    0.5736    0.1490
#   H    2.2817   -0.0475    0.2182
#   H    2.2817    2.5282    0.2184
#   H   -0.2362    3.2504    0.7458
#   H   -0.1320    2.9395   -0.9931
#   H   -0.2361   -0.7697    0.7460
#   H   -0.1321   -0.4590   -0.9930
#   H   -0.6000    1.2404    1.9580
conformer(
    label = 'TS_C6H8_H',
    E0 = (352.7, 'kJ/mol'),
    modes = [
        IdealGasTranslation(mass=(81.0705, 'amu')),
        NonlinearRotor(
            inertia = ([73.7116, 149.245, 208.818], 'amu*angstrom^2'),
            symmetry = 1,
        ),
        HarmonicOscillator(
            frequencies = ([132.315, 330.763, 372.97, 460.862, 489.909, 567.232, 607.312, 625.376, 685.757, 772.437, 814.733, 881.959, 896.714, 918.434, 961.587, 964.955, 975.968, 976.332, 1099.17, 1132.38, 1152.43, 1226.31, 1265.86, 1266.39, 1345.23, 1399.64, 1429.19, 1435.97, 1608.21, 1659.5, 2925.99, 2926.23, 2979.66, 2980.42, 3046.09, 3083.24, 3105.82, 3130.44], 'cm^-1'),
```

```
        ),
    ],
    spinMultiplicity = 2,
    opticalIsomers = 2,
    frequency = (-1106.37, 'cm^-1'),
)

# Coordinates for TS_C6H8_H-c6-13 (angstroms):
#   C    0.0000    0.0000    0.0000
#   C   -1.4265   -0.0987   -0.4744
#   C   -2.1980    1.0158   -0.4922
#   H   -3.2186    0.9760   -0.8693
#   C   -1.5846    2.3394   -0.2458
#   H   -2.2395    3.1949   -0.0924
#   C   -0.2552    2.4828   -0.2486
#   C    0.6526    1.2989   -0.4915
#   H    0.8635    1.2296   -1.5731
#   H    1.6192    1.4466    0.0063
#   H    0.1897    3.4686   -0.1192
#   H   -1.8548   -1.0718   -0.7080
#   H    0.5839   -0.8722   -0.3171
#   H   -0.0036   -0.0022    1.1063
#   H   -3.0073    0.9706    1.2216
conformer(
    label = 'TS_C6H8_H-c6-13',
    E0 = (326.835, 'kJ/mol'),
    modes = [
        IdealGasTranslation(mass=(81.0705, 'amu')),
        NonlinearRotor(
            inertia = ([102.525, 107.414, 191.987], 'amu*angstrom^2'),
            symmetry = 1,
        ),
        HarmonicOscillator(
            frequencies = ([187.603, 251.283, 322.735, 395.399, 459.759, 535.101, 549.177, 689.067, 742.188, 763.562, 852.646,
928.136, 940.793, 971.033, 986.182, 990.161, 1022.83, 1052.09, 1130.94, 1152.47, 1159.51, 1233.01, 1313.81, 1326.96,
1369.06, 1399.15, 1425.48, 1436.66, 1563.19, 1668.88, 2888.87, 2906.44, 2978.21, 2989.42, 3063.92, 3071.21, 3086.31,
3092.03], 'cm^-1'),
        ),
    ],
    spinMultiplicity = 2,
    opticalIsomers = 2,
    frequency = (-1116.88, 'cm^-1'),
)

# Coordinates for TS_C6H8_H-c6-14 (angstroms):
#   C    0.0000    0.0000    0.0000
#   C   -1.3079   -0.3245   -0.0658
#   C   -2.4130    0.6886    0.0096
#   H   -3.0779    0.5862   -0.8647
#   H   -3.0554    0.4665    0.8793
#   C   -1.9047    2.1030    0.1014
#   H   -2.6521    2.8894    0.2079
#   C   -0.6152    2.4298    0.0515
#   C    0.4964    1.4252   -0.0938
#   H    0.9992    1.5659   -1.0656
#   H    1.2704    1.6089    0.6662
#   H   -0.3270    3.4795    0.1130
#   H   -1.5939   -1.3759   -0.0995
#   H    0.7446   -0.7894   -0.1024
#   H    0.2667   -0.1369    1.8637
conformer(
    label = 'TS_C6H8_H-c6-14',
```

```
    E0 = (327.396, 'kJ/mol'),
    modes = [
        IdealGasTranslation(mass=(81.0705, 'amu')),
        NonlinearRotor(
            inertia = ([103.527, 108.342, 197.975], 'amu*angstrom^2'),
            symmetry = 1,
        ),
        HarmonicOscillator(
            frequencies = ([103.248, 239.069, 384.091, 454.44, 476.001, 527.507, 559.785, 641.846, 737.844, 851.286, 885.643,
924.777, 934.992, 953.844, 961.045, 1001.99, 1018.72, 1029.19, 1140.48, 1184.94, 1187.54, 1189.65, 1327, 1354.87, 1384.9,
1401.39, 1427.26, 1434.51, 1612.25, 1712.48, 2897.76, 2906.88, 2923.53, 2944.96, 3048.42, 3049.4, 3069.4, 3070.76], 'cm^-1'),
        ),
    ],
    spinMultiplicity = 2,
    opticalIsomers = 2,
    frequency = (-1053.28, 'cm^-1'),
)

# Coordinates for TS1 (angstroms):
#   C    0.0000    0.0000    0.0000
#   C   -1.4696    0.0002   -0.1664
#   H   -1.9884    0.9385   -0.3371
#   H   -1.9885   -0.9373   -0.3410
#   C    0.8543   -1.2403   -0.1596
#   H    0.6737   -2.0014    0.6153
#   H    0.6701   -1.7394   -1.1307
#   C    2.2552   -0.6659   -0.1025
#   H    3.1472   -1.2876   -0.0899
#   C    2.2549    0.6672   -0.1023
#   C    0.8537    1.2408   -0.1598
#   H    0.6722    2.0022    0.6146
#   H    0.6693    1.7391   -1.1313
#   H    3.1466    1.2892   -0.0897
#   H   -0.8324   -0.0008    0.9851
conformer(
    label = 'TS1',
    E0 = (357.417, 'kJ/mol'),
    modes = [
        IdealGasTranslation(mass=(81.0705, 'amu')),
        NonlinearRotor(
            inertia = ([71.6079, 154.453, 216.624], 'amu*angstrom^2'),
            symmetry = 1,
        ),
        HarmonicOscillator(
            frequencies = ([119.569, 287.029, 348.335, 372.419, 395.94, 569.911, 679.069, 703.881, 770.349, 807.326, 887.081,
913.568, 952.387, 957.863, 973.515, 975.485, 1098.13, 1120.23, 1139.67, 1197.5, 1223.93, 1245.31, 1276.14, 1345.2, 1355.95,
1396.57, 1439.09, 1451.84, 1659.32, 2181.61, 2870.51, 2874.65, 2928.93, 2929.26, 3068.87, 3087.49, 3110.68, 3181.07], 'cm^-
1'),
        ),
    ],
    spinMultiplicity = 2,
    opticalIsomers = 2,
    frequency = (-1814.78, 'cm^-1'),
)

# Coordinates for TS2 (angstroms):
#   C    0.0000    0.0000    0.0000
#   C   -1.4685    0.0094   -0.2722
#   H   -1.9949   -0.7812    0.2781
#   H   -1.9206    0.9717    0.0008
#   C    0.8776    1.2035   -0.1212
#   H    0.5089    2.1851   -0.4031
```

```
#   H    0.4246    0.8313    0.9971
#   C    2.2445    0.7195   -0.2468
#   H    3.1118    1.3702   -0.3085
#   C    2.2783   -0.6307   -0.2196
#   C    0.8860   -1.2222   -0.1174
#   H    0.6198   -1.8101   -1.0233
#   H    0.7757   -1.9272    0.7249
#   H    3.1803   -1.2348   -0.2498
#   H   -1.6658   -0.1499   -1.3482
conformer(
    label = 'TS2',
    E0 = (327.931, 'kJ/mol'),
    modes = [
        IdealGasTranslation(mass=(81.0705, 'amu')),
        NonlinearRotor(
            inertia = ([69.1107, 158.734, 217.342], 'amu*angstrom^2'),
            symmetry = 1,
        ),
        HarmonicOscillator(
            frequencies = ([159.274, 182.097, 283.7, 313.22, 482.896, 569.458, 667.722, 765.266, 793.23, 827.223, 899.147, 912.199, 930.904, 970.284, 1002.12, 1015.33, 1093.25, 1110.8, 1144.15, 1216.22, 1222.88, 1274.06, 1347.24, 1361.81, 1392.07, 1426.25, 1437.87, 1452.19, 1557.77, 2162.49, 2802.8, 2880.65, 2894.69, 2961.87, 3001.07, 3099.49, 3116.79, 3126.42], 'cm^-1'),
        ),
    ],
    spinMultiplicity = 2,
    opticalIsomers = 2,
    frequency = (-1798.49, 'cm^-1'),
)

# Coordinates for TS_C5H6_CH3-c5-2 (angstroms):
#   C    0.0000    0.0000    0.0000
#   C   -0.6930   -1.2709    0.4436
#   H   -1.1734   -1.7454   -0.4306
#   H   -0.0253   -2.0223    0.8842
#   C   -1.7479   -0.7624    1.3913
#   H   -2.4048   -1.4023    1.9717
#   C   -1.7664    0.5892    1.3558
#   C   -0.7287    1.0702    0.4541
#   H   -0.5364    2.1137    0.2239
#   H   -2.4484    1.2285    1.9093
#   H    0.7305    0.0304   -0.8020
#   C    1.7013   -0.0984    1.5889
#   H    0.9939   -0.2741    2.3969
#   H    2.1585    0.8847    1.5220
#   H    2.2766   -0.9451    1.2206
conformer(
    label = 'TS_C5H6_CH3-c5-2',
    E0 = (298.047, 'kJ/mol'),
    modes = [
        IdealGasTranslation(mass=(81.0705, 'amu')),
        NonlinearRotor(
            inertia = ([96.362, 162.736, 187.578], 'amu*angstrom^2'),
            symmetry = 1,
        ),
        HarmonicOscillator(
            frequencies = ([112.897, 180.333, 362.895, 443.283, 493.801, 498.571, 673.616, 716.723, 771.199, 789.296, 799.092, 877.798, 901.463, 925.001, 953.794, 962.536, 1007.84, 1069.36, 1090.74, 1098.79, 1247.24, 1291.34, 1359.49, 1372.61, 1376.51, 1393.49, 1434.01, 1570.38, 2922.24, 2989.65, 3014.46, 3101.72, 3110.08, 3122.62, 3131.89, 3174.8, 3189.65], 'cm^-1'),
        ),
        HinderedRotor(
```

```
            inertia = (2.94805, 'amu*angstrom^2'),
            symmetry = 3,
            fourier = (
                [
                    [-0.0572817, -0.0475977, -2.29159, 0.0320211, -0.0162698],
                    [-0.0550576, 0.0166946, -0.0873755, 0.0751546, -0.00257136],
                ],
                'kJ/mol',
            ),
        ),
    ],
    spinMultiplicity = 2,
    opticalIsomers = 2,
    frequency = (-738.967, 'cm^-1'),
)

# Coordinates for TS_C5H6_CH3-c5 (angstroms):
#   C    0.0000    0.0000    0.0000
#   C   -1.1531    0.9814    0.3152
#   C   -2.2443    0.0803    0.8538
#   C   -1.9475   -1.2236    0.7078
#   C   -0.6071   -1.4130    0.1469
#   H   -1.4968    1.5220   -0.5793
#   H   -0.8386    1.7436    1.0434
#   H   -3.1670    0.4606    1.2858
#   H   -2.5905   -2.0454    1.0133
#   H   -0.3742   -2.2024   -0.5690
#   H    0.3047   -1.5371    1.1574
#   H    0.4971    0.2061   -0.9519
#   C    0.9630   -0.2467    1.1551
#   H    2.0185   -0.4053    0.9361
#   H    0.7276    0.2176    2.1149
conformer(
    label = 'TS_C5H6_CH3-c5',
    E0 = (339.761, 'kJ/mol'),
    modes = [
        IdealGasTranslation(mass=(81.0705, 'amu')),
        NonlinearRotor(
            inertia = ([85.4147, 131.463, 175.181], 'amu*angstrom^2'),
            symmetry = 1,
        ),
        HarmonicOscillator(
            frequencies = ([140.579, 323.769, 364.844, 445.466, 597.747, 677.434, 703.142, 775.697, 835.379, 859.087, 892.085,
902.674, 910.189, 944.507, 964.354, 1004.34, 1060.13, 1062.22, 1094.2, 1160.05, 1196.04, 1239.66, 1275.69, 1283.26, 1292.8,
1354.25, 1381.47, 1445.69, 1584.73, 1736.93, 2928.44, 2957.97, 3002.53, 3015.23, 3063.56, 3082.12, 3103.71, 3125.66], 'cm^-
1'),
        ),
    ],
    spinMultiplicity = 2,
    opticalIsomers = 2,
    frequency = (-2105, 'cm^-1'),
)

#  ======= =========== =========== ========== ===============
#  Temp.   k (TST)     Tunneling   k (TST+T)   Units
#  ======= =========== =========== ========== ===============
#    300 K   1.688e+10           1   1.688e+10 cm^3/(mol*s)
#    400 K   4.209e+10           1   4.209e+10 cm^3/(mol*s)
#    500 K   8.088e+10           1   8.088e+10 cm^3/(mol*s)
#    600 K   1.337e+11           1   1.337e+11 cm^3/(mol*s)
#    800 K   2.837e+11           1   2.837e+11 cm^3/(mol*s)
#   1000 K   5.011e+11           1   5.011e+11 cm^3/(mol*s)
```

```
#    1500 K   1.428e+12          1   1.428e+12 cm^3/(mol*s)
#    2000 K   3.107e+12          1   3.107e+12 cm^3/(mol*s)
#   ======= =========== =========== ========== ===============
kinetics(
    label = 'C2H3 + C4H6 = C6H9',
    kinetics = Arrhenius(
        A = (39134.6, 'cm^3/(mol*s)'),
        n = 2.40428,
        Ea = (1.75909, 'kJ/mol'),
        T0 = (1, 'K'),
        Tmin = (303.03, 'K'),
        Tmax = (2500, 'K'),
        comment = 'Fitted to 59 data points; dA = *|/ 1.18629, dn = +|- 0.0224198, dEa = +|- 0.123331 kJ/mol',
    ),
)

#   ======= =========== =========== ========== ===============
#   Temp.   k (TST)     Tunneling   k (TST+T)   Units
#   ======= =========== =========== ========== ===============
#     300 K   1.748e-19     3.37806   5.904e-19 s^-1
#     400 K   1.228e-11     1.94073   2.384e-11 s^-1
#     500 K   6.820e-07     1.52317   1.039e-06 s^-1
#     600 K   1.049e-03     1.33946   1.405e-03 s^-1
#     800 K   1.113e+01     1.18042   1.314e+01 s^-1
#    1000 K   3.137e+03     1.11346   3.493e+03 s^-1
#    1500 K   6.791e+06     1.05054   7.134e+06 s^-1
#    2000 K   3.539e+08     1.02899   3.642e+08 s^-1
#   ======= =========== =========== ========== ===============
kinetics(
    label = 'C6H9 = C6H8 + H',
    kinetics = Arrhenius(
        A = (2.28967e+06, 's^-1'),
        n = 2.0172,
        Ea = (170.136, 'kJ/mol'),
        T0 = (1, 'K'),
        Tmin = (303.03, 'K'),
        Tmax = (2500, 'K'),
        comment = 'Fitted to 59 data points; dA = *|/ 1.28199, dn = +|- 0.0326017, dEa = +|- 0.179342 kJ/mol',
    ),
)

#   ======= =========== =========== ========== ===============
#   Temp.   k (TST)     Tunneling   k (TST+T)   Units
#   ======= =========== =========== ========== ===============
#     300 K   3.022e-05     1.59243   4.812e-05 s^-1
#     400 K   2.252e-01     1.28929   2.904e-01 s^-1
#     500 K   4.728e+01     1.17509   5.556e+01 s^-1
#     600 K   1.680e+03     1.11852   1.879e+03 s^-1
#     800 K   1.491e+05     1.06555   1.589e+05 s^-1
#    1000 K   2.262e+06     1.04196   2.357e+06 s^-1
#    1500 K   9.184e+07     1.01906   9.359e+07 s^-1
#    2000 K   6.281e+08     1.01105   6.350e+08 s^-1
#   ======= =========== =========== ========== ===============
kinetics(
    label = 'C6H9 = c6-C6H9',
    kinetics = Arrhenius(
        A = (5.04053e+08, 's^-1'),
        n = 0.699681,
        Ea = (84.7108, 'kJ/mol'),
        T0 = (1, 'K'),
        Tmin = (303.03, 'K'),
        Tmax = (2500, 'K'),
```

```
        comment = 'Fitted to 59 data points; dA = *|/ 1.05522, dn = +|- 0.00705411, dEa = +|- 0.0388047 kJ/mol',
    ),
)

#  ======= =========== =========== ========== ===============
#  Temp.   k (TST)     Tunneling   k (TST+T)   Units
#  ======= =========== =========== ========== ===============
#    300 K   3.670e-04     1.5593   5.723e-04 s^-1
#    400 K   1.871e+00    1.27595   2.387e+00 s^-1
#    500 K   3.180e+02    1.16785   3.714e+02 s^-1
#    600 K   9.903e+03    1.11399   1.103e+04 s^-1
#    800 K   7.544e+05    1.06332   8.022e+05 s^-1
#   1000 K   1.052e+07    1.04068   1.095e+07 s^-1
#   1500 K   3.854e+08    1.01861   3.925e+08 s^-1
#   2000 K   2.515e+09    1.01085   2.543e+09 s^-1
#  ======= =========== =========== ========== ===============
kinetics(
    label = 'C6H9 = c5-C6H9',
    kinetics = Arrhenius(
        A = (5.24904e+08, 's^-1'),
        n = 0.846103,
        Ea = (80.7435, 'kJ/mol'),
        T0 = (1, 'K'),
        Tmin = (303.03, 'K'),
        Tmax = (2500, 'K'),
        comment = 'Fitted to 59 data points; dA = *|/ 1.02085, dn = +|- 0.00270819, dEa = +|- 0.0148978 kJ/mol',
    ),
)

#  ======= =========== =========== ========== ===============
#  Temp.   k (TST)     Tunneling   k (TST+T)   Units
#  ======= =========== =========== ========== ===============
#    300 K   5.627e-13     3.23882   1.823e-12 s^-1
#    400 K   1.087e-06     1.91807   2.084e-06 s^-1
#    500 K   6.932e-03     1.51745   1.052e-02 s^-1
#    600 K   2.513e+00     1.33817   3.363e+00 s^-1
#    800 K   4.355e+03     1.18126   5.145e+03 s^-1
#   1000 K   4.106e+05     1.11461   4.576e+05 s^-1
#   1500 K   2.008e+08     1.05156   2.112e+08 s^-1
#   2000 K   4.834e+09      1.0298   4.978e+09 s^-1
#  ======= =========== =========== ========== ===============
kinetics(
    label = 'c5-C6H9 = c5-C6H8 + H',
    kinetics = Arrhenius(
        A = (1.972e+07, 's^-1'),
        n = 1.80161,
        Ea = (135.161, 'kJ/mol'),
        T0 = (1, 'K'),
        Tmin = (303.03, 'K'),
        Tmax = (2500, 'K'),
        comment = 'Fitted to 59 data points; dA = *|/ 1.30856, dn = +|- 0.0352944, dEa = +|- 0.194155 kJ/mol',
    ),
)

#  ======= =========== =========== ========== ===============
#  Temp.   k (TST)     Tunneling   k (TST+T)   Units
#  ======= =========== =========== ========== ===============
#    300 K   6.025e-13     2.80928   1.693e-12 s^-1
#    400 K   1.350e-06     1.80869   2.442e-06 s^-1
#    500 K   9.393e-03     1.47054   1.381e-02 s^-1
#    600 K   3.589e+00     1.31211   4.709e+00 s^-1
#    800 K   6.540e+03     1.16925   7.647e+03 s^-1
```

```
#    1000 K   6.245e+05     1.10728   6.915e+05 s^-1
#    1500 K   2.967e+08     1.04797   3.110e+08 s^-1
#    2000 K   6.762e+09      1.0274   6.947e+09 s^-1
#   ======= =========== =========== =========== ===============
kinetics(
    label = 'c6-C6H9 = C6H8-c6-13 + H',
    kinetics = Arrhenius(
        A = (7.48689e+08, 's^-1'),
        n = 1.39467,
        Ea = (138.623, 'kJ/mol'),
        T0 = (1, 'K'),
        Tmin = (303.03, 'K'),
        Tmax = (2500, 'K'),
        comment = 'Fitted to 59 data points; dA = *|/ 1.32799, dn = +|- 0.0372287, dEa = +|- 0.204795 kJ/mol',
    ),
)

#   ======= =========== =========== =========== ===============
#   Temp.   k (TST)     Tunneling   k (TST+T)   Units
#   ======= =========== =========== =========== ===============
#     300 K   6.828e-13     2.56856   1.754e-12 s^-1
#     400 K   1.620e-06     1.71305   2.776e-06 s^-1
#     500 K   1.159e-02     1.41798   1.644e-02 s^-1
#     600 K   4.493e+00      1.2783   5.743e+00 s^-1
#     800 K   8.284e+03     1.15142   9.539e+03 s^-1
#    1000 K   7.938e+05     1.09611   8.701e+05 s^-1
#    1500 K   3.777e+08     1.04301   3.939e+08 s^-1
#    2000 K   8.607e+09     1.02458   8.819e+09 s^-1
#   ======= =========== =========== =========== ===============
kinetics(
    label = 'c6-C6H9 = C6H8-c6-14 + H',
    kinetics = Arrhenius(
        A = (2.09669e+09, 's^-1'),
        n = 1.29873,
        Ea = (139.719, 'kJ/mol'),
        T0 = (1, 'K'),
        Tmin = (303.03, 'K'),
        Tmax = (2500, 'K'),
        comment = 'Fitted to 59 data points; dA = *|/ 1.29047, dn = +|- 0.0334678, dEa = +|- 0.184107 kJ/mol',
    ),
)

#   ======= =========== =========== =========== ===============
#   Temp.   k (TST)     Tunneling   k (TST+T)   Units
#   ======= =========== =========== =========== ===============
#     300 K   1.072e-13     2791.97   2.992e-10 s^-1
#     400 K   3.305e-07     15.9524   5.272e-06 s^-1
#     500 K   2.709e-03     4.25567   1.153e-02 s^-1
#     600 K   1.135e+00     2.52477   2.865e+00 s^-1
#     800 K   2.269e+03     1.63252   3.704e+03 s^-1
#    1000 K   2.267e+05     1.36089   3.086e+05 s^-1
#    1500 K   1.150e+08     1.14691   1.319e+08 s^-1
#    2000 K   2.764e+09     1.08159   2.989e+09 s^-1
#   ======= =========== =========== =========== ===============
kinetics(
    label = 'c5-C6H9 = c5-C6H9-3',
    kinetics = Arrhenius(
        A = (5.26502e-07, 's^-1'),
        n = 5.63896,
        Ea = (102.679, 'kJ/mol'),
        T0 = (1, 'K'),
        Tmin = (303.03, 'K'),
```

```
        Tmax = (2500, 'K'),
        comment = 'Fitted to 59 data points; dA = *|/ 31.2022, dn = +|- 0.451533, dEa = +|- 2.48388 kJ/mol',
    ),
)

#  ======= =========== =========== ========== ===============
#  Temp.   k (TST)     Tunneling   k (TST+T)   Units
#  ======= =========== =========== ========== ===============
#    300 K   7.775e-11     86860.3   6.753e-06 s^-1
#    400 K   3.615e-05     73.3027   2.650e-03 s^-1
#    500 K   9.421e-02     8.29555   7.816e-01 s^-1
#    600 K   1.838e+01     3.68741   6.778e+01 s^-1
#    800 K   1.423e+04     1.95709   2.785e+04 s^-1
#   1000 K   8.111e+05     1.51874   1.232e+06 s^-1
#   1500 K   1.975e+08     1.20241   2.375e+08 s^-1
#   2000 K   3.312e+09     1.11092   3.679e+09 s^-1
#  ======= =========== =========== ========== ===============
kinetics(
    label = 'c5-C6H9 = c5-C6H9-2',
    kinetics = Arrhenius(
        A = (3.53654e-16, 's^-1'),
        n = 8.13829,
        Ea = (61.0164, 'kJ/mol'),
        T0 = (1, 'K'),
        Tmin = (303.03, 'K'),
        Tmax = (2500, 'K'),
        comment = 'Fitted to 59 data points; dA = *|/ 97.8226, dn = +|- 0.601498, dEa = +|- 3.30884 kJ/mol',
    ),
)

#  ======= =========== =========== ========== ===============
#  Temp.   k (TST)     Tunneling   k (TST+T)   Units
#  ======= =========== =========== ========== ===============
#    300 K   7.690e-16     1.75071   1.346e-15 s^-1
#    400 K   1.333e-08     1.36009   1.813e-08 s^-1
#    500 K   3.154e-04     1.21638   3.837e-04 s^-1
#    600 K   2.695e-01     1.14597   3.089e-01 s^-1
#    800 K   1.300e+03      1.0805   1.404e+03 s^-1
#   1000 K   2.152e+05     1.05148   2.263e+05 s^-1
#   1500 K   1.989e+08     1.02336   2.036e+08 s^-1
#   2000 K   6.055e+09     1.01353   6.137e+09 s^-1
#  ======= =========== =========== ========== ===============
kinetics(
    label = 'c5-C6H9-2 = C5H6 + CH3',
    kinetics = Arrhenius(
        A = (4.96084e+11, 's^-1'),
        n = 0.717063,
        Ea = (163.015, 'kJ/mol'),
        T0 = (1, 'K'),
        Tmin = (303.03, 'K'),
        Tmax = (2500, 'K'),
        comment = 'Fitted to 59 data points; dA = *|/ 1.33396, dn = +|- 0.037817, dEa = +|- 0.208031 kJ/mol',
    ),
)

#  ======= =========== =========== ========== ===============
#  Temp.   k (TST)     Tunneling   k (TST+T)   Units
#  ======= =========== =========== ========== ===============
#    300 K   2.307e-13     2521.82   5.819e-10 s^-1
#    400 K   7.701e-07     15.0446   1.159e-05 s^-1
#    500 K   6.892e-03     4.13168   2.848e-02 s^-1
#    600 K   3.144e+00     2.47895   7.794e+00 s^-1
```

```
#    800 K   7.300e+03     1.61698   1.180e+04 s^-1
#   1000 K   8.247e+05     1.35265   1.116e+06 s^-1
#   1500 K   5.234e+08     1.14368   5.986e+08 s^-1
#   2000 K   1.468e+10     1.07976   1.585e+10 s^-1
#  ======= =========== =========== =========== ===============
kinetics(
    label = 'c5-C6H9-3 = c5-C6H9-2',
    kinetics = Arrhenius(
        A = (3.23947e-08, 's^-1'),
        n = 6.22368,
        Ea = (102.429, 'kJ/mol'),
        T0 = (1, 'K'),
        Tmin = (303.03, 'K'),
        Tmax = (2500, 'K'),
        comment = 'Fitted to 59 data points; dA = *|/ 32.0376, dn = +|- 0.455001, dEa = +|- 2.50296 kJ/mol',
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#       T \ P   1.106e-03   2.191e-03   7.920e-03   4.474e-02   3.204e-01   2.295e+00   1.296e+01   4.686e+01   9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#         300   4.353e-18   4.353e-18   4.353e-18   4.353e-18   4.353e-18   4.353e-18   4.353e-18   4.353e-18   4.353e-18
#         400   6.992e-12   7.051e-12   7.103e-12   7.122e-12   7.125e-12   7.126e-12   7.126e-12   7.126e-12   7.126e-12
#         500   1.910e-07   2.046e-07   2.209e-07   2.296e-07   2.318e-07   2.321e-07   2.322e-07   2.322e-07   2.322e-07
#         600   1.789e-04   2.137e-04   2.710e-04   3.181e-04   3.367e-04   3.405e-04   3.410e-04   3.411e-04   3.411e-04
#         700   1.892e-02   2.533e-02   3.902e-02   5.571e-02   6.592e-02   6.887e-02   6.938e-02   6.947e-02   6.949e-02
#        1000   3.350e+01   5.797e+01   1.448e+02   3.809e+02   7.672e+02   1.059e+03   1.159e+03   1.182e+03   1.187e+03
#        1200   3.214e+02   6.318e+02   2.032e+03   7.629e+03   2.260e+04   4.161e+04   5.182e+04   5.479e+04   5.547e+04
#        1300   5.816e+02   1.214e+03   4.405e+03   1.976e+04   7.212e+04   1.591e+05   2.188e+05   2.393e+05   2.445e+05
#        1400   8.397e+02   1.851e+03   7.514e+03   3.983e+04   1.782e+05   4.750e+05   7.346e+05   8.411e+05   8.700e+05
#        1500   1.005e+03   2.332e+03   1.051e+04   6.520e+04   3.553e+05   1.150e+06   2.033e+06   2.469e+06   2.599e+06
#        1700   9.704e+02   2.466e+03   1.339e+04   1.105e+05   8.677e+05   4.120e+06   9.765e+06   1.379e+07   1.529e+07
#        2000   4.174e+02   1.193e+03   8.246e+03   9.885e+04   1.275e+06   1.058e+07   4.088e+07   7.808e+07   9.786e+07
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
pdepreaction(
    reactants = ['c5-C6H9-2'],
    products = ['c5-C6H9-3'],
    kinetics = Chebyshev(
        coeffs = [
            [-5.78871, 0.622634, -0.137865, 0.00602101],
            [12.1961, 0.951502, -0.24105, -0.0145389],
            [0.0230772, 0.673188, -0.088358, -0.0248137],
            [-0.492816, 0.332862, 0.00424676, -0.0258422],
            [-0.0475947, 0.0883644, 0.0156251, -0.0168986],
            [-0.15587, 0.100107, 0.0263106, 0.00472185],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#       T \ P   1.106e-03   2.191e-03   7.920e-03   4.474e-02   3.204e-01   2.295e+00   1.296e+01   4.686e+01   9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
```

```
#        300  1.037e-17  5.184e-18  1.147e-18  9.535e-20  3.095e-21  6.907e-23  2.214e-24  1.700e-25  4.334e-26
#        400  1.253e-10  8.886e-11  3.635e-11  6.286e-12  3.865e-13  1.179e-14  4.084e-16  3.182e-17  8.133e-18
#        500  1.583e-06  1.472e-06  9.982e-07  3.295e-07  3.782e-08  1.724e-09  6.869e-11  5.522e-12  1.421e-12
#        600  5.168e-04  5.812e-04  5.741e-04  3.245e-04  6.806e-05  4.977e-06  2.456e-07  2.093e-08  5.456e-09
#        700  2.494e-02  3.204e-02  4.136e-02  3.507e-02  1.229e-02  1.460e-03  9.567e-05  8.979e-06  2.398e-06
#       1000  1.692e+01  2.815e+01  6.091e+01  1.135e+02  1.158e+02  4.691e+01  8.314e+00  1.293e+00  4.075e-01
#       1200  1.539e+02  2.943e+02  8.348e+02  2.288e+03  3.808e+03  2.711e+03  8.226e+02  1.833e+02  6.716e+01
#       1300  2.721e+02  5.587e+02  1.823e+03  6.108e+03  1.305e+04  1.229e+04  4.855e+03  1.305e+03  5.208e+02
#       1400  3.881e+02  8.498e+02  3.150e+03  1.268e+04  3.416e+04  4.173e+04  2.117e+04  6.835e+03  2.977e+03
#       1500  4.607e+02  1.069e+03  4.451e+03  2.123e+04  7.088e+04  1.108e+05  7.151e+04  2.766e+04  1.317e+04
#       1700  4.452e+02  1.143e+03  5.819e+03  3.735e+04  1.829e+05  4.469e+05  4.503e+05  2.461e+05  1.400e+05
#       2000  1.741e+02  5.032e+02  3.265e+03  3.027e+04  2.427e+05  1.085e+06  2.067e+06  1.900e+06  1.430e+06
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
pdepreaction(
    reactants = ['c6-C6H9'],
    products = ['c5-C6H9-3'],
    kinetics = Chebyshev(
        coeffs = [
            [-7.68651, -2.13598, -0.623265, 0.0186063],
            [13.344, 2.8222, -0.223849, -0.0984016],
            [-0.322735, 0.938315, 0.132591, -0.0333241],
            [-0.250874, 0.285825, 0.0764728, 0.0130087],
            [0.0102958, 0.0608339, 0.00581386, 0.0182345],
            [-0.238818, 0.084271, 0.00532308, -0.0027011],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#         T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#        300  2.769e-10  2.831e-10  2.915e-10  2.971e-10  2.989e-10  2.992e-10  2.992e-10  2.992e-10  2.992e-10
#        400  1.440e-06  1.802e-06  2.663e-06  3.958e-06  4.918e-06  5.210e-06  5.260e-06  5.269e-06  5.270e-06
#        500  9.166e-04  1.310e-03  2.547e-03  5.503e-03  9.235e-03  1.104e-02  1.143e-02  1.150e-02  1.151e-02
#        600  1.031e-01  1.571e-01  3.439e-01  9.049e-01  1.911e+00  2.613e+00  2.812e+00  2.850e+00  2.858e+00
#        700  2.726e+00  4.437e+00  1.081e+01  3.337e+01  8.734e+01  1.404e+02  1.602e+02  1.646e+02  1.655e+02
#       1000  2.463e+02  4.830e+02  1.620e+03  7.836e+03  4.032e+04  1.335e+05  2.346e+05  2.802e+05  2.929e+05
#       1200  8.013e+02  1.750e+03  6.973e+03  4.068e+04  2.741e+05  1.341e+06  3.359e+06  4.839e+06  5.384e+06
#       1300  9.545e+02  2.214e+03  9.777e+03  6.389e+04  4.909e+05  2.872e+06  8.592e+06  1.384e+07  1.608e+07
#       1400  9.682e+02  2.374e+03  1.158e+04  8.481e+04  7.387e+05  5.101e+06  1.813e+07  3.282e+07  4.003e+07
#       1500  8.678e+02  2.241e+03  1.201e+04  9.840e+04  9.673e+05  7.798e+06  3.268e+07  6.666e+07  8.574e+07
#       1700  5.353e+02  1.512e+03  9.614e+03  9.763e+04  1.209e+06  1.292e+07  7.361e+07  1.901e+08  2.740e+08
#       2000  1.739e+02  5.464e+02  4.286e+03  5.804e+04  9.900e+05  1.530e+07  1.305e+08  4.697e+08  8.052e+08
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
pdepreaction(
    reactants = ['c5-C6H9'],
    products = ['c5-C6H9-3'],
    kinetics = Chebyshev(
        coeffs = [
            [-1.67953, 1.03932, -0.183831, -0.00856721],
            [8.32047, 1.44063, -0.154651, -0.0425081],
            [-0.0677667, 0.571113, 0.0621454, -0.0233052],
            [-0.522539, 0.239689, 0.0398306, 0.0120182],
```

```
            [-0.0994733, 0.102901, 0.00587715, 0.0123211],
            [-0.113118, 0.0193932, 0.00754593, 0.00721637],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#       T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#        300  1.600e-11  1.164e-11  5.623e-12  1.589e-12  2.728e-13  3.986e-14  7.106e-15  1.968e-15  9.934e-16
#        400  7.780e-07  7.425e-07  5.939e-07  3.100e-07  8.452e-08  1.470e-08  2.714e-09  7.563e-10  3.822e-10
#        500  7.063e-04  7.958e-04  8.533e-04  6.505e-04  2.598e-04  5.639e-05  1.109e-05  3.130e-06  1.586e-06
#        600  6.519e-02  8.357e-02  1.123e-01  1.139e-01  6.222e-02  1.703e-02  3.658e-03  1.053e-03  5.360e-04
#        700  1.489e+00  2.125e+00  3.468e+00  4.541e+00  3.323e+00  1.168e+00  2.826e-01  8.408e-02  4.309e-02
#       1000  2.140e+02  3.904e+02  1.017e+03  2.554e+03  4.211e+03  3.558e+03  1.622e+03  6.327e+02  3.507e+02
#       1200  7.399e+02  1.556e+03  5.308e+03  1.923e+04  4.861e+04  6.506e+04  4.512e+04  2.279e+04  1.393e+04
#       1300  8.313e+02  1.879e+03  7.379e+03  3.255e+04  1.038e+05  1.767e+05  1.517e+05  8.839e+04  5.744e+04
#       1400  8.018e+02  1.933e+03  8.621e+03  4.554e+04  1.805e+05  3.867e+05  4.085e+05  2.750e+05  1.908e+05
#       1500  6.882e+02  1.757e+03  8.790e+03  5.475e+04  2.658e+05  7.085e+05  9.148e+05  7.115e+05  5.285e+05
#       1700  3.958e+02  1.114e+03  6.781e+03  5.633e+04  3.927e+05  1.566e+06  2.959e+06  3.056e+06  2.614e+06
#       2000  1.189e+02  3.733e+02  2.848e+03  3.340e+04  3.654e+05  2.453e+06  7.751e+06  1.196e+07  1.263e+07
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
pdepreaction(
    reactants = ['C6H9'],
    products = ['c5-C6H9-3'],
    kinetics = Chebyshev(
        coeffs = [
            [-3.53956, -0.670068, -0.421481, 0.0242832],
            [9.41964, 2.01754, -0.215641, -0.0606825],
            [-0.167405, 0.76957, 0.064936, -0.0269919],
            [-0.325445, 0.336716, 0.0364809, 0.00398741],
            [-0.114831, 0.110047, 0.0135798, 0.00509249],
            [-0.183027, 0.0376307, 0.0108176, 0.00282913],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#       T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#        300  5.359e+06  5.038e+06  3.087e+06  8.524e+05  1.033e+05  5.527e+03  2.297e+02  1.857e+01  4.781e+00
#        400  1.208e+07  1.440e+07  1.397e+07  6.592e+06  1.203e+06  9.228e+04  4.727e+03  4.051e+02  1.057e+02
#        500  1.693e+07  2.340e+07  3.110e+07  2.303e+07  6.507e+06  6.918e+05  4.324e+04  3.966e+03  1.052e+03
#        600  2.105e+07  3.144e+07  5.002e+07  4.946e+07  1.985e+07  2.872e+06  2.189e+05  2.168e+04  5.864e+03
#        700  2.539e+07  3.975e+07  7.109e+07  8.579e+07  4.521e+07  8.727e+06  8.255e+05  8.996e+04  2.500e+04
#       1000  3.149e+07  5.390e+07  1.222e+08  2.274e+08  2.231e+08  9.349e+07  1.906e+07  3.375e+06  1.124e+06
#       1200  2.547e+07  4.605e+07  1.217e+08  3.029e+08  4.429e+08  2.891e+08  8.986e+07  2.175e+07  8.384e+06
```

```
#       1300  1.782e+07  3.301e+07  9.380e+07  2.718e+08  4.981e+08  4.239e+08  1.690e+08  4.887e+07  2.050e+07
#       1400  1.228e+07  2.315e+07  6.958e+07  2.288e+08  5.121e+08  5.558e+08  2.805e+08  9.661e+07  4.417e+07
#       1500  8.372e+06  1.599e+07  5.022e+07  1.835e+08  4.902e+08  6.649e+08  4.193e+08  1.712e+08  8.536e+07
#       1700  3.772e+06  7.331e+06  2.448e+07  1.052e+08  3.784e+08  7.627e+08  7.269e+08  4.124e+08  2.445e+08
#       2000  1.185e+06  2.331e+06  8.163e+06  4.067e+07  1.999e+08  6.406e+08  1.027e+09  9.044e+08  6.843e+08
#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
pdepreaction(
   reactants = ['C2H3', 'C4H6'],
   products = ['c5-C6H9-3'],
   kinetics = Chebyshev(
      coeffs = [
         [6.10548, -1.56987, -0.728015, -0.00185362],
         [2.03429, 2.05809, 0.00571449, -0.0802575],
         [0.0296339, 0.637103, 0.164651, -0.0269716],
         [-0.103617, 0.252629, 0.0803021, 0.00207763],
         [-0.0266244, 0.130024, 0.0057282, 0.000850452],
         [-0.146758, 0.0119034, 0.0262953, -0.00113866],
      ],
      kunits = 'cm^3/(mol*s)',
      Tmin = (300, 'K'),
      Tmax = (2000, 'K'),
      Pmin = (0.00101325, 'bar'),
      Pmax = (101.325, 'bar'),
   ),
)

#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
#      T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
#       300  5.818e-10  5.818e-10  5.819e-10  5.819e-10  5.819e-10  5.819e-10  5.819e-10  5.819e-10  5.819e-10
#       400  1.137e-05  1.146e-05  1.155e-05  1.158e-05  1.158e-05  1.159e-05  1.159e-05  1.159e-05  1.159e-05
#       500  2.342e-02  2.509e-02  2.709e-02  2.815e-02  2.843e-02  2.847e-02  2.848e-02  2.848e-02  2.848e-02
#       600  4.087e+00  4.883e+00  6.191e+00  7.268e+00  7.692e+00  7.778e+00  7.791e+00  7.793e+00  7.793e+00
#       700  1.340e+02  1.794e+02  2.764e+02  3.946e+02  4.669e+02  4.878e+02  4.915e+02  4.921e+02  4.922e+02
#      1000  3.137e+04  5.427e+04  1.356e+05  3.567e+05  7.184e+05  9.913e+05  1.086e+06  1.107e+06  1.111e+06
#      1200  1.424e+05  2.800e+05  9.003e+05  3.381e+06  1.001e+07  1.844e+07  2.296e+07  2.428e+07  2.458e+07
#      1300  1.947e+05  4.063e+05  1.475e+06  6.614e+06  2.415e+07  5.326e+07  7.326e+07  8.013e+07  8.184e+07
#      1400  2.219e+05  4.893e+05  1.986e+06  1.053e+07  4.709e+07  1.255e+08  1.941e+08  2.223e+08  2.299e+08
#      1500  2.171e+05  5.037e+05  2.269e+06  1.408e+07  7.674e+07  2.485e+08  4.391e+08  5.332e+08  5.614e+08
#      1700  1.514e+05  3.847e+05  2.089e+06  1.723e+07  1.354e+08  6.427e+08  1.524e+09  2.151e+09  2.385e+09
#      2000  4.575e+04  1.307e+05  9.038e+05  1.084e+07  1.398e+08  1.160e+09  4.481e+09  8.558e+09  1.073e+10
#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
pdepreaction(
   reactants = ['c5-C6H9-3'],
   products = ['c5-C6H9-2'],
   kinetics = Chebyshev(
      coeffs = [
         [-0.798495, 0.622634, -0.137865, 0.00602101],
         [9.13077, 0.951502, -0.24105, -0.0145389],
         [0.112275, 0.673188, -0.088358, -0.0248137],
         [-0.472403, 0.332862, 0.00424676, -0.0258422],
         [-0.0442566, 0.0883644, 0.0156251, -0.0168986],
         [-0.154234, 0.100107, 0.0263106, 0.00472185],
      ],
      kunits = 's^-1',
      Tmin = (300, 'K'),
      Tmax = (2000, 'K'),
      Pmin = (0.00101325, 'bar'),
```

```
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#         T \ P   1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#         300  2.139e-15  9.159e-16  1.527e-16  9.102e-18  2.364e-19  4.920e-21  1.558e-22  1.194e-23  3.043e-24
#         400  1.025e-08  6.017e-09  1.765e-09  2.072e-10  9.225e-12  2.402e-13  7.990e-15  6.177e-16  1.577e-16
#         500  7.016e-05  5.423e-05  2.642e-05  5.860e-06  4.706e-07  1.731e-08  6.407e-10  5.066e-11  1.299e-11
#         600  1.303e-02  1.258e-02  9.435e-03  3.769e-03  5.614e-04  3.222e-05  1.432e-06  1.186e-07  3.071e-08
#         700  3.596e-01  4.106e-01  4.304e-01  2.797e-01  7.381e-02  6.966e-03  4.036e-04  3.636e-05  9.610e-06
#        1000  8.204e+01  1.270e+02  2.461e+02  4.071e+02  3.650e+02  1.283e+02  2.016e+01  2.932e+00  9.025e-01
#        1200  5.750e+02  1.025e+03  2.615e+03  6.448e+03  9.642e+03  6.081e+03  1.641e+03  3.381e+02  1.198e+02
#        1300  1.081e+03  2.061e+03  5.997e+03  1.779e+04  3.345e+04  2.724e+04  9.347e+03  2.278e+03  8.707e+02
#        1400  1.667e+03  3.386e+03  1.115e+04  3.935e+04  9.161e+04  9.449e+04  4.052e+04  1.159e+04  4.774e+03
#        1500  2.129e+03  4.591e+03  1.698e+04  7.070e+04  2.019e+05  2.617e+05  1.392e+05  4.656e+04  2.068e+04
#        1700  2.376e+03  5.697e+03  2.596e+04  1.458e+05  6.058e+05  1.200e+06  9.574e+05  4.327e+05  2.231e+05
#        2000  9.270e+02  2.535e+03  1.503e+04  1.250e+05  8.749e+05  3.253e+06  4.946e+06  3.700e+06  2.472e+06
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
pdepreaction(
    reactants = ['c6-C6H9'],
    products = ['c5-C6H9-2'],
    kinetics = Chebyshev(
        coeffs = [
            [-6.52446, -2.38475, -0.5685, 0.015076],
            [12.5186, 2.81704, -0.282086, -0.0950136],
            [-0.272523, 0.996068, 0.0960286, -0.0420857],
            [-0.1851, 0.262457, 0.0768567, 0.00890378],
            [0.0633535, 0.00428721, 0.0176341, 0.0191138],
            [-0.207434, 0.0942658, -0.00645336, -0.00102881],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#         T \ P   1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#         300  6.741e-06  6.746e-06  6.750e-06  6.753e-06  6.753e-06  6.753e-06  6.753e-06  6.753e-06  6.753e-06
#         400  2.027e-03  2.156e-03  2.369e-03  2.553e-03  2.630e-03  2.647e-03  2.649e-03  2.650e-03  2.650e-03
#         500  2.399e-01  2.968e-01  4.252e-01  6.040e-01  7.319e-01  7.726e-01  7.799e-01  7.811e-01  7.813e-01
#         600  7.719e+00  1.089e+01  1.976e+01  3.728e+01  5.635e+01  6.526e+01  6.728e+01  6.764e+01  6.771e+01
#         700  8.204e+01  1.293e+02  2.882e+02  7.098e+02  1.379e+03  1.837e+03  1.973e+03  2.000e+03  2.006e+03
#        1000  1.579e+03  3.116e+03  1.085e+04  5.260e+04  2.365e+05  6.487e+05  1.009e+06  1.151e+06  1.188e+06
#        1200  3.288e+03  7.040e+03  2.818e+04  1.694e+05  1.084e+06  4.600e+06  1.012e+07  1.363e+07  1.483e+07
#        1300  3.945e+03  8.808e+03  3.759e+04  2.428e+05  1.747e+06  8.836e+06  2.298e+07  3.420e+07  3.859e+07
#        1400  4.192e+03  9.791e+03  4.493e+04  3.127e+05  2.484e+06  1.460e+07  4.440e+07  7.320e+07  8.608e+07
#        1500  3.968e+03  9.713e+03  4.824e+04  3.654e+05  3.189e+06  2.143e+07  7.531e+07  1.375e+08  1.691e+08
#        1700  2.776e+03  7.435e+03  4.339e+04  3.964e+05  4.191e+06  3.572e+07  1.621e+08  3.592e+08  4.840e+08
#        2000  8.873e+02  2.672e+03  1.953e+04  2.417e+05  3.604e+06  4.499e+07  2.977e+08  8.748e+08  1.356e+09
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
```

```
pdepreaction(
    reactants = ['c5-C6H9'],
    products = ['c5-C6H9-2'],
    kinetics = Chebyshev(
        coeffs = [
            [0.47797, 0.887248, -0.165214, -0.00522622],
            [6.29458, 1.35316, -0.17543, -0.0358811],
            [0.196464, 0.653458, -0.0010266, -0.027088],
            [-0.461764, 0.194129, 0.0566842, -0.0031797],
            [-0.081603, 0.0326209, 0.0348638, 0.00922296],
            [-0.0698607, 0.0261673, -0.0126101, 0.0158395],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#       T \ P   1.106e-03   2.191e-03   7.920e-03   4.474e-02   3.204e-01   2.295e+00   1.296e+01   4.686e+01   9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#         300   8.923e-09   5.661e-09   2.143e-09   4.707e-10   7.077e-11   1.002e-11   1.777e-12   4.917e-13   2.482e-13
#         400   1.387e-04   1.125e-04   6.583e-05   2.316e-05   4.653e-06   7.188e-07   1.295e-07   3.593e-08   1.814e-08
#         500   4.581e-02   4.476e-02   3.675e-02   1.966e-02   5.655e-03   1.033e-03   1.938e-04   5.417e-05   2.739e-05
#         600   1.860e+00   2.132e+00   2.341e+00   1.810e+00   7.424e-01   1.684e-01   3.385e-02   9.603e-03   4.871e-03
#         700   2.113e+01   2.777e+01   3.950e+01   4.318e+01   2.553e+01   7.552e+00   1.692e+00   4.929e-01   2.515e-01
#        1000   9.055e+02   1.570e+03   3.838e+03   9.203e+03   1.444e+04   1.121e+04   4.690e+03   1.749e+03   9.555e+02
#        1200   2.431e+03   4.840e+03   1.536e+04   5.262e+04   1.272e+05   1.589e+05   1.012e+05   4.820e+04   2.879e+04
#        1300   2.947e+03   6.280e+03   2.264e+04   9.204e+04   2.707e+05   4.150e+05   3.184e+05   1.718e+05   1.081e+05
#        1400   3.114e+03   7.070e+03   2.876e+04   1.377e+05   4.885e+05   9.081e+05   8.285e+05   5.044e+05   3.351e+05
#        1500   2.906e+03   6.998e+03   3.189e+04   1.786e+05   7.612e+05   1.709e+06   1.842e+06   1.262e+06   8.860e+05
#        1700   1.960e+03   5.234e+03   2.919e+04   2.174e+05   1.308e+06   4.230e+06   6.294e+06   5.412e+06   4.243e+06
#        2000   5.912e+02   1.784e+03   1.272e+04   1.368e+05   1.326e+06   7.403e+06   1.838e+07   2.282e+07   2.140e+07
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
pdepreaction(
    reactants = ['C6H9'],
    products = ['c5-C6H9-2'],
    kinetics = Chebyshev(
        coeffs = [
            [-2.14535, -0.869031, -0.375751, 0.0180916],
            [8.3103, 2.0091, -0.273409, -0.0518914],
            [-0.0995231, 0.815843, 0.0279159, -0.0385745],
            [-0.230765, 0.282, 0.0424103, 0.000821771],
            [-0.0636837, 0.0505952, 0.0202867, 0.00984508],
            [-0.154545, 0.052514, -0.00323284, 0.0023426],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#       T \ P   1.106e-03   2.191e-03   7.920e-03   4.474e-02   3.204e-01   2.295e+00   1.296e+01   4.686e+01   9.284e+01
```

```
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
#        300  4.350e+07  4.052e+07  2.419e+07  6.394e+06  7.456e+05  3.832e+04  1.562e+03  1.257e+02  3.234e+01
#        400  9.304e+07  1.089e+08  1.001e+08  4.237e+07  6.873e+06  4.858e+05  2.384e+04  2.018e+03  5.248e+02
#        500  9.925e+07  1.356e+08  1.751e+08  1.214e+08  3.039e+07  2.869e+06  1.676e+05  1.503e+04  3.965e+03
#        600  7.748e+07  1.149e+08  1.812e+08  1.794e+08  7.082e+07  9.551e+06  6.808e+05  6.559e+04  1.761e+04
#        700  6.066e+07  9.445e+07  1.683e+08  2.086e+08  1.169e+08  2.301e+07  2.113e+06  2.254e+05  6.221e+04
#       1000  4.804e+07  8.186e+07  1.843e+08  3.452e+08  3.554e+08  1.589e+08  3.308e+07  5.791e+06  1.913e+06
#       1200  4.197e+07  7.562e+07  1.983e+08  4.907e+08  7.216e+08  4.722e+08  1.423e+08  3.299e+07  1.243e+07
#       1300  3.608e+07  6.662e+07  1.877e+08  5.366e+08  9.635e+08  7.793e+08  2.820e+08  7.435e+07  2.981e+07
#       1400  2.998e+07  5.637e+07  1.681e+08  5.432e+08  1.173e+09  1.167e+09  5.073e+08  1.517e+08  6.462e+07
#       1500  2.386e+07  4.548e+07  1.417e+08  5.085e+08  1.300e+09  1.585e+09  8.311e+08  2.832e+08  1.283e+08
#       1700  1.390e+07  2.697e+07  8.955e+07  3.786e+08  1.298e+09  2.316e+09  1.769e+09  7.915e+08  4.088e+08
#       2000  4.742e+06  9.323e+06  3.257e+07  1.608e+08  7.666e+08  2.246e+09  2.993e+09  2.093e+09  1.361e+09
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
pdepreaction(
    reactants = ['C2H3', 'C4H6'],
    products = ['c5-C6H9-2'],
    kinetics = Chebyshev(
        coeffs = [
            [6.6863, -1.60522, -0.731863, -0.00901058],
            [1.76982, 1.99503, -0.0372252, -0.082724],
            [0.0571245, 0.640224, 0.149985, -0.0382539],
            [0.0101266, 0.201093, 0.0758623, 0.00190412],
            [0.0721144, 0.0604535, -0.0136482, 0.00904525],
            [-0.153353, 0.0681449, 0.0292314, -0.0119279],
        ],
        kunits = 'cm^3/(mol*s)',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
#         T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
#        300  4.126e-18  2.063e-18  4.566e-19  3.794e-20  1.232e-21  2.749e-23  8.810e-25  6.766e-26  1.725e-26
#        400  6.630e-11  4.702e-11  1.924e-11  3.327e-12  2.045e-13  6.240e-15  2.161e-16  1.684e-17  4.304e-18
#        500  1.033e-06  9.601e-07  6.512e-07  2.150e-07  2.467e-08  1.125e-09  4.481e-11  3.602e-12  9.267e-13
#        600  3.984e-04  4.481e-04  4.426e-04  2.501e-04  5.247e-05  3.837e-06  1.894e-07  1.614e-08  4.206e-09
#        700  2.212e-02  2.841e-02  3.668e-02  3.110e-02  1.090e-02  1.295e-03  8.484e-05  7.963e-06  2.126e-06
#       1000  2.071e+01  3.444e+01  7.453e+01  1.388e+02  1.417e+02  5.740e+01  1.017e+01  1.582e+00  4.986e-01
#       1200  2.220e+02  4.244e+02  1.204e+03  3.300e+03  5.492e+03  3.909e+03  1.186e+03  2.643e+02  9.685e+01
#       1300  4.218e+02  8.661e+02  2.826e+03  9.469e+03  2.024e+04  1.905e+04  7.526e+03  2.023e+03  8.073e+02
#       1400  6.432e+02  1.409e+03  5.220e+03  2.102e+04  5.661e+04  6.916e+04  3.509e+04  1.133e+04  4.934e+03
#       1500  8.127e+02  1.886e+03  7.852e+03  3.744e+04  1.250e+05  1.955e+05  1.261e+05  4.879e+04  2.324e+04
#       1700  8.796e+02  2.258e+03  1.150e+04  7.380e+04  3.613e+05  8.830e+05  8.897e+05  4.863e+05  2.766e+05
#       2000  3.988e+02  1.153e+03  7.479e+03  6.935e+04  5.560e+05  2.487e+06  4.734e+06  4.353e+06  3.276e+06
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
pdepreaction(
    reactants = ['c5-C6H9-3'],
    products = ['c6-C6H9'],
    kinetics = Chebyshev(
        coeffs = [
            [-7.78727, -2.13598, -0.623265, 0.0186063],
            [13.6954, 2.8222, -0.223849, -0.0984016],
```

```
            [-0.248568, 0.938315, 0.132591, -0.0333241],
            [-0.227007, 0.285825, 0.0764728, 0.0130087],
            [0.0163595, 0.0608339, 0.00581386, 0.0182345],
            [-0.234357, 0.084271, 0.00532308, -0.0027011],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#      T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#        300  6.367e-24  2.726e-24  4.544e-25  2.710e-26  7.038e-28  1.465e-29  4.638e-31  3.555e-32  9.058e-33
#        400  3.337e-15  1.958e-15  5.746e-16  6.745e-17  3.003e-18  7.820e-20  2.600e-21  2.011e-22  5.132e-23
#        500  3.732e-10  2.884e-10  1.406e-10  3.117e-11  2.503e-12  9.206e-14  3.408e-15  2.695e-16  6.909e-17
#        600  4.396e-07  4.244e-07  3.184e-07  1.272e-07  1.894e-08  1.087e-09  4.832e-11  4.001e-12  1.036e-12
#        700  4.503e-05  5.141e-05  5.389e-05  3.502e-05  9.241e-06  8.721e-07  5.053e-08  4.552e-09  1.203e-09
#       1000  1.072e-01  1.659e-01  3.216e-01  5.321e-01  4.770e-01  1.676e-01  2.635e-02  3.832e-03  1.179e-03
#       1200  1.871e+00  3.335e+00  8.512e+00  2.099e+01  3.138e+01  1.979e+01  5.341e+00  1.100e+00  3.901e-01
#       1300  5.005e+00  9.543e+00  2.777e+01  8.238e+01  1.549e+02  1.261e+02  4.328e+01  1.055e+01  4.032e+00
#       1400  1.045e+01  2.124e+01  6.991e+01  2.468e+02  5.745e+02  5.926e+02  2.541e+02  7.268e+01  2.994e+01
#       1500  1.739e+01  3.750e+01  1.387e+02  5.774e+02  1.649e+03  2.137e+03  1.137e+03  3.803e+02  1.689e+02
#       1700  3.009e+01  7.215e+01  3.288e+02  1.847e+03  7.672e+03  1.519e+04  1.213e+04  5.480e+03  2.825e+03
#       2000  1.937e+01  5.299e+01  3.142e+02  2.613e+03  1.828e+04  6.799e+04  1.034e+05  7.732e+04  5.167e+04
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
pdepreaction(
    reactants = ['c5-C6H9-2'],
    products = ['c6-C6H9'],
    kinetics = Chebyshev(
        coeffs = [
            [-11.6154, -2.38475, -0.5685, 0.015076],
            [15.9352, 2.81704, -0.282086, -0.0950136],
            [-0.287554, 0.996068, 0.0960286, -0.0420857],
            [-0.181647, 0.262457, 0.0768567, 0.00890378],
            [0.066079, 0.00428721, 0.0176341, 0.0191138],
            [-0.204609, 0.0942658, -0.00645336, -0.00102881],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#      T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#        300  3.460e-07  2.204e-07  8.176e-08  1.726e-08  2.538e-09  3.575e-10  6.338e-11  1.754e-11  8.851e-12
#        400  2.289e-02  1.778e-02  9.283e-03  2.755e-03  4.854e-04  7.164e-05  1.280e-05  3.545e-06  1.790e-06
#        500  1.413e+01  1.303e+01  9.337e+00  4.049e+00  9.496e-01  1.567e-01  2.865e-02  7.970e-03  4.027e-03
#        600  6.271e+02  6.709e+02  6.415e+02  4.069e+02  1.355e+02  2.695e+01  5.191e+00  1.459e+00  7.387e-01
#        700  6.046e+03  7.322e+03  8.975e+03  8.114e+03  3.951e+03  1.019e+03  2.164e+02  6.221e+01  3.165e+01
```

```
#       1000  6.860e+04  1.077e+05  2.254e+05  4.633e+05  6.378e+05  4.410e+05  1.697e+05  6.092e+04  3.290e+04
#       1200  1.104e+05  1.957e+05  5.212e+05  1.536e+06  3.408e+06  4.036e+06  2.432e+06  1.113e+06  6.538e+05
#       1300  1.167e+05  2.192e+05  6.526e+05  2.255e+06  6.130e+06  9.185e+06  6.866e+06  3.597e+06  2.231e+06
#       1400  1.093e+05  2.169e+05  7.179e+05  2.876e+06  9.404e+06  1.743e+07  1.595e+07  9.584e+06  6.303e+06
#       1500  9.173e+04  1.920e+05  7.034e+05  3.242e+06  1.260e+07  2.845e+07  3.154e+07  2.172e+07  1.520e+07
#       1700  5.175e+04  1.195e+05  5.292e+05  3.162e+06  1.680e+07  5.409e+07  8.502e+07  7.608e+07  6.045e+07
#       2000  1.177e+04  3.088e+04  1.751e+05  1.484e+06  1.218e+07  6.504e+07  1.709e+08  2.289e+08  2.238e+08
#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
pdepreaction(
    reactants = ['c5-C6H9'],
    products = ['c6-C6H9'],
    kinetics = Chebyshev(
        coeffs = [
            [-0.375465, -0.991305, -0.33271, 0.0195019],
            [8.12066, 1.96428, -0.241484, -0.0643821],
            [-0.595777, 0.863497, 0.0303786, -0.043731],
            [-0.308323, 0.286141, 0.0594383, 0.00101115],
            [-0.0038575, 0.0490908, 0.0323449, 0.0111973],
            [-0.119749, 0.0373469, -0.00271808, 0.0114109],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
#         T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
#       300  4.761e-05  4.782e-05  4.802e-05  4.810e-05  4.811e-05  4.811e-05  4.812e-05  4.812e-05  4.812e-05
#       400  2.677e-01  2.759e-01  2.848e-01  2.891e-01  2.902e-01  2.904e-01  2.904e-01  2.904e-01  2.904e-01
#       500  3.973e+01  4.401e+01  4.993e+01  5.390e+01  5.525e+01  5.551e+01  5.555e+01  5.555e+01  5.556e+01
#       600  8.194e+02  1.002e+03  1.334e+03  1.662e+03  1.828e+03  1.870e+03  1.877e+03  1.878e+03  1.879e+03
#       700  5.346e+03  7.184e+03  1.134e+04  1.714e+04  2.154e+04  2.315e+04  2.348e+04  2.354e+04  2.355e+04
#       1000  6.755e+04  1.113e+05  2.598e+05  6.585e+05  1.362e+06  1.990e+06  2.257e+06  2.325e+06  2.340e+06
#       1200  1.058e+05  1.949e+05  5.611e+05  1.889e+06  5.340e+06  1.008e+07  1.306e+07  1.406e+07  1.431e+07
#       1300  1.035e+05  2.016e+05  6.446e+05  2.494e+06  8.234e+06  1.787e+07  2.517e+07  2.800e+07  2.876e+07
#       1400  9.118e+04  1.875e+05  6.642e+05  2.941e+06  1.129e+07  2.816e+07  4.349e+07  5.030e+07  5.226e+07
#       1500  7.286e+04  1.580e+05  6.182e+05  3.125e+06  1.392e+07  4.005e+07  6.840e+07  8.288e+07  8.739e+07
#       1700  3.827e+04  9.159e+04  4.321e+05  2.806e+06  1.662e+07  6.355e+07  1.348e+08  1.828e+08  2.004e+08
#       2000  8.138e+03  2.210e+04  1.332e+05  1.218e+06  1.095e+07  6.624e+07  2.115e+08  3.711e+08  4.519e+08
#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
pdepreaction(
    reactants = ['C6H9'],
    products = ['c6-C6H9'],
    kinetics = Chebyshev(
        coeffs = [
            [1.6983, 0.581594, -0.136529, 0.0077353],
            [5.88262, 0.854621, -0.211129, -0.00861683],
            [-0.454547, 0.571633, -0.0756684, -0.0191914],
            [-0.251799, 0.262295, 0.00166907, -0.0158779],
            [-0.0532867, 0.0549617, 0.0116317, -0.00673999],
            [-0.122271, 0.0899843, 0.0101362, 0.00562527],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
```

```
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#       T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#        300  1.222e+09  1.305e+09  1.165e+09  5.655e+08  1.194e+08  1.819e+07  3.269e+06  9.064e+05  4.577e+05
#        400  2.011e+09  2.485e+09  2.859e+09  2.090e+09  6.690e+08  1.192e+08  2.210e+07  6.164e+06  3.116e+06
#        500  1.745e+09  2.410e+09  3.401e+09  3.384e+09  1.708e+09  4.121e+08  8.331e+07  2.364e+07  1.199e+07
#        600  1.173e+09  1.725e+09  2.769e+09  3.334e+09  2.357e+09  8.176e+08  1.945e+08  5.749e+07  2.942e+07
#        700  8.136e+08  1.246e+09  2.187e+09  2.983e+09  2.581e+09  1.201e+09  3.474e+08  1.097e+08  5.707e+07
#       1000  4.614e+08  7.696e+08  1.658e+09  3.047e+09  3.664e+09  2.635e+09  1.147e+09  4.438e+08  2.459e+08
#       1200  3.361e+08  5.949e+08  1.495e+09  3.537e+09  5.555e+09  5.034e+09  2.672e+09  1.164e+09  6.735e+08
#       1300  2.629e+08  4.782e+08  1.296e+09  3.520e+09  6.519e+09  6.846e+09  4.087e+09  1.912e+09  1.137e+09
#       1400  2.009e+08  3.731e+08  1.074e+09  3.293e+09  7.154e+09  8.752e+09  5.904e+09  2.974e+09  1.821e+09
#       1500  1.483e+08  2.797e+08  8.456e+08  2.878e+09  7.278e+09  1.042e+10  8.012e+09  4.383e+09  2.776e+09
#       1700  7.516e+07  1.449e+08  4.707e+08  1.901e+09  6.327e+09  1.241e+10  1.261e+10  8.300e+09  5.692e+09
#       2000  1.977e+07  3.874e+07  1.338e+08  6.399e+08  2.938e+09  8.916e+09  1.434e+10  1.349e+10  1.103e+10
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
pdepreaction(
    reactants = ['C2H3', 'C4H6'],
    products = ['c6-C6H9'],
    kinetics = Chebyshev(
        coeffs = [
            [8.49877, -0.709162, -0.456759, 0.0407811],
            [0.880771, 1.39175, -0.109562, -0.0959411],
            [-0.149497, 0.450235, 0.0806494, -0.0214873],
            [-0.0322245, 0.16638, 0.0326391, 0.00244741],
            [0.0731329, 0.0776359, -0.0231637, -0.00391509],
            [-0.148168, 0.0962626, 0.0454517, -0.00997423],
        ],
        kunits = 'cm^3/(mol*s)',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#       T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#        300  3.855e-15  3.941e-15  4.058e-15  4.136e-15  4.161e-15  4.165e-15  4.166e-15  4.166e-15  4.166e-15
#        400  4.068e-10  5.093e-10  7.525e-10  1.118e-09  1.390e-09  1.472e-09  1.487e-09  1.489e-09  1.489e-09
#        500  1.652e-06  2.361e-06  4.590e-06  9.917e-06  1.664e-05  1.989e-05  2.060e-05  2.072e-05  2.075e-05
#        600  6.588e-04  1.004e-03  2.197e-03  5.781e-03  1.221e-02  1.669e-02  1.796e-02  1.821e-02  1.826e-02
#        700  4.388e-02  7.142e-02  1.741e-01  5.371e-01  1.406e+00  2.260e+00  2.579e+00  2.649e+00  2.664e+00
#       1000  2.217e+01  4.348e+01  1.458e+02  7.054e+02  3.630e+03  1.202e+04  2.112e+04  2.523e+04  2.637e+04
#       1200  1.447e+02  3.162e+02  1.260e+03  7.348e+03  4.952e+04  2.423e+05  6.067e+05  8.741e+05  9.727e+05
#       1300  2.266e+02  5.255e+02  2.321e+03  1.517e+04  1.165e+05  6.818e+05  2.040e+06  3.286e+06  3.816e+06
#       1400  2.913e+02  7.143e+02  3.485e+03  2.552e+04  2.222e+05  1.535e+06  5.454e+06  9.875e+06  1.205e+07
#       1500  3.214e+02  8.298e+02  4.448e+03  3.644e+04  3.582e+05  2.888e+06  1.210e+07  2.469e+07  3.175e+07
#       1700  2.807e+02  7.930e+02  5.041e+03  5.119e+04  6.337e+05  6.775e+06  3.860e+07  9.969e+07  1.437e+08
#       2000  1.363e+02  4.281e+02  3.358e+03  4.547e+04  7.756e+05  1.198e+07  1.022e+08  3.679e+08  6.308e+08
```

```
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
pdepreaction(
    reactants = ['c5-C6H9-3'],
    products = ['c5-C6H9'],
    kinetics = Chebyshev(
        coeffs = [
            [-4.22675, 1.03932, -0.183831, -0.00856721],
            [10.6796, 1.44063, -0.154651, -0.0425081],
            [-0.00436825, 0.571113, 0.0621454, -0.0233052],
            [-0.508419, 0.239689, 0.0398306, 0.0120182],
            [-0.0970083, 0.102901, 0.00587715, 0.0123211],
            [-0.111453, 0.0193932, 0.00754593, 0.00721637],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
#         T \ P   1.106e-03   2.191e-03   7.920e-03   4.474e-02   3.204e-01   2.295e+00   1.296e+01   4.686e+01   9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
#         300   7.021e-19   7.026e-19   7.031e-19   7.033e-19   7.034e-19   7.034e-19   7.034e-19   7.034e-19   7.034e-19
#         400   3.523e-13   3.748e-13   4.117e-13   4.436e-13   4.572e-13   4.601e-13   4.605e-13   4.606e-13   4.606e-13
#         500   3.525e-09   4.362e-09   6.247e-09   8.875e-09   1.076e-08   1.135e-08   1.146e-08   1.148e-08   1.148e-08
#         600   2.158e-06   3.044e-06   5.526e-06   1.042e-05   1.576e-05   1.825e-05   1.881e-05   1.891e-05   1.893e-05
#         700   1.864e-04   2.938e-04   6.549e-04   1.613e-03   3.135e-03   4.176e-03   4.484e-03   4.546e-03   4.558e-03
#        1000   1.518e-01   2.996e-01   1.043e+00   5.057e+00   2.274e+01   6.237e+01   9.702e+01   1.106e+02   1.142e+02
#        1200   1.341e+00   2.870e+00   1.149e+01   6.907e+01   4.419e+02   1.875e+03   4.124e+03   5.558e+03   6.047e+03
#        1300   2.798e+00   6.245e+00   2.665e+01   1.722e+02   1.239e+03   6.265e+03   1.630e+04   2.425e+04   2.736e+04
#        1400   4.772e+00   1.115e+01   5.115e+01   3.560e+02   2.827e+03   1.662e+04   5.055e+04   8.333e+04   9.800e+04
#        1500   6.804e+00   1.665e+01   8.271e+01   6.265e+02   5.467e+03   3.674e+04   1.291e+05   2.358e+05   2.900e+05
#        1700   9.328e+00   2.499e+01   1.458e+02   1.332e+03   1.409e+04   1.200e+05   5.447e+05   1.207e+06   1.626e+06
#        2000   6.341e+00   1.910e+01   1.396e+02   1.728e+03   2.576e+04   3.216e+05   2.128e+06   6.253e+06   9.692e+06
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
pdepreaction(
    reactants = ['c5-C6H9-2'],
    products = ['c5-C6H9'],
    kinetics = Chebyshev(
        coeffs = [
            [-7.05947, 0.887248, -0.165214, -0.00522622],
            [11.7191, 1.35316, -0.17543, -0.0358811],
            [0.170665, 0.653458, -0.0010266, -0.027088],
            [-0.468057, 0.194129, 0.0566842, -0.0031797],
            [-0.0824761, 0.0326209, 0.0348638, 0.00922296],
            [-0.0698306, 0.0261673, -0.0126101, 0.0158395],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)
```

```
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
#       T \ P   1.106e-03   2.191e-03   7.920e-03   4.474e-02   3.204e-01   2.295e+00   1.296e+01   4.686e+01   9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
#         300   1.211e-11   7.712e-12   2.860e-12   6.038e-13   8.881e-14   1.251e-14   2.217e-15   6.135e-16   3.096e-16
#         400   1.222e-05   9.492e-06   4.957e-06   1.471e-06   2.592e-07   3.826e-08   6.833e-09   1.893e-09   9.556e-10
#         500   3.904e-02   3.599e-02   2.580e-02   1.118e-02   2.623e-03   4.328e-04   7.915e-05   2.202e-05   1.112e-05
#         600   5.196e+00   5.559e+00   5.316e+00   3.372e+00   1.123e+00   2.233e-01   4.302e-02   1.209e-02   6.121e-03
#         700   1.098e+02   1.329e+02   1.629e+02   1.473e+02   7.171e+01   1.851e+01   3.928e+00   1.129e+00   5.746e-01
#        1000   5.047e+03   7.923e+03   1.658e+04   3.409e+04   4.693e+04   3.245e+04   1.249e+04   4.482e+03   2.421e+03
#        1200   1.383e+04   2.451e+04   6.528e+04   1.924e+05   4.268e+05   5.055e+05   3.046e+05   1.394e+05   8.189e+04
#        1300   1.788e+04   3.357e+04   9.993e+04   3.453e+05   9.388e+05   1.407e+06   1.051e+06   5.508e+05   3.416e+05
#        1400   1.984e+04   3.938e+04   1.303e+05   5.220e+05   1.707e+06   3.164e+06   2.896e+06   1.740e+06   1.144e+06
#        1500   1.926e+04   4.030e+04   1.477e+05   6.807e+05   2.644e+06   5.972e+06   6.621e+06   4.559e+06   3.190e+06
#        1700   1.373e+04   3.172e+04   1.404e+05   8.392e+05   4.459e+06   1.435e+07   2.256e+07   2.019e+07   1.604e+07
#        2000   4.025e+03   1.056e+04   5.989e+04   5.074e+05   4.165e+06   2.224e+07   5.844e+07   7.827e+07   7.655e+07
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
pdepreaction(
    reactants = ['c6-C6H9'],
    products = ['c5-C6H9'],
    kinetics = Chebyshev(
        coeffs = [
            [-2.82192, -0.991305, -0.33271, 0.0195019],
            [10.1285, 1.96428, -0.241484, -0.0643821],
            [-0.606546, 0.863497, 0.0303786, -0.043731],
            [-0.31807, 0.286141, 0.0594383, 0.00101115],
            [-0.00745611, 0.0490908, 0.0323449, 0.0111973],
            [-0.122545, 0.0373469, -0.00271808, 0.0114109],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
#       T \ P   1.106e-03   2.191e-03   7.920e-03   4.474e-02   3.204e-01   2.295e+00   1.296e+01   4.686e+01   9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
#         300   5.065e-04   5.312e-04   5.574e-04   5.692e-04   5.718e-04   5.722e-04   5.722e-04   5.723e-04   5.723e-04
#         400   1.510e+00   1.733e+00   2.062e+00   2.294e+00   2.371e+00   2.385e+00   2.387e+00   2.387e+00   2.387e+00
#         500   1.416e+02   1.789e+02   2.500e+02   3.235e+02   3.606e+02   3.696e+02   3.711e+02   3.713e+02   3.713e+02
#         600   2.282e+03   3.147e+03   5.167e+03   8.040e+03   1.016e+04   1.087e+04   1.100e+04   1.102e+04   1.103e+04
#         700   1.291e+04   1.929e+04   3.701e+04   7.040e+04   1.054e+05   1.219e+05   1.257e+05   1.264e+05   1.266e+05
#        1000   6.579e+04   1.208e+05   3.520e+05   1.244e+06   3.772e+06   7.479e+06   9.810e+06   1.056e+07   1.074e+07
#        1200   5.902e+04   1.201e+05   4.261e+05   2.008e+06   8.933e+06   2.669e+07   4.676e+07   5.703e+07   6.017e+07
#        1300   4.693e+04   1.005e+05   3.911e+05   2.083e+06   1.083e+07   3.888e+07   7.969e+07   1.057e+08   1.148e+08
#        1400   3.457e+04   7.787e+04   3.321e+05   1.985e+06   1.185e+07   5.014e+07   1.198e+08   1.745e+08   1.963e+08
#        1500   2.400e+04   5.681e+04   2.651e+05   1.772e+06   1.199e+07   5.881e+07   1.627e+08   2.611e+08   3.058e+08
#        1700   1.013e+04   2.635e+04   1.461e+05   1.212e+06   1.036e+07   6.574e+07   2.369e+08   4.623e+08   5.922e+08
#        2000   2.271e+03   6.654e+03   4.621e+04   5.168e+05   6.139e+06   5.473e+07   2.766e+08   7.089e+08   1.045e+09
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
pdepreaction(
    reactants = ['C6H9'],
    products = ['c5-C6H9'],
    kinetics = Chebyshev(
```

```
        coeffs = [
            [2.33043, 0.752507, -0.16163, 0.0135994],
            [5.28525, 1.17169, -0.177264, -0.0296806],
            [-0.596017, 0.626164, -0.024512, -0.023737],
            [-0.319846, 0.254668, 0.0277677, -0.00389409],
            [-0.105367, 0.0768136, 0.026667, 0.0010852],
            [-0.0831801, 0.00957236, 0.00365477, 0.0169916],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
#      T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
#        300  2.260e+08  2.541e+08  2.819e+08  2.839e+08  2.037e+08  6.709e+07  1.471e+07  4.233e+06  2.153e+06
#        400  6.493e+08  8.240e+08  1.049e+09  1.137e+09  9.251e+08  3.801e+08  9.399e+07  2.785e+07  1.426e+07
#        500  1.224e+09  1.722e+09  2.562e+09  3.054e+09  2.649e+09  1.243e+09  3.392e+08  1.036e+08  5.339e+07
#        600  1.659e+09  2.480e+09  4.138e+09  5.440e+09  5.002e+09  2.605e+09  7.815e+08  2.469e+08  1.283e+08
#        700  1.752e+09  2.728e+09  4.968e+09  7.195e+09  7.131e+09  4.184e+09  1.408e+09  4.662e+08  2.452e+08
#       1000  6.610e+08  1.122e+09  2.523e+09  4.967e+09  6.672e+09  6.049e+09  3.509e+09  1.607e+09  9.424e+08
#       1200  3.184e+08  5.722e+08  1.498e+09  3.823e+09  6.774e+09  7.777e+09  5.912e+09  3.404e+09  2.214e+09
#       1300  2.136e+08  3.936e+08  1.108e+09  3.244e+09  6.792e+09  8.973e+09  7.722e+09  4.953e+09  3.403e+09
#       1400  1.420e+08  2.667e+08  7.945e+08  2.620e+09  6.439e+09  9.850e+09  9.565e+09  6.787e+09  4.922e+09
#       1500  9.395e+07  1.789e+08  5.574e+08  2.034e+09  5.810e+09  1.032e+10  1.131e+10  8.837e+09  6.754e+09
#       1700  4.021e+07  7.801e+07  2.592e+08  1.110e+09  4.138e+09  9.896e+09  1.395e+10  1.317e+10  1.116e+10
#       2000  1.196e+07  2.352e+07  8.221e+07  4.088e+08  2.043e+09  7.193e+09  1.467e+10  1.827e+10  1.798e+10
#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
pdepreaction(
    reactants = ['C2H3', 'C4H6'],
    products = ['c5-C6H9'],
    kinetics = Chebyshev(
        coeffs = [
            [8.68372, -0.254831, -0.470627, -0.0283121],
            [0.839341, 1.09749, 0.0155732, 0.00132926],
            [-0.294739, 0.494532, 0.0589391, -0.0132382],
            [-0.15937, 0.234011, 0.0364223, -0.0138144],
            [0.00556635, 0.0895424, -0.00261702, -0.000606535],
            [-0.0554896, 0.0130651, 0.0171828, -0.00810054],
        ],
        kunits = 'cm^3/(mol*s)',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
#      T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
#        300  3.055e-16  2.222e-16  1.074e-16  3.035e-17  5.208e-18  7.611e-19  1.357e-19  3.757e-20  1.897e-20
#        400  9.127e-10  8.711e-10  6.968e-10  3.636e-10  9.916e-11  1.725e-11  3.184e-12  8.872e-13  4.484e-13
```

```
#        500  1.088e-05  1.226e-05  1.314e-05  1.002e-05  4.002e-06  8.686e-07  1.709e-07  4.821e-08  2.443e-08
#        600  5.921e-03  7.591e-03  1.020e-02  1.034e-02  5.652e-03  1.547e-03  3.323e-04  9.568e-05  4.868e-05
#        700  4.968e-01  7.089e-01  1.157e+00  1.515e+00  1.108e+00  3.898e-01  9.429e-02  2.805e-02  1.438e-02
#       1000  8.017e+02  1.463e+03  3.810e+03  9.569e+03  1.578e+04  1.333e+04  6.077e+03  2.371e+03  1.314e+03
#       1200  7.293e+03  1.533e+04  5.233e+04  1.896e+05  4.792e+05  6.413e+05  4.448e+05  2.246e+05  1.374e+05
#       1300  1.193e+04  2.696e+04  1.059e+05  4.671e+05  1.490e+06  2.536e+06  2.178e+06  1.269e+06  8.244e+05
#       1400  1.590e+04  3.833e+04  1.710e+05  9.031e+05  3.580e+06  7.668e+06  8.101e+06  5.453e+06  3.783e+06
#       1500  1.808e+04  4.618e+04  2.310e+05  1.439e+06  6.983e+06  1.862e+07  2.404e+07  1.869e+07  1.389e+07
#       1700  1.656e+04  4.662e+04  2.837e+05  2.357e+06  1.643e+07  6.553e+07  1.238e+08  1.279e+08  1.094e+08
#       2000  8.418e+03  2.642e+04  2.016e+05  2.365e+06  2.586e+07  1.737e+08  5.487e+08  8.468e+08  8.944e+08
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========  ===========  ===========
pdepreaction(
    reactants = ['c5-C6H9-3'],
    products = ['C6H9'],
    kinetics = Chebyshev(
        coeffs = [
            [-5.06669, -0.670068, -0.421481, 0.0242832],
            [12.6978, 2.01754, -0.215641, -0.0606825],
            [-0.0737803, 0.76957, 0.064936, -0.0269919],
            [-0.317972, 0.336716, 0.0364809, 0.00398741],
            [-0.11587, 0.110047, 0.0135798, 0.00509249],
            [-0.184093, 0.0376307, 0.0108176, 0.00282913],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
#         T \ P   1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
#        300  1.274e-21  8.086e-22  3.060e-22  6.722e-23  1.011e-23  1.431e-24  2.538e-25  7.023e-26  3.545e-26
#        400  1.001e-13  8.116e-14  4.750e-14  1.671e-14  3.357e-15  5.186e-16  9.344e-17  2.592e-17  1.309e-17
#        500  5.754e-09  5.622e-09  4.615e-09  2.470e-09  7.103e-10  1.297e-10  2.434e-11  6.803e-12  3.440e-12
#        600  7.394e-06  8.477e-06  9.306e-06  7.194e-06  2.952e-06  6.694e-07  1.346e-07  3.818e-08  1.937e-08
#        700  9.951e-04  1.308e-03  1.860e-03  2.034e-03  1.202e-03  3.557e-04  7.967e-05  2.321e-05  1.184e-05
#       1000  3.624e+00  6.284e+00  1.536e+01  3.683e+01  5.780e+01  4.486e+01  1.877e+01  6.999e+00  3.824e+00
#       1200  5.407e+01  1.077e+02  3.416e+02  1.171e+03  2.830e+03  3.536e+03  2.252e+03  1.072e+03  6.405e+02
#       1300  1.263e+02  2.692e+02  9.705e+02  3.946e+03  1.160e+04  1.779e+04  1.365e+04  7.364e+03  4.635e+03
#       1400  2.337e+02  5.306e+02  2.158e+03  1.033e+04  3.666e+04  6.815e+04  6.217e+04  3.785e+04  2.515e+04
#       1500  3.535e+02  8.514e+02  3.880e+03  2.173e+04  9.260e+04  2.079e+05  2.241e+05  1.535e+05  1.078e+05
#       1700  5.256e+02  1.404e+03  7.828e+03  5.830e+04  3.507e+05  1.134e+06  1.688e+06  1.451e+06  1.138e+06
#       2000  3.818e+02  1.152e+03  8.215e+03  8.833e+04  8.562e+05  4.781e+06  1.187e+07  1.474e+07  1.382e+07
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========  ===========  ===========
pdepreaction(
    reactants = ['c5-C6H9-2'],
    products = ['C6H9'],
    kinetics = Chebyshev(
        coeffs = [
            [-8.6627, -0.869031, -0.375751, 0.0180916],
            [14.6538, 2.0091, -0.273409, -0.0518914],
            [-0.0950968, 0.815843, 0.0279159, -0.0385745],
            [-0.243705, 0.282, 0.0424103, 0.000821771],
            [-0.0680601, 0.0505952, 0.0202867, 0.00984508],
            [-0.157247, 0.052514, -0.00323284, 0.0023426],
```

```
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#       T \ P   1.106e-03   2.191e-03   7.920e-03   4.474e-02   3.204e-01   2.295e+00   1.296e+01   4.686e+01   9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#        300   2.284e-09   2.295e-09   2.304e-09   2.308e-09   2.308e-09   2.309e-09   2.309e-09   2.309e-09   2.309e-09
#        400   5.935e-04   6.117e-04   6.313e-04   6.408e-04   6.433e-04   6.437e-04   6.438e-04   6.438e-04   6.438e-04
#        500   9.382e-01   1.039e+00   1.179e+00   1.273e+00   1.305e+00   1.311e+00   1.312e+00   1.312e+00   1.312e+00
#        600   9.654e+01   1.181e+02   1.572e+02   1.958e+02   2.154e+02   2.204e+02   2.212e+02   2.213e+02   2.213e+02
#        700   2.011e+03   2.703e+03   4.267e+03   6.447e+03   8.102e+03   8.709e+03   8.834e+03   8.856e+03   8.860e+03
#       1000   2.069e+05   3.409e+05   7.955e+05   2.016e+06   4.170e+06   6.095e+06   6.910e+06   7.120e+06   7.167e+06
#       1200   7.234e+05   1.332e+06   3.835e+06   1.291e+07   3.650e+07   6.892e+07   8.925e+07   9.610e+07   9.781e+07
#       1300   9.584e+05   1.866e+06   5.967e+06   2.309e+07   7.623e+07   1.654e+08   2.330e+08   2.592e+08   2.663e+08
#       1400   1.091e+06   2.244e+06   7.947e+06   3.519e+07   1.351e+08   3.370e+08   5.204e+08   6.019e+08   6.253e+08
#       1500   1.085e+06   2.353e+06   9.208e+06   4.654e+07   2.073e+08   5.966e+08   1.019e+09   1.234e+09   1.302e+09
#       1700   8.103e+05   1.939e+06   9.150e+06   5.942e+07   3.520e+08   1.346e+09   2.855e+09   3.872e+09   4.245e+09
#       2000   2.515e+05   6.830e+05   4.116e+06   3.764e+07   3.385e+08   2.047e+09   6.536e+09   1.147e+10   1.397e+10
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
pdepreaction(
    reactants = ['c6-C6H9'],
    products = ['C6H9'],
    kinetics = Chebyshev(
        coeffs = [
            [0.271931, 0.581594, -0.136529, 0.0077353],
            [8.80946, 0.854621, -0.211129, -0.00861683],
            [-0.43509, 0.571633, -0.0756684, -0.0191914],
            [-0.268193, 0.262295, 0.00166907, -0.0158779],
            [-0.0603887, 0.0549617, 0.0116317, -0.00673999],
            [-0.127798, 0.0899843, 0.0101362, 0.00562527],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#       T \ P   1.106e-03   2.191e-03   7.920e-03   4.474e-02   3.204e-01   2.295e+00   1.296e+01   4.686e+01   9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#        300   6.947e-04   7.285e-04   7.644e-04   7.806e-04   7.842e-04   7.847e-04   7.848e-04   7.848e-04   7.848e-04
#        400   6.271e+00   7.195e+00   8.561e+00   9.523e+00   9.844e+00   9.902e+00   9.910e+00   9.911e+00   9.911e+00
#        500   1.211e+03   1.529e+03   2.137e+03   2.765e+03   3.082e+03   3.159e+03   3.172e+03   3.174e+03   3.174e+03
#        600   3.245e+04   4.474e+04   7.347e+04   1.143e+05   1.444e+05   1.545e+05   1.564e+05   1.567e+05   1.568e+05
#        700   2.676e+05   3.998e+05   7.670e+05   1.459e+06   2.184e+06   2.525e+06   2.606e+06   2.620e+06   2.623e+06
#       1000   2.738e+06   5.027e+06   1.465e+07   5.176e+07   1.570e+08   3.113e+08   4.083e+08   4.396e+08   4.471e+08
#       1200   3.220e+06   6.552e+06   2.325e+07   1.096e+08   4.875e+08   1.456e+09   2.552e+09   3.112e+09   3.283e+09
#       1300   2.837e+06   6.074e+06   2.365e+07   1.260e+08   6.549e+08   2.351e+09   4.818e+09   6.391e+09   6.941e+09
#       1400   2.279e+06   5.133e+06   2.189e+07   1.308e+08   7.809e+08   3.305e+09   7.899e+09   1.150e+10   1.294e+10
```

```
#       1500  1.702e+06  4.031e+06  1.881e+07  1.257e+08  8.507e+08  4.172e+09  1.154e+10  1.853e+10  2.170e+10
#       1700  8.083e+05  2.102e+06  1.166e+07  9.675e+07  8.269e+08  5.246e+09  1.890e+10  3.689e+10  4.726e+10
#       2000  2.052e+05  6.013e+05  4.176e+06  4.670e+07  5.548e+08  4.945e+09  2.499e+10  6.406e+10  9.439e+10
#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
pdepreaction(
    reactants = ['c5-C6H9'],
    products = ['C6H9'],
    kinetics = Chebyshev(
        coeffs = [
            [3.35052, 0.752507, -0.16163, 0.0135994],
            [6.20426, 1.17169, -0.177264, -0.0296806],
            [-0.565791, 0.626164, -0.024512, -0.023737],
            [-0.326494, 0.254668, 0.0277677, -0.00389409],
            [-0.108871, 0.0768136, 0.026667, 0.0010852],
            [-0.085912, 0.00957236, 0.00365477, 0.0169916],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
#       T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
#        300  1.176e+10  1.327e+10  1.489e+10  1.598e+10  1.656e+10  1.680e+10  1.687e+10  1.688e+10  1.688e+10
#        400  2.048e+10  2.611e+10  3.362e+10  3.815e+10  4.045e+10  4.159e+10  4.198e+10  4.206e+10  4.207e+10
#        500  2.655e+10  3.758e+10  5.673e+10  7.047e+10  7.613e+10  7.920e+10  8.045e+10  8.075e+10  8.081e+10
#        600  3.227e+10  4.858e+10  8.240e+10  1.127e+11  1.247e+11  1.301e+11  1.327e+11  1.333e+11  1.335e+11
#        700  3.721e+10  5.837e+10  1.082e+11  1.625e+11  1.866e+11  1.951e+11  1.992e+11  2.004e+11  2.007e+11
#       1000  3.876e+10  6.625e+10  1.516e+11  3.070e+11  4.351e+11  4.822e+11  4.947e+11  4.986e+11  4.997e+11
#       1200  2.425e+10  4.383e+10  1.165e+11  3.060e+11  5.661e+11  7.262e+11  7.772e+11  7.904e+11  7.939e+11
#       1300  1.666e+10  3.086e+10  8.804e+10  2.650e+11  5.785e+11  8.357e+11  9.378e+11  9.656e+11  9.726e+11
#       1400  1.133e+10  2.137e+10  6.444e+10  2.181e+11  5.583e+11  9.213e+11  1.103e+12  1.158e+12  1.173e+12
#       1500  7.663e+09  1.464e+10  4.610e+10  1.724e+11  5.121e+11  9.729e+11  1.263e+12  1.365e+12  1.392e+12
#       1700  3.427e+09  6.662e+09  2.230e+10  9.743e+10  3.762e+11  9.519e+11  1.510e+12  1.784e+12  1.870e+12
#       2000  1.088e+09  2.140e+09  7.512e+09  3.782e+10  1.942e+11  7.154e+11  1.580e+12  2.264e+12  2.553e+12
#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
pdepreaction(
    reactants = ['C2H3', 'C4H6'],
    products = ['C6H9'],
    kinetics = Chebyshev(
        coeffs = [
            [10.7762, 0.463961, -0.141565, 0.0322192],
            [0.622153, 0.595338, -0.187498, -0.00010096],
            [-0.120828, 0.348971, -0.0205171, -0.0362142],
            [-0.136137, 0.201066, 0.0141352, -0.0278014],
            [-0.060671, 0.0996424, -0.00875327, -0.0127666],
            [-0.0798317, 0.0521536, 0.0387642, -0.00442428],
        ],
        kunits = 'cm^3/(mol*s)',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
```

```
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
#       T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
#        300  6.847e-28  6.437e-28  3.945e-28  1.089e-28  1.321e-29  7.063e-31  2.935e-32  2.372e-33  6.109e-34
#        400  7.322e-18  8.729e-18  8.464e-18  3.995e-18  7.291e-19  5.592e-20  2.864e-21  2.455e-22  6.403e-23
#        500  7.101e-12  9.818e-12  1.305e-11  9.662e-12  2.730e-12  2.902e-13  1.814e-14  1.664e-15  4.412e-16
#        600  7.174e-08  1.071e-07  1.704e-07  1.685e-07  6.765e-08  9.784e-09  7.458e-10  7.386e-11  1.998e-11
#        700  5.439e-05  8.515e-05  1.523e-04  1.838e-04  9.685e-05  1.869e-05  1.768e-06  1.927e-07  5.356e-08
#       1000  7.203e+00  1.233e+01  2.795e+01  5.201e+01  5.105e+01  2.139e+01  4.361e+00  7.720e-01  2.571e-01
#       1200  5.037e+02  9.106e+02  2.406e+03  5.990e+03  8.758e+03  5.716e+03  1.777e+03  4.301e+02  1.658e+02
#       1300  1.929e+03  3.573e+03  1.015e+04  2.942e+04  5.392e+04  4.588e+04  1.829e+04  5.290e+03  2.219e+03
#       1400  5.651e+03  1.066e+04  3.203e+04  1.053e+05  2.357e+05  2.558e+05  1.291e+05  4.447e+04  2.033e+04
#       1500  1.339e+04  2.558e+04  8.033e+04  2.935e+05  7.842e+05  1.064e+06  6.707e+05  2.739e+05  1.365e+05
#       1700  4.587e+04  8.915e+04  2.977e+05  1.280e+06  4.601e+06  9.275e+06  8.840e+06  5.015e+06  2.973e+06
#       2000  1.348e+05  2.651e+05  9.286e+05  4.627e+06  2.274e+07  7.288e+07  1.169e+08  1.029e+08  7.785e+07
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
pdepreaction(
    reactants = ['c5-C6H9-3'],
    products = ['C2H3', 'C4H6'],
    kinetics = Chebyshev(
        coeffs = [
            [-11.2864, -1.56987, -0.728015, -0.00185362],
            [18.565, 2.05809, 0.00571449, -0.0802575],
            [0.0208479, 0.637103, 0.164651, -0.0269716],
            [-0.14458, 0.252629, 0.0803021, 0.00207763],
            [-0.043538, 0.130024, 0.0057282, 0.000850452],
            [-0.160642, 0.0119034, 0.0262953, -0.00113866],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
#       T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
#        300  4.158e-35  3.874e-35  2.312e-35  6.113e-36  7.127e-37  3.663e-38  1.493e-39  1.202e-40  3.091e-41
#        400  3.468e-23  4.057e-23  3.733e-23  1.579e-23  2.562e-24  1.811e-25  8.885e-27  7.520e-28  1.956e-28
#        500  3.395e-16  4.638e-16  5.988e-16  4.153e-16  1.040e-16  9.814e-18  5.732e-19  5.142e-20  1.356e-20
#        600  1.156e-11  1.714e-11  2.703e-11  2.676e-11  1.056e-11  1.424e-12  1.015e-13  9.782e-15  2.627e-15
#        700  1.834e-08  2.856e-08  5.090e-08  6.308e-08  3.534e-08  6.958e-09  6.390e-10  6.815e-11  1.881e-11
#       1000  1.174e-02  2.000e-02  4.502e-02  8.434e-02  8.682e-02  3.882e-02  8.081e-03  1.415e-03  4.673e-04
#       1200  1.873e+00  3.375e+00  8.847e+00  2.190e+01  3.220e+01  2.107e+01  6.350e+00  1.472e+00  5.546e-01
#       1300  1.166e+01  2.154e+01  6.070e+01  1.735e+02  3.115e+02  2.520e+02  9.118e+01  2.404e+01  9.637e+00
#       1400  5.222e+01  9.819e+01  2.928e+02  9.461e+02  2.042e+03  2.032e+03  8.836e+02  2.643e+02  1.126e+02
#       1500  1.767e+02  3.368e+02  1.050e+03  3.766e+03  9.629e+03  1.174e+04  6.155e+03  2.097e+03  9.500e+02
#       1700  1.083e+03  2.102e+03  6.980e+03  2.951e+04  1.012e+05  1.805e+05  1.379e+05  6.170e+04  3.186e+04
#       2000  4.921e+03  9.676e+03  3.381e+04  1.669e+05  7.957e+05  2.332e+06  3.106e+06  2.173e+06  1.412e+06
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
pdepreaction(
    reactants = ['c5-C6H9-2'],
```

```
    products = ['C2H3', 'C4H6'],
    kinetics = Chebyshev(
        coeffs = [
            [-15.6958, -1.60522, -0.731863, -0.00901058],
            [21.3659, 1.99503, -0.0372252, -0.082724],
            [-0.0408597, 0.640224, 0.149985, -0.0382539],
            [-0.051249, 0.201093, 0.0758623, 0.00190412],
            [0.0518626, 0.0604535, -0.0136482, 0.00904525],
            [-0.168872, 0.0681449, 0.0292314, -0.0119279],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#       T \ P   1.106e-03   2.191e-03   7.920e-03   4.474e-02   3.204e-01   2.295e+00   1.296e+01   4.686e+01   9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#        300   3.925e-25   4.192e-25   3.741e-25   1.816e-25   3.835e-26   5.842e-27   1.050e-27   2.911e-28   1.470e-28
#        400   2.303e-15   2.846e-15   3.274e-15   2.393e-15   7.661e-16   1.365e-16   2.531e-17   7.059e-18   3.568e-18
#        500   1.122e-09   1.550e-09   2.188e-09   2.176e-09   1.099e-09   2.650e-10   5.358e-11   1.520e-11   7.712e-12
#        600   5.183e-06   7.623e-06   1.224e-05   1.474e-05   1.042e-05   3.614e-06   8.596e-07   2.541e-07   1.300e-07
#        700   1.965e-03   3.009e-03   5.282e-03   7.206e-03   6.234e-03   2.900e-03   8.391e-04   2.650e-04   1.378e-04
#       1000   8.626e+01   1.439e+02   3.100e+02   5.695e+02   6.849e+02   4.925e+02   2.144e+02   8.296e+01   4.596e+01
#       1200   4.609e+03   8.157e+03   2.049e+04   4.849e+04   7.616e+04   6.902e+04   3.664e+04   1.596e+04   9.234e+03
#       1300   1.836e+04   3.339e+04   9.050e+04   2.458e+05   4.552e+05   4.780e+05   2.854e+05   1.335e+05   7.937e+04
#       1400   5.580e+04   1.036e+05   2.984e+05   9.145e+05   1.987e+06   2.431e+06   1.640e+06   8.260e+05   5.058e+05
#       1500   1.344e+05   2.536e+05   7.667e+05   2.610e+06   6.599e+06   9.449e+06   7.265e+06   3.974e+06   2.517e+06
#       1700   4.626e+05   8.917e+05   2.897e+06   1.170e+07   3.894e+07   7.635e+07   7.761e+07   5.108e+07   3.503e+07
#       2000   9.816e+05   1.924e+06   6.643e+06   3.178e+07   1.459e+08   4.428e+08   7.124e+08   6.699e+08   5.478e+08
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
pdepreaction(
    reactants = ['c6-C6H9'],
    products = ['C2H3', 'C4H6'],
    kinetics = Chebyshev(
        coeffs = [
            [-8.79238, -0.709162, -0.456759, 0.0407811],
            [17.0602, 1.39175, -0.109562, -0.0959411],
            [-0.23245, 0.450235, 0.0806494, -0.0214873],
            [-0.097054, 0.16638, 0.0326391, 0.00244741],
            [0.0501556, 0.0776359, -0.0231637, -0.00391509],
            [-0.166513, 0.0962626, 0.0454517, -0.00997423],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#       T \ P   1.106e-03   2.191e-03   7.920e-03   4.474e-02   3.204e-01   2.295e+00   1.296e+01   4.686e+01   9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
```

```
#        300  2.074e-21  2.333e-21  2.588e-21  2.606e-21  1.870e-21  6.158e-22  1.351e-22  3.885e-23  1.976e-23
#        400  1.393e-12  1.767e-12  2.249e-12  2.439e-12  1.984e-12  8.151e-13  2.016e-13  5.973e-14  3.057e-14
#        500  2.849e-07  4.008e-07  5.964e-07  7.109e-07  6.167e-07  2.893e-07  7.897e-08  2.412e-08  1.243e-08
#        600  8.850e-04  1.323e-03  2.207e-03  2.902e-03  2.668e-03  1.390e-03  4.168e-04  1.317e-04  6.842e-05
#        700  2.332e-01  3.630e-01  6.611e-01  9.574e-01  9.488e-01  5.567e-01  1.874e-01  6.204e-02  3.262e-02
#       1000  1.679e+03  2.851e+03  6.412e+03  1.262e+04  1.695e+04  1.537e+04  8.917e+03  4.083e+03  2.395e+03
#       1200  3.486e+04  6.264e+04  1.640e+05  4.185e+05  7.415e+05  8.513e+05  6.471e+05  3.727e+05  2.424e+05
#       1300  9.737e+04  1.795e+05  5.051e+05  1.479e+06  3.097e+06  4.091e+06  3.521e+06  2.259e+06  1.552e+06
#       1400  2.173e+05  4.080e+05  1.216e+06  4.008e+06  9.852e+06  1.507e+07  1.463e+07  1.038e+07  7.530e+06
#       1500  4.058e+05  7.727e+05  2.408e+06  8.786e+06  2.510e+07  4.458e+07  4.887e+07  3.817e+07  2.917e+07
#       1700  9.325e+05  1.809e+06  6.011e+06  2.575e+07  9.596e+07  2.295e+08  3.236e+08  3.054e+08  2.588e+08
#       2000  1.737e+06  3.415e+06  1.194e+07  5.936e+07  2.967e+08  1.045e+09  2.130e+09  2.653e+09  2.611e+09
#        ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
pdepreaction(
    reactants = ['c5-C6H9'],
    products = ['C2H3', 'C4H6'],
    kinetics = Chebyshev(
        coeffs = [
            [-6.16096, -0.254831, -0.470627, -0.0283121],
            [15.0109, 1.09749, 0.0155732, 0.00132926],
            [-0.366923, 0.494532, 0.0589391, -0.0132382],
            [-0.214453, 0.234011, 0.0364223, -0.0138144],
            [-0.0138123, 0.0895424, -0.00261702, -0.000606535],
            [-0.0710389, 0.0130651, 0.0171828, -0.00810054],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#        ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#      T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#        ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#        300  7.870e-20  8.878e-20  9.964e-20  1.069e-19  1.108e-19  1.124e-19  1.129e-19  1.130e-19  1.130e-19
#        400  1.058e-11  1.349e-11  1.737e-11  1.971e-11  2.090e-11  2.148e-11  2.168e-11  2.172e-11  2.173e-11
#        500  7.232e-07  1.024e-06  1.545e-06  1.919e-06  2.074e-06  2.157e-06  2.191e-06  2.199e-06  2.201e-06
#        600  1.211e-03  1.822e-03  3.091e-03  4.228e-03  4.677e-03  4.881e-03  4.977e-03  5.002e-03  5.008e-03
#        700  2.389e-01  3.748e-01  6.945e-01  1.043e+00  1.198e+00  1.253e+00  1.279e+00  1.287e+00  1.288e+00
#       1000  2.366e+03  4.045e+03  9.254e+03  1.874e+04  2.656e+04  2.944e+04  3.020e+04  3.044e+04  3.051e+04
#       1200  4.865e+04  8.792e+04  2.337e+05  6.138e+05  1.136e+06  1.457e+06  1.559e+06  1.586e+06  1.593e+06
#       1300  1.257e+05  2.327e+05  6.641e+05  1.999e+06  4.363e+06  6.303e+06  7.073e+06  7.282e+06  7.336e+06
#       1400  2.631e+05  4.960e+05  1.496e+06  5.062e+06  1.296e+07  2.138e+07  2.560e+07  2.689e+07  2.722e+07
#       1500  4.665e+05  8.913e+05  2.807e+06  1.049e+07  3.117e+07  5.923e+07  7.688e+07  8.309e+07  8.475e+07
#       1700  9.960e+05  1.936e+06  6.482e+06  2.832e+07  1.093e+08  2.767e+08  4.389e+08  5.186e+08  5.436e+08
#       2000  1.748e+06  3.440e+06  1.207e+07  6.078e+07  3.121e+08  1.150e+09  2.539e+09  3.638e+09  4.103e+09
#        ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
pdepreaction(
    reactants = ['C6H9'],
    products = ['C2H3', 'C4H6'],
    kinetics = Chebyshev(
        coeffs = [
            [-5.08853, 0.463961, -0.141565, 0.0322192],
            [13.8747, 0.595338, -0.187498, -0.00010096],
            [-0.223238, 0.348971, -0.0205171, -0.0362142],
            [-0.184572, 0.201066, 0.0141352, -0.0278014],
```

```
            [-0.0765463, 0.0996424, -0.00875327, -0.0127666],
            [-0.0926491, 0.0521536, 0.0387642, -0.00442428],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#      T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#        300  2.232e-27  1.753e-27  8.147e-28  1.790e-28  1.757e-29  7.570e-31  2.890e-32  2.294e-33  5.885e-34
#        400  7.515e-18  7.803e-18  5.953e-18  2.182e-18  3.273e-19  2.119e-20  9.916e-22  8.290e-23  2.151e-23
#        500  3.731e-12  4.653e-12  5.118e-12  3.033e-12  7.046e-13  6.442e-14  3.695e-15  3.298e-16  8.687e-17
#        600  2.388e-08  3.298e-08  4.523e-08  3.729e-08  1.257e-08  1.585e-09  1.115e-10  1.073e-11  2.882e-12
#        700  1.316e-05  1.937e-05  3.068e-05  3.182e-05  1.443e-05  2.460e-06  2.156e-07  2.280e-08  6.286e-09
#       1000  1.021e+00  1.694e+00  3.583e+00  6.060e+00  5.397e+00  2.084e+00  4.020e-01  6.910e-02  2.277e-02
#       1200  5.935e+01  1.053e+02  2.653e+02  6.139e+02  8.292e+02  5.063e+02  1.505e+02  3.555e+01  1.357e+01
#       1300  2.142e+02  3.910e+02  1.069e+03  2.899e+03  4.929e+03  3.932e+03  1.499e+03  4.229e+02  1.756e+02
#       1400  5.919e+02  1.104e+03  3.217e+03  9.998e+03  2.091e+04  2.137e+04  1.034e+04  3.477e+03  1.574e+03
#       1500  1.325e+03  2.510e+03  7.698e+03  2.685e+04  6.762e+04  8.692e+04  5.274e+04  2.107e+04  1.041e+04
#       1700  4.209e+03  8.143e+03  2.678e+04  1.113e+05  3.809e+05  7.317e+05  6.725e+05  3.734e+05  2.193e+05
#       2000  1.137e+04  2.233e+04  7.769e+04  3.796e+05  1.801e+06  5.547e+06  8.608e+06  7.421e+06  5.562e+06
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
pdepreaction(
    reactants = ['c5-C6H9-3'],
    products = ['C6H8', 'H'],
    kinetics = Chebyshev(
        coeffs = [
            [-11.8132, -1.74746, -0.688991, -0.00246999],
            [17.9214, 2.16863, -0.032842, -0.0737918],
            [0.078036, 0.667577, 0.157259, -0.0285577],
            [-0.13908, 0.252705, 0.0828753, 0.000171095],
            [-0.0381007, 0.126294, 0.00626709, 0.00260667],
            [-0.16393, 0.0129025, 0.0252288, -0.00186348],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#      T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#        300  1.715e-34  1.344e-34  6.171e-35  1.316e-35  1.228e-36  5.004e-38  1.870e-39  1.477e-40  3.787e-41
#        400  4.070e-23  4.133e-23  2.983e-23  9.899e-24  1.335e-24  7.905e-26  3.535e-27  2.919e-28  7.553e-29
#        500  1.970e-16  2.418e-16  2.572e-16  1.420e-16  2.927e-17  2.375e-18  1.273e-19  1.111e-20  2.913e-21
#        600  4.154e-12  5.686e-12  7.731e-12  6.387e-12  2.101e-12  2.449e-13  1.607e-14  1.505e-15  4.014e-16
#        700  4.707e-09  6.880e-09  1.088e-08  1.166e-08  5.604e-09  9.624e-10  8.132e-11  8.405e-12  2.301e-12
#       1000  1.707e-03  2.813e-03  5.901e-03  1.007e-02  9.443e-03  3.884e-03  7.608e-04  1.290e-04  4.211e-05
#       1200  2.241e-01  3.956e-01  9.877e-01  2.270e+00  3.086e+00  1.888e+00  5.432e-01  1.228e-01  4.582e-02
```

```
#       1300  1.311e+00  2.384e+00  6.448e+00  1.722e+01  2.865e+01  2.169e+01  7.505e+00  1.932e+00  7.674e-01
#       1400  5.523e+00  1.026e+01  2.961e+01  9.023e+01  1.816e+02  1.698e+02  7.075e+01  2.070e+01  8.742e+00
#       1500  1.762e+01  3.329e+01  1.011e+02  3.455e+02  8.303e+02  9.567e+02  4.827e+02  1.612e+02  7.247e+01
#       1700  9.991e+01  1.929e+02  6.303e+02  2.569e+03  8.361e+03  1.417e+04  1.043e+04  4.573e+03  2.343e+03
#       2000  4.164e+02  8.170e+02  2.833e+03  1.370e+04  6.290e+04  1.766e+05  2.273e+05  1.557e+05  1.004e+05
#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
pdepreaction(
   reactants = ['c5-C6H9-2'],
   products = ['C6H8', 'H'],
   kinetics = Chebyshev(
      coeffs = [
         [-16.177, -1.78347, -0.695788, -0.00888187],
         [20.6675, 2.10304, -0.0711592, -0.0771097],
         [0.0249082, 0.671287, 0.140766, -0.0386516],
         [-0.0470158, 0.203194, 0.0786402, -0.00102705],
         [0.0564251, 0.0546286, -0.0106542, 0.0113712],
         [-0.170341, 0.069072, 0.0257257, -0.0123455],
      ],
      kunits = 's^-1',
      Tmin = (300, 'K'),
      Tmax = (2000, 'K'),
      Pmin = (0.00101325, 'bar'),
      Pmax = (101.325, 'bar'),
   ),
)

#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
#      T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
#        300  2.613e-24  2.484e-24  1.755e-24  6.203e-25  1.100e-25  1.610e-26  2.873e-27  7.959e-28  4.018e-28
#        400  3.624e-15  4.026e-15  3.895e-15  2.232e-15  5.721e-16  9.399e-17  1.714e-17  4.767e-18  2.408e-18
#        500  8.016e-10  1.007e-09  1.225e-09  1.024e-09  4.206e-10  8.947e-11  1.744e-11  4.913e-12  2.488e-12
#        600  2.194e-06  2.980e-06  4.206e-06  4.442e-06  2.687e-06  8.107e-07  1.817e-07  5.289e-08  2.698e-08
#        700  5.781e-04  8.278e-04  1.296e-03  1.583e-03  1.219e-03  4.996e-04  1.343e-04  4.143e-05  2.143e-05
#       1000  1.364e+01  2.188e+01  4.366e+01  7.349e+01  8.202e+01  5.478e+01  2.247e+01  8.452e+00  4.641e+00
#       1200  5.875e+02  1.014e+03  2.409e+03  5.285e+03  7.738e+03  6.606e+03  3.348e+03  1.424e+03  8.170e+02
#       1300  2.189e+03  3.903e+03  1.008e+04  2.549e+04  4.397e+04  4.351e+04  2.485e+04  1.135e+04  6.692e+03
#       1400  6.225e+03  1.138e+04  3.150e+04  9.058e+04  1.839e+05  2.125e+05  1.375e+05  6.773e+04  4.113e+04
#       1500  1.406e+04  2.621e+04  7.676e+04  2.474e+05  5.880e+05  7.986e+05  5.911e+05  3.168e+05  1.991e+05
#       1700  4.452e+04  8.521e+04  2.710e+05  1.049e+06  3.303e+06  6.158e+06  6.034e+06  3.891e+06  2.647e+06
#       2000  8.617e+04  1.684e+05  5.750e+05  2.678e+06  1.179e+07  3.424e+07  5.323e+07  4.902e+07  3.972e+07
#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
pdepreaction(
   reactants = ['c6-C6H9'],
   products = ['C6H8', 'H'],
   kinetics = Chebyshev(
      coeffs = [
         [-9.13935, -0.850646, -0.413789, 0.0391622],
         [16.2264, 1.45883, -0.154793, -0.0877309],
         [-0.16035, 0.479113, 0.0793867, -0.0268637],
         [-0.0895928, 0.169026, 0.0355768, 0.00407956],
         [0.0558803, 0.0725534, -0.0230245, -0.000561009],
         [-0.166022, 0.098572, 0.0423112, -0.0120783],
      ],
      kunits = 's^-1',
      Tmin = (300, 'K'),
      Tmax = (2000, 'K'),
      Pmin = (0.00101325, 'bar'),
```

```
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#       T \ P   1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#        300  1.307e-20  1.388e-20  1.461e-20  1.359e-20  7.651e-21  1.934e-21  3.887e-22  1.099e-22  5.571e-23
#        400  2.014e-12  2.345e-12  2.708e-12  2.746e-12  1.924e-12  6.379e-13  1.431e-13  4.146e-14  2.112e-14
#        500  1.867e-07  2.409e-07  3.176e-07  3.476e-07  2.705e-07  1.074e-07  2.674e-08  7.966e-09  4.083e-09
#        600  3.452e-04  4.792e-04  7.110e-04  8.509e-04  7.163e-04  3.276e-04  9.040e-05  2.784e-05  1.438e-05
#        700  6.360e-02  9.304e-02  1.523e-01  2.006e-01  1.844e-01  9.749e-02  3.039e-02  9.792e-03  5.115e-03
#       1000  2.516e+02  4.126e+02  8.652e+02  1.571e+03  1.993e+03  1.723e+03  9.487e+02  4.206e+02  2.439e+02
#       1200  4.254e+03  7.482e+03  1.864e+04  4.443e+04  7.420e+04  8.186e+04  6.009e+04  3.371e+04  2.168e+04
#       1300  1.114e+04  2.019e+04  5.450e+04  1.497e+05  2.948e+05  3.734e+05  3.112e+05  1.949e+05  1.324e+05
#       1400  2.332e+04  4.325e+04  1.246e+05  3.883e+05  8.996e+05  1.319e+06  1.243e+06  8.636e+05  6.199e+05
#       1500  4.095e+04  7.727e+04  2.346e+05  8.162e+05  2.209e+06  3.766e+06  4.017e+06  3.081e+06  2.333e+06
#       1700  8.684e+04  1.676e+05  5.476e+05  2.264e+06  8.046e+06  1.847e+07  2.534e+07  2.351e+07  1.976e+07
#       2000  1.479e+05  2.902e+05  1.007e+06  4.902e+06  2.366e+07  8.033e+07  1.594e+08  1.953e+08  1.907e+08
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
pdepreaction(
    reactants = ['c5-C6H9'],
    products = ['C6H8', 'H'],
    kinetics = Chebyshev(
        coeffs = [
            [-6.49294, -0.385153, -0.462013, -0.0185916],
            [14.1455, 1.1727, 0.0154697, -0.0129419],
            [-0.28377, 0.510767, 0.0513467, -0.00569626],
            [-0.203702, 0.237768, 0.0325614, -0.0124786],
            [-0.0090311, 0.0865456, -0.00108098, -0.000179131],
            [-0.072978, 0.0141506, 0.0159338, -0.00893771],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#       T \ P   1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#        300  4.665e-19  4.980e-19  5.363e-19  5.670e-19  5.825e-19  5.886e-19  5.901e-19  5.903e-19  5.903e-19
#        400  1.458e-11  1.708e-11  2.005e-11  2.198e-11  2.310e-11  2.364e-11  2.379e-11  2.382e-11  2.383e-11
#        500  4.547e-07  5.915e-07  7.941e-07  9.247e-07  9.868e-07  1.022e-06  1.035e-06  1.038e-06  1.038e-06
#        600  4.556e-04  6.382e-04  9.663e-04  1.220e-03  1.321e-03  1.375e-03  1.397e-03  1.403e-03  1.404e-03
#        700  6.313e-02  9.324e-02  1.559e-01  2.150e-01  2.394e-01  2.493e-01  2.538e-01  2.551e-01  2.554e-01
#       1000  3.469e+02  5.739e+02  1.228e+03  2.300e+03  3.100e+03  3.378e+03  3.454e+03  3.478e+03  3.485e+03
#       1200  5.837e+03  1.034e+04  2.623e+04  6.446e+04  1.127e+05  1.406e+05  1.493e+05  1.515e+05  1.521e+05
#       1300  1.415e+04  2.580e+04  7.078e+04  2.003e+05  4.122e+05  5.753e+05  6.377e+05  6.546e+05  6.590e+05
#       1400  2.782e+04  5.186e+04  1.516e+05  4.860e+05  1.175e+06  1.868e+06  2.202e+06  2.302e+06  2.328e+06
#       1500  4.646e+04  8.802e+04  2.706e+05  9.669e+05  2.728e+06  4.991e+06  6.365e+06  6.840e+06  6.966e+06
#       1700  9.163e+04  1.773e+05  5.845e+05  2.470e+06  9.117e+06  2.220e+07  3.444e+07  4.033e+07  4.216e+07
#       2000  1.472e+05  2.892e+05  1.008e+06  4.980e+06  2.476e+07  8.812e+07  1.899e+08  2.686e+08  3.016e+08
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
```

```
pdepreaction(
    reactants = ['C6H9'],
    products = ['C6H8', 'H'],
    kinetics = Chebyshev(
        coeffs = [
            [-5.36484, 0.426189, -0.123088, 0.024884],
            [12.9471, 0.579498, -0.190569, 0.00692701],
            [-0.139451, 0.361528, -0.03394, -0.0294992],
            [-0.172356, 0.206702, 0.00978877, -0.0281808],
            [-0.069993, 0.0981742, -0.00876636, -0.0138073],
            [-0.0934125, 0.0558341, 0.0386722, -0.00569583],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#       T \ P   1.106e-03   2.191e-03   7.920e-03   4.474e-02   3.204e-01   2.295e+00   1.296e+01   4.686e+01   9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#         300   3.520e+05   2.200e+05   7.530e+04   1.480e+04   2.165e+03   3.079e+02   5.485e+01   1.519e+01   7.671e+00
#         400   7.344e+06   5.575e+06   2.569e+06   6.032e+05   9.246e+04   1.340e+04   2.408e+03   6.688e+02   3.378e+02
#         500   6.519e+07   5.560e+07   3.297e+07   9.972e+06   1.674e+06   2.470e+05   4.484e+04   1.251e+04   6.324e+03
#         600   3.391e+08   3.048e+08   2.083e+08   7.739e+07   1.469e+07   2.219e+06   4.052e+05   1.133e+05   5.737e+04
#         700   1.235e+09   1.142e+09   8.503e+08   3.708e+08   8.082e+07   1.275e+07   2.341e+06   6.561e+05   3.323e+05
#        1000   1.421e+10   1.373e+10   1.191e+10   7.463e+09   2.596e+09   5.407e+08   1.062e+08   3.010e+07   1.528e+07
#        1200   3.556e+10   3.501e+10   3.269e+10   2.519e+10   1.247e+10   3.611e+09   8.287e+08   2.443e+08   1.252e+08
#        1300   4.973e+10   4.926e+10   4.717e+10   3.944e+10   2.305e+10   8.105e+09   2.108e+09   6.489e+08   3.359e+08
#        1400   6.578e+10   6.540e+10   6.364e+10   5.638e+10   3.769e+10   1.587e+10   4.735e+09   1.545e+09   8.124e+08
#        1500   8.349e+10   8.320e+10   8.179e+10   7.546e+10   5.610e+10   2.774e+10   9.543e+09   3.343e+09   1.797e+09
#        1700   1.236e+11   1.234e+11   1.226e+11   1.185e+11   1.017e+11   6.536e+10   2.965e+10   1.234e+10   7.063e+09
#        2000   1.971e+11   1.971e+11   1.967e+11   1.949e+11   1.851e+11   1.515e+11   9.572e+10   5.198e+10   3.368e+10
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
pdepreaction(
    reactants = ['C2H3', 'C4H6'],
    products = ['C6H8', 'H'],
    kinetics = Chebyshev(
        coeffs = [
            [6.6792, -1.80845, -0.196315, 0.040658],
            [3.88336, 0.901089, -0.162162, -0.0538319],
            [0.474631, 0.359441, 0.055788, -0.0542496],
            [0.059377, 0.157939, 0.0619517, -0.0169056],
            [0.0434196, 0.0989454, 0.0156975, -0.00895258],
            [-0.0307807, -0.0125166, 0.0375684, 0.0179681],
        ],
        kunits = 'cm^3/(mol*s)',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#       T \ P   1.106e-03   2.191e-03   7.920e-03   4.474e-02   3.204e-01   2.295e+00   1.296e+01   4.686e+01   9.284e+01
```

```
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
#        300  2.394e-22  1.894e-22  1.309e-22  6.866e-23  1.857e-23  3.132e-24  5.727e-25  1.593e-25  8.047e-26
#        400  2.895e-14  2.336e-14  1.551e-14  9.157e-15  3.625e-15  7.953e-16  1.562e-16  4.404e-17  2.231e-17
#        500  2.322e-09  2.159e-09  1.676e-09  1.086e-09  5.345e-10  1.498e-10  3.250e-11  9.372e-12  4.770e-12
#        600  3.942e-06  4.173e-06  3.977e-06  3.104e-06  1.879e-06  6.628e-07  1.620e-07  4.829e-08  2.476e-08
#        700  7.666e-04  8.959e-04  1.017e-03  9.662e-04  7.291e-04  3.284e-04  9.320e-05  2.916e-05  1.512e-05
#       1000  7.873e+00  1.126e+01  1.872e+01  2.886e+01  3.973e+01  3.942e+01  2.234e+01  9.843e+00  5.685e+00
#       1200  2.102e+02  3.346e+02  6.877e+02  1.379e+03  2.464e+03  3.435e+03  2.862e+03  1.657e+03  1.072e+03
#       1300  5.667e+02  9.466e+02  2.161e+03  5.021e+03  1.046e+04  1.742e+04  1.758e+04  1.175e+04  8.119e+03
#       1400  1.212e+03  2.105e+03  5.254e+03  1.399e+04  3.382e+04  6.645e+04  8.025e+04  6.174e+04  4.567e+04
#       1500  2.165e+03  3.879e+03  1.044e+04  3.151e+04  8.788e+04  2.014e+05  2.877e+05  2.536e+05  2.009e+05
#       1700  4.730e+03  8.854e+03  2.676e+04  9.956e+04  3.608e+05  1.092e+06  2.106e+06  2.393e+06  2.170e+06
#       2000  8.742e+03  1.696e+04  5.698e+04  2.646e+05  1.313e+06  5.591e+06  1.556e+07  2.452e+07  2.677e+07
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
pdepreaction(
    reactants = ['c5-C6H9-3'],
    products = ['H', 'c5-C6H8'],
    kinetics = Chebyshev(
        coeffs = [
            [-8.60921, -0.693143, -0.341046, -0.0223554],
            [14.8239, 1.55832, -0.00650143, -0.0417203],
            [0.102675, 0.660428, 0.0449477, 0.00855428],
            [-0.180338, 0.232439, 0.0495083, -0.00210181],
            [-0.0762401, 0.0505914, 0.0199324, 0.0108358],
            [-0.142129, 0.0180059, -0.000365297, -0.00281166],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
#         T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
#        300  8.950e-29  7.369e-29  5.135e-29  2.396e-29  5.572e-30  8.846e-31  1.599e-31  4.438e-32  2.241e-32
#        400  3.926e-19  3.199e-19  2.175e-19  1.222e-19  4.107e-20  8.023e-21  1.524e-21  4.270e-22  2.160e-22
#        500  2.329e-13  2.147e-13  1.671e-13  1.062e-13  4.598e-14  1.126e-14  2.316e-15  6.598e-16  3.350e-16
#        600  1.143e-09  1.213e-09  1.199e-09  9.885e-10  5.671e-10  1.774e-10  4.065e-11  1.190e-11  6.077e-12
#        700  4.092e-07  4.810e-07  5.769e-07  6.207e-07  4.920e-07  2.065e-07  5.511e-08  1.688e-08  8.708e-09
#       1000  1.571e-02  2.230e-02  3.750e-02  6.315e-02  9.961e-02  1.033e-01  5.659e-02  2.411e-02  1.375e-02
#       1200  8.865e-01  1.395e+00  2.838e+00  5.810e+00  1.103e+01  1.570e+01  1.253e+01  6.924e+00  4.383e+00
#       1300  3.790e+00  6.256e+00  1.402e+01  3.225e+01  6.711e+01  1.070e+02  9.875e+01  6.132e+01  4.099e+01
#       1400  1.215e+01  2.087e+01  5.100e+01  1.323e+02  3.069e+02  5.464e+02  5.735e+02  3.961e+02  2.792e+02
#       1500  3.054e+01  5.418e+01  1.429e+02  4.170e+02  1.093e+03  2.189e+03  2.596e+03  1.980e+03  1.468e+03
#       1700  1.167e+02  2.171e+02  6.451e+02  2.321e+03  7.821e+03  2.001e+04  3.001e+04  2.743e+04  2.234e+04
#       2000  3.259e+02  6.306e+02  2.102e+03  9.582e+03  4.548e+04  1.713e+05  3.781e+05  4.642e+05  4.385e+05
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
pdepreaction(
    reactants = ['c5-C6H9-2'],
    products = ['H', 'c5-C6H8'],
    kinetics = Chebyshev(
        coeffs = [
            [-12.6512, -0.734788, -0.366545, -0.0176105],
            [17.2203, 1.50407, -0.028601, -0.054758],
```

```
            [0.0665877, 0.639187, 0.0329417, -0.00132882],
            [-0.0949243, 0.180608, 0.0415634, 0.000158993],
            [0.000643373, -0.0289819, 0.020932, 0.0194438],
            [-0.132404, 0.0660623, -0.0189892, -0.0101255],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#      T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#        300  3.226e-18  1.918e-18  5.550e-19  5.982e-20  2.256e-21  5.258e-23  1.698e-24  1.306e-25  3.330e-26
#        400  1.033e-10  7.753e-11  3.475e-11  6.617e-12  4.379e-13  1.382e-14  4.826e-16  3.766e-17  9.630e-18
#        500  2.267e-06  2.031e-06  1.321e-06  4.300e-07  4.989e-08  2.303e-09  9.221e-11  7.421e-12  1.910e-12
#        600  1.173e-03  1.181e-03  9.939e-04  4.976e-04  9.906e-05  7.138e-06  3.509e-07  2.987e-08  7.785e-09
#        700  8.563e-02  9.349e-02  9.318e-02  6.283e-02  1.947e-02  2.210e-03  1.425e-04  1.331e-05  3.551e-06
#       1000  1.751e+02  2.285e+02  3.179e+02  3.549e+02  2.466e+02  8.264e+01  1.363e+01  2.068e+00  6.471e-01
#       1200  3.022e+03  4.422e+03  7.632e+03  1.121e+04  1.078e+04  5.542e+03  1.459e+03  3.084e+02  1.111e+02
#       1300  7.997e+03  1.236e+04  2.380e+04  4.058e+04  4.603e+04  2.857e+04  9.227e+03  2.286e+03  8.879e+02
#       1400  1.681e+04  2.719e+04  5.777e+04  1.135e+05  1.516e+05  1.125e+05  4.376e+04  1.259e+04  5.267e+03
#       1500  2.891e+04  4.863e+04  1.125e+05  2.526e+05  3.963e+05  3.503e+05  1.629e+05  5.411e+04  2.437e+04
#       1700  5.657e+04  1.008e+05  2.677e+05  7.568e+05  1.604e+06  1.982e+06  1.286e+06  5.592e+05  2.904e+05
#       2000  5.867e+04  1.103e+05  3.367e+05  1.243e+06  3.907e+06  7.825e+06  8.454e+06  5.614e+06  3.673e+06
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
pdepreaction(
    reactants = ['c6-C6H9'],
    products = ['H', 'c5-C6H8'],
    kinetics = Chebyshev(
        coeffs = [
            [-7.37987, -2.34366, -0.590291, 0.0171028],
            [13.931, 2.29142, -0.0984562, -0.0966069],
            [-0.118318, 0.725204, 0.133946, -0.0210735],
            [-0.103276, 0.193537, 0.0626255, 0.0172003],
            [0.0540306, 0.0289723, -0.00764118, 0.0230832],
            [-0.189994, 0.0728011, 0.00343631, -0.0139583],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#      T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#        300  1.692e-13  2.713e-13  6.213e-13  1.277e-12  1.704e-12  1.804e-12  1.819e-12  1.822e-12  1.822e-12
#        400  1.385e-07  1.989e-07  4.358e-07  1.071e-06  1.770e-06  2.027e-06  2.074e-06  2.081e-06  2.083e-06
#        500  6.578e-04  8.536e-04  1.617e-03  4.064e-03  7.880e-03  9.933e-03  1.040e-02  1.049e-02  1.050e-02
#        600  1.814e-01  2.285e-01  3.935e-01  9.712e-01  2.152e+00  3.035e+00  3.293e+00  3.343e+00  3.353e+00
#        700  8.535e+00  1.089e+01  1.818e+01  4.440e+01  1.125e+02  1.826e+02  2.094e+02  2.153e+02  2.165e+02
```

```
#       1000  2.829e+03  4.039e+03  7.358e+03  1.808e+04  6.619e+04  2.018e+05  3.493e+05  4.162e+05  4.347e+05
#       1200  1.933e+04  3.030e+04  6.321e+04  1.577e+05  5.682e+05  2.227e+06  5.279e+06  7.509e+06  8.330e+06
#       1300  3.624e+04  5.949e+04  1.349e+05  3.551e+05  1.244e+06  5.168e+06  1.401e+07  2.199e+07  2.537e+07
#       1400  5.683e+04  9.705e+04  2.383e+05  6.785e+05  2.378e+06  1.020e+07  3.098e+07  5.358e+07  6.454e+07
#       1500  7.756e+04  1.369e+05  3.613e+05  1.125e+06  4.067e+06  1.780e+07  5.927e+07  1.125e+08  1.417e+08
#       1700  1.083e+05  2.007e+05  5.954e+05  2.214e+06  9.062e+06  4.152e+07  1.576e+08  3.512e+08  4.835e+08
#       2000  1.199e+05  2.317e+05  7.704e+05  3.547e+06  1.830e+07  9.479e+07  4.068e+08  1.077e+09  1.661e+09
#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
pdepreaction(
    reactants = ['c5-C6H9'],
    products = ['H', 'c5-C6H8'],
    kinetics = Chebyshev(
        coeffs = [
            [-2.01313, 0.927848, -0.204489, 0.000499374],
            [9.90227, 0.659202, 0.125515, -0.0598011],
            [-0.313738, 0.331313, 0.0365529, 0.0225285],
            [-0.223578, 0.151484, -0.00504446, 0.0302152],
            [-0.061939, 0.0190835, 0.0104195, 0.0227911],
            [-0.0489561, 0.00473997, -0.0221638, -0.00471135],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
#         T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
#         300  1.135e-12  1.090e-12  8.639e-13  3.964e-13  8.624e-14  1.333e-14  2.397e-15  6.649e-16  3.357e-16
#         400  4.105e-07  4.136e-07  3.801e-07  2.408e-07  7.536e-08  1.377e-08  2.568e-09  7.167e-10  3.624e-10
#         500  9.368e-04  9.769e-04  9.661e-04  7.340e-04  3.061e-04  6.830e-05  1.354e-05  3.826e-06  1.939e-06
#         600  1.620e-01  1.776e-01  1.888e-01  1.619e-01  8.405e-02  2.295e-02  4.938e-03  1.422e-03  7.239e-04
#         700  6.162e+00  7.162e+00  8.312e+00  7.962e+00  4.993e+00  1.683e+00  4.034e-01  1.198e-01  6.138e-02
#        1000  3.120e+03  4.309e+03  6.686e+03  8.924e+03  8.955e+03  6.022e+03  2.564e+03  9.826e+02  5.424e+02
#        1200  2.175e+04  3.361e+04  6.465e+04  1.120e+05  1.431e+05  1.282e+05  7.662e+04  3.706e+04  2.240e+04
#        1300  3.782e+04  6.148e+04  1.316e+05  2.639e+05  3.891e+05  3.971e+05  2.738e+05  1.486e+05  9.467e+04
#        1400  5.536e+04  9.383e+04  2.204e+05  5.079e+05  8.694e+05  1.012e+06  7.952e+05  4.816e+05  3.239e+05
#        1500  7.077e+04  1.241e+05  3.155e+05  8.270e+05  1.645e+06  2.194e+06  1.951e+06  1.311e+06  9.304e+05
#        1700  8.664e+04  1.594e+05  4.582e+05  1.494e+06  3.948e+06  6.961e+06  7.882e+06  6.429e+06  5.066e+06
#        2000  7.453e+04  1.429e+05  4.610e+05  1.907e+06  7.196e+06  1.890e+07  3.059e+07  3.279e+07  2.999e+07
#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
pdepreaction(
    reactants = ['C6H9'],
    products = ['H', 'c5-C6H8'],
    kinetics = Chebyshev(
        coeffs = [
            [-3.33453, -0.88123, -0.396374, 0.0255967],
            [10.2417, 1.34778, -0.038539, -0.0608698],
            [-0.0286965, 0.550773, 0.0469106, -0.00329073],
            [-0.150456, 0.239108, 0.0169695, 0.00602101],
            [-0.0742394, 0.0740814, 0.000132583, 0.00772617],
            [-0.130736, 0.025022, 0.00749341, -0.011612],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
```

```
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#       T \ P   1.106e-03   2.191e-03   7.920e-03   4.474e-02   3.204e-01   2.295e+00   1.296e+01   4.686e+01   9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#        300   3.877e+07   2.282e+07   7.272e+06   1.330e+06   1.438e+05   7.576e+03   3.146e+02   2.543e+01   6.549e+00
#        400   2.636e+08   1.834e+08   7.293e+07   1.515e+07   1.900e+06   1.343e+05   6.799e+03   5.817e+02   1.517e+02
#        500   9.412e+08   7.428e+08   3.724e+08   9.351e+07   1.298e+07   1.090e+06   6.489e+04   5.897e+03   1.561e+03
#        600   2.317e+09   1.956e+09   1.144e+09   3.435e+08   5.314e+07   5.050e+06   3.444e+05   3.327e+04   8.950e+03
#        700   4.613e+09   4.053e+09   2.629e+09   9.217e+08   1.616e+08   1.740e+07   1.368e+06   1.423e+05   3.913e+04
#       1000   1.572e+10   1.477e+10   1.171e+10   6.070e+09   1.672e+09   2.790e+08   3.755e+07   5.848e+06   1.885e+06
#       1200   2.261e+10   2.192e+10   1.933e+10   1.288e+10   5.091e+09   1.177e+09   2.076e+08   4.084e+07   1.486e+07
#       1300   2.483e+10   2.433e+10   2.235e+10   1.660e+10   7.884e+09   2.208e+09   4.511e+08   9.900e+07   3.821e+07
#       1400   2.625e+10   2.591e+10   2.448e+10   1.976e+10   1.098e+10   3.699e+09   8.781e+08   2.144e+08   8.760e+07
#       1500   2.703e+10   2.681e+10   2.583e+10   2.219e+10   1.408e+10   5.632e+09   1.554e+09   4.218e+08   1.823e+08
#       1700   2.731e+10   2.722e+10   2.680e+10   2.493e+10   1.925e+10   1.037e+10   3.846e+09   1.296e+09   6.263e+08
#       2000   2.685e+10   2.683e+10   2.672e+10   2.615e+10   2.367e+10   1.733e+10   9.336e+09   4.277e+09   2.441e+09
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
pdepreaction(
    reactants = ['C2H3', 'C4H6'],
    products = ['H', 'c5-C6H8'],
    kinetics = Chebyshev(
        coeffs = [
            [7.03723, -2.49467, -0.465934, -0.0321309],
            [2.78575, 1.32249, 0.0298486, -0.0174021],
            [0.326843, 0.474717, 0.09139, -0.0201718],
            [0.0414546, 0.192606, 0.0624393, -0.0145524],
            [0.0316899, 0.0892865, 0.00877387, -0.00635135],
            [-0.0637897, -0.024337, 0.0235093, 0.00496257],
        ],
        kunits = 'cm^3/(mol*s)',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#       T \ P   1.106e-03   2.191e-03   7.920e-03   4.474e-02   3.204e-01   2.295e+00   1.296e+01   4.686e+01   9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#        300   2.158e-20   7.556e-21   7.956e-22   2.174e-23   1.642e-25   6.368e-28   3.789e-30   8.118e-32   1.046e-32
#        400   2.922e-12   1.514e-12   3.243e-13   2.099e-14   3.609e-16   2.393e-18   1.706e-20   3.798e-22   4.934e-23
#        500   1.882e-07   1.306e-07   4.948e-08   7.030e-09   2.756e-10   3.385e-12   3.183e-14   7.644e-16   1.010e-16
#        600   2.307e-04   1.939e-04   1.082e-04   2.749e-05   2.203e-06   5.199e-08   7.095e-10   1.932e-11   2.633e-12
#        700   3.197e-02   3.065e-02   2.227e-02   8.454e-03   1.160e-03   4.895e-05   1.016e-06   3.311e-08   4.747e-09
#       1000   1.436e+02   1.774e+02   2.132e+02   1.708e+02   6.451e+01   9.384e+00   6.193e-01   4.049e-02   7.519e-03
#       1200   2.639e+03   3.727e+03   5.853e+03   6.898e+03   4.221e+03   1.069e+03   1.224e+02   1.201e+01   2.687e+00
#       1300   6.119e+03   9.196e+03   1.646e+04   2.365e+04   1.867e+04   6.322e+03   9.586e+02   1.160e+02   2.876e+01
#       1400   1.131e+04   1.790e+04   3.582e+04   6.138e+04   6.109e+04   2.708e+04   5.352e+03   7.931e+02   2.176e+02
#       1500   1.750e+04   2.889e+04   6.363e+04   1.275e+05   1.570e+05   8.949e+04   2.278e+04   4.114e+03   1.250e+03
#       1700   2.844e+04   5.002e+04   1.281e+05   3.331e+05   5.925e+05   5.291e+05   2.139e+05   5.608e+04   2.079e+04
#       2000   3.144e+04   5.860e+04   1.746e+05   6.077e+05   1.690e+06   2.698e+06   2.067e+06   9.358e+05   4.709e+05
```

```
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
pdepreaction(
    reactants = ['c5-C6H9-3'],
    products = ['H', 'C6H8-c6-13'],
    kinetics = Chebyshev(
        coeffs = [
            [-9.66241, -3.77018, -0.750581, 0.00332112],
            [15.9135, 3.22017, -0.148093, -0.1148],
            [-0.138056, 0.881368, 0.192621, -0.0175047],
            [-0.255711, 0.219938, 0.0869974, 0.018726],
            [-0.0235118, 0.0685446, -0.0106379, 0.0126027],
            [-0.146448, 0.0788741, 0.0229919, -0.0095684],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
#         T \ P   1.106e-03   2.191e-03   7.920e-03   4.474e-02   3.204e-01   2.295e+00   1.296e+01   4.686e+01   9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
#         300   9.107e-27   2.831e-27   2.418e-28   5.120e-30   3.079e-32   1.074e-34   6.241e-37   1.331e-38   1.714e-39
#         400   4.880e-17   2.242e-17   3.839e-18   1.882e-19   2.498e-21   1.401e-23   9.404e-26   2.066e-27   2.676e-28
#         500   2.440e-11   1.544e-11   4.895e-12   5.415e-13   1.618e-14   1.615e-16   1.381e-18   3.229e-20   4.240e-21
#         600   8.758e-08   6.973e-08   3.521e-08   7.693e-09   5.034e-10   9.739e-12   1.181e-13   3.087e-15   4.163e-16
#         700   2.189e-05   2.033e-05   1.413e-05   5.065e-06   6.283e-07   2.305e-08   4.286e-10   1.330e-11   1.880e-12
#        1000   3.284e-01   3.967e-01   4.657e-01   3.741e-01   1.434e-01   2.043e-02   1.270e-03   7.891e-05   1.434e-05
#        1200   1.222e+01   1.688e+01   2.569e+01   2.967e+01   1.793e+01   4.368e+00   4.650e-01   4.268e-02   9.246e-03
#        1300   4.425e+01   6.502e+01   1.122e+02   1.551e+02   1.168e+02   3.643e+01   4.922e+00   5.393e-01   1.273e-01
#        1400   1.213e+02   1.879e+02   3.622e+02   5.911e+02   5.488e+02   2.164e+02   3.663e+01   4.746e+00   1.216e+00
#        1500   2.620e+02   4.243e+02   9.010e+02   1.713e+03   1.944e+03   9.652e+02   2.041e+02   3.126e+01   8.699e+00
#        1700   7.375e+02   1.278e+03   3.173e+03   7.835e+03   1.274e+04   9.720e+03   3.149e+03   6.675e+02   2.190e+02
#        2000   1.219e+03   2.255e+03   6.589e+03   2.212e+04   5.756e+04   8.099e+04   5.093e+04   1.864e+04   8.200e+03
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
pdepreaction(
    reactants = ['c5-C6H9-2'],
    products = ['H', 'C6H8-c6-13'],
    kinetics = Chebyshev(
        coeffs = [
            [-13.7935, -3.9244, -0.7304, 0.000704993],
            [18.4052, 3.22716, -0.210529, -0.114655],
            [-0.161327, 0.913647, 0.173537, -0.0295811],
            [-0.181815, 0.177395, 0.0902705, 0.0157778],
            [0.0609874, -0.0103644, -0.00987151, 0.0207065],
            [-0.137829, 0.121936, 0.010794, -0.0134343],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)
```

```
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
#       T \ P   1.106e-03   2.191e-03   7.920e-03   4.474e-02   3.204e-01   2.295e+00   1.296e+01   4.686e+01   9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
#        300   1.643e-12   1.666e-12   1.685e-12   1.691e-12   1.692e-12   1.693e-12   1.693e-12   1.693e-12   1.693e-12
#        400   2.042e-06   2.183e-06   2.343e-06   2.420e-06   2.438e-06   2.441e-06   2.442e-06   2.442e-06   2.442e-06
#        500   7.692e-03   9.048e-03   1.127e-02   1.303e-02   1.367e-02   1.379e-02   1.381e-02   1.381e-02   1.381e-02
#        600   1.345e+00   1.750e+00   2.643e+00   3.770e+00   4.468e+00   4.667e+00   4.702e+00   4.707e+00   4.708e+00
#        700   4.218e+01   5.911e+01   1.052e+02   1.886e+02   2.702e+02   3.063e+02   3.146e+02   3.161e+02   3.164e+02
#       1000   1.383e+04   2.111e+04   4.723e+04   1.315e+05   3.225e+05   5.382e+05   6.463e+05   6.768e+05   6.838e+05
#       1200   1.127e+05   1.768e+05   4.138e+05   1.304e+06   4.088e+06   8.833e+06   1.236e+07   1.368e+07   1.402e+07
#       1300   2.305e+05   3.699e+05   8.888e+05   2.911e+06   1.005e+07   2.462e+07   3.768e+07   4.328e+07   4.485e+07
#       1400   3.981e+05   6.566e+05   1.637e+06   5.572e+06   2.087e+07   5.744e+07   9.635e+07   1.155e+08   1.212e+08
#       1500   5.904e+05   1.002e+06   2.614e+06   9.309e+06   3.752e+07   1.154e+08   2.129e+08   2.679e+08   2.858e+08
#       1700   9.558e+05   1.712e+06   4.913e+06   1.944e+07   8.937e+07   3.339e+08   7.426e+08   1.040e+09   1.153e+09
#       2000   9.478e+05   1.800e+06   5.838e+06   2.728e+07   1.522e+08   7.504e+08   2.295e+09   4.030e+09   4.923e+09
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
pdepreaction(
    reactants = ['c6-C6H9'],
    products = ['H', 'C6H8-c6-13'],
    kinetics = Chebyshev(
        coeffs = [
            [-1.55849, 0.54638, -0.116951, 0.000801956],
            [10.1654, 0.764416, -0.126873, -0.036163],
            [-0.283868, 0.41961, -0.00826341, -0.0300908],
            [-0.163762, 0.134255, 0.0404668, -0.0114976],
            [-0.0174988, -0.00545237, 0.0308966, -0.000504856],
            [-0.0879932, 0.0576707, -0.00460253, 0.015857],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
#       T \ P   1.106e-03   2.191e-03   7.920e-03   4.474e-02   3.204e-01   2.295e+00   1.296e+01   4.686e+01   9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
#        300   2.962e-11   1.395e-11   2.697e-12   1.839e-13   5.112e-15   1.083e-16   3.438e-18   2.637e-19   6.719e-20
#        400   2.705e-05   1.647e-05   5.152e-06   6.512e-07   3.072e-08   8.212e-10   2.748e-11   2.127e-12   5.430e-13
#        500   1.096e-01   8.267e-02   3.926e-02   8.702e-03   7.153e-04   2.689e-05   1.004e-06   7.954e-08   2.040e-08
#        600   2.040e+01   1.793e+01   1.172e+01   4.207e+00   6.001e-01   3.436e-02   1.533e-03   1.272e-04   3.296e-05
#        700   6.117e+02   5.977e+02   4.882e+02   2.517e+02   5.802e+01   5.211e+00   2.985e-01   2.684e-02   7.093e-03
#       1000   6.871e+04   8.278e+04   1.012e+05   9.748e+04   5.730e+04   1.617e+04   2.347e+03   3.336e+02   1.021e+02
#       1200   2.983e+05   4.074e+05   6.263e+05   8.081e+05   6.811e+05   3.064e+05   7.223e+04   1.430e+04   5.023e+03
#       1300   4.685e+05   6.800e+05   1.174e+06   1.765e+06   1.766e+06   9.698e+05   2.826e+05   6.569e+04   2.485e+04
#       1400   6.228e+05   9.531e+05   1.830e+06   3.182e+06   3.760e+06   2.485e+06   8.782e+05   2.375e+05   9.676e+04
#       1500   7.258e+05   1.162e+06   2.452e+06   4.894e+06   6.812e+06   5.387e+06   2.285e+06   7.146e+05   3.134e+05
#       1700   7.403e+05   1.272e+06   3.135e+06   7.977e+06   1.508e+07   1.674e+07   9.961e+06   4.087e+06   2.067e+06
#       2000   4.836e+05   8.896e+05   2.581e+06   8.762e+06   2.488e+07   4.513e+07   4.489e+07   2.816e+07   1.792e+07
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
pdepreaction(
    reactants = ['c5-C6H9'],
    products = ['H', 'C6H8-c6-13'],
    kinetics = Chebyshev(
```

```
        coeffs = [
            [-3.41079, -2.60968, -0.516406, 0.0155777],
            [11.1305, 2.38451, -0.166336, -0.086944],
            [-0.376929, 0.782777, 0.120294, -0.0281153],
            [-0.30934, 0.200766, 0.0675105, 0.0155398],
            [-0.00747584, 0.0165238, 0.00285285, 0.0241798],
            [-0.0436288, 0.0703031, -0.00359591, -0.00947177],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#         T \ P   1.106e-03   2.191e-03   7.920e-03   4.474e-02   3.204e-01   2.295e+00   1.296e+01   4.686e+01   9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#         300   9.928e-10   5.399e-10   1.609e-10   2.947e-11   4.153e-12   5.807e-13   1.028e-13   2.845e-14   1.436e-14
#         400   1.645e-04   1.070e-04   4.093e-05   8.874e-06   1.326e-06   1.878e-07   3.332e-08   9.220e-09   4.654e-09
#         500   2.204e-01   1.742e-01   9.433e-02   2.938e-02   5.393e-03   8.109e-04   1.455e-04   4.033e-05   2.036e-05
#         600   2.215e+01   2.022e+01   1.465e+01   6.770e+00   1.754e+00   3.095e-01   5.780e-02   1.615e-02   8.165e-03
#         700   5.005e+02   5.043e+02   4.461e+02   2.793e+02   1.021e+02   2.283e+01   4.644e+00   1.324e+00   6.724e-01
#        1000   8.010e+04   9.852e+04   1.253e+05   1.294e+05   8.910e+04   3.669e+04   1.068e+04   3.458e+03   1.816e+03
#        1200   3.522e+05   4.908e+05   7.830e+05   1.065e+06   9.847e+05   5.483e+05   2.007e+05   7.249e+04   3.940e+04
#        1300   5.148e+05   7.617e+05   1.364e+06   2.156e+06   2.333e+06   1.515e+06   6.266e+05   2.415e+05   1.342e+05
#        1400   6.455e+05   1.006e+06   1.999e+06   3.652e+06   4.631e+06   3.506e+06   1.642e+06   6.780e+05   3.864e+05
#        1500   7.172e+05   1.168e+06   2.547e+06   5.333e+06   7.926e+06   7.029e+06   3.752e+06   1.673e+06   9.815e+05
#        1700   6.824e+05   1.189e+06   3.014e+06   8.023e+06   1.611e+07   1.958e+07   1.370e+07   7.237e+06   4.548e+06
#        2000   4.205e+05   7.804e+05   2.313e+06   8.161e+06   2.446e+07   4.773e+07   5.319e+07   3.942e+07   2.900e+07
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
pdepreaction(
    reactants = ['C6H9'],
    products = ['H', 'C6H8-c6-13'],
    kinetics = Chebyshev(
        coeffs = [
            [-1.97166, -1.42391, -0.239695, 0.00748731],
            [9.51721, 1.40689, -0.280108, -0.0156966],
            [-0.171151, 0.646985, 0.00282147, -0.0444025],
            [-0.262554, 0.198635, 0.0486177, -0.00865579],
            [-0.0649378, 0.0283007, -0.00234736, 0.0153455],
            [-0.0639209, 0.114525, 0.0141026, -0.00882527],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#         T \ P   1.106e-03   2.191e-03   7.920e-03   4.474e-02   3.204e-01   2.295e+00   1.296e+01   4.686e+01   9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#         300   1.506e+09   8.405e+08   2.211e+08   2.119e+07   6.871e+05   1.502e+04   4.802e+02   3.687e+01   9.398e+00
#         400   7.687e+09   5.126e+09   1.831e+09   2.776e+08   1.524e+07   4.235e+05   1.428e+04   1.107e+03   2.829e+02
```

```
#        500  2.046e+10  1.555e+10  7.163e+09  1.532e+09  1.393e+08  5.919e+06  2.319e+05  1.859e+04  4.781e+03
#        600  3.798e+10  3.101e+10  1.678e+10  4.493e+09  5.695e+08  3.730e+07  1.888e+06  1.636e+05  4.284e+04
#        700  5.853e+10  4.992e+10  3.010e+10  9.478e+09  1.468e+09  1.302e+08  8.602e+06  8.353e+05  2.257e+05
#       1000  1.119e+11  1.030e+11  7.698e+10  3.568e+10  8.549e+09  1.195e+09  1.258e+08  1.623e+07  4.851e+06
#       1200  1.215e+11  1.162e+11  9.820e+10  5.922e+10  2.016e+10  3.826e+09  5.066e+08  7.542e+07  2.387e+07
#       1300  1.175e+11  1.141e+11  1.013e+11  6.895e+10  2.829e+10  6.481e+09  9.903e+08  1.607e+08  5.268e+07
#       1400  1.102e+11  1.080e+11  9.942e+10  7.451e+10  3.607e+10  9.941e+09  1.764e+09  3.139e+08  1.069e+08
#       1500  1.012e+11  9.988e+10  9.433e+10  7.622e+10  4.262e+10  1.402e+10  2.910e+09  5.730e+08  2.036e+08
#       1700  8.218e+10  8.171e+10  7.960e+10  7.127e+10  4.993e+10  2.259e+10  6.413e+09  1.576e+09  6.191e+08
#       2000  6.025e+10  6.015e+10  5.970e+10  5.753e+10  4.945e+10  3.225e+10  1.431e+10  5.157e+09  2.484e+09
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
pdepreaction(
   reactants = ['C2H3', 'C4H6'],
   products = ['H', 'C6H8-c6-13'],
   kinetics = Chebyshev(
      coeffs = [
         [7.7788, -2.95523, -0.463598, 0.0349173],
         [2.55725, 1.64706, -0.0702741, -0.119938],
         [0.116333, 0.443876, 0.118138, -0.0170259],
         [-0.0390234, 0.132009, 0.0486008, 0.00279274],
         [0.036369, 0.0848189, -0.015681, -0.0141185],
         [-0.0324022, 0.0540737, 0.0561018, 0.00407778],
      ],
      kunits = 'cm^3/(mol*s)',
      Tmin = (300, 'K'),
      Tmax = (2000, 'K'),
      Pmin = (0.00101325, 'bar'),
      Pmax = (101.325, 'bar'),
   ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#       T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#        300  2.625e-20  9.216e-21  9.746e-22  2.675e-23  2.028e-25  7.879e-28  4.690e-30  1.005e-31  1.295e-32
#        400  3.596e-12  1.868e-12  4.017e-13  2.611e-14  4.504e-16  2.993e-18  2.134e-20  4.754e-22  6.175e-23
#        500  2.331e-07  1.620e-07  6.163e-08  8.789e-09  3.457e-10  4.254e-12  4.004e-14  9.616e-16  1.270e-16
#        600  2.870e-04  2.417e-04  1.353e-04  3.447e-05  2.771e-06  6.552e-08  8.950e-10  2.438e-11  3.323e-12
#        700  3.993e-02  3.834e-02  2.792e-02  1.063e-02  1.462e-03  6.179e-05  1.284e-06  4.185e-08  6.001e-09
#       1000  1.806e+02  2.234e+02  2.687e+02  2.156e+02  8.156e+01  1.188e+01  7.844e-01  5.130e-02  9.529e-03
#       1200  3.327e+03  4.702e+03  7.391e+03  8.722e+03  5.343e+03  1.354e+03  1.551e+02  1.523e+01  3.408e+00
#       1300  7.721e+03  1.161e+04  2.080e+04  2.991e+04  2.364e+04  8.011e+03  1.216e+03  1.472e+02  3.649e+01
#       1400  1.428e+04  2.261e+04  4.529e+04  7.767e+04  7.738e+04  3.433e+04  6.788e+03  1.006e+03  2.762e+02
#       1500  2.211e+04  3.651e+04  8.047e+04  1.614e+05  1.989e+05  1.135e+05  2.890e+04  5.221e+03  1.587e+03
#       1700  3.596e+04  6.327e+04  1.621e+05  4.219e+05  7.510e+05  6.711e+05  2.715e+05  7.121e+04  2.640e+04
#       2000  3.980e+04  7.420e+04  2.211e+05  7.701e+05  2.143e+06  3.424e+06  2.625e+06  1.189e+06  5.982e+05
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
pdepreaction(
   reactants = ['c5-C6H9-3'],
   products = ['H', 'C6H8-c6-14'],
   kinetics = Chebyshev(
      coeffs = [
         [-9.56516, -3.76752, -0.751394, 0.00339792],
         [15.9199, 3.21875, -0.147373, -0.1149],
         [-0.138547, 0.880822, 0.192764, -0.0174951],
         [-0.255669, 0.219927, 0.0869804, 0.0187332],
         [-0.0235988, 0.0687238, -0.0106959, 0.0125856],
         [-0.14643, 0.0788513, 0.0230286, -0.00957023],
```

```
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#      T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#        300  1.094e-26  3.414e-27  2.934e-28  6.253e-30  3.778e-32  1.321e-34  7.676e-37  1.638e-38  2.109e-39
#        400  5.961e-17  2.748e-17  4.733e-18  2.333e-19  3.109e-21  1.748e-23  1.174e-25  2.580e-27  3.341e-28
#        500  3.005e-11  1.907e-11  6.076e-12  6.756e-13  2.026e-14  2.027e-16  1.735e-18  4.058e-20  5.328e-21
#        600  1.085e-07  8.657e-08  4.390e-08  9.631e-09  6.325e-10  1.227e-11  1.489e-13  3.893e-15  5.250e-16
#        700  2.724e-05  2.535e-05  1.767e-05  6.358e-06  7.910e-07  2.908e-08  5.413e-10  1.680e-11  2.375e-12
#       1000  4.125e-01  4.987e-01  5.864e-01  4.719e-01  1.812e-01  2.584e-02  1.609e-03  9.998e-05  1.817e-05
#       1200  1.539e+01  2.128e+01  3.243e+01  3.750e+01  2.269e+01  5.533e+00  5.895e-01  5.412e-02  1.173e-02
#       1300  5.580e+01  8.205e+01  1.417e+02  1.962e+02  1.479e+02  4.617e+01  6.241e+00  6.842e-01  1.615e-01
#       1400  1.531e+02  2.373e+02  4.577e+02  7.479e+02  6.951e+02  2.744e+02  4.646e+01  6.022e+00  1.543e+00
#       1500  3.309e+02  5.361e+02  1.139e+03  2.169e+03  2.463e+03  1.224e+03  2.590e+02  3.967e+01  1.104e+01
#       1700  9.324e+02  1.617e+03  4.015e+03  9.923e+03  1.615e+04  1.233e+04  3.996e+03  8.476e+02  2.782e+02
#       2000  1.544e+03  2.855e+03  8.345e+03  2.803e+04  7.300e+04  1.028e+05  6.467e+04  2.368e+04  1.042e+04
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
pdepreaction(
    reactants = ['c5-C6H9-2'],
    products = ['H', 'C6H8-c6-14'],
    kinetics = Chebyshev(
        coeffs = [
            [-13.6977, -3.92102, -0.731536, 0.00084246],
            [18.4134, 3.22512, -0.209519, -0.114816],
            [-0.162191, 0.912982, 0.173729, -0.0295869],
            [-0.181667, 0.177354, 0.0902597, 0.0157908],
            [0.0609089, -0.010154, -0.00998508, 0.0207162],
            [-0.137874, 0.121988, 0.0108361, -0.0134566],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#      T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#        300  1.697e-12  1.723e-12  1.745e-12  1.752e-12  1.754e-12  1.754e-12  1.754e-12  1.754e-12  1.754e-12
#        400  2.298e-06  2.465e-06  2.657e-06  2.750e-06  2.772e-06  2.775e-06  2.775e-06  2.775e-06  2.775e-06
#        500  8.993e-03  1.062e-02  1.332e-02  1.547e-02  1.626e-02  1.641e-02  1.643e-02  1.643e-02  1.643e-02
#        600  1.605e+00  2.096e+00  3.188e+00  4.577e+00  5.443e+00  5.690e+00  5.733e+00  5.740e+00  5.742e+00
#        700  5.104e+01  7.173e+01  1.284e+02  2.317e+02  3.334e+02  3.787e+02  3.891e+02  3.910e+02  3.913e+02
#       1000  1.719e+04  2.625e+04  5.885e+04  1.644e+05  4.046e+05  6.765e+05  8.130e+05  8.515e+05  8.604e+05
#       1200  1.413e+05  2.218e+05  5.195e+05  1.639e+06  5.151e+06  1.115e+07  1.561e+07  1.728e+07  1.771e+07
#       1300  2.897e+05  4.651e+05  1.118e+06  3.666e+06  1.268e+07  3.110e+07  4.763e+07  5.473e+07  5.672e+07
#       1400  5.012e+05  8.270e+05  2.063e+06  7.030e+06  2.636e+07  7.263e+07  1.219e+08  1.462e+08  1.535e+08
```

```
#       1500  7.444e+05  1.264e+06  3.299e+06  1.176e+07  4.744e+07  1.460e+08  2.696e+08  3.393e+08  3.620e+08
#       1700  1.207e+06  2.163e+06  6.211e+06  2.460e+07  1.131e+08  4.229e+08  9.413e+08  1.318e+09  1.462e+09
#       2000  1.200e+06  2.279e+06  7.394e+06  3.457e+07  1.930e+08  9.516e+08  2.911e+09  5.115e+09  6.248e+09
#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
pdepreaction(
    reactants = ['c6-C6H9'],
    products = ['H', 'C6H8-c6-14'],
    kinetics = Chebyshev(
        coeffs = [
            [-1.49108, 0.548426, -0.117783, 0.000966357],
            [10.2097, 0.764772, -0.126819, -0.0362503],
            [-0.292441, 0.418074, -0.00733824, -0.0303874],
            [-0.164014, 0.133429, 0.0406823, -0.011388],
            [-0.0172895, -0.00538738, 0.030574, -0.000243899],
            [-0.0881938, 0.0582199, -0.00473699, 0.0157441],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
#       T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
#        300  3.424e-11  1.623e-11  3.173e-12  2.186e-13  6.114e-15  1.297e-16  4.120e-18  3.159e-19  8.051e-20
#        400  3.232e-05  1.978e-05  6.237e-06  7.951e-07  3.774e-08  1.012e-09  3.387e-11  2.622e-12  6.694e-13
#        500  1.331e-01  1.008e-01  4.817e-02  1.075e-02  8.890e-04  3.352e-05  1.253e-06  9.925e-08  2.546e-08
#        600  2.502e+01  2.206e+01  1.450e+01  5.234e+00  7.504e-01  4.308e-02  1.925e-03  1.597e-04  4.139e-05
#        700  7.565e+02  7.408e+02  6.074e+02  3.145e+02  7.279e+01  6.556e+00  3.760e-01  3.382e-02  8.937e-03
#       1000  8.613e+04  1.039e+05  1.272e+05  1.228e+05  7.228e+04  2.043e+04  2.968e+03  4.222e+02  1.292e+02
#       1200  3.753e+05  5.131e+05  7.898e+05  1.020e+06  8.611e+05  3.877e+05  9.148e+04  1.812e+04  6.366e+03
#       1300  5.903e+05  8.573e+05  1.482e+06  2.230e+06  2.234e+06  1.228e+06  3.580e+05  8.327e+04  3.151e+04
#       1400  7.855e+05  1.203e+06  2.311e+06  4.023e+06  4.759e+06  3.149e+06  1.113e+06  3.012e+05  1.227e+05
#       1500  9.160e+05  1.468e+06  3.099e+06  6.192e+06  8.626e+06  6.827e+06  2.897e+06  9.065e+05  3.976e+05
#       1700  9.355e+05  1.608e+06  3.965e+06  1.010e+07  1.911e+07  2.123e+07  1.264e+07  5.187e+06  2.624e+06
#       2000  6.120e+05  1.126e+06  3.268e+06  1.110e+07  3.155e+07  5.726e+07  5.698e+07  3.576e+07  2.276e+07
#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
pdepreaction(
    reactants = ['c5-C6H9'],
    products = ['H', 'C6H8-c6-14'],
    kinetics = Chebyshev(
        coeffs = [
            [-3.31993, -2.60506, -0.518179, 0.0158414],
            [11.1449, 2.38117, -0.164548, -0.0873271],
            [-0.379159, 0.781934, 0.120413, -0.0279876],
            [-0.309227, 0.200865, 0.0674227, 0.0155411],
            [-0.00758008, 0.016825, 0.00267599, 0.0242046],
            [-0.0436554, 0.0703395, -0.00351607, -0.00952954],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
```

```
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
#       T \ P   1.106e-03   2.191e-03   7.920e-03   4.474e-02   3.204e-01   2.295e+00   1.296e+01   4.686e+01   9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
#        300   1.138e-09   6.204e-10   1.854e-10   3.400e-11   4.792e-12   6.702e-13   1.187e-13   3.283e-14   1.657e-14
#        400   1.963e-04   1.282e-04   4.928e-05   1.072e-05   1.605e-06   2.272e-07   4.032e-08   1.116e-08   5.632e-09
#        500   2.676e-01   2.122e-01   1.155e-01   3.616e-02   6.656e-03   1.001e-03   1.797e-04   4.982e-05   2.516e-05
#        600   2.719e+01   2.489e+01   1.810e+01   8.406e+00   2.185e+00   3.862e-01   7.213e-02   2.015e-02   1.019e-02
#        700   6.194e+02   6.253e+02   5.549e+02   3.487e+02   1.279e+02   2.863e+01   5.829e+00   1.662e+00   8.440e-01
#       1000   1.005e+05   1.237e+05   1.576e+05   1.629e+05   1.124e+05   4.634e+04   1.350e+04   4.371e+03   2.295e+03
#       1200   4.435e+05   6.184e+05   9.876e+05   1.345e+06   1.245e+06   6.938e+05   2.541e+05   9.180e+04   4.989e+04
#       1300   6.489e+05   9.606e+05   1.722e+06   2.725e+06   2.952e+06   1.918e+06   7.938e+05   3.060e+05   1.701e+05
#       1400   8.144e+05   1.270e+06   2.526e+06   4.619e+06   5.862e+06   4.441e+06   2.081e+06   8.595e+05   4.898e+05
#       1500   9.055e+05   1.475e+06   3.220e+06   6.748e+06   1.004e+07   8.907e+06   4.757e+06   2.122e+06   1.245e+06
#       1700   8.626e+05   1.503e+06   3.814e+06   1.016e+07   2.041e+07   2.482e+07   1.738e+07   9.184e+06   5.771e+06
#       2000   5.322e+05   9.879e+05   2.930e+06   1.034e+07   3.101e+07   6.056e+07   6.752e+07   5.005e+07   3.683e+07
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
pdepreaction(
    reactants = ['C6H9'],
    products = ['H', 'C6H8-c6-14'],
    kinetics = Chebyshev(
        coeffs = [
            [-1.88501, -1.42203, -0.240506, 0.00775169],
            [9.53766, 1.40685, -0.279762, -0.015982],
            [-0.175363, 0.645702, 0.0034581, -0.0444966],
            [-0.262252, 0.198493, 0.0485273, -0.0085231],
            [-0.0650529, 0.02869, -0.00258445, 0.015363],
            [-0.0639403, 0.114547, 0.0142175, -0.00889846],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
#       T \ P   1.106e-03   2.191e-03   7.920e-03   4.474e-02   3.204e-01   2.295e+00   1.296e+01   4.686e+01   9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
#        300   1.887e+09   1.053e+09   2.772e+08   2.658e+07   8.620e+05   1.885e+04   6.025e+02   4.626e+01   1.179e+01
#        400   9.650e+09   6.437e+09   2.300e+09   3.489e+08   1.916e+07   5.326e+05   1.796e+04   1.393e+03   3.558e+02
#        500   2.573e+10   1.957e+10   9.016e+09   1.929e+09   1.755e+08   7.461e+06   2.924e+05   2.344e+04   6.029e+03
#        600   4.786e+10   3.909e+10   2.115e+10   5.668e+09   7.187e+08   4.710e+07   2.385e+06   2.067e+05   5.412e+04
#        700   7.385e+10   6.300e+10   3.800e+10   1.197e+10   1.855e+09   1.646e+08   1.088e+07   1.056e+06   2.854e+05
#       1000   1.416e+11   1.303e+11   9.742e+10   4.517e+10   1.083e+10   1.514e+09   1.594e+08   2.058e+07   6.148e+06
#       1200   1.539e+11   1.472e+11   1.244e+11   7.504e+10   2.555e+10   4.852e+09   6.426e+08   9.568e+07   3.028e+07
#       1300   1.489e+11   1.445e+11   1.283e+11   8.739e+10   3.586e+10   8.220e+09   1.256e+09   2.040e+08   6.686e+07
#       1400   1.396e+11   1.369e+11   1.260e+11   9.446e+10   4.575e+10   1.261e+10   2.239e+09   3.985e+08   1.357e+08
#       1500   1.283e+11   1.266e+11   1.196e+11   9.666e+10   5.406e+10   1.780e+10   3.693e+09   7.274e+08   2.586e+08
#       1700   1.042e+11   1.037e+11   1.010e+11   9.042e+10   6.336e+10   2.868e+10   8.143e+09   2.001e+09   7.864e+08
#       2000   7.649e+10   7.637e+10   7.580e+10   7.304e+10   6.279e+10   4.096e+10   1.817e+10   6.553e+09   3.156e+09
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
========== ========== ==========
pdepreaction(
    reactants = ['C2H3', 'C4H6'],
```

```
    products = ['H', 'C6H8-c6-14'],
    kinetics = Chebyshev(
        coeffs = [
            [7.87958, -2.95484, -0.46366, 0.0349086],
            [2.55999, 1.6471, -0.0701866, -0.119953],
            [0.116663, 0.443723, 0.11818, -0.0170142],
            [-0.0391004, 0.131982, 0.048601, 0.00279131],
            [0.036352, 0.0848513, -0.0156729, -0.0141277],
            [-0.0323543, 0.0540387, 0.0561069, 0.00409548],
        ],
        kunits = 'cm^3/(mol*s)',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#       T \ P   1.106e-03   2.191e-03   7.920e-03   4.474e-02   3.204e-01   2.295e+00   1.296e+01   4.686e+01   9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#        300   1.864e-14   9.519e-15   2.658e-15   4.721e-16   6.596e-17   9.210e-18   1.631e-18   4.511e-19   2.277e-19
#        400   1.417e-07   8.045e-08   2.532e-08   4.770e-09   6.759e-10   9.458e-11   1.675e-11   4.634e-12   2.339e-12
#        500   2.735e-03   1.910e-03   8.248e-04   1.999e-04   3.132e-05   4.474e-06   7.947e-07   2.200e-07   1.110e-07
#        600   1.675e+00   1.433e+00   8.922e-01   3.239e-01   6.590e-02   1.025e-02   1.850e-03   5.134e-04   2.593e-04
#        700   1.259e+02   1.265e+02   1.072e+02   5.813e+01   1.683e+01   3.115e+00   5.886e-01   1.648e-01   8.338e-02
#       1000   1.097e+05   1.479e+05   2.266e+05   2.872e+05   2.113e+05   7.861e+04   2.025e+04   6.188e+03   3.195e+03
#       1200   8.373e+05   1.283e+06   2.553e+06   4.809e+06   5.765e+06   3.387e+06   1.157e+06   3.943e+05   2.097e+05
#       1300   1.392e+06   2.255e+06   5.048e+06   1.145e+07   1.751e+07   1.322e+07   5.405e+06   2.000e+06   1.091e+06
#       1400   1.962e+06   3.327e+06   8.230e+06   2.195e+07   4.182e+07   4.010e+07   1.976e+07   8.041e+06   4.527e+06
#       1500   2.454e+06   4.323e+06   1.163e+07   3.574e+07   8.310e+07   1.000e+08   5.967e+07   2.701e+07   1.581e+07
#       1700   3.040e+06   5.656e+06   1.726e+07   6.627e+07   2.151e+08   3.884e+08   3.354e+08   1.914e+08   1.230e+08
#       2000   3.138e+06   6.095e+06   2.074e+07   9.917e+07   4.687e+08   1.420e+09   2.093e+09   1.757e+09   1.348e+09
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
pdepreaction(
    reactants = ['c5-C6H9-3'],
    products = ['C5H6', 'CH3'],
    kinetics = Chebyshev(
        coeffs = [
            [-3.78911, -1.42309, -0.235033, 0.00495059],
            [12.5941, 1.6331, -0.329157, -0.0334799],
            [-0.0709658, 0.843543, -0.0313877, -0.0547206],
            [-0.340183, 0.274193, 0.0757829, -0.0287359],
            [-0.111966, 0.0478351, 0.0373954, -0.00119936],
            [-0.0433372, 0.0572425, 0.0272875, 0.00955773],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#       T \ P   1.106e-03   2.191e-03   7.920e-03   4.474e-02   3.204e-01   2.295e+00   1.296e+01   4.686e+01   9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
```

```
#        300  1.346e-15  1.346e-15  1.346e-15  1.346e-15  1.346e-15  1.346e-15  1.346e-15  1.346e-15  1.346e-15
#        400  1.802e-08  1.807e-08  1.811e-08  1.812e-08  1.812e-08  1.813e-08  1.813e-08  1.813e-08  1.813e-08
#        500  3.629e-04  3.711e-04  3.793e-04  3.828e-04  3.836e-04  3.837e-04  3.837e-04  3.837e-04  3.837e-04
#        600  2.413e-01  2.612e-01  2.872e-01  3.031e-01  3.079e-01  3.087e-01  3.088e-01  3.089e-01  3.089e-01
#        700  2.041e+01  2.391e+01  2.975e+01  3.485e+01  3.710e+01  3.761e+01  3.769e+01  3.771e+01  3.771e+01
#       1000  2.649e+04  3.807e+04  6.878e+04  1.246e+05  1.843e+05  2.156e+05  2.240e+05  2.256e+05  2.260e+05
#       1200  2.669e+05  4.232e+05  9.281e+05  2.195e+06  4.246e+06  5.909e+06  6.547e+06  6.701e+06  6.734e+06
#       1300  5.672e+05  9.374e+05  2.236e+06  5.975e+06  1.325e+07  2.045e+07  2.375e+07  2.464e+07  2.483e+07
#       1400  1.007e+06  1.726e+06  4.437e+06  1.327e+07  3.358e+07  5.784e+07  7.102e+07  7.497e+07  7.590e+07
#       1500  1.539e+06  2.722e+06  7.481e+06  2.482e+07  7.147e+07  1.383e+08  1.812e+08  1.958e+08  1.994e+08
#       1700  2.679e+06  4.971e+06  1.520e+07  6.010e+07  2.188e+08  5.345e+08  8.147e+08  9.350e+08  9.687e+08
#       2000  3.294e+06  6.385e+06  2.166e+07  1.041e+08  5.149e+08  1.815e+09  3.729e+09  4.987e+09  5.440e+09
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
pdepreaction(
    reactants = ['c5-C6H9-2'],
    products = ['C5H6', 'CH3'],
    kinetics = Chebyshev(
        coeffs = [
            [-2.90069, 0.361941, -0.0885907, 0.00334851],
            [11.9078, 0.588929, -0.175266, -0.00352281],
            [-0.265622, 0.411812, -0.0715154, -0.015067],
            [-0.190865, 0.204973, -0.0067106, -0.0191072],
            [-0.0546009, 0.0584179, 0.00500765, -0.013695],
            [-0.067284, 0.0383776, 0.0269946, -0.00278727],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#      T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#        300  3.494e-17  9.873e-18  7.238e-19  1.297e-20  6.867e-23  2.278e-25  1.309e-27  2.788e-29  3.589e-30
#        400  1.100e-09  4.582e-10  6.706e-11  2.785e-12  3.221e-14  1.666e-16  1.089e-18  2.380e-20  3.079e-21
#        500  2.665e-05  1.536e-05  4.168e-06  3.881e-07  9.998e-09  9.065e-11  7.450e-13  1.724e-14  2.258e-15
#        600  1.306e-02  9.566e-03  4.191e-03  7.770e-04  4.378e-05  7.617e-07  8.778e-09  2.257e-10  3.032e-11
#        700  7.829e-01  6.769e-01  4.159e-01  1.290e-01  1.392e-02  4.595e-04  8.061e-06  2.448e-07  3.441e-08
#       1000  8.188e+02  9.437e+02  1.025e+03  7.522e+02  2.638e+02  3.483e+01  2.059e+00  1.247e-01  2.245e-02
#       1200  1.067e+04  1.419e+04  2.028e+04  2.177e+04  1.225e+04  2.814e+03  2.876e+02  2.583e+01  5.550e+00
#       1300  2.557e+04  3.633e+04  5.916e+04  7.644e+04  5.394e+04  1.593e+04  2.074e+03  2.227e+02  5.215e+01
#       1400  4.926e+04  7.409e+04  1.355e+05  2.078e+05  1.815e+05  6.805e+04  1.113e+04  1.416e+03  3.600e+02
#       1500  7.850e+04  1.239e+05  2.512e+05  4.507e+05  4.828e+05  2.286e+05  4.683e+04  7.047e+03  1.948e+03
#       1700  1.345e+05  2.288e+05  5.473e+05  1.287e+06  1.990e+06  1.455e+06  4.578e+05  9.557e+04  3.117e+04
#       2000  1.182e+05  2.163e+05  6.170e+05  1.997e+06  4.987e+06  6.770e+06  4.152e+06  1.499e+06  6.556e+05
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
pdepreaction(
    reactants = ['c6-C6H9'],
    products = ['C5H6', 'CH3'],
    kinetics = Chebyshev(
        coeffs = [
            [-8.13109, -4.04337, -0.696953, -0.000688601],
            [14.6921, 3.2618, -0.232572, -0.111238],
            [-0.134999, 0.949702, 0.164437, -0.0301662],
            [-0.197656, 0.187209, 0.0900593, 0.0154309],
```

```
            [0.0481972, -0.0146331, -0.0059249, 0.0208057],
            [-0.137856, 0.118445, 0.00894443, -0.0123653],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#      T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#        300  2.442e-11  1.559e-11  6.055e-12  1.378e-12  2.112e-13  3.003e-14  5.330e-15  1.475e-15  7.445e-16
#        400  3.284e-06  2.472e-06  1.370e-06  4.953e-07  1.054e-07  1.674e-08  3.034e-09  8.427e-10  4.256e-10
#        500  9.952e-03  8.091e-03  5.259e-03  2.549e-03  7.632e-04  1.467e-04  2.799e-05  7.849e-06  3.972e-06
#        600  2.240e+00  2.062e+00  1.650e+00  1.050e+00  4.337e-01  1.053e-01  2.186e-02  6.250e-03  3.176e-03
#        700  8.082e+01  8.354e+01  8.252e+01  7.008e+01  4.084e+01  1.318e+01  3.115e+00  9.221e-01  4.722e-01
#       1000  1.265e+04  1.630e+04  2.379e+04  3.505e+04  4.655e+04  3.927e+04  1.849e+04  7.341e+03  4.094e+03
#       1200  6.413e+04  9.298e+04  1.650e+05  2.946e+05  4.917e+05  6.033e+05  4.250e+05  2.186e+05  1.347e+05
#       1300  1.082e+05  1.659e+05  3.266e+05  6.515e+05  1.193e+06  1.669e+06  1.379e+06  8.005e+05  5.208e+05
#       1400  1.547e+05  2.493e+05  5.405e+05  1.216e+06  2.475e+06  3.903e+06  3.706e+06  2.406e+06  1.651e+06
#       1500  1.944e+05  3.266e+05  7.734e+05  1.965e+06  4.514e+06  8.043e+06  8.695e+06  6.260e+06  4.526e+06
#       1700  2.337e+05  4.187e+05  1.146e+06  3.648e+06  1.081e+07  2.475e+07  3.411e+07  2.962e+07  2.358e+07
#       2000  2.102e+05  3.993e+05  1.269e+06  5.315e+06  2.277e+07  7.808e+07  1.597e+08  1.867e+08  1.726e+08
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
pdepreaction(
    reactants = ['c5-C6H9'],
    products = ['C5H6', 'CH3'],
    kinetics = Chebyshev(
        coeffs = [
            [-2.71172, -1.04042, -0.286722, -0.00678192],
            [10.2504, 1.66107, -0.115584, -0.0570555],
            [-0.0351864, 0.646929, 0.0520175, -0.01728],
            [-0.328577, 0.202679, 0.0306289, 0.0135281],
            [-0.0866758, -0.0173706, 0.0273376, 0.0147199],
            [0.0140797, 0.0514335, -0.0200407, -0.00470769],
        ],
        kunits = 's^-1',
        Tmin = (300, 'K'),
        Tmax = (2000, 'K'),
        Pmin = (0.00101325, 'bar'),
        Pmax = (101.325, 'bar'),
    ),
)

#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#      T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ===========  ===========  ===========  ===========  ===========  ===========  ===========
=========== =========== ===========
#        300  2.616e-11  1.119e-11  1.914e-12  1.211e-13  3.307e-15  6.996e-17  2.222e-18  1.704e-19  4.342e-20
#        400  5.263e-06  2.863e-06  7.704e-07  8.962e-08  4.261e-09  1.170e-10  3.950e-12  3.063e-13  7.823e-14
#        500  1.129e-02  7.628e-03  2.998e-03  5.565e-04  4.286e-05  1.638e-06  6.211e-08  4.942e-09  1.269e-09
#        600  1.715e+00  1.406e+00  7.913e-01  2.320e-01  2.835e-02  1.539e-03  6.836e-05  5.674e-06  1.470e-06
#        700  5.131e+01  4.867e+01  3.642e+01  1.592e+01  3.053e+00  2.441e-01  1.336e-02  1.185e-03  3.122e-04
#       1000  1.307e+04  1.627e+04  2.049e+04  1.885e+04  9.417e+03  2.181e+03  2.794e+02  3.779e+01  1.140e+01
#       1200  6.950e+04  9.938e+04  1.634e+05  2.157e+05  1.641e+05  5.999e+04  1.186e+04  2.163e+03  7.402e+02
```

```
#       1300  1.097e+05  1.669e+05  3.112e+05  4.918e+05  4.621e+05  2.096e+05  5.010e+04  1.046e+04  3.815e+03
#       1400  1.475e+05  2.364e+05  4.920e+05  9.176e+05  1.056e+06  5.921e+05  1.702e+05  4.043e+04  1.568e+04
#       1500  1.750e+05  2.926e+05  6.695e+05  1.452e+06  2.033e+06  1.408e+06  4.872e+05  1.316e+05  5.431e+04
#       1700  1.880e+05  3.348e+05  8.885e+05  2.487e+06  4.945e+06  5.119e+06  2.565e+06  8.979e+05  4.197e+05
#       2000  1.371e+05  2.582e+05  7.941e+05  2.962e+06  9.168e+06  1.661e+07  1.469e+07  7.901e+06  4.575e+06
#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
pdepreaction(
   reactants = ['C6H9'],
   products = ['C5H6', 'CH3'],
   kinetics = Chebyshev(
      coeffs = [
         [-4.11349, -2.68444, -0.507843, 0.0112187],
         [10.9194, 2.35686, -0.224445, -0.076004],
         [0.0552658, 0.822109, 0.0794227, -0.0295997],
         [-0.256797, 0.250213, 0.0616261, -0.00138108],
         [-0.0868713, 0.0218932, 0.0159211, 0.00995648],
         [-0.0759369, 0.0727382, 0.0055156, -0.0068999],
      ],
      kunits = 's^-1',
      Tmin = (300, 'K'),
      Tmax = (2000, 'K'),
      Pmin = (0.00101325, 'bar'),
      Pmax = (101.325, 'bar'),
   ),
)

#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
#       T \ P  1.106e-03  2.191e-03  7.920e-03  4.474e-02  3.204e-01  2.295e+00  1.296e+01  4.686e+01  9.284e+01
#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
#        300  1.954e+08  9.678e+07  1.760e+07  9.082e+05  1.609e+04  1.291e+02  9.892e-01  2.234e-02  2.910e-03
#        400  1.211e+09  7.744e+08  2.321e+08  2.156e+07  5.865e+05  6.935e+03  6.854e+01  1.673e+00  2.219e-01
#        500  3.702e+09  2.790e+09  1.211e+09  1.979e+08  9.444e+06  1.631e+05  2.037e+03  5.433e+01  7.365e+00
#        600  7.727e+09  6.331e+09  3.394e+09  8.070e+08  6.457e+07  1.761e+06  2.871e+04  8.487e+02  1.183e+02
#        700  1.325e+10  1.138e+10  6.934e+09  2.087e+09  2.398e+08  1.007e+07  2.257e+05  7.666e+03  1.112e+03
#       1000  3.295e+10  3.058e+10  2.335e+10  1.106e+10  2.462e+09  2.406e+08  1.289e+07  7.776e+05  1.409e+05
#       1200  4.116e+10  3.960e+10  3.404e+10  2.112e+10  7.028e+09  1.063e+09  8.465e+07  6.839e+06  1.428e+06
#       1300  4.252e+10  4.145e+10  3.733e+10  2.611e+10  1.065e+10  2.047e+09  2.018e+08  1.877e+07  4.184e+06
#       1400  4.248e+10  4.177e+10  3.888e+10  2.985e+10  1.450e+10  3.489e+09  4.250e+08  4.566e+07  1.087e+07
#       1500  4.150e+10  4.105e+10  3.909e+10  3.225e+10  1.818e+10  5.384e+09  8.096e+08  1.012e+08  2.583e+07
#       1700  3.801e+10  3.783e+10  3.701e+10  3.357e+10  2.377e+10  1.007e+10  2.253e+09  3.848e+08  1.143e+08
#       2000  3.290e+10  3.286e+10  3.266e+10  3.163e+10  2.737e+10  1.727e+10  6.564e+09  1.806e+09  6.965e+08
#       ==========  ==========  ==========  ==========  ==========  ==========  ==========
========== ========== ==========
pdepreaction(
   reactants = ['C2H3', 'C4H6'],
   products = ['C5H6', 'CH3'],
   kinetics = Chebyshev(
      coeffs = [
         [6.50286, -3.79188, -0.727139, -0.0197028],
         [3.33487, 2.2357, 0.00669546, -0.109736],
         [0.27081, 0.597812, 0.191779, -0.0316626],
         [-0.014768, 0.151357, 0.0915703, 0.0104976],
         [0.0259598, 0.0625963, -0.0102749, 0.00311971],
         [-0.0325689, 0.0334033, 0.0385803, -0.000923795],
      ],
      kunits = 'cm^3/(mol*s)',
      Tmin = (300, 'K'),
      Tmax = (2000, 'K'),
      Pmin = (0.00101325, 'bar'),
```

```
        Pmax = (101.325, 'bar'),
    ),
)
```

2. *Chemkin ready Chebyshev rate coefficients for reactions in Helium and N_2 bath gases.*

Below; rates in Nitrogen
High pressure limit rate coefficents:

C2H3 + C4H6 <=> C6H9	3.913e+04	2.404	0.420
C6H9 <=> C6H8 + H	2.290e+06	2.017	40.664
C6H9 <=> c6-C6H9	5.041e+08	0.700	20.246
C6H9 <=> c5-C6H9	5.249e+08	0.846	19.298
c5-C6H9 <=> H + c5-C6H8	1.972e+07	1.802	32.304
c6-C6H9 <=> H + C6H8-c6-13	7.487e+08	1.395	33.132
c6-C6H9 <=> H + C6H8-c6-14	2.097e+09	1.299	33.394
c5-C6H9 <=> c5-C6H9-3	5.265e-07	5.639	24.541
c5-C6H9 <=> c5-C6H9-2	3.537e-16	8.138	14.583
c5-C6H9-2 <=> C5H6 + CH3	4.961e+11	0.717	38.962
c5-C6H9-3 <=> c5-C6H9-2	3.239e-08	6.224	24.481

Pressure dependent and well-skipping reactions:

```
c5-C6H9-2 <=> c5-C6H9-3                 1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
```

PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -5.789e+00 6.226e-01 -1.379e-01 6.021e-03 /
CHEB/ 1.220e+01 9.515e-01 -2.410e-01 -1.454e-02 /
CHEB/ 2.308e-02 6.732e-01 -8.836e-02 -2.481e-02 /
CHEB/ -4.928e-01 3.329e-01 4.247e-03 -2.584e-02 /
CHEB/ -4.759e-02 8.836e-02 1.563e-02 -1.690e-02 /
CHEB/ -1.559e-01 1.001e-01 2.631e-02 4.722e-03 /

c6-C6H9 <=> c5-C6H9-3 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -7.687e+00 -2.136e+00 -6.233e-01 1.861e-02 /
CHEB/ 1.334e+01 2.822e+00 -2.238e-01 -9.840e-02 /
CHEB/ -3.227e-01 9.383e-01 1.326e-01 -3.332e-02 /
CHEB/ -2.509e-01 2.858e-01 7.647e-02 1.301e-02 /
CHEB/ 1.030e-02 6.083e-02 5.814e-03 1.823e-02 /
CHEB/ -2.388e-01 8.427e-02 5.323e-03 -2.701e-03 /

c5-C6H9 <=> c5-C6H9-3 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -1.680e+00 1.039e+00 -1.838e-01 -8.567e-03 /
CHEB/ 8.320e+00 1.441e+00 -1.547e-01 -4.251e-02 /
CHEB/ -6.777e-02 5.711e-01 6.215e-02 -2.331e-02 /
CHEB/ -5.225e-01 2.397e-01 3.983e-02 1.202e-02 /
CHEB/ -9.947e-02 1.029e-01 5.877e-03 1.232e-02 /
CHEB/ -1.131e-01 1.939e-02 7.546e-03 7.216e-03 /

C6H9 <=> c5-C6H9-3 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -3.540e+00 -6.701e-01 -4.215e-01 2.428e-02 /
CHEB/ 9.420e+00 2.018e+00 -2.156e-01 -6.068e-02 /
CHEB/ -1.674e-01 7.696e-01 6.494e-02 -2.699e-02 /
CHEB/ -3.254e-01 3.367e-01 3.648e-02 3.987e-03 /
CHEB/ -1.148e-01 1.100e-01 1.358e-02 5.092e-03 /
CHEB/ -1.830e-01 3.763e-02 1.082e-02 2.829e-03 /

C2H3 + C4H6 <=> c5-C6H9-3 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ 6.105e+00 -1.570e+00 -7.280e-01 -1.854e-03 /
CHEB/ 2.034e+00 2.058e+00 5.714e-03 -8.026e-02 /
CHEB/ 2.963e-02 6.371e-01 1.647e-01 -2.697e-02 /
CHEB/ -1.036e-01 2.526e-01 8.030e-02 2.078e-03 /
CHEB/ -2.662e-02 1.300e-01 5.728e-03 8.505e-04 /
CHEB/ -1.468e-01 1.190e-02 2.630e-02 -1.139e-03 /

c5-C6H9-3 <=> c5-C6H9-2 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -7.985e-01 6.226e-01 -1.379e-01 6.021e-03 /
CHEB/ 9.131e+00 9.515e-01 -2.410e-01 -1.454e-02 /
CHEB/ 1.123e-01 6.732e-01 -8.836e-02 -2.481e-02 /
CHEB/ -4.724e-01 3.329e-01 4.247e-03 -2.584e-02 /
CHEB/ -4.426e-02 8.836e-02 1.563e-02 -1.690e-02 /

CHEB/ -1.542e-01 1.001e-01 2.631e-02 4.722e-03 /

c6-C6H9 <=> c5-C6H9-2 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -6.524e+00 -2.385e+00 -5.685e-01 1.508e-02 /
CHEB/ 1.252e+01 2.817e+00 -2.821e-01 -9.501e-02 /
CHEB/ -2.725e-01 9.961e-01 9.603e-02 -4.209e-02 /
CHEB/ -1.851e-01 2.625e-01 7.686e-02 8.904e-03 /
CHEB/ 6.335e-02 4.287e-03 1.763e-02 1.911e-02 /
CHEB/ -2.074e-01 9.427e-02 -6.453e-03 -1.029e-03 /

c5-C6H9 <=> c5-C6H9-2 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ 4.780e-01 8.872e-01 -1.652e-01 -5.226e-03 /
CHEB/ 6.295e+00 1.353e+00 -1.754e-01 -3.588e-02 /
CHEB/ 1.965e-01 6.535e-01 -1.027e-03 -2.709e-02 /
CHEB/ -4.618e-01 1.941e-01 5.668e-02 -3.180e-03 /
CHEB/ -8.160e-02 3.262e-02 3.486e-02 9.223e-03 /
CHEB/ -6.986e-02 2.617e-02 -1.261e-02 1.584e-02 /

C6H9 <=> c5-C6H9-2 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -2.145e+00 -8.690e-01 -3.758e-01 1.809e-02 /
CHEB/ 8.310e+00 2.009e+00 -2.734e-01 -5.189e-02 /
CHEB/ -9.952e-02 8.158e-01 2.792e-02 -3.857e-02 /
CHEB/ -2.308e-01 2.820e-01 4.241e-02 8.218e-04 /
CHEB/ -6.368e-02 5.060e-02 2.029e-02 9.845e-03 /
CHEB/ -1.545e-01 5.251e-02 -3.233e-03 2.343e-03 /

C2H3 + C4H6 <=> c5-C6H9-2 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ 6.686e+00 -1.605e+00 -7.319e-01 -9.011e-03 /
CHEB/ 1.770e+00 1.995e+00 -3.723e-02 -8.272e-02 /
CHEB/ 5.712e-02 6.402e-01 1.500e-01 -3.825e-02 /
CHEB/ 1.013e-02 2.011e-01 7.586e-02 1.904e-03 /
CHEB/ 7.211e-02 6.045e-02 -1.365e-02 9.045e-03 /
CHEB/ -1.534e-01 6.814e-02 2.923e-02 -1.193e-02 /

c5-C6H9-3 <=> c6-C6H9 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -7.787e+00 -2.136e+00 -6.233e-01 1.861e-02 /
CHEB/ 1.370e+01 2.822e+00 -2.238e-01 -9.840e-02 /
CHEB/ -2.486e-01 9.383e-01 1.326e-01 -3.332e-02 /
CHEB/ -2.270e-01 2.858e-01 7.647e-02 1.301e-02 /
CHEB/ 1.636e-02 6.083e-02 5.814e-03 1.823e-02 /
CHEB/ -2.344e-01 8.427e-02 5.323e-03 -2.701e-03 /

c5-C6H9-2 <=> c6-C6H9 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -1.162e+01 -2.385e+00 -5.685e-01 1.508e-02 /

CHEB/ 1.594e+01 2.817e+00 -2.821e-01 -9.501e-02 /
CHEB/ -2.876e-01 9.961e-01 9.603e-02 -4.209e-02 /
CHEB/ -1.816e-01 2.625e-01 7.686e-02 8.904e-03 /
CHEB/ 6.608e-02 4.287e-03 1.763e-02 1.911e-02 /
CHEB/ -2.046e-01 9.427e-02 -6.453e-03 -1.029e-03 /

c5-C6H9 <=> c6-C6H9 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -3.755e-01 -9.913e-01 -3.327e-01 1.950e-02 /
CHEB/ 8.121e+00 1.964e+00 -2.415e-01 -6.438e-02 /
CHEB/ -5.958e-01 8.635e-01 3.038e-02 -4.373e-02 /
CHEB/ -3.083e-01 2.861e-01 5.944e-02 1.011e-03 /
CHEB/ -3.858e-03 4.909e-02 3.234e-02 1.120e-02 /
CHEB/ -1.197e-01 3.735e-02 -2.718e-03 1.141e-02 /

C6H9 <=> c6-C6H9 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ 1.698e+00 5.816e-01 -1.365e-01 7.735e-03 /
CHEB/ 5.883e+00 8.546e-01 -2.111e-01 -8.617e-03 /
CHEB/ -4.545e-01 5.716e-01 -7.567e-02 -1.919e-02 /
CHEB/ -2.518e-01 2.623e-01 1.669e-03 -1.588e-02 /
CHEB/ -5.329e-02 5.496e-02 1.163e-02 -6.740e-03 /
CHEB/ -1.223e-01 8.998e-02 1.014e-02 5.625e-03 /

C2H3 + C4H6 <=> c6-C6H9 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ 8.499e+00 -7.092e-01 -4.568e-01 4.078e-02 /
CHEB/ 8.808e-01 1.392e+00 -1.096e-01 -9.594e-02 /
CHEB/ -1.495e-01 4.502e-01 8.065e-02 -2.149e-02 /
CHEB/ -3.222e-02 1.664e-01 3.264e-02 2.447e-03 /
CHEB/ 7.313e-02 7.764e-02 -2.316e-02 -3.915e-03 /
CHEB/ -1.482e-01 9.626e-02 4.545e-02 -9.974e-03 /

c5-C6H9-3 <=> c5-C6H9 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -4.227e+00 1.039e+00 -1.838e-01 -8.567e-03 /
CHEB/ 1.068e+01 1.441e+00 -1.547e-01 -4.251e-02 /
CHEB/ -4.368e-03 5.711e-01 6.215e-02 -2.331e-02 /
CHEB/ -5.084e-01 2.397e-01 3.983e-02 1.202e-02 /
CHEB/ -9.701e-02 1.029e-01 5.877e-03 1.232e-02 /
CHEB/ -1.115e-01 1.939e-02 7.546e-03 7.216e-03 /

c5-C6H9-2 <=> c5-C6H9 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -7.059e+00 8.872e-01 -1.652e-01 -5.226e-03 /
CHEB/ 1.172e+01 1.353e+00 -1.754e-01 -3.588e-02 /
CHEB/ 1.707e-01 6.535e-01 -1.027e-03 -2.709e-02 /
CHEB/ -4.681e-01 1.941e-01 5.668e-02 -3.180e-03 /
CHEB/ -8.248e-02 3.262e-02 3.486e-02 9.223e-03 /
CHEB/ -6.983e-02 2.617e-02 -1.261e-02 1.584e-02 /

c6-C6H9 <=> c5-C6H9 1.0 0.0 0.0

TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001   100.000 /
CHEB/ 6 4/
CHEB/ -2.822e+00   -9.913e-01   -3.327e-01   1.950e-02   /
CHEB/ 1.013e+01   1.964e+00   -2.415e-01   -6.438e-02 /
CHEB/ -6.065e-01   8.635e-01   3.038e-02   -4.373e-02 /
CHEB/ -3.181e-01   2.861e-01   5.944e-02   1.011e-03   /
CHEB/ -7.456e-03   4.909e-02   3.234e-02   1.120e-02   /
CHEB/ -1.225e-01   3.735e-02   -2.718e-03   1.141e-02   /

C6H9 <=> c5-C6H9   1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001   100.000 /
CHEB/ 6 4/
CHEB/ 2.330e+00   7.525e-01   -1.616e-01   1.360e-02   /
CHEB/ 5.285e+00   1.172e+00   -1.773e-01   -2.968e-02 /
CHEB/ -5.960e-01   6.262e-01   -2.451e-02   -2.374e-02 /
CHEB/ -3.198e-01   2.547e-01   2.777e-02   -3.894e-03 /
CHEB/ -1.054e-01   7.681e-02   2.667e-02   1.085e-03   /
CHEB/ -8.318e-02   9.572e-03   3.655e-03   1.699e-02   /

C2H3 + C4H6 <=> c5-C6H9   1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001   100.000 /
CHEB/ 6 4/
CHEB/ 8.684e+00   -2.548e-01   -4.706e-01   -2.831e-02 /
CHEB/ 8.393e-01   1.097e+00   1.557e-02   1.329e-03   /
CHEB/ -2.947e-01   4.945e-01   5.894e-02   -1.324e-02 /
CHEB/ -1.594e-01   2.340e-01   3.642e-02   -1.381e-02 /
CHEB/ 5.566e-03   8.954e-02   -2.617e-03   -6.065e-04 /
CHEB/ -5.549e-02   1.307e-02   1.718e-02   -8.101e-03 /

c5-C6H9-3 <=> C6H9   1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001   100.000 /
CHEB/ 6 4/
CHEB/ -5.067e+00   -6.701e-01   -4.215e-01   2.428e-02   /
CHEB/ 1.270e+01   2.018e+00   -2.156e-01   -6.068e-02 /
CHEB/ -7.378e-02   7.696e-01   6.494e-02   -2.699e-02 /
CHEB/ -3.180e-01   3.367e-01   3.648e-02   3.987e-03   /
CHEB/ -1.159e-01   1.100e-01   1.358e-02   5.092e-03   /
CHEB/ -1.841e-01   3.763e-02   1.082e-02   2.829e-03   /

c5-C6H9-2 <=> C6H9   1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001   100.000 /
CHEB/ 6 4/
CHEB/ -8.663e+00   -8.690e-01   -3.758e-01   1.809e-02   /
CHEB/ 1.465e+01   2.009e+00   -2.734e-01   -5.189e-02 /
CHEB/ -9.510e-02   8.158e-01   2.792e-02   -3.857e-02 /
CHEB/ -2.437e-01   2.820e-01   4.241e-02   8.218e-04   /
CHEB/ -6.806e-02   5.060e-02   2.029e-02   9.845e-03   /
CHEB/ -1.572e-01   5.251e-02   -3.233e-03   2.343e-03   /

c6-C6H9 <=> C6H9   1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001   100.000 /
CHEB/ 6 4/
CHEB/ 2.719e-01   5.816e-01   -1.365e-01   7.735e-03   /
CHEB/ 8.809e+00   8.546e-01   -2.111e-01   -8.617e-03 /
CHEB/ -4.351e-01   5.716e-01   -7.567e-02   -1.919e-02 /
CHEB/ -2.682e-01   2.623e-01   1.669e-03   -1.588e-02 /

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CHEB/ -6.039e-02   5.496e-02    1.163e-02    -6.740e-03  /
CHEB/ -1.278e-01   8.998e-02    1.014e-02    5.625e-03   /

c5-C6H9 <=> C6H9                              1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ 3.351e+00    7.525e-01    -1.616e-01   1.360e-02   /
CHEB/ 6.204e+00    1.172e+00    -1.773e-01   -2.968e-02  /
CHEB/ -5.658e-01   6.262e-01    -2.451e-02   -2.374e-02  /
CHEB/ -3.265e-01   2.547e-01    2.777e-02    -3.894e-03  /
CHEB/ -1.089e-01   7.681e-02    2.667e-02    1.085e-03   /
CHEB/ -8.591e-02   9.572e-03    3.655e-03    1.699e-02   /

C2H3 + C4H6 <=> C6H9                          1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ 1.078e+01    4.640e-01    -1.416e-01   3.222e-02   /
CHEB/ 6.222e-01    5.953e-01    -1.875e-01   -1.010e-04  /
CHEB/ -1.208e-01   3.490e-01    -2.052e-02   -3.621e-02  /
CHEB/ -1.361e-01   2.011e-01    1.414e-02    -2.780e-02  /
CHEB/ -6.067e-02   9.964e-02    -8.753e-03   -1.277e-02  /
CHEB/ -7.983e-02   5.215e-02    3.876e-02    -4.424e-03  /

c5-C6H9-3 <=> C2H3 + C4H6                     1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -1.129e+01   -1.570e+00   -7.280e-01   -1.854e-03  /
CHEB/ 1.857e+01    2.058e+00    5.714e-03    -8.026e-02  /
CHEB/ 2.085e-02    6.371e-01    1.647e-01    -2.697e-02  /
CHEB/ -1.446e-01   2.526e-01    8.030e-02    2.078e-03   /
CHEB/ -4.354e-02   1.300e-01    5.728e-03    8.505e-04   /
CHEB/ -1.606e-01   1.190e-02    2.630e-02    -1.139e-03  /

c5-C6H9-2 <=> C2H3 + C4H6                     1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -1.570e+01   -1.605e+00   -7.319e-01   -9.011e-03  /
CHEB/ 2.137e+01    1.995e+00    -3.723e-02   -8.272e-02  /
CHEB/ -4.086e-02   6.402e-01    1.500e-01    -3.825e-02  /
CHEB/ -5.125e-02   2.011e-01    7.586e-02    1.904e-03   /
CHEB/ 5.186e-02    6.045e-02    -1.365e-02   9.045e-03   /
CHEB/ -1.689e-01   6.814e-02    2.923e-02    -1.193e-02  /

c6-C6H9 <=> C2H3 + C4H6                       1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -8.792e+00   -7.092e-01   -4.568e-01   4.078e-02   /
CHEB/ 1.706e+01    1.392e+00    -1.096e-01   -9.594e-02  /
CHEB/ -2.325e-01   4.502e-01    8.065e-02    -2.149e-02  /
CHEB/ -9.705e-02   1.664e-01    3.264e-02    2.447e-03   /
CHEB/ 5.016e-02    7.764e-02    -2.316e-02   -3.915e-03  /
CHEB/ -1.665e-01   9.626e-02    4.545e-02    -9.974e-03  /

c5-C6H9 <=> C2H3 + C4H6                       1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
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CHEB/ -6.161e+00   -2.548e-01   -4.706e-01   -2.831e-02  /
CHEB/ 1.501e+01    1.097e+00    1.557e-02    1.329e-03  /
CHEB/ -3.669e-01   4.945e-01    5.894e-02    -1.324e-02  /
CHEB/ -2.145e-01   2.340e-01    3.642e-02    -1.381e-02  /
CHEB/ -1.381e-02   8.954e-02    -2.617e-03   -6.065e-04  /
CHEB/ -7.104e-02   1.307e-02    1.718e-02    -8.101e-03  /

C6H9 <=> C2H3 + C4H6                          1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -5.089e+00   4.640e-01    -1.416e-01   3.222e-02   /
CHEB/ 1.387e+01    5.953e-01    -1.875e-01   -1.010e-04  /
CHEB/ -2.232e-01   3.490e-01    -2.052e-02   -3.621e-02  /
CHEB/ -1.846e-01   2.011e-01    1.414e-02    -2.780e-02  /
CHEB/ -7.655e-02   9.964e-02    -8.753e-03   -1.277e-02  /
CHEB/ -9.265e-02   5.215e-02    3.876e-02    -4.424e-03  /

c5-C6H9-3 <=> C6H8 + H                        1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -1.181e+01   -1.747e+00   -6.890e-01   -2.470e-03  /
CHEB/ 1.792e+01    2.169e+00    -3.284e-02   -7.379e-02  /
CHEB/ 7.804e-02    6.676e-01    1.573e-01    -2.856e-02  /
CHEB/ -1.391e-01   2.527e-01    8.288e-02    1.711e-04   /
CHEB/ -3.810e-02   1.263e-01    6.267e-03    2.607e-03   /
CHEB/ -1.639e-01   1.290e-02    2.523e-02    -1.863e-03  /

c5-C6H9-2 <=> C6H8 + H                        1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -1.618e+01   -1.783e+00   -6.958e-01   -8.882e-03  /
CHEB/ 2.067e+01    2.103e+00    -7.116e-02   -7.711e-02  /
CHEB/ 2.491e-02    6.713e-01    1.408e-01    -3.865e-02  /
CHEB/ -4.702e-02   2.032e-01    7.864e-02    -1.027e-03  /
CHEB/ 5.643e-02    5.463e-02    -1.065e-02   1.137e-02   /
CHEB/ -1.703e-01   6.907e-02    2.573e-02    -1.235e-02  /

c6-C6H9 <=> C6H8 + H                          1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -9.139e+00   -8.506e-01   -4.138e-01   3.916e-02   /
CHEB/ 1.623e+01    1.459e+00    -1.548e-01   -8.773e-02  /
CHEB/ -1.603e-01   4.791e-01    7.939e-02    -2.686e-02  /
CHEB/ -8.959e-02   1.690e-01    3.558e-02    4.080e-03   /
CHEB/ 5.588e-02    7.255e-02    -2.302e-02   -5.610e-04  /
CHEB/ -1.660e-01   9.857e-02    4.231e-02    -1.208e-02  /

c5-C6H9 <=> C6H8 + H                          1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -6.493e+00   -3.852e-01   -4.620e-01   -1.859e-02  /
CHEB/ 1.415e+01    1.173e+00    1.547e-02    -1.294e-02  /
CHEB/ -2.838e-01   5.108e-01    5.135e-02    -5.696e-03  /
CHEB/ -2.037e-01   2.378e-01    3.256e-02    -1.248e-02  /
CHEB/ -9.031e-03   8.655e-02    -1.081e-03   -1.791e-04  /
CHEB/ -7.298e-02   1.415e-02    1.593e-02    -8.938e-03  /
```

```
C6H9 <=> C6H8 + H                          1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -5.365e+00   4.262e-01    -1.231e-01   2.488e-02   /
CHEB/ 1.295e+01    5.795e-01    -1.906e-01   6.927e-03   /
CHEB/ -1.395e-01   3.615e-01    -3.394e-02   -2.950e-02  /
CHEB/ -1.724e-01   2.067e-01    9.789e-03    -2.818e-02  /
CHEB/ -6.999e-02   9.817e-02    -8.766e-03   -1.381e-02  /
CHEB/ -9.341e-02   5.583e-02    3.867e-02    -5.696e-03  /

C2H3 + C4H6 <=> C6H8 + H                    1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ 6.679e+00    -1.808e+00   -1.963e-01   4.066e-02   /
CHEB/ 3.883e+00    9.011e-01    -1.622e-01   -5.383e-02  /
CHEB/ 4.746e-01    3.594e-01    5.579e-02    -5.425e-02  /
CHEB/ 5.938e-02    1.579e-01    6.195e-02    -1.691e-02  /
CHEB/ 4.342e-02    9.895e-02    1.570e-02    -8.953e-03  /
CHEB/ -3.078e-02   -1.252e-02   3.757e-02    1.797e-02   /

c5-C6H9-3 <=> H + c5-C6H8                   1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -8.609e+00   -6.931e-01   -3.410e-01   -2.236e-02  /
CHEB/ 1.482e+01    1.558e+00    -6.501e-03   -4.172e-02  /
CHEB/ 1.027e-01    6.604e-01    4.495e-02    8.554e-03   /
CHEB/ -1.803e-01   2.324e-01    4.951e-02    -2.102e-03  /
CHEB/ -7.624e-02   5.059e-02    1.993e-02    1.084e-02   /
CHEB/ -1.421e-01   1.801e-02    -3.653e-04   -2.812e-03  /

c5-C6H9-2 <=> H + c5-C6H8                   1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -1.265e+01   -7.348e-01   -3.665e-01   -1.761e-02  /
CHEB/ 1.722e+01    1.504e+00    -2.860e-02   -5.476e-02  /
CHEB/ 6.659e-02    6.392e-01    3.294e-02    -1.329e-03  /
CHEB/ -9.492e-02   1.806e-01    4.156e-02    1.590e-04   /
CHEB/ 6.434e-04    -2.898e-02   2.093e-02    1.944e-02   /
CHEB/ -1.324e-01   6.606e-02    -1.899e-02   -1.013e-02  /

c6-C6H9 <=> H + c5-C6H8                     1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -7.380e+00   -2.344e+00   -5.903e-01   1.710e-02   /
CHEB/ 1.393e+01    2.291e+00    -9.846e-02   -9.661e-02  /
CHEB/ -1.183e-01   7.252e-01    1.339e-01    -2.107e-02  /
CHEB/ -1.033e-01   1.935e-01    6.263e-02    1.720e-02   /
CHEB/ 5.403e-02    2.897e-02    -7.641e-03   2.308e-02   /
CHEB/ -1.900e-01   7.280e-02    3.436e-03    -1.396e-02  /

c5-C6H9 <=> H + c5-C6H8                     1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -2.013e+00   9.278e-01    -2.045e-01   4.994e-04   /
CHEB/ 9.902e+00    6.592e-01    1.255e-01    -5.980e-02  /
CHEB/ -3.137e-01   3.313e-01    3.655e-02    2.253e-02   /
```

CHEB/ -2.236e-01 1.515e-01 -5.044e-03 3.022e-02 /
CHEB/ -6.194e-02 1.908e-02 1.042e-02 2.279e-02 /
CHEB/ -4.896e-02 4.740e-03 -2.216e-02 -4.711e-03 /

C6H9 <=> H + c5-C6H8 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -3.335e+00 -8.812e-01 -3.964e-01 2.560e-02 /
CHEB/ 1.024e+01 1.348e+00 -3.854e-02 -6.087e-02 /
CHEB/ -2.870e-02 5.508e-01 4.691e-02 -3.291e-03 /
CHEB/ -1.505e-01 2.391e-01 1.697e-02 6.021e-03 /
CHEB/ -7.424e-02 7.408e-02 1.326e-04 7.726e-03 /
CHEB/ -1.307e-01 2.502e-02 7.493e-03 -1.161e-02 /

C2H3 + C4H6 <=> H + c5-C6H8 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ 7.037e+00 -2.495e+00 -4.659e-01 -3.213e-02 /
CHEB/ 2.786e+00 1.322e+00 2.985e-02 -1.740e-02 /
CHEB/ 3.268e-01 4.747e-01 9.139e-02 -2.017e-02 /
CHEB/ 4.145e-02 1.926e-01 6.244e-02 -1.455e-02 /
CHEB/ 3.169e-02 8.929e-02 8.774e-03 -6.351e-03 /
CHEB/ -6.379e-02 -2.434e-02 2.351e-02 4.963e-03 /

c5-C6H9-3 <=> H + C6H8-c6-13 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -9.662e+00 -3.770e+00 -7.506e-01 3.321e-03 /
CHEB/ 1.591e+01 3.220e+00 -1.481e-01 -1.148e-01 /
CHEB/ -1.381e-01 8.814e-01 1.926e-01 -1.750e-02 /
CHEB/ -2.557e-01 2.199e-01 8.700e-02 1.873e-02 /
CHEB/ -2.351e-02 6.854e-02 -1.064e-02 1.260e-02 /
CHEB/ -1.464e-01 7.887e-02 2.299e-02 -9.568e-03 /

c5-C6H9-2 <=> H + C6H8-c6-13 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -1.379e+01 -3.924e+00 -7.304e-01 7.050e-04 /
CHEB/ 1.841e+01 3.227e+00 -2.105e-01 -1.147e-01 /
CHEB/ -1.613e-01 9.136e-01 1.735e-01 -2.958e-02 /
CHEB/ -1.818e-01 1.774e-01 9.027e-02 1.578e-02 /
CHEB/ 6.099e-02 -1.036e-02 -9.872e-03 2.071e-02 /
CHEB/ -1.378e-01 1.219e-01 1.079e-02 -1.343e-02 /

c6-C6H9 <=> H + C6H8-c6-13 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -1.558e+00 5.464e-01 -1.170e-01 8.020e-04 /
CHEB/ 1.017e+01 7.644e-01 -1.269e-01 -3.616e-02 /
CHEB/ -2.839e-01 4.196e-01 -8.263e-03 -3.009e-02 /
CHEB/ -1.638e-01 1.343e-01 4.047e-02 -1.150e-02 /
CHEB/ -1.750e-02 -5.452e-03 3.090e-02 -5.049e-04 /
CHEB/ -8.799e-02 5.767e-02 -4.603e-03 1.586e-02 /

c5-C6H9 <=> H + C6H8-c6-13 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /

```
CHEB/ 6 4/
CHEB/ -3.411e+00   -2.610e+00   -5.164e-01   1.558e-02   /
CHEB/ 1.113e+01    2.385e+00    -1.663e-01   -8.694e-02  /
CHEB/ -3.769e-01   7.828e-01    1.203e-01    -2.812e-02  /
CHEB/ -3.093e-01   2.008e-01    6.751e-02    1.554e-02   /
CHEB/ -7.476e-03   1.652e-02    2.853e-03    2.418e-02   /
CHEB/ -4.363e-02   7.030e-02    -3.596e-03   -9.472e-03  /

C6H9 <=> H + C6H8-c6-13                          1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -1.972e+00   -1.424e+00   -2.397e-01   7.487e-03   /
CHEB/ 9.517e+00    1.407e+00    -2.801e-01   -1.570e-02  /
CHEB/ -1.712e-01   6.470e-01    2.821e-03    -4.440e-02  /
CHEB/ -2.626e-01   1.986e-01    4.862e-02    -8.656e-03  /
CHEB/ -6.494e-02   2.830e-02    -2.347e-03   1.535e-02   /
CHEB/ -6.392e-02   1.145e-01    1.410e-02    -8.825e-03  /

C2H3 + C4H6 <=> H + C6H8-c6-13                   1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ 7.779e+00    -2.955e+00   -4.636e-01   3.492e-02   /
CHEB/ 2.557e+00    1.647e+00    -7.027e-02   -1.199e-01  /
CHEB/ 1.163e-01    4.439e-01    1.181e-01    -1.703e-02  /
CHEB/ -3.902e-02   1.320e-01    4.860e-02    2.793e-03   /
CHEB/ 3.637e-02    8.482e-02    -1.568e-02   -1.412e-02  /
CHEB/ -3.240e-02   5.407e-02    5.610e-02    4.078e-03   /

c5-C6H9-3 <=> H + C6H8-c6-14                     1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -9.565e+00   -3.768e+00   -7.514e-01   3.398e-03   /
CHEB/ 1.592e+01    3.219e+00    -1.474e-01   -1.149e-01  /
CHEB/ -1.385e-01   8.808e-01    1.928e-01    -1.750e-02  /
CHEB/ -2.557e-01   2.199e-01    8.698e-02    1.873e-02   /
CHEB/ -2.360e-02   6.872e-02    -1.070e-02   1.259e-02   /
CHEB/ -1.464e-01   7.885e-02    2.303e-02    -9.570e-03  /

c5-C6H9-2 <=> H + C6H8-c6-14                     1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -1.370e+01   -3.921e+00   -7.315e-01   8.425e-04   /
CHEB/ 1.841e+01    3.225e+00    -2.095e-01   -1.148e-01  /
CHEB/ -1.622e-01   9.130e-01    1.737e-01    -2.959e-02  /
CHEB/ -1.817e-01   1.774e-01    9.026e-02    1.579e-02   /
CHEB/ 6.091e-02    -1.015e-02   -9.985e-03   2.072e-02   /
CHEB/ -1.379e-01   1.220e-01    1.084e-02    -1.346e-02  /

c6-C6H9 <=> H + C6H8-c6-14                       1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -1.491e+00   5.484e-01    -1.178e-01   9.664e-04   /
CHEB/ 1.021e+01    7.648e-01    -1.268e-01   -3.625e-02  /
CHEB/ -2.924e-01   4.181e-01    -7.338e-03   -3.039e-02  /
CHEB/ -1.640e-01   1.334e-01    4.068e-02    -1.139e-02  /
CHEB/ -1.729e-02   -5.387e-03   3.057e-02    -2.439e-04  /
CHEB/ -8.819e-02   5.822e-02    -4.737e-03   1.574e-02   /
```

c5-C6H9 <=> H + C6H8-c6-14 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -3.320e+00 -2.605e+00 -5.182e-01 1.584e-02 /
CHEB/ 1.114e+01 2.381e+00 -1.645e-01 -8.733e-02 /
CHEB/ -3.792e-01 7.819e-01 1.204e-01 -2.799e-02 /
CHEB/ -3.092e-01 2.009e-01 6.742e-02 1.554e-02 /
CHEB/ -7.580e-03 1.683e-02 2.676e-03 2.420e-02 /
CHEB/ -4.366e-02 7.034e-02 -3.516e-03 -9.530e-03 /

C6H9 <=> H + C6H8-c6-14 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -1.885e+00 -1.422e+00 -2.405e-01 7.752e-03 /
CHEB/ 9.538e+00 1.407e+00 -2.798e-01 -1.598e-02 /
CHEB/ -1.754e-01 6.457e-01 3.458e-03 -4.450e-02 /
CHEB/ -2.623e-01 1.985e-01 4.853e-02 -8.523e-03 /
CHEB/ -6.505e-02 2.869e-02 -2.584e-03 1.536e-02 /
CHEB/ -6.394e-02 1.145e-01 1.422e-02 -8.898e-03 /

C2H3 + C4H6 <=> H + C6H8-c6-14 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ 7.880e+00 -2.955e+00 -4.637e-01 3.491e-02 /
CHEB/ 2.560e+00 1.647e+00 -7.019e-02 -1.200e-01 /
CHEB/ 1.167e-01 4.437e-01 1.182e-01 -1.701e-02 /
CHEB/ -3.910e-02 1.320e-01 4.860e-02 2.791e-03 /
CHEB/ 3.635e-02 8.485e-02 -1.567e-02 -1.413e-02 /
CHEB/ -3.235e-02 5.404e-02 5.611e-02 4.095e-03 /

c5-C6H9-3 <=> C5H6 + CH3 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -3.789e+00 -1.423e+00 -2.350e-01 4.951e-03 /
CHEB/ 1.259e+01 1.633e+00 -3.292e-01 -3.348e-02 /
CHEB/ -7.097e-02 8.435e-01 -3.139e-02 -5.472e-02 /
CHEB/ -3.402e-01 2.742e-01 7.578e-02 -2.874e-02 /
CHEB/ -1.120e-01 4.784e-02 3.740e-02 -1.199e-03 /
CHEB/ -4.334e-02 5.724e-02 2.729e-02 9.558e-03 /

c5-C6H9-2 <=> C5H6 + CH3 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -2.901e+00 3.619e-01 -8.859e-02 3.349e-03 /
CHEB/ 1.191e+01 5.889e-01 -1.753e-01 -3.523e-03 /
CHEB/ -2.656e-01 4.118e-01 -7.152e-02 -1.507e-02 /
CHEB/ -1.909e-01 2.050e-01 -6.711e-03 -1.911e-02 /
CHEB/ -5.460e-02 5.842e-02 5.008e-03 -1.369e-02 /
CHEB/ -6.728e-02 3.838e-02 2.699e-02 -2.787e-03 /

c6-C6H9 <=> C5H6 + CH3 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -8.131e+00 -4.043e+00 -6.970e-01 -6.886e-04 /
CHEB/ 1.469e+01 3.262e+00 -2.326e-01 -1.112e-01 /

```
CHEB/ -1.350e-01   9.497e-01    1.644e-01    -3.017e-02  /
CHEB/ -1.977e-01   1.872e-01    9.006e-02    1.543e-02   /
CHEB/ 4.820e-02    -1.463e-02   -5.925e-03   2.081e-02   /
CHEB/ -1.379e-01   1.184e-01    8.944e-03    -1.237e-02  /

c5-C6H9 <=> C5H6 + CH3                          1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -2.712e+00   -1.040e+00   -2.867e-01   -6.782e-03  /
CHEB/ 1.025e+01    1.661e+00    -1.156e-01   -5.706e-02  /
CHEB/ -3.519e-02   6.469e-01    5.202e-02    -1.728e-02  /
CHEB/ -3.286e-01   2.027e-01    3.063e-02    1.353e-02   /
CHEB/ -8.668e-02   -1.737e-02   2.734e-02    1.472e-02   /
CHEB/ 1.408e-02    5.143e-02    -2.004e-02   -4.708e-03  /

C6H9 <=> C5H6 + CH3                             1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -4.113e+00   -2.684e+00   -5.078e-01   1.122e-02   /
CHEB/ 1.092e+01    2.357e+00    -2.244e-01   -7.600e-02  /
CHEB/ 5.527e-02    8.221e-01    7.942e-02    -2.960e-02  /
CHEB/ -2.568e-01   2.502e-01    6.163e-02    -1.381e-03  /
CHEB/ -8.687e-02   2.189e-02    1.592e-02    9.956e-03   /
CHEB/ -7.594e-02   7.274e-02    5.516e-03    -6.900e-03  /

C2H3 + C4H6 <=> C5H6 + CH3                      1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ 6.503e+00    -3.792e+00   -7.271e-01   -1.970e-02  /
CHEB/ 3.335e+00    2.236e+00    6.695e-03    -1.097e-01  /
CHEB/ 2.708e-01    5.978e-01    1.918e-01    -3.166e-02  /
CHEB/ -1.477e-02   1.514e-01    9.157e-02    1.050e-02   /
CHEB/ 2.596e-02    6.260e-02    -1.027e-02   3.120e-03   /
CHEB/ -3.257e-02   3.340e-02    3.858e-02    -9.238e-04  /
```

Below: pressure-dependent and well skipping rates for Helium bath gas

```
c5-C6H9-2 <=> c5-C6H9-3                         1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -5.741e+00   5.816e-01    -1.359e-01   6.427e-03   /
CHEB/ 1.227e+01    8.816e-01    -2.444e-01   -8.981e-03  /
CHEB/ 6.958e-02    6.453e-01    -9.848e-02   -2.297e-02  /
CHEB/ -4.720e-01   3.310e-01    -6.707e-03   -2.639e-02  /
CHEB/ -4.345e-02   9.081e-02    9.197e-03    -1.779e-02  /
CHEB/ -1.483e-01   1.054e-01    2.607e-02    1.061e-03   /

c6-C6H9 <=> c5-C6H9-3                           1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -7.803e+00   -2.298e+00   -6.197e-01   2.432e-02   /
CHEB/ 1.348e+01    2.722e+00    -2.593e-01   -1.018e-01  /
CHEB/ -2.452e-01   9.587e-01    1.131e-01    -4.336e-02  /
CHEB/ -2.239e-01   3.080e-01    7.751e-02    8.277e-03   /
CHEB/ 1.829e-02    6.590e-02    1.150e-02    1.786e-02   /
CHEB/ -2.324e-01   8.873e-02    6.620e-03    -4.716e-05  /
```

```
c5-C6H9 <=> c5-C6H9-3                          1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -1.605e+00   9.883e-01    -1.874e-01   -6.029e-03  /
CHEB/ 8.422e+00    1.383e+00    -1.717e-01   -4.764e-02  /
CHEB/ -2.466e-02   5.746e-01    5.215e-02    -3.195e-02  /
CHEB/ -5.029e-01   2.476e-01    4.075e-02    6.286e-03   /
CHEB/ -9.100e-02   1.041e-01    7.685e-03    1.001e-02   /
CHEB/ -1.098e-01   2.497e-02    1.088e-02    9.980e-03   /

C6H9 <=> c5-C6H9-3                             1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -3.568e+00   -7.804e-01   -4.147e-01   2.815e-02   /
CHEB/ 9.529e+00    1.933e+00    -2.368e-01   -6.276e-02  /
CHEB/ -1.068e-01   7.744e-01    5.100e-02    -3.417e-02  /
CHEB/ -2.988e-01   3.476e-01    3.436e-02    1.251e-03   /
CHEB/ -1.056e-01   1.145e-01    1.411e-02    4.239e-03   /
CHEB/ -1.791e-01   4.336e-02    1.336e-02    4.548e-03   /

C2H3 + C4H6 <=> c5-C6H9-3                      1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ 6.016e+00    -1.753e+00   -7.279e-01   2.016e-03   /
CHEB/ 2.126e+00    2.011e+00    -3.049e-02   -8.302e-02  /
CHEB/ 8.234e-02    6.777e-01    1.485e-01    -3.343e-02  /
CHEB/ -8.184e-02   2.778e-01    7.909e-02    -8.807e-04  /
CHEB/ -1.638e-02   1.354e-01    5.975e-03    2.164e-03   /
CHEB/ -1.452e-01   1.963e-02    2.763e-02    -1.153e-03  /

c5-C6H9-3 <=> c5-C6H9-2                        1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -7.513e-01   5.816e-01    -1.359e-01   6.427e-03   /
CHEB/ 9.200e+00    8.816e-01    -2.444e-01   -8.981e-03  /
CHEB/ 1.588e-01    6.453e-01    -9.848e-02   -2.297e-02  /
CHEB/ -4.516e-01   3.310e-01    -6.707e-03   -2.639e-02  /
CHEB/ -4.012e-02   9.081e-02    9.197e-03    -1.779e-02  /
CHEB/ -1.466e-01   1.054e-01    2.607e-02    1.061e-03   /

c6-C6H9 <=> c5-C6H9-2                          1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -6.657e+00   -2.536e+00   -5.661e-01   2.009e-02   /
CHEB/ 1.265e+01    2.708e+00    -3.166e-01   -9.541e-02  /
CHEB/ -1.924e-01   1.006e+00    7.446e-02    -5.085e-02  /
CHEB/ -1.603e-01   2.830e-01    7.609e-02    3.663e-03   /
CHEB/ 6.741e-02    1.180e-02    2.338e-02    1.773e-02   /
CHEB/ -2.004e-01   9.549e-02    -4.787e-03   1.572e-03   /

c5-C6H9 <=> c5-C6H9-2                          1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ 5.429e-01    8.398e-01    -1.673e-01   -2.752e-03  /
CHEB/ 6.390e+00    1.293e+00    -1.902e-01   -3.923e-02  /
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CHEB/ 2.434e-01   6.441e-01   -1.201e-02  -3.099e-02  /
CHEB/ -4.467e-01  2.047e-01   5.348e-02   -8.498e-03  /
CHEB/ -7.834e-02  3.963e-02   3.585e-02   4.124e-03   /
CHEB/ -6.532e-02  2.606e-02   -6.716e-03  1.804e-02   /

C6H9 <=> c5-C6H9-2                          1.0 0.0 0.0
TCHEB/ 300.000  2000.000 /
PCHEB/ 0.001    100.000  /
CHEB/ 6 4/
CHEB/ -2.187e+00  -9.709e-01  -3.705e-01  2.133e-02   /
CHEB/ 8.417e+00   1.916e+00   -2.923e-01  -5.077e-02  /
CHEB/ -3.764e-02  8.110e-01   1.138e-02   -4.333e-02  /
CHEB/ -2.080e-01  2.920e-01   3.941e-02   -3.079e-03  /
CHEB/ -5.824e-02  5.660e-02   2.215e-02   7.947e-03   /
CHEB/ -1.500e-01  5.435e-02   -1.022e-03  4.356e-03   /

C2H3 + C4H6 <=> c5-C6H9-2                   1.0 0.0 0.0
TCHEB/ 300.000  2000.000 /
PCHEB/ 0.001    100.000  /
CHEB/ 6 4/
CHEB/ 6.593e+00   -1.791e+00  -7.343e-01  -5.613e-03  /
CHEB/ 1.855e+00   1.938e+00   -7.353e-02  -8.283e-02  /
CHEB/ 1.075e-01   6.748e-01   1.298e-01   -4.529e-02  /
CHEB/ 2.792e-02   2.230e-01   7.399e-02   -2.277e-03  /
CHEB/ 7.820e-02   6.203e-02   -1.078e-02  1.169e-02   /
CHEB/ -1.498e-01  7.518e-02   2.647e-02   -1.278e-02  /

c5-C6H9-3 <=> c6-C6H9                       1.0 0.0 0.0
TCHEB/ 300.000  2000.000 /
PCHEB/ 0.001    100.000  /
CHEB/ 6 4/
CHEB/ -7.904e+00  -2.298e+00  -6.197e-01  2.432e-02   /
CHEB/ 1.383e+01   2.722e+00   -2.593e-01  -1.018e-01  /
CHEB/ -1.710e-01  9.587e-01   1.131e-01   -4.336e-02  /
CHEB/ -2.000e-01  3.080e-01   7.751e-02   8.277e-03   /
CHEB/ 2.435e-02   6.590e-02   1.150e-02   1.786e-02   /
CHEB/ -2.279e-01  8.873e-02   6.620e-03   -4.716e-05  /

c5-C6H9-2 <=> c6-C6H9                       1.0 0.0 0.0
TCHEB/ 300.000  2000.000 /
PCHEB/ 0.001    100.000  /
CHEB/ 6 4/
CHEB/ -1.175e+01  -2.536e+00  -5.661e-01  2.009e-02   /
CHEB/ 1.606e+01   2.708e+00   -3.166e-01  -9.541e-02  /
CHEB/ -2.074e-01  1.006e+00   7.446e-02   -5.085e-02  /
CHEB/ -1.568e-01  2.830e-01   7.609e-02   3.663e-03   /
CHEB/ 7.014e-02   1.180e-02   2.338e-02   1.773e-02   /
CHEB/ -1.976e-01  9.549e-02   -4.787e-03  1.572e-03   /

c5-C6H9 <=> c6-C6H9                         1.0 0.0 0.0
TCHEB/ 300.000  2000.000 /
PCHEB/ 0.001    100.000  /
CHEB/ 6 4/
CHEB/ -4.217e-01  -1.083e+00  -3.270e-01  2.145e-02   /
CHEB/ 8.223e+00   1.881e+00   -2.662e-01  -6.319e-02  /
CHEB/ -5.314e-01  8.608e-01   1.177e-02   -4.764e-02  /
CHEB/ -2.846e-01  2.993e-01   5.639e-02   -4.323e-03  /
CHEB/ 1.647e-03   5.686e-02   3.394e-02   7.385e-03   /
CHEB/ -1.148e-01  4.034e-02   2.738e-03   1.366e-02   /

C6H9 <=> c6-C6H9                            1.0 0.0 0.0
TCHEB/ 300.000  2000.000 /
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PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ 1.743e+00    5.414e-01    -1.337e-01   8.284e-03   /
CHEB/ 5.946e+00    7.918e-01    -2.129e-01   -5.331e-03  /
CHEB/ -4.144e-01   5.471e-01    -8.349e-02   -1.798e-02  /
CHEB/ -2.345e-01   2.599e-01    -5.388e-03   -1.714e-02  /
CHEB/ -5.013e-02   5.623e-02    8.706e-03    -8.575e-03  /
CHEB/ -1.153e-01   9.211e-02    1.077e-02    3.650e-03   /

C2H3 + C4H6 <=> c6-C6H9                          1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ 8.469e+00    -8.267e-01   -4.465e-01   4.144e-02   /
CHEB/ 9.448e-01    1.335e+00    -1.384e-01   -9.287e-02  /
CHEB/ -1.151e-01   4.649e-01    6.516e-02    -2.728e-02  /
CHEB/ -1.904e-02   1.775e-01    2.981e-02    1.368e-03   /
CHEB/ 7.809e-02    7.532e-02    -2.395e-02   -5.997e-04  /
CHEB/ -1.423e-01   1.064e-01    4.227e-02    -1.271e-02  /

c5-C6H9-3 <=> c5-C6H9                            1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -4.152e+00   9.883e-01    -1.874e-01   -6.029e-03  /
CHEB/ 1.078e+01    1.383e+00    -1.717e-01   -4.764e-02  /
CHEB/ 3.874e-02    5.746e-01    5.215e-02    -3.195e-02  /
CHEB/ -4.888e-01   2.476e-01    4.075e-02    6.286e-03   /
CHEB/ -8.853e-02   1.041e-01    7.685e-03    1.001e-02   /
CHEB/ -1.081e-01   2.497e-02    1.088e-02    9.980e-03   /

c5-C6H9-2 <=> c5-C6H9                            1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -6.995e+00   8.398e-01    -1.673e-01   -2.752e-03  /
CHEB/ 1.181e+01    1.293e+00    -1.902e-01   -3.923e-02  /
CHEB/ 2.176e-01    6.441e-01    -1.201e-02   -3.099e-02  /
CHEB/ -4.530e-01   2.047e-01    5.348e-02    -8.498e-03  /
CHEB/ -7.921e-02   3.963e-02    3.585e-02    4.124e-03   /
CHEB/ -6.529e-02   2.606e-02    -6.716e-03   1.804e-02   /

c6-C6H9 <=> c5-C6H9                              1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -2.868e+00   -1.083e+00   -3.270e-01   2.145e-02   /
CHEB/ 1.023e+01    1.881e+00    -2.662e-01   -6.319e-02  /
CHEB/ -5.421e-01   8.608e-01    1.177e-02    -4.764e-02  /
CHEB/ -2.943e-01   2.993e-01    5.639e-02    -4.323e-03  /
CHEB/ -1.952e-03   5.686e-02    3.394e-02    7.385e-03   /
CHEB/ -1.176e-01   4.034e-02    2.738e-03    1.366e-02   /

C6H9 <=> c5-C6H9                                 1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ 2.388e+00    7.065e-01    -1.570e-01   1.402e-02   /
CHEB/ 5.368e+00    1.114e+00    -1.891e-01   -3.031e-02  /
CHEB/ -5.520e-01   6.143e-01    -3.448e-02   -2.451e-02  /
CHEB/ -3.012e-01   2.591e-01    2.448e-02    -7.390e-03  /
CHEB/ -9.978e-02   8.105e-02    2.529e-02    -3.122e-03  /
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CHEB/ -7.971e-02   1.310e-02    9.662e-03    1.782e-02   /

C2H3 + C4H6 <=> c5-C6H9                          1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ 8.671e+00    -3.709e-01   -4.760e-01   -2.428e-02  /
CHEB/ 9.033e-01    1.064e+00    6.704e-03    -6.710e-03  /
CHEB/ -2.576e-01   5.127e-01    4.917e-02    -1.361e-02  /
CHEB/ -1.428e-01   2.476e-01    3.151e-02    -1.227e-02  /
CHEB/ 1.278e-02    9.209e-02    -2.450e-03   1.603e-03   /
CHEB/ -5.510e-02   1.781e-02    1.613e-02    -8.175e-03  /

c5-C6H9-3 <=> C6H9                               1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -5.096e+00   -7.804e-01   -4.147e-01   2.815e-02   /
CHEB/ 1.281e+01    1.933e+00    -2.368e-01   -6.276e-02  /
CHEB/ -1.322e-02   7.744e-01    5.100e-02    -3.417e-02  /
CHEB/ -2.913e-01   3.476e-01    3.436e-02    1.251e-03   /
CHEB/ -1.066e-01   1.145e-01    1.411e-02    4.239e-03   /
CHEB/ -1.802e-01   4.336e-02    1.336e-02    4.548e-03   /

c5-C6H9-2 <=> C6H9                               1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -8.705e+00   -9.709e-01   -3.705e-01   2.133e-02   /
CHEB/ 1.476e+01    1.916e+00    -2.923e-01   -5.077e-02  /
CHEB/ -3.321e-02   8.110e-01    1.138e-02    -4.333e-02  /
CHEB/ -2.209e-01   2.920e-01    3.941e-02    -3.079e-03  /
CHEB/ -6.261e-02   5.660e-02    2.215e-02    7.947e-03   /
CHEB/ -1.527e-01   5.435e-02    -1.022e-03   4.356e-03   /

c6-C6H9 <=> C6H9                                 1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ 3.164e-01    5.414e-01    -1.337e-01   8.284e-03   /
CHEB/ 8.873e+00    7.918e-01    -2.129e-01   -5.331e-03  /
CHEB/ -3.949e-01   5.471e-01    -8.349e-02   -1.798e-02  /
CHEB/ -2.509e-01   2.599e-01    -5.388e-03   -1.714e-02  /
CHEB/ -5.723e-02   5.623e-02    8.706e-03    -8.575e-03  /
CHEB/ -1.208e-01   9.211e-02    1.077e-02    3.650e-03   /

c5-C6H9 <=> C6H9                                 1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ 3.408e+00    7.065e-01    -1.570e-01   1.402e-02   /
CHEB/ 6.287e+00    1.114e+00    -1.891e-01   -3.031e-02  /
CHEB/ -5.217e-01   6.143e-01    -3.448e-02   -2.451e-02  /
CHEB/ -3.078e-01   2.591e-01    2.448e-02    -7.390e-03  /
CHEB/ -1.033e-01   8.105e-02    2.529e-02    -3.122e-03  /
CHEB/ -8.245e-02   1.310e-02    9.662e-03    1.782e-02   /

C2H3 + C4H6 <=> C6H9                             1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ 1.081e+01    4.216e-01    -1.294e-01   2.771e-02   /
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CHEB/ 6.669e-01    5.442e-01    -1.861e-01   7.552e-03   /
CHEB/ -1.009e-01   3.440e-01    -3.474e-02   -3.110e-02  /
CHEB/ -1.261e-01   2.042e-01    3.383e-03    -2.730e-02  /
CHEB/ -5.558e-02   9.742e-02    -1.323e-02   -1.203e-02  /
CHEB/ -7.691e-02   5.965e-02    3.606e-02    -8.368e-03  /

c5-C6H9-3 <=> C2H3 + C4H6                    1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -1.138e+01   -1.753e+00   -7.279e-01   2.016e-03   /
CHEB/ 1.866e+01    2.011e+00    -3.049e-02   -8.302e-02  /
CHEB/ 7.356e-02    6.777e-01    1.485e-01    -3.343e-02  /
CHEB/ -1.228e-01   2.778e-01    7.909e-02    -8.807e-04  /
CHEB/ -3.330e-02   1.354e-01    5.975e-03    2.164e-03   /
CHEB/ -1.591e-01   1.963e-02    2.763e-02    -1.153e-03  /

c5-C6H9-2 <=> C2H3 + C4H6                    1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -1.579e+01   -1.791e+00   -7.343e-01   -5.613e-03  /
CHEB/ 2.145e+01    1.938e+00    -7.353e-02   -8.283e-02  /
CHEB/ 9.536e-03    6.748e-01    1.298e-01    -4.529e-02  /
CHEB/ -3.346e-02   2.230e-01    7.399e-02    -2.277e-03  /
CHEB/ 5.795e-02    6.203e-02    -1.078e-02   1.169e-02   /
CHEB/ -1.653e-01   7.518e-02    2.647e-02    -1.278e-02  /

c6-C6H9 <=> C2H3 + C4H6                      1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -8.823e+00   -8.267e-01   -4.465e-01   4.144e-02   /
CHEB/ 1.712e+01    1.335e+00    -1.384e-01   -9.287e-02  /
CHEB/ -1.980e-01   4.649e-01    6.516e-02    -2.728e-02  /
CHEB/ -8.387e-02   1.775e-01    2.981e-02    1.368e-03   /
CHEB/ 5.511e-02    7.532e-02    -2.395e-02   -5.997e-04  /
CHEB/ -1.606e-01   1.064e-01    4.227e-02    -1.271e-02  /

c5-C6H9 <=> C2H3 + C4H6                      1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -6.174e+00   -3.709e-01   -4.760e-01   -2.428e-02  /
CHEB/ 1.507e+01    1.064e+00    6.704e-03    -6.710e-03  /
CHEB/ -3.297e-01   5.127e-01    4.917e-02    -1.361e-02  /
CHEB/ -1.979e-01   2.476e-01    3.151e-02    -1.227e-02  /
CHEB/ -6.596e-03   9.209e-02    -2.450e-03   1.603e-03   /
CHEB/ -7.065e-02   1.781e-02    1.613e-02    -8.175e-03  /

C6H9 <=> C2H3 + C4H6                         1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -5.050e+00   4.216e-01    -1.294e-01   2.771e-02   /
CHEB/ 1.392e+01    5.442e-01    -1.861e-01   7.552e-03   /
CHEB/ -2.033e-01   3.440e-01    -3.474e-02   -3.110e-02  /
CHEB/ -1.745e-01   2.042e-01    3.383e-03    -2.730e-02  /
CHEB/ -7.145e-02   9.742e-02    -1.323e-02   -1.203e-02  /
CHEB/ -8.973e-02   5.965e-02    3.606e-02    -8.368e-03  /

c5-C6H9-3 <=> C6H8 + H                       1.0 0.0 0.0
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TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -1.191e+01   -1.921e+00   -6.890e-01   1.934e-03   /
CHEB/ 1.802e+01    2.113e+00    -6.640e-02   -7.799e-02  /
CHEB/ 1.332e-01    7.058e-01    1.403e-01    -3.418e-02  /
CHEB/ -1.173e-01   2.783e-01    8.111e-02    -2.709e-03  /
CHEB/ -2.793e-02   1.318e-01    6.877e-03    3.713e-03   /
CHEB/ -1.624e-01   2.066e-02    2.638e-02    -1.539e-03  /

c5-C6H9-2 <=> C6H8 + H                          1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -1.628e+01   -1.960e+00   -6.982e-01   -4.468e-03  /
CHEB/ 2.076e+01    2.038e+00    -1.048e-01   -7.912e-02  /
CHEB/ 7.795e-02    7.031e-01    1.200e-01    -4.483e-02  /
CHEB/ -2.921e-02   2.257e-01    7.601e-02    -5.001e-03  /
CHEB/ 6.241e-02    5.661e-02    -7.259e-03   1.339e-02   /
CHEB/ -1.668e-01   7.581e-02    2.284e-02    -1.251e-02  /

c6-C6H9 <=> C6H8 + H                            1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -9.178e+00   -9.598e-01   -4.036e-01   3.871e-02   /
CHEB/ 1.629e+01    1.395e+00    -1.816e-01   -8.284e-02  /
CHEB/ -1.237e-01   4.912e-01    6.346e-02    -3.334e-02  /
CHEB/ -7.600e-02   1.802e-01    3.275e-02    2.308e-03   /
CHEB/ 6.078e-02    7.050e-02    -2.328e-02   2.741e-03   /
CHEB/ -1.602e-01   1.084e-01    3.873e-02    -1.408e-02  /

c5-C6H9 <=> C6H8 + H                            1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -6.513e+00   -4.969e-01   -4.660e-01   -1.252e-02  /
CHEB/ 1.421e+01    1.138e+00    5.059e-03    -2.308e-02  /
CHEB/ -2.442e-01   5.258e-01    4.307e-02    -7.324e-03  /
CHEB/ -1.867e-01   2.509e-01    2.776e-02    -1.023e-02  /
CHEB/ -1.953e-03   8.954e-02    -8.606e-04   2.144e-03   /
CHEB/ -7.261e-02   1.896e-02    1.475e-02    -8.618e-03  /

C6H9 <=> C6H8 + H                               1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -5.330e+00   3.891e-01    -1.136e-01   2.130e-02   /
CHEB/ 1.299e+01    5.269e-01    -1.863e-01   1.282e-02   /
CHEB/ -1.178e-01   3.528e-01    -4.595e-02   -2.469e-02  /
CHEB/ -1.620e-01   2.091e-01    -1.224e-03   -2.682e-02  /
CHEB/ -6.508e-02   9.611e-02    -1.349e-02   -1.274e-02  /
CHEB/ -9.045e-02   6.336e-02    3.553e-02    -9.574e-03  /

C2H3 + C4H6 <=> C6H8 + H                        1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ 6.575e+00    -1.863e+00   -1.832e-01   3.799e-02   /
CHEB/ 3.905e+00    8.544e-01    -1.805e-01   -4.471e-02  /
CHEB/ 4.972e-01    3.702e-01    3.573e-02    -5.386e-02  /
CHEB/ 6.984e-02    1.701e-01    5.423e-02    -2.283e-02  /
```

```
CHEB/ 4.910e-02   1.007e-01   1.127e-02   -1.219e-02  /
CHEB/ -2.915e-02  -3.749e-03  4.216e-02   1.457e-02   /

c5-C6H9-3 <=> H + c5-C6H8                      1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -8.649e+00  -7.777e-01  -3.495e-01  -1.640e-02  /
CHEB/ 1.491e+01   1.517e+00   -2.345e-02  -5.912e-02  /
CHEB/ 1.565e-01   6.691e-01   3.897e-02   3.242e-03   /
CHEB/ -1.614e-01  2.497e-01   4.672e-02   -6.477e-04  /
CHEB/ -7.007e-02  5.705e-02   2.289e-02   9.755e-03   /
CHEB/ -1.407e-01  2.233e-02   5.851e-04   1.049e-03   /

c5-C6H9-2 <=> H + c5-C6H8                      1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -1.269e+01  -8.258e-01  -3.747e-01  -1.025e-02  /
CHEB/ 1.730e+01   1.459e+00   -4.747e-02  -6.875e-02  /
CHEB/ 1.175e-01   6.419e-01   2.453e-02   -7.695e-03  /
CHEB/ -7.982e-02  1.944e-01   3.898e-02   6.170e-04   /
CHEB/ 2.359e-03   -2.260e-02  2.696e-02   1.759e-02   /
CHEB/ -1.292e-01  6.576e-02   -2.108e-02  -4.944e-03  /

c6-C6H9 <=> H + c5-C6H8                        1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -7.514e+00  -2.494e+00  -5.877e-01  2.253e-02   /
CHEB/ 1.403e+01   2.224e+00   -1.330e-01  -1.021e-01  /
CHEB/ -5.684e-02  7.497e-01   1.185e-01   -3.131e-02  /
CHEB/ -8.274e-02  2.130e-01   6.578e-02   1.372e-02   /
CHEB/ 6.019e-02   3.171e-02   -2.886e-04  2.433e-02   /
CHEB/ -1.863e-01  7.730e-02   9.919e-04   -9.699e-03  /

c5-C6H9 <=> H + c5-C6H8                        1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -1.951e+00  8.831e-01   -2.078e-01  7.053e-03   /
CHEB/ 9.952e+00   6.628e-01   1.058e-01   -7.544e-02  /
CHEB/ -2.852e-01  3.337e-01   4.091e-02   1.105e-02   /
CHEB/ -2.087e-01  1.523e-01   2.106e-03   2.960e-02   /
CHEB/ -5.796e-02  2.233e-02   1.480e-02   2.211e-02   /
CHEB/ -4.849e-02  6.713e-03   -2.147e-02  3.837e-03   /

C6H9 <=> H + c5-C6H8                           1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ -3.382e+00  -9.788e-01  -3.903e-01  3.014e-02   /
CHEB/ 1.031e+01   1.307e+00   -5.816e-02  -6.630e-02  /
CHEB/ 1.600e-02   5.568e-01   4.044e-02   -1.033e-02  /
CHEB/ -1.308e-01  2.468e-01   1.669e-02   6.413e-03   /
CHEB/ -6.737e-02  7.729e-02   1.617e-03   9.857e-03   /
CHEB/ -1.298e-01  3.000e-02   5.892e-03   -8.547e-03  /

C2H3 + C4H6 <=> H + c5-C6H8                    1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
```

CHEB/ 6.880e+00 -2.612e+00 -4.742e-01 -3.085e-02 /
CHEB/ 2.826e+00 1.296e+00 1.318e-02 -2.213e-02 /
CHEB/ 3.662e-01 5.026e-01 8.036e-02 -2.005e-02 /
CHEB/ 5.719e-02 2.114e-01 5.833e-02 -1.568e-02 /
CHEB/ 3.875e-02 9.362e-02 7.750e-03 -5.774e-03 /
CHEB/ -6.475e-02 -1.959e-02 2.542e-02 2.514e-03 /

c5-C6H9-3 <=> H + C6H8-c6-13 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -9.886e+00 -3.964e+00 -7.531e-01 8.452e-03 /
CHEB/ 1.604e+01 3.128e+00 -1.918e-01 -1.214e-01 /
CHEB/ -5.796e-02 9.200e-01 1.761e-01 -2.914e-02 /
CHEB/ -2.309e-01 2.487e-01 9.092e-02 1.568e-02 /
CHEB/ -1.542e-02 7.235e-02 -5.298e-03 1.544e-02 /
CHEB/ -1.417e-01 8.667e-02 2.154e-02 -7.912e-03 /

c5-C6H9-2 <=> H + C6H8-c6-13 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -1.403e+01 -4.115e+00 -7.342e-01 6.097e-03 /
CHEB/ 1.853e+01 3.122e+00 -2.533e-01 -1.194e-01 /
CHEB/ -8.107e-02 9.448e-01 1.529e-01 -4.102e-02 /
CHEB/ -1.606e-01 2.050e-01 9.269e-02 1.154e-02 /
CHEB/ 6.449e-02 -6.879e-03 -1.974e-03 2.241e-02 /
CHEB/ -1.310e-01 1.266e-01 7.674e-03 -1.114e-02 /

c6-C6H9 <=> H + C6H8-c6-13 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -1.518e+00 5.127e-01 -1.173e-01 2.328e-03 /
CHEB/ 1.022e+01 7.236e-01 -1.390e-01 -3.457e-02 /
CHEB/ -2.563e-01 4.129e-01 -2.033e-02 -3.043e-02 /
CHEB/ -1.550e-01 1.411e-01 3.499e-02 -1.576e-02 /
CHEB/ -1.771e-02 -6.367e-04 3.040e-02 -5.533e-03 /
CHEB/ -8.206e-02 5.711e-02 -6.770e-04 1.513e-02 /

c5-C6H9 <=> H + C6H8-c6-13 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -3.562e+00 -2.744e+00 -5.141e-01 1.993e-02 /
CHEB/ 1.123e+01 2.306e+00 -1.979e-01 -9.112e-02 /
CHEB/ -3.116e-01 8.018e-01 1.035e-01 -3.754e-02 /
CHEB/ -2.883e-01 2.206e-01 6.971e-02 1.156e-02 /
CHEB/ -1.859e-03 2.078e-02 1.051e-02 2.373e-02 /
CHEB/ -3.950e-02 7.359e-02 -4.613e-03 -4.771e-03 /

C6H9 <=> H + C6H8-c6-13 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -2.054e+00 -1.493e+00 -2.368e-01 8.223e-03 /
CHEB/ 9.581e+00 1.320e+00 -2.864e-01 -1.397e-02 /
CHEB/ -1.245e-01 6.397e-01 -1.468e-02 -4.530e-02 /
CHEB/ -2.470e-01 2.082e-01 4.288e-02 -1.292e-02 /
CHEB/ -6.092e-02 2.774e-02 8.945e-04 1.305e-02 /
CHEB/ -5.708e-02 1.206e-01 1.098e-02 -6.828e-03 /

C2H3 + C4H6 <=> H + C6H8-c6-13 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ 7.602e+00 -3.074e+00 -4.570e-01 3.458e-02 /
CHEB/ 2.597e+00 1.597e+00 -1.095e-01 -1.184e-01 /
CHEB/ 1.547e-01 4.688e-01 1.029e-01 -2.392e-02 /
CHEB/ -2.590e-02 1.482e-01 4.708e-02 1.353e-03 /
CHEB/ 4.131e-02 8.394e-02 -1.844e-02 -1.125e-02 /
CHEB/ -2.761e-02 6.589e-02 5.694e-02 -7.121e-04 /

c5-C6H9-3 <=> H + C6H8-c6-14 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -9.789e+00 -3.961e+00 -7.539e-01 8.527e-03 /
CHEB/ 1.605e+01 3.126e+00 -1.911e-01 -1.215e-01 /
CHEB/ -5.850e-02 9.195e-01 1.762e-01 -2.913e-02 /
CHEB/ -2.308e-01 2.487e-01 9.090e-02 1.569e-02 /
CHEB/ -1.550e-02 7.252e-02 -5.360e-03 1.543e-02 /
CHEB/ -1.416e-01 8.665e-02 2.157e-02 -7.918e-03 /

c5-C6H9-2 <=> H + C6H8-c6-14 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -1.393e+01 -4.112e+00 -7.353e-01 6.233e-03 /
CHEB/ 1.854e+01 3.120e+00 -2.524e-01 -1.195e-01 /
CHEB/ -8.200e-02 9.442e-01 1.531e-01 -4.102e-02 /
CHEB/ -1.604e-01 2.050e-01 9.269e-02 1.155e-02 /
CHEB/ 6.442e-02 -6.694e-03 -2.084e-03 2.242e-02 /
CHEB/ -1.310e-01 1.267e-01 7.708e-03 -1.116e-02 /

c6-C6H9 <=> H + C6H8-c6-14 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -1.450e+00 5.145e-01 -1.181e-01 2.495e-03 /
CHEB/ 1.026e+01 7.240e-01 -1.390e-01 -3.464e-02 /
CHEB/ -2.650e-01 4.116e-01 -1.951e-02 -3.073e-02 /
CHEB/ -1.553e-01 1.403e-01 3.525e-02 -1.569e-02 /
CHEB/ -1.747e-02 -6.645e-04 3.017e-02 -5.299e-03 /
CHEB/ -8.224e-02 5.765e-02 -8.560e-04 1.507e-02 /

c5-C6H9 <=> H + C6H8-c6-14 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -3.471e+00 -2.740e+00 -5.158e-01 2.022e-02 /
CHEB/ 1.124e+01 2.303e+00 -1.962e-01 -9.152e-02 /
CHEB/ -3.139e-01 8.011e-01 1.037e-01 -3.743e-02 /
CHEB/ -2.882e-01 2.207e-01 6.964e-02 1.156e-02 /
CHEB/ -1.940e-03 2.104e-02 1.034e-02 2.377e-02 /
CHEB/ -3.953e-02 7.364e-02 -4.553e-03 -4.828e-03 /

C6H9 <=> H + C6H8-c6-14 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -1.967e+00 -1.491e+00 -2.375e-01 8.453e-03 /
CHEB/ 9.601e+00 1.320e+00 -2.862e-01 -1.420e-02 /
CHEB/ -1.288e-01 6.386e-01 -1.408e-02 -4.541e-02 /

CHEB/ -2.467e-01 2.081e-01 4.283e-02 -1.280e-02 /
CHEB/ -6.101e-02 2.809e-02 6.622e-04 1.310e-02 /
CHEB/ -5.711e-02 1.206e-01 1.107e-02 -6.903e-03 /

C2H3 + C4H6 <=> H + C6H8-c6-14 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ 7.703e+00 -3.074e+00 -4.571e-01 3.457e-02 /
CHEB/ 2.600e+00 1.597e+00 -1.094e-01 -1.185e-01 /
CHEB/ 1.550e-01 4.686e-01 1.029e-01 -2.391e-02 /
CHEB/ -2.598e-02 1.482e-01 4.708e-02 1.351e-03 /
CHEB/ 4.130e-02 8.397e-02 -1.844e-02 -1.127e-02 /
CHEB/ -2.756e-02 6.586e-02 5.695e-02 -6.953e-04 /

c5-C6H9-3 <=> C5H6 + CH3 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -3.870e+00 -1.491e+00 -2.332e-01 7.174e-03 /
CHEB/ 1.267e+01 1.534e+00 -3.416e-01 -2.907e-02 /
CHEB/ -1.202e-02 8.283e-01 -5.307e-02 -5.314e-02 /
CHEB/ -3.217e-01 2.897e-01 6.272e-02 -3.300e-02 /
CHEB/ -1.084e-01 5.474e-02 3.465e-02 -6.206e-03 /
CHEB/ -3.811e-02 6.619e-02 2.956e-02 8.582e-03 /

c5-C6H9-2 <=> C5H6 + CH3 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -2.873e+00 3.354e-01 -8.717e-02 3.499e-03 /
CHEB/ 1.195e+01 5.399e-01 -1.747e-01 1.945e-03 /
CHEB/ -2.372e-01 3.903e-01 -7.725e-02 -1.323e-02 /
CHEB/ -1.786e-01 2.017e-01 -1.435e-02 -1.860e-02 /
CHEB/ -5.220e-02 5.955e-02 8.277e-05 -1.285e-02 /
CHEB/ -6.529e-02 4.374e-02 2.484e-02 -5.929e-03 /

c6-C6H9 <=> C5H6 + CH3 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -8.371e+00 -4.226e+00 -7.013e-01 4.549e-03 /
CHEB/ 1.482e+01 3.153e+00 -2.741e-01 -1.158e-01 /
CHEB/ -5.190e-02 9.776e-01 1.440e-01 -4.160e-02 /
CHEB/ -1.756e-01 2.145e-01 9.226e-02 1.113e-02 /
CHEB/ 5.150e-02 -1.038e-02 1.946e-03 2.216e-02 /
CHEB/ -1.312e-01 1.228e-01 6.244e-03 -9.979e-03 /

c5-C6H9 <=> C5H6 + CH3 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /
CHEB/ 6 4/
CHEB/ -2.770e+00 -1.117e+00 -2.908e-01 -3.758e-03 /
CHEB/ 1.033e+01 1.607e+00 -1.371e-01 -6.365e-02 /
CHEB/ 1.690e-02 6.488e-01 4.177e-02 -2.561e-02 /
CHEB/ -3.102e-01 2.118e-01 3.162e-02 1.098e-02 /
CHEB/ -8.508e-02 -8.797e-03 3.109e-02 1.372e-02 /
CHEB/ 1.719e-02 5.076e-02 -2.014e-02 7.841e-05 /

C6H9 <=> C5H6 + CH3 1.0 0.0 0.0
TCHEB/ 300.000 2000.000 /
PCHEB/ 0.001 100.000 /

```
CHEB/ 6 4/
CHEB/ -4.273e+00   -2.817e+00   -5.066e-01   1.607e-02   /
CHEB/ 1.101e+01    2.265e+00    -2.508e-01   -7.796e-02  /
CHEB/ 1.223e-01    8.310e-01    6.220e-02    -3.686e-02  /
CHEB/ -2.353e-01   2.684e-01    5.788e-02    -3.793e-03  /
CHEB/ -8.261e-02   2.851e-02    1.919e-02    9.510e-03   /
CHEB/ -7.183e-02   7.653e-02    3.989e-03    -4.882e-03  /

C2H3 + C4H6 <=> C5H6 + CH3                    1.0 0.0 0.0
TCHEB/ 300.000   2000.000 /
PCHEB/ 0.001     100.000  /
CHEB/ 6 4/
CHEB/ 6.267e+00    -3.978e+00   -7.355e-01   -1.860e-02  /
CHEB/ 3.396e+00    2.188e+00    -4.081e-02   -1.111e-01  /
CHEB/ 3.235e-01    6.427e-01    1.733e-01    -4.115e-02  /
CHEB/ 2.499e-03    1.776e-01    9.270e-02    5.021e-03   /
CHEB/ 3.190e-02    6.503e-02    -8.671e-03   5.676e-03   /
CHEB/ -2.984e-02   4.194e-02    3.925e-02    -3.454e-03  /

================================================================================================
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```

3. *Cantherm example input file (python files corresponding to individual species not included)*

```
#!/usr/bin/env python
# -*- coding: utf-8 -*-

modelChemistry = "CCSD(T)-F12/cc-pVTZ-F12"
frequencyScaleFactor = 0.985
useHinderedRotors = True
useBondCorrections = False

species('C6H9', './species/C6H9.py',
      collisionModel = TransportData(sigma=(5.72,'angstrom'), epsilon=(3.28969,'kJ/mol')), #from Joback method
      energyTransferModel = SingleExponentialDown(alpha0=(4.78,'kJ/mol'), T0=(300,'K'), n=0.7,),# assumed equal to N2-benzene from Miller
      molecularWeight = (81.135,'amu'),
      )
species('C2H3', './species/C2H3.py')
species('C4H6', './species/C4H6.py')
species('C6H8', './species/nC6H8.py')
species('H', './species/H.py')
species('c6-C6H9', './species/c6-C6H9.py',
      collisionModel = TransportData(sigma=(6.35,'angstrom'), epsilon=(3.63058,'kJ/mol')), #from Joback method, cyclohexene
      energyTransferModel = SingleExponentialDown(alpha0=(4.78,'kJ/mol'), T0=(300,'K'), n=0.7,), #assumed equal to N2-benzene from Miller
      molecularWeight = (81.135,'amu'),
      )
species('c5-C6H9', './species/c5-C6H9.py',
      collisionModel = TransportData(sigma=(6.14 ,'angstrom'), epsilon=(3.51103,'kJ/mol')), #from Joback method
      energyTransferModel = SingleExponentialDown(alpha0=(4.78,'kJ/mol'), T0=(300,'K'), n=0.7,), #assumed equal to N2-benzene from Miller
      molecularWeight = (81.135,'amu'),
      )
species('c5-C6H9-3', './species/c5-C6H9-3.py',
      collisionModel = TransportData(sigma=(6.14 ,'angstrom'), epsilon=(3.51103,'kJ/mol')), #from Joback method
      energyTransferModel = SingleExponentialDown(alpha0=(4.78,'kJ/mol'), T0=(300,'K'), n=0.7,), #assumed equal to N2-benzene from Miller
      molecularWeight = (81.135,'amu'),
      )
species('c5-C6H9-2', './species/c5-C6H9-2.py',
      collisionModel = TransportData(sigma=(6.14,'angstrom'), epsilon=(3.51103,'kJ/mol')), #from Joback method
      energyTransferModel = SingleExponentialDown(alpha0=(4.78,'kJ/mol'), T0=(300,'K'), n=0.7,), #assumed equal to N2-benzene from Miller
      molecularWeight = (81.135,'amu'),
      )
species('c5-C6H8', './species/c5-C6H8.py')
species('C6H8-c6-13', './species/C6H8-c6-13.py')
species('C6H8-c6-14', './species/C6H8-c6-14.py')
species('C5H6', './species/C5H6.py')
species('CH3', './species/CH3.py')
species(
   label = 'N2',
   molecularWeight = (28.01,'amu'),
   collisionModel = TransportData(sigma=(3.621e-10,'m'), epsilon=(0.810904,'kJ/mol')),
   energyTransferModel = SingleExponentialDown(alpha0=(4.78,'kJ/mol'), T0=(300,'K'), n=0.7),
)
transitionState('TSadd', './species/add-C6H9correct.py')
```

```
#transitionState('TSaddi', './species/add-C6H9i.py')
#transitionState('TSi_beta', './species/iC6H9c3_beta.py')
transitionState('TS_C6H8_H-l', './species/C6H8_H.py')
transitionState('TSendo', './species/tsendo.py')
transitionState('TSexo', './species/tsexo.py')
transitionState('TS_C6H8_H', './species/C6H8_H-c5.py')
transitionState('TS_C6H8_H-c6-13', './species/TS_C6H8_H-c6-13.py')
transitionState('TS_C6H8_H-c6-14', './species/TS_C6H8_H-c6-14.py')
transitionState('TS1', './species/TS1.py')
transitionState('TS2', './species/TS2.py')
transitionState('TS_C5H6_CH3-c5-2', './species/TS_C5H6_CH3-c5-2b.py')
transitionState('TS_C5H6_CH3-c5', './species/TS_C5H6_CH3-c5.py')
reaction(
    label = 'C2H3 + C4H6 = C6H9',
    reactants = ['C2H3','C4H6'],
    products = ['C6H9'],
    transitionState = 'TSadd',
#    tunneling='Eckart'
)
'''
reaction(
    label = 'C2H3 + C4H6 = iC6H9',
    reactants = ['C2H3','C4H6'],
    products = ['iC6H9'],
    transitionState = 'TSaddi',
#    tunneling='Eckart'
)
reaction(
    label = 'iC6H9 = iC6H9c3',
    reactants = ['iC6H9'],
    products = ['iC6H9c3'],
    transitionState = 'TSendo',   #fake TS, qchem running
#    tunneling='Eckart',
)
reaction(
    label = 'iC6H9c3 = C6H9',
    reactants = ['iC6H9c3'],
    products = ['C6H9'],
    transitionState = 'TSi_beta',
    tunneling='Eckart',
)'''
reaction(
    label = 'C6H9 = C6H8 + H',
    reactants = ['C6H9'],
    products = ['C6H8','H'],
    transitionState = 'TS_C6H8_H-l',
    tunneling='Eckart',
)
reaction(
    label = 'C6H9 = c6-C6H9',
    reactants = ['C6H9'],
    products = ['c6-C6H9'],
    transitionState = 'TSendo',
    tunneling='Eckart',
)
reaction(
    label = 'C6H9 = c5-C6H9',
    reactants = ['C6H9'],
    products = ['c5-C6H9'],
    transitionState = 'TSexo',
    tunneling='Eckart',
)
```

```
reaction(
    label = 'c5-C6H9 = c5-C6H8 + H',
    reactants = ['c5-C6H9'],
    products = ['c5-C6H8','H'],
    transitionState = 'TS_C6H8_H',
    tunneling='Eckart',
)
reaction(
    label = 'c6-C6H9 = C6H8-c6-13 + H',
    reactants = ['c6-C6H9'],
    products = ['C6H8-c6-13','H'],
    transitionState = 'TS_C6H8_H-c6-13',
    tunneling='Eckart',
)
reaction(
    label = 'c6-C6H9 = C6H8-c6-14 + H',
    reactants = ['c6-C6H9'],
    products = ['C6H8-c6-14','H'],
    transitionState = 'TS_C6H8_H-c6-14',
    tunneling='Eckart',
)
reaction(
    label = 'c5-C6H9 = c5-C6H9-2',
    reactants = ['c5-C6H9'],
    products = ['c5-C6H9-2'],
    transitionState = 'TS_C5H6_CH3-c5',
    tunneling='Eckart',
)
reaction(
    label = 'c5-C6H9 = c5-C6H9-3',
    reactants = ['c5-C6H9'],
    products = ['c5-C6H9-3'],
    transitionState = 'TS1',
    tunneling='Eckart',
)
reaction(
    label = 'c5-C6H9-3 = c5-C6H9-2',
    reactants = ['c5-C6H9-3'],
    products = ['c5-C6H9-2'],
    transitionState = 'TS2',
    tunneling='Eckart',
)
reaction(
    label = 'c5-C6H9-2 = C5H6 + CH3',
    reactants = ['c5-C6H9-2'],
    products = ['C5H6','CH3'],
    transitionState = 'TS_C5H6_CH3-c5-2',
    tunneling='Eckart',
)

statmech('TSadd')
#statmech('TSaddi')
#statmech('TSi_beta')
statmech('TS_C6H8_H-l')
statmech('TSendo')
statmech('TSexo')
statmech('TS_C6H8_H')
statmech('TS_C6H8_H-c6-13')
statmech('TS_C6H8_H-c6-14')
statmech('TS1')
statmech('TS2')
statmech('H')
```

```
statmech('TS_C5H6_CH3-c5-2')
statmech('TS_C5H6_CH3-c5')

kinetics('C2H3 + C4H6 = C6H9')
#kinetics('C2H3 + C4H6 = iC6H9')
#kinetics('iC6H9 = iC6H9c3')
#kinetics('iC6H9c3 = C6H9')
kinetics('C6H9 = C6H8 + H')
kinetics('C6H9 = c6-C6H9')
kinetics('C6H9 = c5-C6H9')
kinetics('c5-C6H9 = c5-C6H8 + H')
kinetics('c6-C6H9 = C6H8-c6-13 + H')
kinetics('c6-C6H9 = C6H8-c6-14 + H')
kinetics('c5-C6H9 = c5-C6H9-3')
kinetics('c5-C6H9 = c5-C6H9-2')
kinetics('c5-C6H9-2 = C5H6 + CH3')
kinetics('c5-C6H9-3 = c5-C6H9-2')



network(
    label = 'vinyl+butadiene',
    isomers = [
    'c5-C6H9-3',
    'c5-C6H9-2',
    'c6-C6H9',
    'c5-C6H9',
    'C6H9',
#     'iC6H9',
#     'iC6H9c3',
            ],

    reactants = [
    ('C2H3','C4H6'),
#     ('C6H8','H'),
    ],
#     products = [
#     ('C6H8','H'),
#     ],
    bathGas = {
        'N2': 1,
    },
)

pressureDependence(
    label = 'vinyl+butadiene',
    Tmin = (300,'K'), Tmax = (2000,'K'), Tcount = 12,
    Tlist = ([300,400,500,600,700,1000,1200,1300,1400,1500,1700,2000],'K'),
    Pmin = (0.0001,'atm'), Pmax = (100,'atm'), Pcount = 9,
    maximumGrainSize = (.5,'kcal/mol'), #0.057 = 20 cm-1
    minimumGrainCount = 800, #max is 500 in my MW simulations
    method = 'modified strong collision',
    interpolationModel = ('Chebyshev', 6, 4),
    activeKRotor = True,
    rmgmode = False,
)
================================================================================================
=============================================
```

4. High-pressure limit rate coefficients for H-abstraction reactions from 1,3-butadiene + vinyl

```
C2H3 + C4H6 <=> C2H4 + nC4H5                 3.437e-04     4.732     6.579

C2H3 + C4H6 <=> C2H4 + iC4H5                 6.210e-04     4.814     4.902
Units: cm, mol, s

# Coordinates for C2H3 (angstroms):
#   C    0.0000    0.0000    0.0000
#   H    0.9087    0.5894   -0.0000
#   C   -1.2940    0.1702    0.0000
#   H   -1.9868   -0.6734   -0.0000
#   H   -1.7421    1.1707   -0.0000
conformer(
    label = 'C2H3',
    E0 = (294.699, 'kJ/mol'),
    modes = [
        IdealGasTranslation(mass=(27.0235, 'amu')),
        NonlinearRotor(
            inertia = ([2.13743, 15.509, 17.6464], 'amu*angstrom^2'),
            symmetry = 1,
        ),
        HarmonicOscillator(
            frequencies = ([678.291, 813.039, 913.725, 1009.14, 1352.92, 1634.06, 2971.51, 3059.2, 3193.55], 'cm^-1'),
        ),
    ],
    spinMultiplicity = 2,
    opticalIsomers = 1,
)

# Coordinates for C2H4 (angstroms):
#   C    0.0000    0.0000    0.0000
#   C   -1.3281    0.0000    0.0000
#   H    0.5699    0.9277    0.0000
#   H    0.5699   -0.9277    0.0000
#   H   -1.8980    0.9277    0.0000
#   H   -1.8980   -0.9277    0.0000
conformer(
    label = 'C2H4',
    E0 = (50.9608, 'kJ/mol'),
    modes = [
        IdealGasTranslation(mass=(28.0313, 'amu')),
        NonlinearRotor(
            inertia = ([3.46974, 16.722, 20.1917], 'amu*angstrom^2'),
            symmetry = 2,
        ),
        HarmonicOscillator(
            frequencies = ([803.799, 965.684, 986.566, 1034.79, 1205.2, 1344.11, 1429.56, 1663.97, 3033.54, 3050.24, 3106.39,
3131.32], 'cm^-1'),
        ),
    ],
    spinMultiplicity = 1,
    opticalIsomers = 1,
)

# Coordinates for nC4H5 (angstroms):
#   C    0.0000    0.0000    0.0000
#   C   -1.2311    0.4600    0.0006
#   C   -2.4386   -0.3853    0.0005
#   C   -3.6756    0.1150    0.0001
#   H    0.5221   -0.9493    0.0001
```

```
#   H   -1.4009    1.5423    0.0009
#   H   -2.2825   -1.4645    0.0008
#   H   -3.8475    1.1908   -0.0002
#   H   -4.5502   -0.5303    0.0000
conformer(
    label = 'nC4H5',
    E0 = (362.99, 'kJ/mol'),
    modes = [
        IdealGasTranslation(mass=(53.0391, 'amu')),
        NonlinearRotor(
            inertia = ([11.5447, 107.232, 118.777], 'amu*angstrom^2'),
            symmetry = 1,
        ),
        HarmonicOscillator(
            frequencies = ([163.934, 275.051, 465.944, 578.293, 733.254, 794.107, 887.347, 908.554, 947.836, 1009.6, 1125.99,
1213.79, 1276.89, 1401.74, 1619.8, 1662.34, 3002.63, 3043.15, 3060.18, 3133.48, 3176.06], 'cm^-1'),
        ),
    ],
    spinMultiplicity = 2,
    opticalIsomers = 1,
)

# Coordinates for iC4H5 (angstroms):
#   C    0.0000    0.0000    0.0000
#   C   -1.2564    0.3360   -0.0009
#   C   -2.5585    0.6862    0.0011
#   C   -3.6269   -0.2131   -0.0002
#   H    0.5479   -0.1502    0.9329
#   H    0.5527   -0.1474   -0.9306
#   H   -2.7763    1.7566    0.0024
#   H   -3.4535   -1.2854    0.0024
#   H   -4.6507    0.1466   -0.0039
conformer(
    label = 'iC4H5',
    E0 = (306.966, 'kJ/mol'),
    modes = [
        IdealGasTranslation(mass=(53.0391, 'amu')),
        NonlinearRotor(inertia=([12.24, 113.919, 122.66], 'amu*angstrom^2'), symmetry=1),
        HarmonicOscillator(
            frequencies = ([204.988, 228.973, 488.422, 513.786, 561.125, 740.681, 884.057, 888.933, 925.496, 956.317, 1045.9,
1141.9, 1330.33, 1405.76, 1444.36, 1870.72, 2996.57, 3027.68, 3064.66, 3084.96, 3190.82], 'cm^-1'),
        ),
    ],
    spinMultiplicity = 2,
    opticalIsomers = 1,
)

# Coordinates for C4H6 (angstroms):
#   C    0.0000    0.0000    0.0000
#   H   -0.1360    1.0836    0.0000
#   C    1.2311   -0.5167    0.0000
#   H    1.3870   -1.5952    0.0000
#   H    2.1161    0.1143    0.0000
#   C   -1.2195   -0.8107    0.0000
#   H   -1.0835   -1.8944    0.0000
#   C   -2.4506   -0.2941    0.0000
#   H   -2.6065    0.7845    0.0000
#   H   -3.3356   -0.9250    0.0000
conformer(
    label = 'C4H6',
    E0 = (110.815, 'kJ/mol'),
    modes = [
```

```
        IdealGasTranslation(mass=(54.047, 'amu')),
        NonlinearRotor(
            inertia = ([12.1052, 113.723, 125.828], 'amu*angstrom^2'),
            symmetry = 2,
        ),
        HarmonicOscillator(
            frequencies = ([168.415, 278.489, 496.598, 529.585, 767.985, 875.173, 943.512, 948.181, 969.89, 993.747, 1034.98,
1191.38, 1275.58, 1276.14, 1377.53, 1430.47, 1630.83, 1690.89, 3038.9, 3042.89, 3047.46, 3051.84, 3133.21, 3133.27], 'cm^-
1'),
        ),
    ],
    spinMultiplicity = 1,
    opticalIsomers = 1,
)

# Coordinates for H (angstroms):
conformer(
    label = 'H',
    E0 = (211.794, 'kJ/mol'),
    modes = [],
    spinMultiplicity = 2,
    opticalIsomers = 1,
)

# Coordinates for Habtr1 (angstroms):
#   C    0.0000    0.0000    0.0000
#   H   -0.8657    0.5720    0.3385
#   C    1.1964    0.5831   -0.1068
#   H    2.0678    0.0215   -0.4433
#   H    1.3436    1.6322    0.1365
#   C   -0.2340   -1.4128   -0.3193
#   H    0.6439   -1.9868   -0.6406
#   C   -1.4134   -2.0164   -0.2426
#   H   -2.4770   -1.2717    0.1207
#   H   -1.6450   -3.0545   -0.4684
#   C   -3.4821   -0.4224    0.3067
#   H   -4.0828   -0.5831    1.2003
#   C   -3.6296    0.5036   -0.6210
#   H   -2.9524    0.5562   -1.4760
#   H   -4.4269    1.2484   -0.5756
conformer(
    label = 'Habtr1',
    E0 = (454.46, 'kJ/mol'),
    modes = [
        IdealGasTranslation(mass=(81.0705, 'amu')),
        NonlinearRotor(
            inertia = ([96.7038, 285.961, 361.681], 'amu*angstrom^2'),
            symmetry = 1,
        ),
        HarmonicOscillator(
            frequencies = ([59.7304, 82.5725, 117.245, 155.876, 242.231, 302.021, 369.405, 501.917, 559.569, 573.713, 759.189,
828.336, 879.871, 933.672, 936.036, 955.371, 959.341, 975.189, 1023.8, 1135.3, 1169.85, 1181.17, 1244.76, 1275.99, 1306.27,
1371.55, 1408.83, 1610.02, 1638.2, 1673.63, 2991.5, 3000.18, 3040.88, 3054.87, 3073.61, 3096.11, 3110.9, 3130.66], 'cm^-1'),
        ),
    ],
    spinMultiplicity = 2,
    opticalIsomers = 2,
    frequency = (-1602.22, 'cm^-1'),
)

# Coordinates for Habtr2 (angstroms):
#   C    0.0000    0.0000    0.0000
```

```
#   H   -0.8657    0.5720    0.3385
#   C    1.1964    0.5831   -0.1068
#   H    2.0678    0.0215   -0.4433
#   H    1.3436    1.6322    0.1365
#   C   -0.2340   -1.4128   -0.3193
#   H    0.6439   -1.9868   -0.6406
#   C   -1.4134   -2.0164   -0.2426
#   H   -2.4770   -1.2717    0.1207
#   H   -1.6450   -3.0545   -0.4684
#   C   -3.4821   -0.4224    0.3067
#   H   -4.0828   -0.5831    1.2003
#   C   -3.6296    0.5036   -0.6210
#   H   -2.9524    0.5562   -1.4760
#   H   -4.4269    1.2484   -0.5756
conformer(
    label = 'Habtr2',
    E0 = (454.46, 'kJ/mol'),
    modes = [
        IdealGasTranslation(mass=(81.0705, 'amu')),
        NonlinearRotor(
            inertia = ([96.7038, 285.961, 361.681], 'amu*angstrom^2'),
            symmetry = 1,
        ),
        HarmonicOscillator(
            frequencies = ([59.7304, 82.5725, 117.245, 155.876, 242.231, 302.021, 369.405, 501.917, 559.569, 573.713, 759.189,
828.336, 879.871, 933.672, 936.036, 955.371, 959.341, 975.189, 1023.8, 1135.3, 1169.85, 1181.17, 1244.76, 1275.99, 1306.27,
1371.55, 1408.83, 1610.02, 1638.2, 1673.63, 2991.5, 3000.18, 3040.88, 3054.87, 3073.61, 3096.11, 3110.9, 3130.66], 'cm^-1'),
        ),
    ],
    spinMultiplicity = 2,
    opticalIsomers = 2,
    frequency = (-1602.22, 'cm^-1'),
)

#   ======= =========== =========== =========== ===============
#   Temp.   k (TST)     Tunneling   k (TST+T)   Units
#   ======= =========== =========== =========== ===============
#     300 K   1.271e+02     20.3667   2.588e+03 cm^3/(mol*s)
#     400 K   2.680e+04     4.78656   1.283e+05 cm^3/(mol*s)
#     500 K   7.761e+05     2.65554   2.061e+06 cm^3/(mol*s)
#     600 K   8.172e+06     1.96625   1.607e+07 cm^3/(mol*s)
#     800 K   1.907e+08     1.47301   2.809e+08 cm^3/(mol*s)
#    1000 K   1.510e+09     1.29055   1.949e+09 cm^3/(mol*s)
#    1500 K   3.493e+10     1.13035   3.949e+10 cm^3/(mol*s)
#    2000 K   2.247e+11     1.07705   2.420e+11 cm^3/(mol*s)
#   ======= =========== =========== =========== ===============
kinetics(
    label = 'C2H3 + C4H6 = C2H4 + nC4H5',
    kinetics = Arrhenius(
        A = (0.000343722, 'cm^3/(mol*s)'),
        n = 4.73167,
        Ea = (28.3623, 'kJ/mol'),
        T0 = (1, 'K'),
        Tmin = (303.03, 'K'),
        Tmax = (2500, 'K'),
        comment = 'Fitted to 59 data points; dA = *|/ 1.74926, dn = +|- 0.0733891, dEa = +|- 0.403714 kJ/mol',
    ),
)

#   ======= =========== =========== =========== ===============
#   Temp.   k (TST)     Tunneling   k (TST+T)   Units
#   ======= =========== =========== =========== ===============
```

```
#     300 K   1.271e+02     29.0119   3.687e+03 cm^3/(mol*s)
#     400 K   2.680e+04     5.17304   1.387e+05 cm^3/(mol*s)
#     500 K   7.761e+05     2.70086   2.096e+06 cm^3/(mol*s)
#     600 K   8.172e+06     1.96405   1.605e+07 cm^3/(mol*s)
#     800 K   1.907e+08     1.45839   2.781e+08 cm^3/(mol*s)
#    1000 K   1.510e+09     1.27657   1.928e+09 cm^3/(mol*s)
#    1500 K   3.493e+10     1.12016   3.913e+10 cm^3/(mol*s)
#    2000 K   2.247e+11     1.06927   2.403e+11 cm^3/(mol*s)
#   ======= ============ ============ ============ ===============
kinetics(
    label = 'C2H3 + C4H6 = C2H4 + iC4H5',
    kinetics = Arrhenius(
        A = (3.56454e-05, 'cm^3/(mol*s)'),
        n = 5.01404,
        Ea = (26.0766, 'kJ/mol'),
        T0 = (1, 'K'),
        Tmin = (303.03, 'K'),
        Tmax = (2500, 'K'),
        comment = 'Fitted to 59 data points; dA = *|/ 2.1404, dn = +|- 0.0998737, dEa = +|- 0.549405 kJ/mol',
    ),
)
================================================================================================
================
```

5. *Hindered rotor potential scan lists used in the RRKM/ME simulations, computed at the BMK/6-311+G(d,p) level of theory.*

TS_add_rotor (addition of vinyl to terminal end of 1,3-butadiene)

Angle (radians)	Energy (kJ/mol)
0	0
0.1745329252	0.3347302279
0.3490658504	1.1523791468
0.5235987756	2.2304960301
0.6981317008	3.4089647691
0.872664626	4.2767108508
1.0471975512	4.8641743206
1.2217304764	5.0499888221
1.3962634016	4.976354053
1.5707963268	4.8554550355
1.745329252	4.6328310261
1.9198621772	4.3969141108
2.0943951024	4.2190574993
2.2689280276	3.9212155445
2.4434609528	3.7217668222
2.617993878	3.5968560409
2.7925268032	3.5203043416
2.9670597284	3.5070035593
3.1415926536	3.4306645254
3.3161255788	3.503104692
3.490658504	3.6589753676
3.6651914292	3.84542524
3.8397243544	4.0545830608
4.0142572796	4.2175872195
4.1887902048	4.4276482121
4.36332313	4.7097844269
4.5378560552	4.8609449557
4.7123889804	4.9917578607
4.8869219056	4.9014432911
5.0614548308	4.6259312124
5.235987756	4.0663085431
5.4105206812	3.3105295284
5.5850536064	2.3673580867
5.7595865316	1.4733044965
5.9341194568	0.6870539304
6.108652382	0.60217152
6.2831853072	0

nC6H9-rotor1, middle rotor

Angle (radians)	Energy (kJ/mol)
0	0
0.1795195802	0.1615128748
0.3590391604	0.6487400111
0.5385587406	2.1155595229
0.7180783208	5.1659781549
0.897597901	9.870438068
1.0771174812	14.9837093132
1.2566370614	16.8091169703
1.4361566416	16.5588490727
1.6156762218	15.5168223104
1.7951958021	14.1590555607
1.9747153823	12.5958618255
2.1542349625	10.9644707316
2.3337545427	9.6712098878
2.5132741229	8.4508775536
2.6927937031	6.9936384908
2.8723132833	5.3619454642

3.0518328635	3.7932250519
3.2313524437	3.0515817284
3.4108720239	2.7732944964
3.5903916041	2.9003634385
3.7699111843	2.9479453725
3.9494307645	2.8044959368
4.1289503447	2.6200020617
4.3084699249	2.501581516
4.4879895051	2.2907906345
4.6675090853	2.2152287485
4.8470286655	1.7620123375
5.0265482457	1.49194292
5.2060678259	1.3216319953
5.3855874062	0.945951846
5.5651069864	0.936822983
5.7446265666	0.4108067118
5.9241461468	0.1880776824
6.103665727	0.0933181415
6.2831853072	0

nC6H9-rotor2, c2h3 rotor

Angle (radians)	Energy (kJ/mol)
0.0000000000	0.0000000000
0.1847995679	0.6749635036
0.3695991357	2.4097756625
0.5543987036	4.7547986220
0.7391982714	7.6314905538
0.9239978393	9.0679592873
1.1087974071	9.1004629756
1.2935969750	7.6277150850
1.4783965429	3.4070192737
1.6631961107	2.3118497688
1.8479956786	2.1580821186
2.0327952464	2.9823000381
2.2175948143	4.6569856247
2.4023943822	7.2385451175
2.5871939500	9.7631128849
2.7719935179	11.9930680620
2.9567930857	13.1329524550
3.1415926536	9.2065147914
3.3263922214	8.1629468606
3.5111917893	5.4368142182
3.6959913572	2.9200468109
3.8807909250	1.0257670417
4.0655904929	0.0470909655
4.2503900607	0.2516935439
4.4351896286	1.4288521585
4.6199891965	3.3167808436
4.8047887643	5.6462450909
4.9895883322	7.8766282246
5.1743879000	9.4852798643
5.3591874679	8.7302149855
5.5439870357	7.0324486297
5.7287866036	5.2312270773
5.9135861715	3.7295383018
6.0983857393	2.8909352686
6.2831853072	0.2159353168

c5-C6H9 rotor ch2. rotor

Angle (radians)	Energy (kJ/mol)
0.0000000000	0.0903381991
0.1745329252	0.0680818369

0.3490658504	0.3535393089
0.5235987756	0.9337852796
0.6981317008	1.7228792621
0.8726646260	2.2333578250
1.0471975512	2.2660032903
1.2217304764	2.2486277322
1.3962634016	2.2662238323
1.5707963268	2.2954771517
1.7453292520	2.1892835589
1.9198621772	1.9583550934
2.0943951024	1.5359567997
2.2689280276	0.8804587520
2.4434609528	0.4469913509
2.6179938780	0.0637602640
2.7925268032	0.0288857495
2.9670597284	0.0165879081
3.1415926536	0.0650205040
3.3161255788	0.4063958721
3.4906585040	0.8403988752
3.6651914292	1.4824753675
3.8397243544	1.9395013789
4.0142572796	2.1700570234
4.1887902048	2.2976983246
4.3633231300	2.2659560313
4.5378560552	2.2499037251
4.7123889804	2.2660347963
4.8869219056	2.2630653559
5.0614548308	1.7927411878
5.2359877560	0.9901836421
5.4105206812	0.3884427041
5.5850536064	0.0753098379
5.7595865316	0.0970831083
5.9341194568	0.0000000000
6.1086523820	0.0003859485
6.2831853072	0.0900178882

c5b-C6H9 ch3 rotor

Angle (radians)	Energy (kJ/mol)
0.0000000000	0.0015385429
0.1745329252	0.9814433530
0.3490658504	3.6115535892
0.5235987756	7.5273737314
0.6981317008	11.6365803168
0.8726646260	14.7931531590
1.0471975512	15.7221337739
1.2217304764	14.5454792553
1.3962634016	11.3912431080
1.5707963268	7.5230232782
1.7453292520	3.8120840174
1.9198621772	1.0961015574
2.0943951024	0.0000000000
2.2689280276	0.9815194925
2.4434609528	3.5441281273
2.6179938780	7.3930085252
2.7925268032	11.5181965281
2.9670597284	14.7122431298
3.1415926536	15.7246542537
3.3161255788	14.5416985355
3.4906585040	11.3693411882
3.6651914292	7.5250370366
3.8397243544	3.8066282287
4.0142572796	1.1293193816

4.1887902048	0.0020452644
4.3633231300	0.9152072426
4.5378560552	3.4248542942
4.7123889804	7.2256539132
4.8869219056	11.4167892216
5.0614548308	14.6654409693
5.2359877560	15.7285216150
5.4105206812	14.6290069078
5.5850536064	11.4771914714
5.7595865316	7.6235274127
5.9341194568	3.8344060172
6.1086523820	1.1115526241
6.2831853072	0.0002966815

c5c-C6H9 ch3 rotor

Angle (radians)	Energy (kJ/mol)
0.0000000000	0.0370405520
0.1745329252	0.0128386943
0.3490658504	0.2514835039
0.5235987756	0.6592656399
0.6981317008	0.1852053855
0.8726646260	0.0022080454
1.0471975512	0.0676039959
1.2217304764	0.3454343908
1.3962634016	0.6177669891
1.5707963268	0.6882695368
1.7453292520	0.5707180317
1.9198621772	0.2623688263
2.0943951024	0.0336457807
2.2689280276	0.0171235100
2.4434609528	0.2917350423
2.6179938780	0.6215870915
2.7925268032	0.1569313775
2.9670597284	0.0008244070
3.1415926536	0.0716367636
3.3161255788	0.3424124405
3.4906585040	0.6134742969
3.6651914292	0.6888812783
3.8397243544	0.5850453844
4.0142572796	0.2892644469
4.1887902048	0.0443788241
4.3633231300	0.0099663974
4.5378560552	0.2515543924
4.7123889804	0.6294609655
4.8869219056	0.1532057932
5.0614548308	0.0000000000
5.2359877560	0.0836458000
5.4105206812	0.3711879190
5.5850536064	0.6284737776
5.7595865316	0.6867336194
5.9341194568	0.5664122119
6.1086523820	0.2612923714
6.2831853072	0.0368462650

TS-C5H6_CH3-c5-2 from species 'c' to 'b', ch3-rotor

Angle (radians)	Energy (kJ/mol)
0.0000000000	0.0000000000
0.1745329252	0.2949407776
0.3490658504	1.1973329555
0.5235987756	2.3833605085
0.6981317008	3.4585237044
0.8726646260	4.2519497616
1.0471975512	4.5905394744
1.2217304764	4.3117035129

1.3962634016	3.5898407054
1.5707963268	2.5784010164
1.7453292520	1.4985329247
1.9198621772	0.5626918787
2.0943951024	0.1565112976
2.2689280276	0.3532321255
2.4434609528	1.1038520329
2.6179938780	2.2688860891
2.7925268032	3.4857711420
2.9670597284	4.3555152291
3.1415926536	4.7190078079
3.3161255788	4.5236916225
3.4906585040	3.7802524571
3.6651914292	2.6789707885
3.8397243544	1.4930955144
4.0142572796	0.5393275554
4.1887902048	0.0642197266
4.3633231300	0.4445312576
4.5378560552	1.3401916537
4.7123889804	2.5611672354
4.8869219056	3.6938104997
5.0614548308	4.4150431873
5.2359877560	4.7369819800
5.4105206812	4.4817728917
5.5850536064	3.5938235886
5.7595865316	2.4241502743
5.9341194568	1.2196313257
6.1086523820	0.3301356032
6.2831853072	0.1275546596

6. *Extended PES figure showing H-abstraction channels*

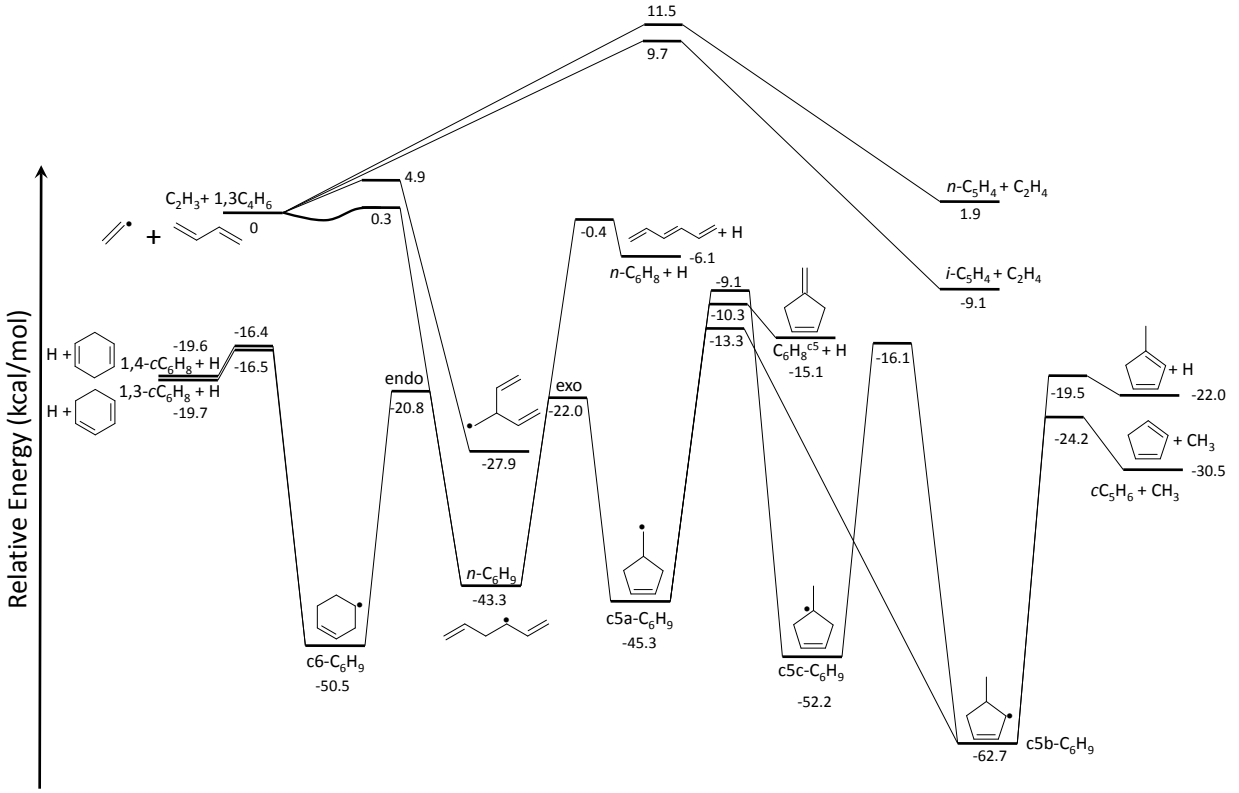

Figure S15: Zero Kelvin relative energy diagram (ZPE included) for the reaction of vinyl + 1,3-butadiene, with selected channels shown. All energies calculated at the CCSD(T)-F12a/cc-pVTZ-F12 level of theory.

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