Supporting Information

Gas-Phase Formation of Fulvenallene (C_7H_6) via the Jahn-Teller Distorted Tropyl (C_7H_7) Radical Intermediate under Single-Collision Conditions

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Computational Details

Geometries of all species involved in various chemical reactions accessing the C_7H_7 PES including reactants, intermediates, transition states, and products were optimized using the B3LYP density functional[1-2] with the 6-311G(d,p) basis set. Calculations of vibrational frequencies were performed at the same B3LYP/6-311G(d,p) level to compute zero-point vibrational energy corrections (ZPE) and for rate constant evaluation. Single-point energies were refined using the explicitly-correlated coupled clusters CCSD(T)-F12 method[3-4] with Dunning's correlation-consistent cc-pVTZ-f12 basis set.[5-6] The CCSD(T)-F12/cc-pVTZ-f12//B3LYP/6-311G(d,p) + ZPE(B3LYP/6-311G(d,p)) relative energies are normally accurate within 4 kJ mol^{-1} or better.[7] The GAUSSIAN 09[8] and MOLPRO 2010[6] program packages were utilized for the ab initio calculations. Rice-Ramsperger-Kassel-Marcus (RRKM) theory,[9-11] was used to compute energy-dependent rate constants of all unimolecular reaction steps on the C_7H_7 PES following the initial association of the CH radical with benzene. Rate constants were computed as functions of the available internal energy of each intermediate or transition state within the harmonic approximation using B3LYP/6-311G(d,p) frequencies and employing our in-house code,[12] which automatically processes GAUSSIAN 09 log files to assess numbers of states for transition states and densities of states for local minima employing the direct count method. The internal energy was assumed to be equal to the sum of the collision energy and the chemical activation energy, that is, negative of the relative energy of a species with respect to the reactants. Only one energy level was considered throughout as at a zero-pressure limit corresponding to crossed molecular beams conditions. RRKM rate constants were then utilized to compute product branching ratios by solving first-order kinetic equations within steady-state approximation.[12-13]

In addition to the zero-pressure limit RRKM calculations pertinent to the conditions of the crossed molecular beams apparatus and cold molecular clouds, RRKM-Master Equation (ME) calculations[14] were carried out to evaluate temperature- and pressure-dependent rate constants for various reaction on the C_7H_7 PES relevant to combustion and/or chemistry of planetary atmospheres. Here, the RRKM-ME calculations covered the temperature range from 500 to 2500 K and pressures of 30 Torr and 1, 10, and 100 atm. The MESS program package[15-16] was used for the calculations where the rigid rotor-harmonic oscillator approximation (RRHO) was employed in the evaluation of partition function. We used the collision parameters for RRKM-ME calculations derived earlier for a similar C_6H_5 + C_2H_2 system,[17] where the Lennard-Jones parameters ε and σ were 317 cm^{-1} and 4.46 Å, respectively, and collisional energy transfer was described using the "exponential down" model,[18] where the temperature dependence of the range parameter α for the deactivating wing of the energy transfer function was expressed as $\alpha(T) = \alpha_{300}(T/300\ \mathrm{K})^n$, with $n = 0.61$ and $\alpha_{300} = 375$ cm^{-1}.

E,J-resolved rate constant for the barierrless CH + benzene addition entrance channel at the high pressure limit was computed using variable reaction coordinate-transition state theory (VRC-TST).[19-21] A multifaceted spherical dividing surface[19] used in the calculations was built as the equidistant surface between the pivot points assigned to the associating fragments. At short-range distances (below 5 Å) the pivot points were assigned to the interacting carbon atoms. Centers of mass of the reacting fragments served as the pivot points at long-range distances. A complex of interacting fragments on a dividing surface was generated using the geometries of CH and benzene optimized as separate fragments at the B3LYP/6-311G(d,p) level of theory. The notation "rigid" is used here to denote lack of the geometrical relaxation in a complex on a dividing surface. Single-point energies of "rigid" structures were probed at the at CCSD(T)/cc-pvdz level of theory. Then, these single-point energies were further refined with one-dimensional geometry relaxation[19] and complete basis set (CBS) corrections. The one-dimensional geometry relaxation correction was calculated for the minimum energy path (MEP) "rigid" structures undergone partial geometry optimization (with the distance between the pivot points kept frozen) using the B3LYP/6-311G(d,p) method. CBS correction was calculated using the CCSD(T)/cc-pV*n*Z (n = D, T, Q) energies of the "rigid" MEP structures. To summarize, in the VRC-TST flux calculations the energies of the "rigid" structures sampled on a dividing surface were first probed at the CCSD(T)/cc-pVDZ level of theory followed by *ad hoc* one-dimensional relaxation and CBS corrections:

$$E = E_{rigid}[\mathrm{CCSD(T)/cc\text{-}pVDZ}] + \Delta E[\mathrm{geom}] + \Delta E[\mathrm{CBS}],$$

where E_{rigid} is the single-point energy of the interacting "rigid" fragments, ΔE[geom] is the geometry relaxation correction computed as the difference of the CCSD(T)/cc-pVDZ energy of the optimized MEP structure corresponding to a particular value of the R_{CC} distance and the "rigid" structure at the same R_{CC}. ΔE[CBS] was calculated as follows:

$\Delta E[pVTZ] = E_{rigid}[CCSD(T)/cc\text{-}VTZ] - E_{rigid}[CCSD(T)/cc\text{-}VDZ]$,

$\Delta E[pVQZ] = E_{rigid}[CCSD(T)/cc\text{-}VQZ] - E_{rigid}[CCSD(T)/cc\text{-}VTZ]$,

$\Delta E[CBS] = \Delta E[pVQZ] + 0.69377\times(\Delta E[pVQZ] - \Delta E[pVTZ])$.

Product branching ratios at zero-pressure limit

Product branching ratios calculated using RRKM theory under single-collision conditions are shown in Table S2. Overall, C_5H_5 + C_2H_2 (**p6**) are predicted to be the prevalent products constituting 98% of the total yield under the experimental conditions, with the H loss products contributing 2%. Among the **p1-p5** products observable experimentally, the results predict that fulvenallene (**p1**), 1-ethynylcyclopenta-1,3-diene (**p2**) and cyclohepta-1,2,4,6-tetraene (**p3**) contribute 92.56%, 7.37% and 0.07% of the total C_7H_6 yield at E_C = 18.6 kJ mol^{-1}, respectively. For the main H loss product fulvenallene (**p1**), dissociation from intermediate **i10**, **i12**, and **i13** supplies 55.26%, 0.92%, and 43.82% of the total yield, respectively.

Rate constant for the barrierless CH addition to C_6H_6

The VRC-TST calculated high pressure limit rate constant of the CH + benzene addition is illustrated in Figure S3. In the considered temperature range of 100-2500 K, its values first slightly increase from 9×10^{-10} to 1.1×10^{-9} cm^3 molecule^{-1} s^{-1} at 250 K, but then steadily decrease at higher temperatures reaching 3×10^{-10} cm^3 molecule^{-1} s^{-1} at 2500 K.

Rate constants and product branching ratios at finite pressures

Table S3 shows phenomenological rate constants and product branching ratios for various reactions accessing the C_7H_7 PES including CH + C_6H_6, C_5H_5 + C_2H_2, fulvenallene (**p1**) + H, 1-ethynylcyclopenta-1,3-diene (**p2**) + H and cyclohepta-1,2,4,6-tetraene (**p3**) + H, as well as unimolecular thermal decomposition of tropyl (**i2**), benzyl (**i8**), vinylcyclopentadienyl (**i10**), and **i13** computes computed using the RRKM-ME approach in the temperatures range of 500-2500 K at pressures of 30 Torr and 1,10, and 100 atm.

$CH + C_6H_6$

Rate constants for this reaction are shown in Figure S4. The main products include the stabilized tropyl radical **i2** favored at lower temperatures and higher pressures, followed by $C_5H_5 + C_2H_2$ (**p6**), cyclohepta-1,2,4,6-tetraene (**p3**) + H, and fulvenallene (**p1**) + H. At 1 atm, stabilization of **i2** prevails up to 1500 K and at higher temperatures the bimolecular products take over; the yields of **p6** and **p3** nearly equalize at 2500 K (Table S3). The branching ratio of **p1** does not exceed few percent. The higher pressure, the higher temperature at which the yield of **p6** exceeds that of **i2**. Interestingly, on the contrary to zero pressure limit, at finite pressures considered, **p1** is not predicted to be the major H loss product.

$C_5H_5 + C_2H_2$

This reaction has a high relevance to combustion as it is often considered as an important step in the formation of small prototype PAH, such as indene. In rate constant calculations, special care has to be taken of the partition function of the cyclopentadienyl radical C_5H_5. This Jahn-Teller-distorted radical is a subject to very fast pseudorotation and this pseudorotation mode cannot be treated as a harmonic oscillator. Here, we followed Sharma and Green[29] who proposed to replace the pseudorotation normal mode with a free rotor with the rotational constant of 230 cm^{-1} and showed that this approach provides rather accurate values for the entropy of C_5H_5. Calculated rate constants are presented in Figure S5a and product branching ratios at 1 atm are shown in Fig. S5b. The reaction is predicted to be moderately fast with rate constants in the 10^{-15}-10^{-13} cm^3 $molecule^{-1}$ s^{-1} range above 1000 K. At low temperatures, the reaction mostly produces the collisionally stabilized tropyl radical **i2**, which constitutes more than 50% of the total product yield up to 1650, 1800, 2000, and 2250 K at 30 Torr, 1, 10, and 100 atm, respectively. Among bimolecular products, 1-ethynylcyclopenta-1,3-diene (**p2**) + H are the most favorable; for instance, at 1 atm their relative yield grows from 6% at 1500 K to 61% at 2500 K. Fulvenallene (**p1**) and cyclohepta-1,2,4,6-tetraene (**p3**) are predicted as minor products, with branching ratios of **p1** being normally slightly higher.

Fulvenallene (p1) + H

This reaction is computed to be rather fast with rate constants in the 10^{-11}-10^{-10} cm^3 $molecule^{-1}$ s^{-1} range (Figure S6). At lower temperatures, stabilization of the initial complex **i13** and then of vinylcyclopentadienyl radical **i10** prevail. With increasing temperatures, the contribution of the stabilized benzyl radical **i8** also becomes significant peaking, for example, at 1800 K at 1 atm (Table S3). 1-Ethynylcyclopenta-1,3-diene (**p2**) + H is the most important bimolecular product followed by C_5H_5 + C_2H_2 (**p6**), with their respective branching ratios at 1 atm reaching 51% and 22% at the highest considered temperature of 2500 K.

1-Ethynylcyclopenta-1,3-diene (p2) + H

The rate constants for the **p2** + H reaction are in the 10^{-12}-10^{-11} cm^3 $molecule^{-1}$ s^{-1} range (Figure S7) and are thus lower than those for **p1** + H. At low temperatures, the reaction mostly forms the collisionally stabilized initial complex **i9**, then stabilization of **i10** takes over, whereas at higher temperatures the bimolecular products C_5H_5 + C_2H_2 (**p6**) and fulvenallene (**p1**) + H prevail. For example, at 2000 K and 1 atm their computed branching ratios are 55% and 39%, respectively (Table S3).

Cyclohepta-1,2,4,6-tetraene (p3) + H

This reaction is barrierless and the rate constant remains nearly unchanged regardless of temperature, at ~4×10^{-10} cm^3 $molecule^{-1}$ s^{-1} (Figure S8). Tropyl (**i2**) is the main product at lower temperatures (e.g., up to 1800 K at 1 atm, Table S3) and at higher temperatures the reaction mostly forms C_5H_5 + C_2H_2 (**p6**), with a minor yield of **p1** + H.

Unimolecular decomposition of the C_7H_7 radicals i2, i8, i10, and i13

The tropyl radical **i2** predominantly dissociates to C_5H_5 + C_2H_2 (**p6**) also giving a minor yield of **p3** and a trace amount of **p1**. The decomposition rate of **i2** increases from 2.2 s^{-1} at 1000 K, to 4.3×10^4 and 2.6×10^6 s^{-1} at 1500 and 2000 K, respectively (Figure S9), and **i2** is predicted to become unstable (i.e., to fully equilibrate with its dissociation products) at 2500 K and 1 atm. The dissociation rate constants of benzyl radical (**i8**) are plotted in Figure S10. Benzyl decomposes to fulvenallene (**p1**) + H nearly exclusively, with a very minor yield of C_5H_5 + C_2H_2. **i8** is more stable than tropyl as the calculated rate constants for its thermal decomposition are only 6.8×10^2, 4.5×10^5, and 6.8×10^6 s^{-1} at 1 atm and at 1500, 2000, 2500 K, respectively. Therefore, at typical combustion conditions benzyl can survive and participate in bimolecular reactions. Alternatively, the vinylcyclopentadienyl radical (**i10**) is much less stable, with its decomposition rate constants at 1 atm being ~10^5 s^{-1} at 1500 K and 5.7×10^6 s^{-1} at 2000 K (Figure S11). **i10** is predicted to fully equilibrate with its dissociation products at 2500 K. The main dissociation product is fulvenallene (**p1**) + H but the contributions of C_5H_5 + C_2H_2 (**p6**) and 1-ethynylcyclopenta-1,3-diene (**p2**) + H are also significant (Table S3). Finally, the C_7H_7 complex **i13**, which can be formed at low temperatures in the fulvenallene (**p1**) + H reaction, is predicted to rapidly decompose back to these reactants with calculated rate constants at 1 atm of 3.8×10^3 and 2.5×10^6 at 1000 and 1500 K, respectively (Figure S12); **i13** is unstable above 1375, 1650, 1800, and 2000 K at the pressures of 30 Torr, 1, 10, and 100 atm, respectively.

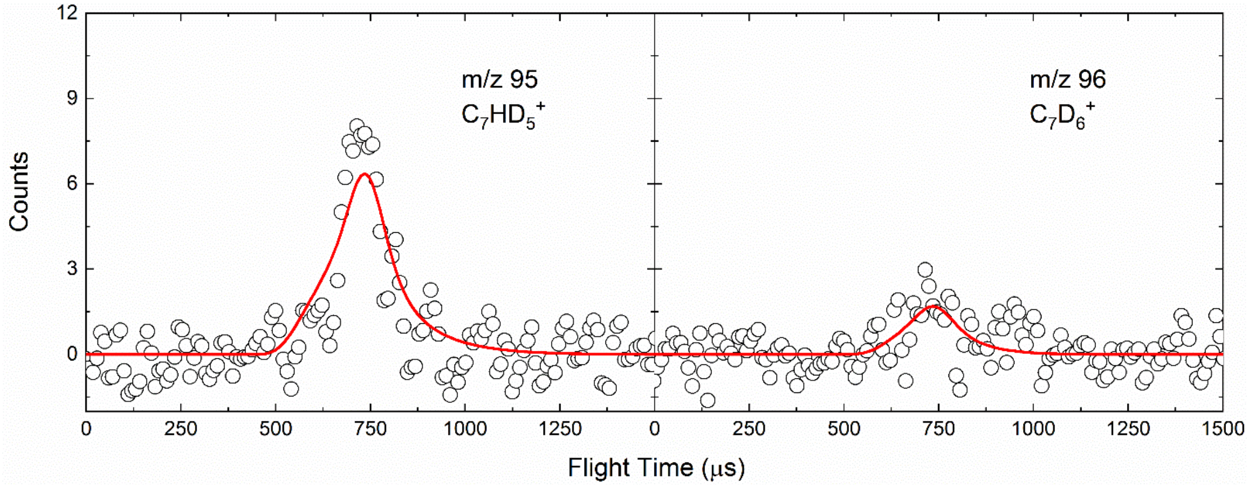

Figure S1. Time-of-flight (TOF) spectra for the reaction of the methylidyne radical (CH; $X^2\Pi$) with benzene-d$_6$ (C_6D_6; X^1A_{1g}), leading to D- and H-loss products at m/z = 95 and 96, respectively. The open circles represent the experimental data, and the red line represents the fit obtained from the forward-convolution routine. Note that ions at m/z = 96 cannot fragment to ions at m/z = 95.

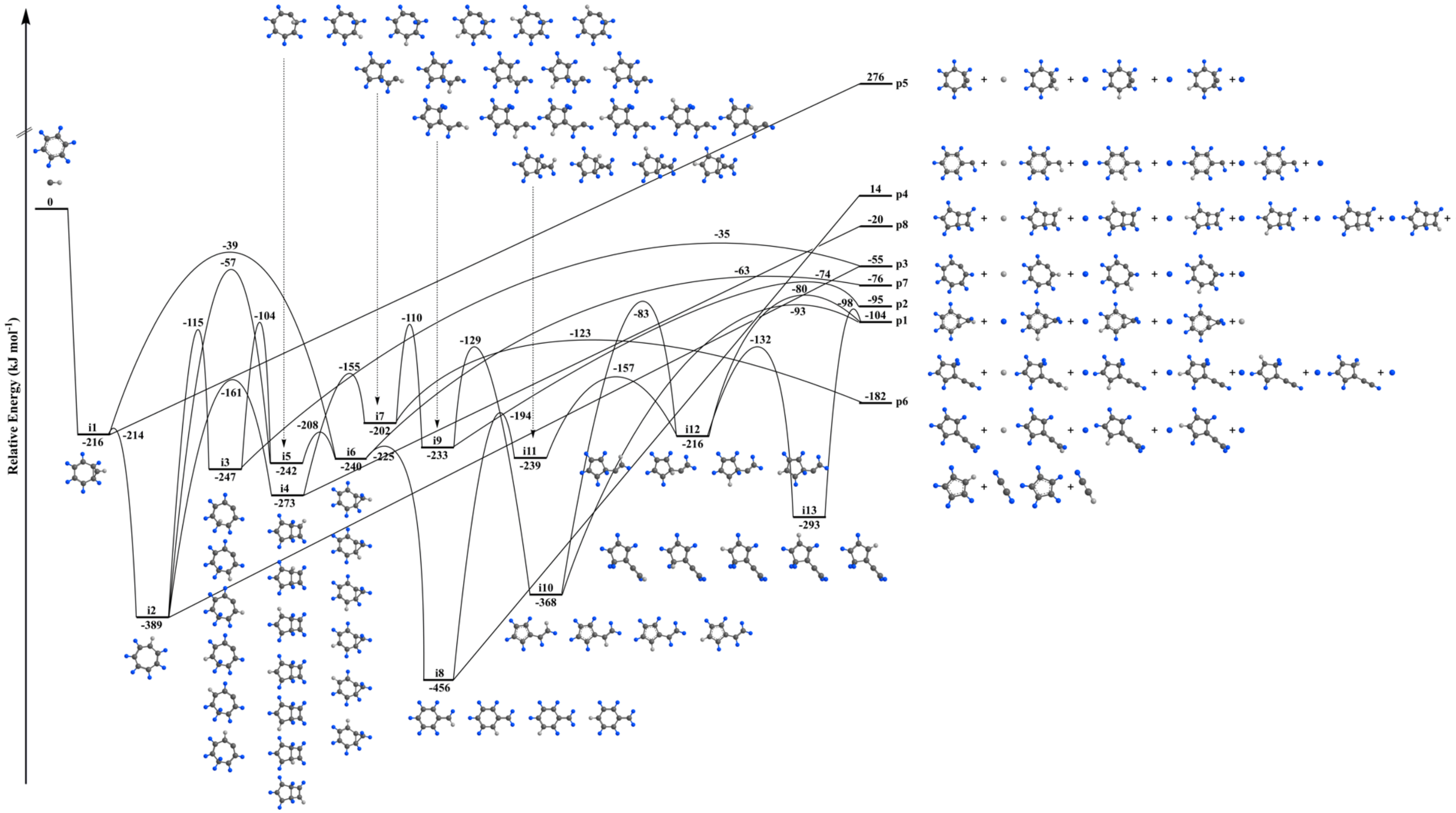

Figure S2. Schematic representation of the potential energy surface of the reaction of the methylidyne radical with benzene-d_6. Energies are given for the fully hydrogenated reactant; energies of the (partially) deuterated species differ by a few kJ mol^{-1} at most.

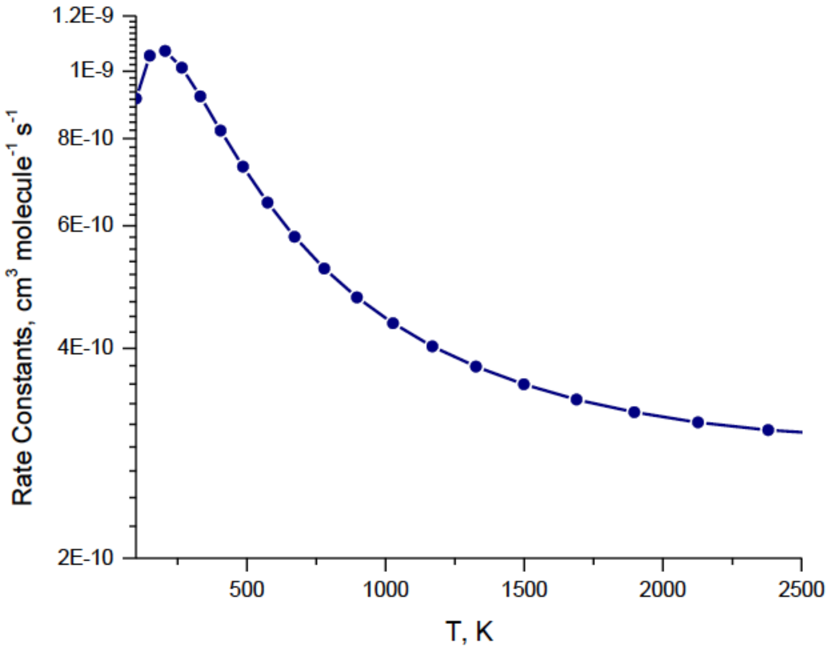

Figure S3. VRC-TST calculated temperature dependence of the total rate constant for the CH + benzene reaction at the high pressure limit.

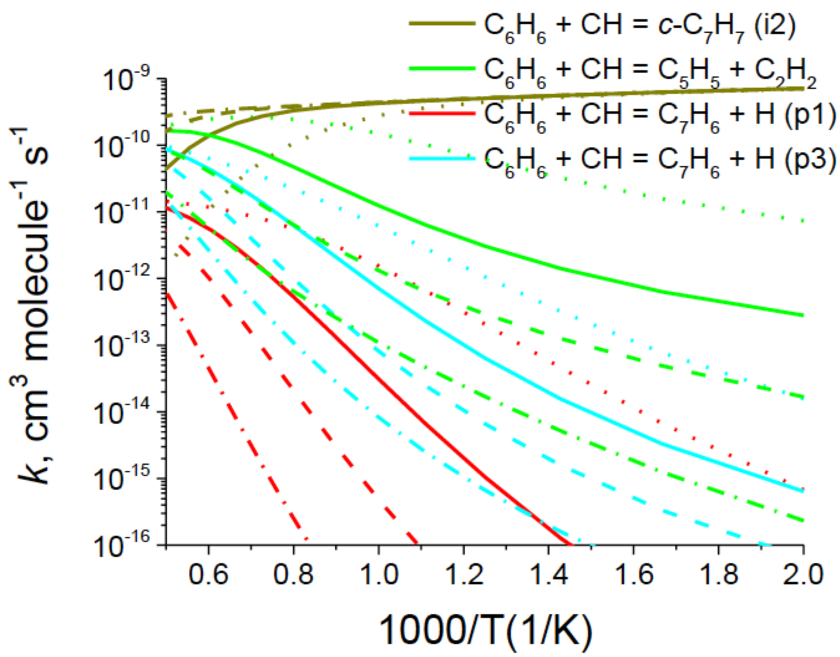

Figure S4. Calculated rate constants for various product channels of the CH + C_6H_6 reaction. Dotted, solid, dashed, and dash-dotted lines show the values computed at the pressures of 30 Torr, 1, 10, and 100 atm, respectively.

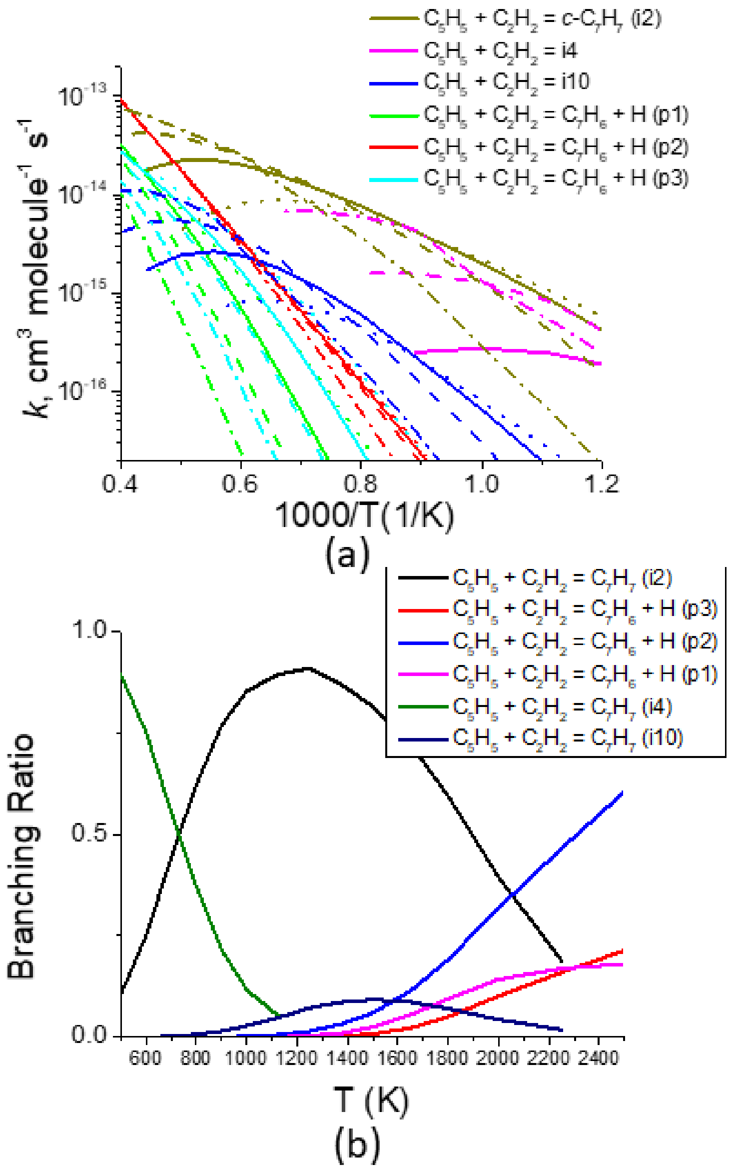

Figure S5. (a) Calculated rate constants for various product channels of the $C_5H_5 + C_2H_2$ reaction. Dotted, solid, dashed, and dash-dotted lines show the values computed at the pressures of 30 Torr, 1, 10, and 100 atm, respectively. (b) Product branching ratios at 1 atm.

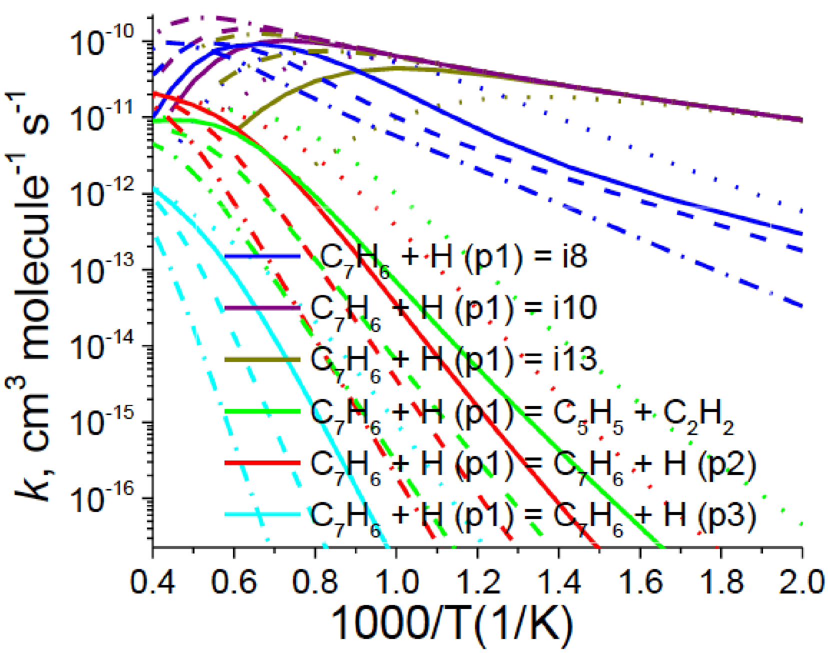

Figure S6. Calculated rate constants for various product channels of the fulvenallene (**p1**) + H reaction. Dotted, solid, dashed, and dash-dotted lines show the values computed at the pressures of 30 Torr, 1, 10, and 100 atm, respectively.

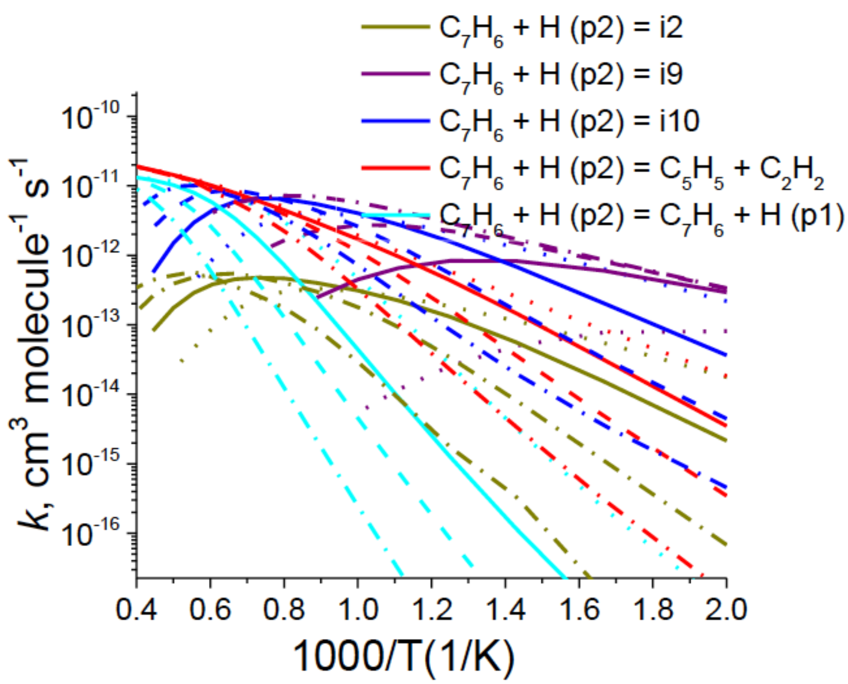

Figure S7. Calculated rate constants for various product channels of the 1-ethynylcyclopenta-1,3-diene (**p2**) + H reaction. Dotted, solid, dashed, and dash-dotted lines show the values computed at the pressures of 30 Torr, 1, 10, and 100 atm, respectively.

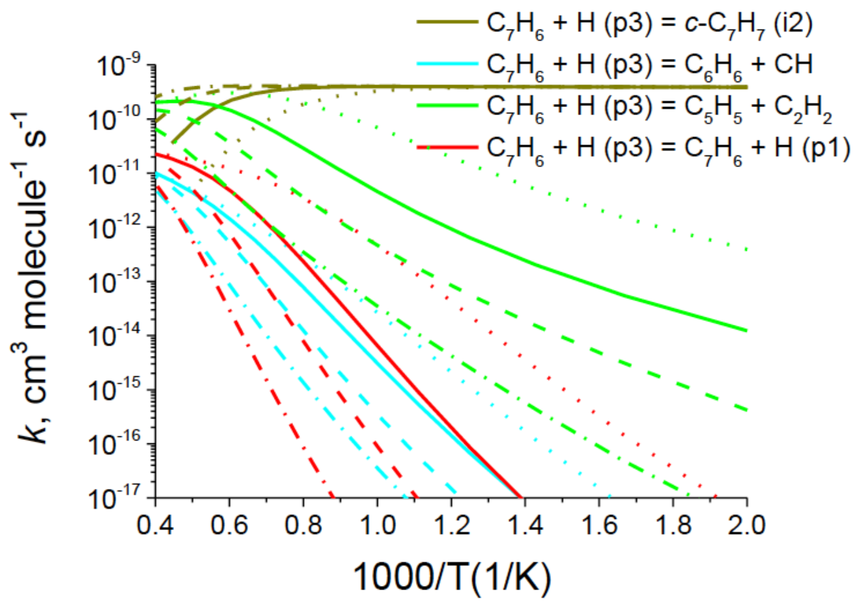

Figure S8. Calculated rate constants for various product channels of the cyclohepta-1,2,4,6-tetraene (**p3**) + H reaction. Dotted, solid, dashed, and dash-dotted lines show the values computed at the pressures of 30 Torr, 1, 10, and 100 atm, respectively.

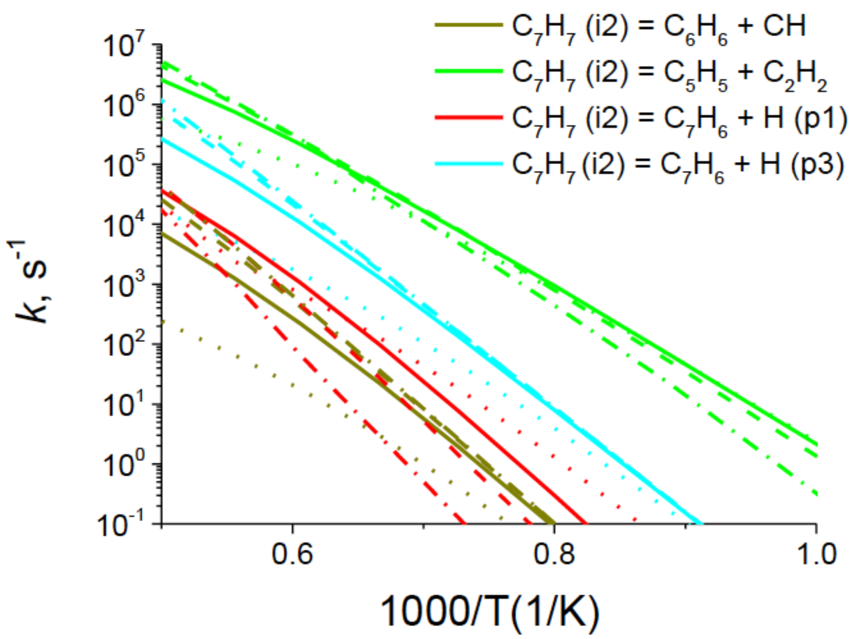

Figure S9. Calculated rate constants for various product channels of unimolecular decomposition of the tropyl radical (**i2**). Dotted, solid, dashed, and dash-dotted lines show the values computed at the pressures of 30 Torr, 1, 10, and 100 atm, respectively.

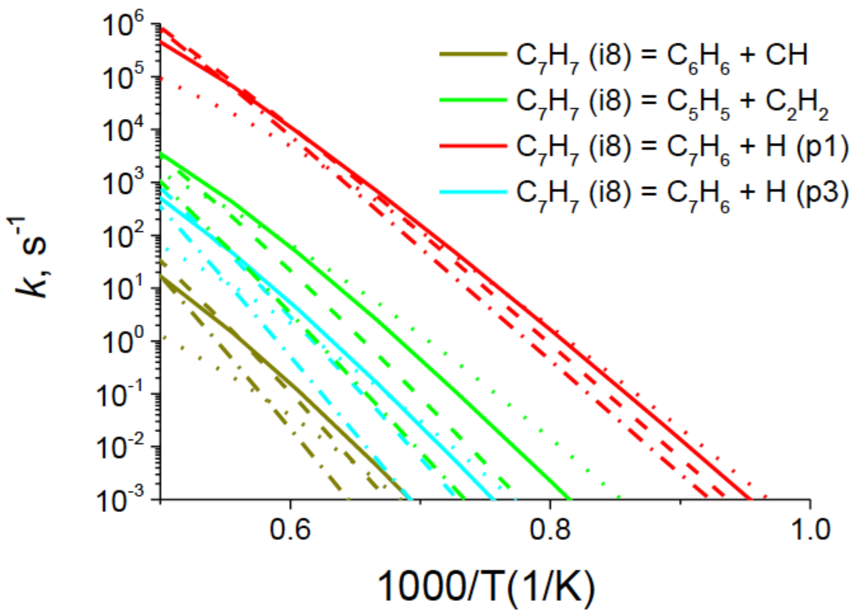

Figure S10. Calculated rate constants for various product channels of unimolecular decomposition of the benzyl radical (**i8**). Dotted, solid, dashed, and dash-dotted lines show the values computed at the pressures of 30 Torr, 1, 10, and 100 atm, respectively.

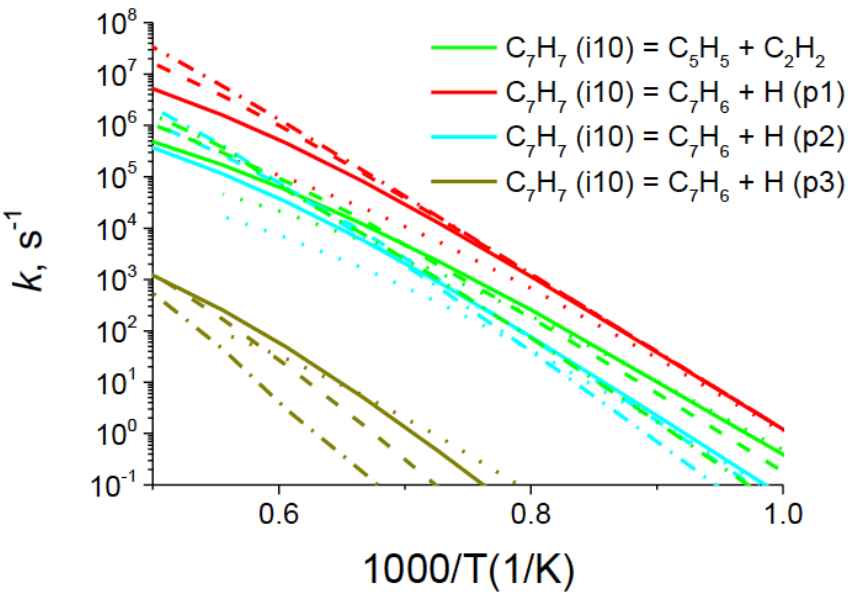

Figure S11. Calculated rate constants for various product channels of unimolecular decomposition of the vinylcyclopentadienyl radical (**i10**). Dotted, solid, dashed, and dash-dotted lines show the values computed at the pressures of 30 Torr, 1, 10, and 100 atm, respectively.

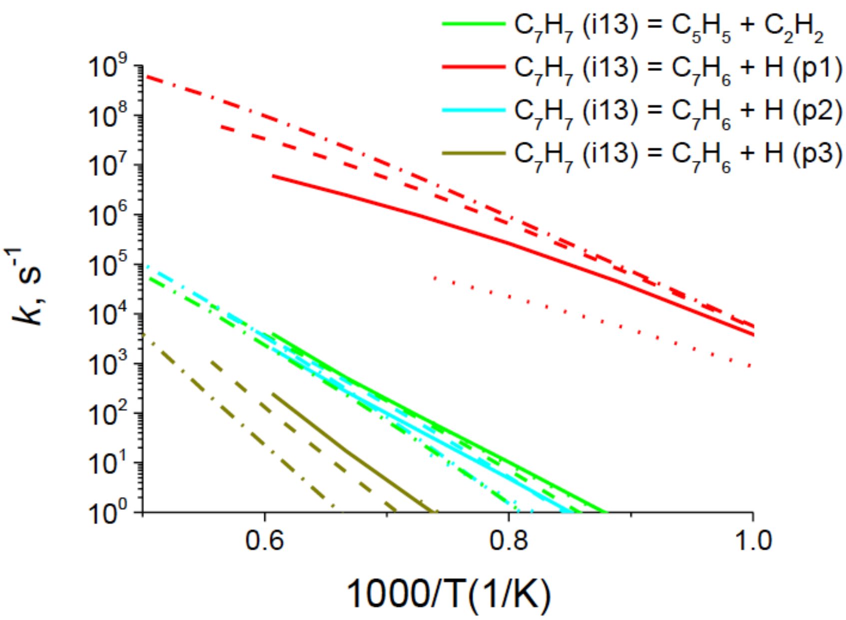

Figure S12. Calculated rate constants for various product channels of unimolecular decomposition of **i13**. Dotted, solid, dashed, and dash-dotted lines show the values computed at the pressures of 30 Torr, 1, 10, and 100 atm, respectively.

Table S1. Peak velocities (V_p) and speed ratios (S) of the methylidyne (CH), benzene (C_6H_6), benzene-d$_6$ (C_6D_6) beams along with the corresponding collision energies (E_C) and center-of-mass angles (Θ_{CM}) for each reactive scattering experiment.

Beam	V_p (m s^{-1})	S	E_C (kJ mol^{-1})	Θ_{CM} (degree)
CH ($X^2\Pi$)	1772 ± 10	13.0 ± 0.4		
C_6H_6 ($^1A_{1g}$)	471 ± 10	14.0 ± 0.3	18.7 ± 0.4	58.6 ± 0.3
C_6D_6 ($^1A_{1g}$)	461 ± 10	14.0 ± 0.3	18.9 ± 0.4	60.0 ± 0.3

Table S2. Statistical branching ratios (%) for the reaction of the methylidyne (CH) with benzene (C_6H_6) at a collision energy of 18.7 kJ mol^{-1}.[a]

p1	**p2**	**p3**	**p4**	**p5**	**p6**	**p7**	**p8**
1.8148	0.1445	0.0013	0	0	98.0394	0	0

p1	**p2**	**p3**	**p4**	**p5**
92.56	7.37	0.07	0	0

p1	from **i10**	from **i12**	from **i13**
92.56	51.15	0.85	40.56
100	55.26	0.92	43.82

[a]Here, **p1-p6** denote fulvenallene, 1-ethynylcyclopenta-1,3-diene, cyclohepta-1,2,4,6-tetraene, phenylcarbene, noncaradienylidene, cyclopentadienyl (C_5H_5) plus acetylene (C_2H_2), benzocyclopropene and bicyclo[3.2.0]hepta-1,3,6-triene.

Table S3. Rate constants (in cm^3 $molecule^{-1}$ s^{-1} for bimolecular reactions and in s^{-1} for unimolecular reactions) and product branching ratios (in %) for various reactions accessing the C_7H_7 PES calculated using the RRKM-ME approach for temperatures in the 500-2500 K range and for pressures of 30 Torr, 1, 10, and 100 atm.

	$CH+C_6H_6 \rightarrow i2$	$CH+C_6H_6 \rightarrow p3$	$CH+C_6H_6 \rightarrow p1$	$CH+C_6H_6 \rightarrow C_5H_5+C_2H_2$	$CH+C_6H_6 \rightarrow i2$	$CH+C_6H_6 \rightarrow p3$	$CH+C_6H_6 \rightarrow p1$	$CH+C_6H_6 \rightarrow C_5H_5+C_2H_2$
1000/T, K^{-1}	30 Torr	30 Torr	30 Torr	30 Torr	1 atm	1 atm	1 atm	1 atm
2	7.07E-10	1.57E-14	6.72E-16	7.39E-12	7.14E-10	6.38E-16	7.85E-19	2.80E-13
1.66667	6.11E-10	7.73E-14	6.75E-15	1.57E-11	6.26E-10	3.31E-15	1.15E-17	6.33E-13
1.42857	5.28E-10	3.20E-13	4.60E-14	3.24E-11	5.60E-10	1.56E-14	1.27E-16	1.42E-12
1.25	4.47E-10	1.07E-12	2.08E-13	6.09E-11	5.08E-10	6.42E-14	1.05E-15	3.07E-12
1.11111	3.64E-10	2.83E-12	6.56E-13	1.02E-10	4.65E-10	2.30E-13	6.58E-15	6.36E-12
1	2.80E-10	6.16E-12	1.55E-12	1.50E-10	4.28E-10	7.11E-13	3.12E-14	1.24E-11
0.88889	1.84E-10	1.29E-11	3.34E-12	2.07E-10	3.82E-10	2.36E-12	1.53E-13	2.59E-11
0.8	1.09E-10	2.23E-11	5.59E-12	2.46E-10	3.32E-10	6.27E-12	5.32E-13	4.76E-11
0.72727	5.82E-11	3.37E-11	7.85E-12	2.64E-10	2.75E-10	1.36E-11	1.39E-12	7.62E-11
0.66667	2.89E-11	4.63E-11	9.81E-12	2.64E-10	2.15E-10	2.48E-11	2.86E-12	1.08E-10
0.60606	1.17E-11	6.19E-11	1.17E-11	2.49E-10	1.47E-10	4.23E-11	5.33E-12	1.40E-10
0.55556	4.61E-12	7.75E-11	1.31E-11	2.27E-10	9.18E-11	6.20E-11	8.14E-12	1.60E-10
0.5	1.34E-12	9.73E-11	1.45E-11	1.97E-10	4.47E-11	8.76E-11	1.16E-11	1.66E-10
0.44444		1.19E-10	1.60E-11	1.63E-10	1.68E-11	1.15E-10	1.47E-11	1.52E-10
0.4		1.38E-10	1.73E-11	1.36E-10		1.37E-10	1.69E-11	1.37E-10
Branching Ratios								
	$CH+C_6H_6 \rightarrow i2$	$CH+C_6H_6 \rightarrow p3$	$CH+C_6H_6 \rightarrow p1$	$CH+C_6H_6 \rightarrow C_5H_5+C_2H_2$	$CH+C_6H_6 \rightarrow i2$	$CH+C_6H_6 \rightarrow p3$	$CH+C_6H_6 \rightarrow p1$	$CH+C_6H_6 \rightarrow C_5H_5+C_2H_2$
T, K	30 Torr	30 Torr	30 Torr	30 Torr	1 atm	1 atm	1 atm	1 atm
500	98.96%	0.00%	0.00%	1.03%	99.96%	0.00%	0.00%	0.04%
600	97.47%	0.01%	0.00%	2.51%	99.90%	0.00%	0.00%	0.10%
700	94.16%	0.06%	0.01%	5.78%	99.75%	0.00%	0.00%	0.25%
800	87.79%	0.21%	0.04%	11.96%	99.39%	0.01%	0.00%	0.60%
900	77.57%	0.60%	0.14%	21.68%	98.60%	0.05%	0.00%	1.35%
1000	64.01%	1.41%	0.35%	34.23%	97.01%	0.16%	0.01%	2.82%

1125	45.22%	3.17%	0.82%	50.78%	93.07%	0.58%	0.04%	6.32%
1250	28.38%	5.83%	1.46%	64.33%	85.92%	1.62%	0.14%	12.32%
1375	16.01%	9.27%	2.16%	72.57%	75.10%	3.71%	0.38%	20.81%
1500	8.29%	13.27%	2.81%	75.62%	61.40%	7.07%	0.82%	30.71%
1650	3.50%	18.55%	3.49%	74.45%	43.86%	12.66%	1.59%	41.89%
1800	1.43%	24.08%	4.05%	70.44%	28.52%	19.27%	2.53%	49.68%
2000	0.43%	31.42%	4.68%	63.47%	14.44%	28.31%	3.74%	53.51%
2250		39.96%	5.36%	54.68%	5.63%	38.41%	4.93%	51.04%
2500		47.37%	5.95%	46.68%		47.00%	5.82%	47.18%
	$CH+C_6H_6 \rightarrow$ i2	$CH+C_6H_6 \rightarrow$ p3	$CH+C_6H_6 \rightarrow$ p1	$CH+C_6H_6 \rightarrow C_5H_5+C_2H_2$	$CH+C_6H_6 \rightarrow$ i2	$CH+C_6H_6 \rightarrow$ p3	$CH+C_6H_6 \rightarrow$ p1	$CH+C_6H_6 \rightarrow C_5H_5+C_2H_2$
1000/T, K^{-1}	10 atm	10 atm	10 atm	10 atm	100 atm	100 atm	100 atm	100 atm
2	7.14E-10	6.38E-17	1.93E-21	1.68E-14	7.14E-10	6.38E-18	6.81E-25	2.33E-16
1.66667	6.27E-10	3.32E-16	5.23E-20	4.88E-14	6.27E-10	3.32E-17	4.62E-23	1.25E-15
1.42857	5.61E-10	1.57E-15	8.37E-19	1.25E-13	5.61E-10	1.57E-16	1.56E-21	5.16E-15
1.25	5.11E-10	6.60E-15	9.09E-18	2.92E-13	5.11E-10	6.62E-16	2.95E-20	1.69E-14
1.11111	4.71E-10	2.45E-14	7.43E-17	6.38E-13	4.72E-10	2.47E-15	3.54E-19	4.62E-14
1	4.40E-10	8.09E-14	4.81E-16	1.32E-12	4.41E-10	8.23E-15	3.04E-18	1.09E-13
0.88889	4.08E-10	3.08E-13	3.70E-15	3.02E-12	4.11E-10	3.21E-14	3.18E-17	2.83E-13
0.8	3.80E-10	9.93E-13	2.10E-14	6.40E-12	3.87E-10	1.09E-13	2.49E-16	6.44E-13
0.72727	3.54E-10	2.73E-12	8.97E-14	1.25E-11	3.68E-10	3.23E-13	1.53E-15	1.35E-12
0.66667	3.25E-10	6.42E-12	2.97E-13	2.21E-11	3.51E-10	8.57E-13	7.53E-15	2.62E-12
0.60606	2.83E-10	1.49E-11	9.28E-13	3.88E-11	3.32E-10	2.40E-12	3.85E-14	5.43E-12
0.55556	2.35E-10	2.86E-11	2.21E-12	5.91E-11	3.12E-10	5.81E-12	1.50E-13	1.01E-11
0.5	1.67E-10	5.39E-11	5.05E-12	8.51E-11	2.80E-10	1.52E-11	6.31E-13	1.98E-11
0.44444	9.60E-11	8.92E-11	9.49E-12	1.04E-10	2.28E-10	3.73E-11	2.33E-12	3.61E-11
0.4	5.01E-11	1.20E-10	1.35E-11	1.08E-10	1.69E-10	6.81E-11	5.46E-12	5.16E-11
Branching Ratios								
	$CH+C_6H_6 \rightarrow$ i2	$CH+C_6H_6 \rightarrow$ p3	$CH+C_6H_6 \rightarrow$ p1	$CH+C_6H_6 \rightarrow C_5H_5+C_2H_2$	$CH+C_6H_6 \rightarrow$ i2	$CH+C_6H_6 \rightarrow$ p3	$CH+C_6H_6 \rightarrow$ p1	$CH+C_6H_6 \rightarrow C_5H_5+C_2H_2$
T, K	10 atm	10 atm	10 atm	10 atm	100 atm	100 atm	100 atm	100 atm

500	100.00%	0.00%	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%
600	99.99%	0.00%	0.00%	0.01%	100.00%	0.00%	0.00%	0.00%
700	99.98%	0.00%	0.00%	0.02%	100.00%	0.00%	0.00%	0.00%
800	99.94%	0.00%	0.00%	0.06%	100.00%	0.00%	0.00%	0.00%
900	99.86%	0.01%	0.00%	0.14%	99.99%	0.00%	0.00%	0.01%
1000	99.68%	0.02%	0.00%	0.30%	99.97%	0.00%	0.00%	0.02%
1125	99.19%	0.07%	0.00%	0.73%	99.92%	0.01%	0.00%	0.07%
1250	98.09%	0.26%	0.01%	1.65%	99.81%	0.03%	0.00%	0.17%
1375	95.85%	0.74%	0.02%	3.38%	99.55%	0.09%	0.00%	0.36%
1500	91.83%	1.82%	0.08%	6.27%	99.02%	0.24%	0.00%	0.74%
1650	83.84%	4.40%	0.27%	11.48%	97.69%	0.71%	0.01%	1.60%
1800	72.32%	8.81%	0.68%	18.20%	95.11%	1.77%	0.05%	3.07%
2000	53.71%	17.33%	1.62%	27.34%	88.69%	4.83%	0.20%	6.28%
2250	32.09%	29.81%	3.17%	34.92%	75.06%	12.29%	0.77%	11.89%
2500	17.20%	41.19%	4.63%	36.97%	57.43%	23.17%	1.86%	17.55%

	$C_5H_5+C_2H_2\rightarrow$ i2	$C_5H_5+C_2H_2\rightarrow$ p3	$C_5H_5+C_2H_2\rightarrow$ p2	$C_5H_5+C_2H_2\rightarrow$ p1	$C_5H_5+C_2H_2\rightarrow$ i4	$C_5H_5+C_2H_2\rightarrow$ i10
1000/T, K^{-1}	30 Torr	30 Torr	30 Torr	30 Torr	30 Torr	30 Torr
2	1.09E-18	3.93E-28	5.14E-25	5.10E-27	6.14E-19	1.09E-18
1.66667	1.73E-17	2.70E-25	9.95E-23	2.87E-24	3.39E-18	1.73E-17
1.42857	1.11E-16	3.76E-23	4.43E-21	3.53E-22	7.62E-18	1.11E-16
1.25	4.09E-16	1.79E-21	7.90E-20	1.53E-20	9.94E-18	4.09E-16
1.11111	1.06E-15	3.90E-20	7.66E-19	2.99E-19	9.43E-18	1.06E-15
1	2.18E-15	4.62E-19	4.83E-18	3.12E-18	7.52E-18	2.18E-15
0.88889	4.18E-15	5.24E-18	3.10E-17	2.93E-17		4.18E-15
0.8	6.44E-15	3.39E-17	1.37E-16	1.55E-16		6.44E-15
0.72727	8.22E-15	1.44E-16	4.59E-16	5.38E-16		8.22E-15
0.66667	8.90E-15	4.51E-16	1.24E-15	1.36E-15		8.90E-15
0.60606	8.23E-15	1.32E-15	3.31E-15	3.11E-15		8.23E-15
0.55556	6.64E-15	3.06E-15	7.46E-15	5.72E-15		6.64E-15

0.5	4.35E-15	7.38E-15	1.82E-14	1.07E-14		4.35E-15
0.44444		1.71E-14	4.47E-14	1.84E-14		
0.4		3.24E-14	9.27E-14	2.81E-14		
Branching Ratios						
	C_5H_5+C_2H_2→ i2	C_5H_5+C_2H_2→ p3	C_5H_5+C_2H_2→ p2	C_5H_5+C_2H_2→ p1	C_5H_5+C_2H_2→ i4	C_5H_5+C_2H_2→ i10
T, K	30 Torr	30 Torr	30 Torr	30 Torr	30 Torr	30 Torr
500	63.97%	0.00%	0.00%	0.00%	35.97%	0.06%
600	83.39%	0.00%	0.00%	0.00%	16.35%	0.26%
700	92.89%	0.00%	0.00%	0.00%	6.40%	0.71%
800	96.22%	0.00%	0.02%	0.00%	2.34%	1.42%
900	96.66%	0.00%	0.07%	0.03%	0.86%	2.38%
1000	95.76%	0.02%	0.21%	0.14%	0.33%	3.54%
1125	93.45%	0.12%	0.69%	0.66%		5.09%
1250	89.17%	0.47%	1.90%	2.15%		6.32%
1375	81.78%	1.44%	4.57%	5.35%		6.86%
1500	69.62%	3.53%	9.70%	10.66%		6.48%
1650	49.04%	7.85%	19.72%	18.51%		4.88%
1800	28.20%	12.99%	31.65%	24.26%		2.90%
2000	10.69%	18.14%	44.79%	26.38%		
2250		21.33%	55.71%	22.96%		
2500		21.17%	60.50%	18.33%		
	C_5H_5+C_2H_2→ i2	C_5H_5+C_2H_2→ p3	C_5H_5+C_2H_2→ p2	C_5H_5+C_2H_2→ p1	C_5H_5+C_2H_2→ i4	C_5H_5+C_2H_2→ i10
1000/T, K^{-1}	1 atm	1 atm	1 atm	1 atm	1 atm	1 atm
2	1.46E-19	1.24E-29	9.83E-26	6.00E-29	1.24E-18	7.25E-23
1.66667	4.87E-18	9.90E-27	3.69E-23	6.28E-26	1.47E-17	8.28E-21
1.42857	5.28E-17	1.51E-24	2.56E-21	1.11E-23	6.60E-17	2.46E-19
1.25	2.76E-16	7.96E-23	5.88E-20	6.16E-22	1.65E-16	2.86E-18
1.11111	8.75E-16	2.03E-21	6.45E-19	1.55E-20	2.45E-16	1.72E-17

1	2.01E-15	3.03E-20	4.26E-18	2.19E-19	2.75E-16	6.57E-17
0.88889	4.27E-15	4.99E-19	2.76E-17	3.15E-18	2.49E-16	2.27E-16
0.8	7.61E-15	4.92E-18	1.23E-16	2.57E-17		6.04E-16
0.72727	1.14E-14	3.18E-17	4.15E-16	1.32E-16		1.13E-15
0.66667	1.55E-14	1.45E-16	1.14E-15	4.76E-16		1.76E-15
0.60606	1.98E-14	6.16E-16	3.13E-15	1.51E-15		2.38E-15
0.55556	2.23E-14	1.88E-15	7.21E-15	3.56E-15		2.64E-15
0.5	2.21E-14	5.72E-15	1.79E-14	8.02E-15		2.44E-15
0.44444	1.80E-14	1.53E-14	4.45E-14	1.61E-14		1.73E-15
0.4		3.27E-14	9.27E-14	2.76E-14		

Branching Ratios

	$C_5H_5+C_2H_2\rightarrow$ i2	$C_5H_5+C_2H_2\rightarrow$ p3	$C_5H_5+C_2H_2\rightarrow$ p2	$C_5H_5+C_2H_2\rightarrow$ p1	$C_5H_5+C_2H_2\rightarrow$ i4	$C_5H_5+C_2H_2\rightarrow$ i10
T, K	1 atm	1 atm	1 atm	1 atm	1 atm	1 atm
500	10.51%	0.00%	0.00%	0.00%	89.49%	0.01%
600	24.85%	0.00%	0.00%	0.00%	75.11%	0.04%
700	44.34%	0.00%	0.00%	0.00%	55.45%	0.21%
800	62.22%	0.00%	0.01%	0.00%	37.12%	0.64%
900	76.89%	0.00%	0.06%	0.00%	21.54%	1.51%
1000	85.34%	0.00%	0.18%	0.01%	11.68%	2.79%
1125	89.37%	0.01%	0.58%	0.07%	5.22%	4.76%
1250	90.95%	0.06%	1.47%	0.31%		7.22%
1375	86.96%	0.24%	3.16%	1.01%		8.63%
1500	81.51%	0.76%	6.00%	2.50%		9.22%
1650	72.17%	2.25%	11.40%	5.52%		8.66%
1800	59.34%	5.01%	19.17%	9.45%		7.03%
2000	39.38%	10.16%	31.86%	14.27%		4.33%
2250	18.81%	15.97%	46.52%	16.88%		1.82%
2500		21.38%	60.57%	18.04%		

	$C_5H_5+C_2H_2 \rightarrow$ i2	$C_5H_5+C_2H_2 \rightarrow$ p3	$C_5H_5+C_2H_2 \rightarrow$ p2	$C_5H_5+C_2H_2 \rightarrow$ p1	$C_5H_5+C_2H_2 \rightarrow$ i4	$C_5H_5+C_2H_2 \rightarrow$ i10
1000/T, K^{-1}	10 atm	10 atm	10 atm	10 atm	10 atm	10 atm
2	8.63E-21	4.24E-31	9.76E-27	7.87E-31	4.85E-19	4.62E-24
1.66667	5.58E-19	5.58E-28	5.75E-24	1.45E-27	1.03E-17	7.98E-22
1.42857	1.07E-17	1.14E-25	6.32E-22	4.26E-25	7.67E-17	3.58E-20
1.25	8.76E-17	7.00E-24	2.21E-20	3.51E-23	2.85E-16	6.37E-19
1.11111	4.26E-16	1.95E-22	3.40E-19	1.17E-21	8.36E-16	5.72E-18
1	1.27E-15	3.08E-21	2.86E-18	2.03E-20	1.27E-15	3.02E-17
0.88889	3.31E-15	5.50E-20	2.23E-17	3.68E-19	1.58E-15	1.41E-16
0.8	6.52E-15	6.12E-19	1.09E-16	3.81E-18	1.58E-15	4.34E-16
0.72727	1.19E-14	4.71E-18	3.83E-16	2.55E-17		9.95E-16
0.66667	1.68E-14	2.66E-17	1.10E-15	1.22E-16		2.16E-15
0.60606	2.36E-14	1.50E-16	3.02E-15	5.25E-16		3.46E-15
0.55556	3.07E-14	6.15E-16	6.99E-15	1.60E-15		4.66E-15
0.5	3.85E-14	2.64E-15	1.75E-14	4.72E-15		5.52E-15
0.44444	4.28E-14	9.64E-15	4.39E-14	1.18E-14		5.24E-15
0.4	4.02E-14	2.37E-14	9.20E-14	2.22E-14		4.07E-15
Branching Ratios						
	$C_5H_5+C_2H_2 \rightarrow$ i2	$C_5H_5+C_2H_2 \rightarrow$ p3	$C_5H_5+C_2H_2 \rightarrow$ p2	$C_5H_5+C_2H_2 \rightarrow$ p1	$C_5H_5+C_2H_2 \rightarrow$ i4	$C_5H_5+C_2H_2 \rightarrow$ i10
T, K	10 atm	10 atm	10 atm	10 atm	10 atm	10 atm
500	1.75%	0.00%	0.00%	0.00%	98.25%	0.00%
600	5.16%	0.00%	0.00%	0.00%	94.83%	0.01%
700	12.19%	0.00%	0.00%	0.00%	87.77%	0.04%
800	23.50%	0.00%	0.01%	0.00%	76.32%	0.17%
900	33.61%	0.00%	0.03%	0.00%	65.91%	0.45%
1000	49.22%	0.00%	0.11%	0.00%	49.49%	1.17%
1125	65.45%	0.00%	0.44%	0.01%	31.31%	2.79%
1250	75.39%	0.01%	1.26%	0.04%	18.28%	5.02%

1375	89.40%	0.04%	2.89%	0.19%		7.49%
1500	83.13%	0.13%	5.44%	0.60%		10.69%
1650	76.74%	0.49%	9.82%	1.70%		11.25%
1800	68.87%	1.38%	15.70%	3.59%		10.46%
2000	55.89%	3.82%	25.43%	6.84%		8.01%
2250	37.72%	8.50%	38.74%	10.42%		4.62%
2500	22.08%	13.03%	50.49%	12.17%		2.23%
	$C_5H_5+C_2H_2\rightarrow$ i2	$C_5H_5+C_2H_2\rightarrow$ p3	$C_5H_5+C_2H_2\rightarrow$ p2	$C_5H_5+C_2H_2\rightarrow$ p1	$C_5H_5+C_2H_2\rightarrow$ i4	$C_5H_5+C_2H_2\rightarrow$ i10
1000/T, K^{-1}	100 atm	100 atm	100 atm	100 atm	100 atm	100 atm
2	1.52E-22	3.16E-33	3.79E-28	4.08E-33	7.21E-20	1.13E-25
1.66667	1.84E-20	8.64E-30	3.59E-25	1.25E-29	2.27E-18	3.23E-23
1.42857	6.28E-19	3.22E-27	5.94E-23	5.83E-27	2.69E-17	2.25E-21
1.25	8.90E-18	3.13E-25	3.04E-21	7.49E-25	1.57E-16	5.83E-20
1.11111	6.51E-17	1.19E-23	6.81E-20	3.78E-23	5.46E-16	7.44E-19
1	2.88E-16	2.30E-22	8.17E-19	9.33E-22	1.31E-15	5.56E-18
0.88889	1.40E-15	4.88E-21	9.55E-18	2.43E-20	4.49E-15	4.07E-17
0.8	3.64E-15	5.93E-20	6.20E-17	3.30E-19	5.98E-15	1.74E-16
0.72727	7.32E-15	4.89E-19	2.67E-16	2.80E-18	6.74E-15	5.21E-16
0.66667	1.25E-14	3.00E-18	8.51E-16	1.64E-17	6.76E-15	1.21E-15
0.60606	2.44E-14	1.99E-17	2.58E-15	9.24E-17		2.56E-15
0.55556	3.31E-14	9.77E-17	6.88E-15	4.09E-16		5.97E-15
0.5	4.62E-14	5.65E-16	1.73E-14	1.70E-15		8.68E-15
0.44444	6.28E-14	3.06E-15	4.34E-14	5.91E-15		1.08E-14
0.4	7.54E-14	1.05E-14	9.12E-14	1.39E-14		1.10E-14
Branching Ratios						
	$C_5H_5+C_2H_2\rightarrow$ i2	$C_5H_5+C_2H_2\rightarrow$ p3	$C_5H_5+C_2H_2\rightarrow$ p2	$C_5H_5+C_2H_2\rightarrow$ p1	$C_5H_5+C_2H_2\rightarrow$ i4	$C_5H_5+C_2H_2\rightarrow$ i10
T, K	100 atm	100 atm	100 atm	100 atm	100 atm	100 atm
500	0.21%	0.00%	0.00%	0.00%	99.79%	0.00%

600	0.81%	0.00%	0.00%	0.00%	99.19%	0.00%
700	2.28%	0.00%	0.00%	0.00%	97.71%	0.01%
800	5.37%	0.00%	0.00%	0.00%	94.59%	0.04%
900	10.64%	0.00%	0.01%	0.00%	89.22%	0.12%
1000	17.91%	0.00%	0.05%	0.00%	81.70%	0.35%
1125	23.61%	0.00%	0.16%	0.00%	75.55%	0.68%
1250	36.93%	0.00%	0.63%	0.00%	60.67%	1.76%
1375	49.28%	0.00%	1.79%	0.02%	45.40%	3.51%
1500	58.51%	0.01%	3.99%	0.08%	31.73%	5.67%
1650	82.31%	0.07%	8.70%	0.31%		8.61%
1800	71.26%	0.21%	14.80%	0.88%		12.84%
2000	62.10%	0.76%	23.21%	2.28%		11.66%
2250	49.85%	2.43%	34.43%	4.69%		8.61%
2500	37.34%	5.22%	45.11%	6.88%		5.45%

	p1→i13	p1→i10	p1→i8	p1→p3	p1→p2	p1→ C_5H_5+C_2H_2	p1→i13	p1→i10	p1→i8	p1→p3	p1→p2	p1→ C_5H_5+C_2H_2
1000/T, K^{-1}	30 Torr	30 Torr	30 Torr	30 Torr	30 Torr	30 Torr	1 atm	1 atm	1 atm	1 atm	1 atm	1 atm
2	8.95E-12	9.22E-12	5.82E-13	3.92E-23	2.12E-18	4.53E-17	9.23E-12	9.22E-12	2.93E-13	3.55E-26	3.45E-20	5.33E-19
1.66667	1.45E-11	1.63E-11	2.62E-12	8.16E-21	8.44E-17	8.95E-16	1.63E-11	1.63E-11	8.65E-13	1.15E-23	2.25E-18	1.96E-17
1.42857	1.83E-11	2.55E-11	8.53E-12	5.16E-19	1.57E-15	9.77E-15	2.50E-11	2.55E-11	2.19E-12	1.11E-21	5.65E-17	3.07E-16
1.25	1.83E-11	3.63E-11	2.01E-11	1.27E-17	1.58E-14	6.72E-14	3.42E-11	3.66E-11	5.31E-12	4.70E-20	7.45E-16	2.71E-15
1.11111	1.47E-11	4.77E-11	3.61E-11	1.48E-16	9.49E-14	3.07E-13	4.15E-11	4.95E-11	1.19E-11	1.04E-18	6.15E-15	1.60E-14
1	9.84E-12	5.74E-11	5.28E-11	9.81E-16	3.71E-13	9.85E-13	4.41E-11	6.37E-11	2.36E-11	1.36E-17	3.48E-14	6.92E-14
0.88889	5.06E-12	6.24E-11	6.91E-11	5.79E-15	1.28E-12	2.80E-12	3.96E-11	8.18E-11	4.43E-11	1.84E-16	1.95E-13	3.00E-13
0.8	2.38E-12	5.69E-11	7.56E-11	2.11E-14	3.01E-12	5.59E-12	2.98E-11	9.63E-11	6.63E-11	1.43E-15	7.24E-13	9.24E-13
0.72727	1.13E-12	4.39E-11	7.11E-11	5.46E-14	5.40E-12	8.59E-12	1.99E-11	1.02E-10	8.31E-11	7.13E-15	1.92E-12	2.12E-12
0.66667		2.94E-11	5.89E-11	1.11E-13	8.02E-12	1.09E-11	1.23E-11	9.60E-11	9.08E-11	2.50E-14	3.93E-12	3.82E-12
0.60606		1.60E-11	3.95E-11	2.08E-13	1.10E-11	1.24E-11	6.73E-12	7.70E-11	8.71E-11	7.83E-14	7.12E-12	6.04E-12
0.55556		7.96E-12	2.31E-11	3.34E-13	1.35E-11	1.26E-11		5.41E-11	7.54E-11	1.81E-13	1.05E-11	7.82E-12
0.5			9.82E-12	5.38E-13	1.64E-11	1.21E-11		2.94E-11	4.87E-11	3.98E-13	1.44E-11	9.05E-12

0.44444			2.96E-12	8.52E-13	1.89E-11	1.05E-11		1.21E-11	2.31E-11	7.55E-13	1.80E-11	9.17E-12
0.4				1.22E-12	2.09E-11	9.10E-12			9.84E-12	1.18E-12	2.08E-11	8.95E-12
Branching Ratios												
	p1→i13	p1→i10	p1→i8	p1→p3	p1→p2	p1→ C_5H_5+C_2H_2	p1→i13	p1→i10	p1→i8	p1→p3	p1→p2	p1→ C_5H_5+C_2H_2
T, K	30 Torr	30 Torr	30 Torr	30 Torr	30 Torr	30 Torr	1 atm	1 atm	1 atm	1 atm	1 atm	1 atm
500	47.71%	49.19%	3.10%	0.00%	0.00%	0.00%	49.24%	49.19%	1.56%	0.00%	0.00%	0.00%
600	43.33%	48.83%	7.84%	0.00%	0.00%	0.00%	48.66%	48.76%	2.58%	0.00%	0.00%	0.00%
700	35.05%	48.64%	16.29%	0.00%	0.00%	0.02%	47.49%	48.35%	4.16%	0.00%	0.00%	0.00%
800	24.43%	48.52%	26.94%	0.00%	0.02%	0.09%	44.96%	48.07%	6.97%	0.00%	0.00%	0.00%
900	14.82%	48.28%	36.49%	0.00%	0.10%	0.31%	40.31%	48.07%	11.60%	0.00%	0.01%	0.02%
1000	8.11%	47.29%	43.49%	0.00%	0.31%	0.81%	33.54%	48.45%	17.93%	0.00%	0.03%	0.05%
1125	3.60%	44.38%	49.11%	0.00%	0.91%	1.99%	23.82%	49.24%	26.64%	0.00%	0.12%	0.18%
1250	1.66%	39.65%	52.68%	0.01%	2.10%	3.89%	15.36%	49.62%	34.17%	0.00%	0.37%	0.48%
1375	0.86%	33.72%	54.63%	0.04%	4.15%	6.60%	9.51%	48.79%	39.77%	0.00%	0.92%	1.01%
1500		27.41%	54.82%	0.10%	7.47%	10.19%	5.96%	46.40%	43.89%	0.01%	1.90%	1.85%
1650		20.21%	49.96%	0.26%	13.90%	15.67%	3.66%	41.83%	47.32%	0.04%	3.87%	3.28%
1800		13.86%	40.15%	0.58%	23.53%	21.88%		36.53%	50.96%	0.12%	7.10%	5.28%
2000			25.28%	1.39%	42.17%	31.16%		28.83%	47.75%	0.39%	14.16%	8.87%
2250			8.94%	2.57%	56.87%	31.62%		19.13%	36.60%	1.20%	28.55%	14.52%
2500				3.90%	66.91%	29.19%			24.12%	2.89%	51.04%	21.95%
	p1→i13	p1→i10	p1→i8	p1→p3	p1→p2	p1→ C_5H_5+C_2H_2	p1→i13	p1→i10	p1→i8	p1→p3	p1→p2	p1→ C_5H_5+C_2H_2
1000/T, K^{-1}	10 atm	10 atm	10 atm	10 atm	10 atm	10 atm	100 atm	100 atm	100 atm	100 atm	100 atm	100 atm
2	9.24E-12	9.22E-12	1.77E-13	5.99E-29	6.35E-22	6.99E-21	9.23E-12	9.22E-12	3.32E-14	1.50E-32	7.12E-24	3.63E-23
1.66667	1.64E-11	1.63E-11	6.26E-13	4.13E-26	6.81E-20	4.52E-19	1.64E-11	1.63E-11	1.81E-13	2.73E-29	9.36E-22	3.91E-21
1.42857	2.56E-11	2.55E-11	1.52E-12	6.42E-24	2.68E-18	1.18E-17	2.56E-11	2.55E-11	6.39E-13	9.50E-27	5.07E-20	1.61E-19
1.25	3.67E-11	3.66E-11	3.03E-12	3.68E-22	4.94E-17	1.54E-16	3.68E-11	3.66E-11	1.62E-12	1.01E-24	1.36E-18	3.29E-18
1.11111	4.90E-11	4.96E-11	5.55E-12	1.06E-20	5.19E-16	1.21E-15	5.00E-11	4.96E-11	3.29E-12	4.53E-23	2.06E-17	3.88E-17
1	6.10E-11	6.42E-11	9.99E-12	1.86E-19	3.60E-15	6.43E-15	6.49E-11	6.43E-11	5.66E-12	1.09E-21	1.96E-16	2.95E-16

0.88889	7.23E-11	8.46E-11	1.97E-11	3.85E-18	2.60E-14	3.51E-14	8.48E-11	8.49E-11	9.87E-12	3.08E-20	1.95E-15	2.32E-15
0.8	7.50E-11	1.06E-10	3.53E-11	4.80E-17	1.28E-13	1.37E-13	1.04E-10	1.08E-10	1.75E-11	5.26E-19	1.25E-14	1.19E-14
0.72727	6.84E-11	1.26E-10	5.45E-11	3.90E-16	4.56E-13	4.07E-13	1.18E-10	1.32E-10	2.68E-11	6.07E-18	5.71E-14	4.47E-14
0.66667	5.60E-11	1.40E-10	7.28E-11	2.20E-15	1.25E-12	9.77E-13	1.24E-10	1.57E-10	3.92E-11	5.03E-17	2.00E-13	1.32E-13
0.60606	3.98E-11	1.44E-10	8.82E-11	1.17E-14	3.08E-12	2.09E-12	1.19E-10	1.85E-10	5.61E-11	4.33E-16	6.73E-13	3.68E-13
0.55556	2.63E-11	1.30E-10	9.30E-11	4.29E-14	5.87E-12	3.52E-12	1.03E-10	2.02E-10	7.16E-11	2.60E-15	1.78E-12	9.00E-13
0.5		9.75E-11	9.23E-11	1.55E-13	1.03E-11	5.32E-12	7.57E-11	2.02E-10	8.47E-11	1.74E-14	4.47E-12	1.91E-12
0.44444		5.63E-11	6.19E-11	4.52E-13	1.53E-11	6.72E-12		1.68E-10	1.02E-10	1.01E-13	9.30E-12	3.36E-12
0.4		2.88E-11	3.56E-11	8.90E-13	1.90E-11	7.18E-12		1.19E-10	7.91E-11	3.33E-13	1.43E-11	4.50E-12
Branching Ratios												
	p1$\rightarrow$i13	p1$\rightarrow$i10	p1$\rightarrow$i8	p1$\rightarrow$p3	p1$\rightarrow$p2	p1$\rightarrow$ C_5H_5+C_2H_2	p1$\rightarrow$i13	p1$\rightarrow$i10	p1$\rightarrow$i8	p1$\rightarrow$p3	p1$\rightarrow$p2	p1$\rightarrow$ C_5H_5+C_2H_2
T, K	10 atm	10 atm	10 atm	10 atm	10 atm	10 atm	100 atm	100 atm	100 atm	100 atm	100 atm	100 atm
500	49.56%	49.49%	0.95%	0.00%	0.00%	0.00%	49.93%	49.89%	0.18%	0.00%	0.00%	0.00%
600	49.13%	48.99%	1.88%	0.00%	0.00%	0.00%	49.76%	49.69%	0.55%	0.00%	0.00%	0.00%
700	48.65%	48.46%	2.89%	0.00%	0.00%	0.00%	49.45%	49.31%	1.23%	0.00%	0.00%	0.00%
800	48.05%	47.98%	3.97%	0.00%	0.00%	0.00%	49.06%	48.78%	2.16%	0.00%	0.00%	0.00%
900	47.04%	47.63%	5.33%	0.00%	0.00%	0.00%	48.61%	48.19%	3.19%	0.00%	0.00%	0.00%
1000	45.13%	47.48%	7.38%	0.00%	0.00%	0.00%	48.12%	47.68%	4.20%	0.00%	0.00%	0.00%
1125	40.91%	47.87%	11.18%	0.00%	0.01%	0.02%	47.23%	47.27%	5.50%	0.00%	0.00%	0.00%
1250	34.62%	48.97%	16.29%	0.00%	0.06%	0.06%	45.38%	47.00%	7.61%	0.00%	0.01%	0.01%
1375	27.37%	50.47%	21.82%	0.00%	0.18%	0.16%	42.66%	47.67%	9.63%	0.00%	0.02%	0.02%
1500	20.63%	51.70%	26.85%	0.00%	0.46%	0.36%	38.69%	49.01%	12.19%	0.00%	0.06%	0.04%
1650	14.37%	51.89%	31.87%	0.00%	1.11%	0.76%	32.92%	51.21%	15.58%	0.00%	0.19%	0.10%
1800	10.16%	50.30%	35.90%	0.02%	2.26%	1.36%	27.07%	53.33%	18.89%	0.00%	0.47%	0.24%
2000		47.42%	44.91%	0.08%	5.00%	2.59%	20.52%	54.81%	22.94%	0.00%	1.21%	0.52%
2250		40.02%	44.01%	0.32%	10.88%	4.77%		59.33%	36.16%	0.04%	3.28%	1.19%
2500		31.43%	38.94%	0.97%	20.81%	7.84%		54.72%	36.47%	0.15%	6.58%	2.08%

	p2→i2	p2→i9	p2→i10	p2→p1	p2→ $C_5H_5+C_2H_2$	p2→i2	p2→i9	p2→i10	p2→p1	p2→ $C_5H_5+C_2H_2$
1000/T, K^{-1}	30 Torr	30 Torr	30 Torr	30 Torr	30 Torr	1 atm	1 atm	1 atm	1 atm	1 atm
2	1.76E-14	8.07E-14	2.18E-13	8.48E-18	1.82E-14	2.14E-15	2.92E-13	3.64E-14	1.38E-19	3.49E-15
1.66667	5.50E-14	7.75E-14	6.36E-13	2.31E-16	8.49E-14	1.53E-14	6.00E-13	2.05E-13	6.15E-18	3.15E-14
1.42857	1.14E-13	4.97E-14	1.30E-12	3.26E-15	2.55E-13	5.61E-14	8.28E-13	6.88E-13	1.17E-16	1.47E-13
1.25	1.84E-13	2.54E-14	2.14E-12	2.67E-14	5.87E-13	1.30E-13	8.29E-13	1.58E-12	1.26E-15	4.36E-13
1.11111	2.53E-13	1.18E-14	3.03E-12	1.37E-13	1.13E-12	2.22E-13	6.56E-13	2.75E-12	8.85E-15	9.54E-13
1	3.06E-13	5.41E-15	3.74E-12	4.70E-13	1.93E-12	3.11E-13	4.47E-13	4.02E-12	4.41E-14	1.70E-12
0.88889	3.30E-13		4.04E-12	1.43E-12	3.29E-12	4.00E-13	2.47E-13	5.45E-12	2.17E-13	2.93E-12
0.8	3.01E-13		3.57E-12	3.02E-12	4.96E-12	4.64E-13		6.48E-12	7.26E-13	4.45E-12
0.72727	2.35E-13		2.64E-12	4.98E-12	6.77E-12	4.76E-13		6.57E-12	1.77E-12	6.12E-12
0.66667	1.61E-13		1.69E-12	6.90E-12	8.56E-12	4.52E-13		5.89E-12	3.38E-12	7.89E-12
0.60606	8.99E-14		8.74E-13	8.81E-12	1.06E-11	3.81E-13		4.44E-12	5.71E-12	1.00E-11
0.55556	4.60E-14		4.15E-13	1.02E-11	1.24E-11	2.89E-13		2.94E-12	7.95E-12	1.20E-11
0.5	2.26E-14			1.16E-11	1.46E-11	1.75E-13		1.49E-12	1.02E-11	1.43E-11
0.44444				1.25E-11	1.69E-11	8.19E-14		5.66E-13	1.20E-11	1.68E-11
0.4				1.32E-11	1.90E-11				1.32E-11	1.90E-11
Branching Ratios										
	p2→i2	p2→i9	p2→i10	p2→p1	p2→ $C_5H_5+C_2H_2$	p2→i2	p2→i9	p2→i10	p2→p1	p2→ $C_5H_5+C_2H_2$
T, K	30 Torr	30 Torr	30 Torr	30 Torr	30 Torr	1 atm	1 atm	1 atm	1 atm	1 atm
500	5.27%	24.10%	65.18%	0.00%	5.45%	0.64%	87.44%	10.88%	0.00%	1.05%
600	6.44%	9.08%	74.50%	0.03%	9.95%	1.80%	70.49%	24.02%	0.00%	3.69%
700	6.62%	2.89%	75.45%	0.19%	14.85%	3.26%	48.16%	40.02%	0.01%	8.55%
800	6.22%	0.86%	72.22%	0.90%	19.80%	4.38%	27.90%	53.00%	0.04%	14.68%
900	5.54%	0.26%	66.40%	2.99%	24.81%	4.84%	14.28%	59.93%	0.19%	20.76%
1000	4.73%	0.08%	58.00%	7.28%	29.91%	4.76%	6.85%	61.61%	0.67%	26.10%
1125	3.63%		44.48%	15.69%	36.20%	4.32%	2.67%	58.94%	2.35%	31.73%
1250	2.54%		30.12%	25.50%	41.83%	3.83%		53.48%	5.99%	36.70%

1375	1.61%		18.06%	34.05%	46.27%	3.19%		43.99%	11.87%	40.95%
1500	0.93%		9.79%	39.84%	49.44%	2.57%		33.45%	19.19%	44.80%
1650	0.44%		4.30%	43.29%	51.97%	1.86%		21.63%	27.81%	48.70%
1800	0.20%		1.80%	44.28%	53.72%	1.25%		12.71%	34.32%	51.73%
2000	0.09%			44.31%	55.60%	0.67%		5.68%	39.04%	54.61%
2250				42.57%	57.43%	0.28%		1.92%	40.72%	57.08%
2500				40.98%	59.02%				40.92%	59.08%
	p2→i2	p2→i9	p2→i10	p2→p1	p2→ C_5H_5+C_2H_2	p2→i2	p2→i9	p2→i10	p2→p1	p2→ C_5H_5+C_2H_2
1000/T, K^{-1}	10 atm	10 atm	10 atm	10 atm	10 atm	100 atm	100 atm	100 atm	100 atm	100 atm
2	6.81E-17	3.30E-13	4.43E-15	2.54E-21	3.46E-16	3.83E-19	3.35E-13	4.55E-16	2.85E-23	1.35E-17
1.66667	1.11E-15	8.16E-13	3.28E-14	1.86E-19	4.90E-15	1.38E-17	8.53E-13	3.58E-15	2.56E-21	3.06E-16
1.42857	8.15E-15	1.52E-12	1.61E-13	5.57E-18	3.63E-14	3.39E-16	1.71E-12	1.99E-14	1.05E-19	3.42E-15
1.25	3.39E-14	2.25E-12	5.46E-13	8.34E-17	1.64E-13	1.74E-15	2.92E-12	8.40E-14	2.30E-18	2.26E-14
1.11111	9.19E-14	2.70E-12	1.36E-12	7.46E-16	5.04E-13	8.69E-15	4.36E-12	2.77E-13	2.96E-17	1.01E-13
1	1.80E-13	2.71E-12	2.59E-12	4.55E-15	1.15E-12	2.91E-14	5.77E-12	7.26E-13	2.48E-16	3.27E-13
0.88889	3.01E-13	2.25E-12	4.46E-12	2.90E-14	2.37E-12	8.74E-14	6.99E-12	1.81E-12	2.17E-15	1.01E-12
0.8	4.02E-13	1.63E-12	6.25E-12	1.28E-13	3.93E-12	1.75E-13	7.25E-12	3.43E-12	1.25E-14	2.24E-12
0.72727	4.88E-13	1.08E-12	7.60E-12	4.20E-13	5.65E-12	2.70E-13	6.65E-12	5.29E-12	5.27E-14	3.93E-12
0.66667	5.46E-13		8.72E-12	1.07E-12	7.60E-12	3.53E-13	5.57E-12	7.04E-12	1.72E-13	5.87E-12
0.60606	5.29E-13		8.26E-12	2.47E-12	9.65E-12	4.90E-13	4.13E-12	8.60E-12	5.40E-13	8.25E-12
0.55556	4.84E-13		6.96E-12	4.44E-12	1.16E-11	5.71E-13		1.07E-11	1.35E-12	1.14E-11
0.5	3.90E-13		4.76E-12	7.29E-12	1.40E-11	5.22E-13		9.46E-12	3.17E-12	1.38E-11
0.44444	2.59E-13		2.50E-12	1.02E-11	1.66E-11	4.40E-13		6.91E-12	6.19E-12	1.64E-11
0.4	1.54E-13			1.20E-11	1.88E-11	3.44E-13		4.40E-12	9.03E-12	1.87E-11
Branching Ratios										
	p2→i2	p2→i9	p2→i10	p2→p1	p2→ C_5H_5+C_2H_2	p2→i2	p2→i9	p2→i10	p2→p1	p2→ C_5H_5+C_2H_2
T, K	10 atm	10 atm	10 atm	10 atm	10 atm	100 atm	100 atm	100 atm	100 atm	100 atm
500	0.02%	98.55%	1.32%	0.00%	0.10%	0.00%	99.86%	0.14%	0.00%	0.00%

600	0.13%	95.45%	3.84%	0.00%	0.57%	0.00%	99.55%	0.42%	0.00%	0.04%
700	0.47%	88.13%	9.30%	0.00%	2.10%	0.02%	98.64%	1.15%	0.00%	0.20%
800	1.13%	75.15%	18.24%	0.00%	5.48%	0.06%	96.42%	2.77%	0.00%	0.75%
900	1.98%	58.05%	29.13%	0.02%	10.83%	0.18%	91.86%	5.83%	0.00%	2.12%
1000	2.71%	40.83%	39.11%	0.07%	17.28%	0.42%	84.21%	10.59%	0.00%	4.77%
1125	3.19%	23.93%	47.39%	0.31%	25.18%	0.88%	70.60%	18.26%	0.02%	10.24%
1250	3.26%	13.22%	50.66%	1.04%	31.83%	1.33%	55.30%	26.17%	0.10%	17.10%
1375	3.20%	7.10%	49.88%	2.76%	37.06%	1.67%	41.05%	32.70%	0.33%	24.26%
1500	3.05%		48.60%	5.97%	42.39%	1.86%	29.29%	37.05%	0.91%	30.89%
1650	2.53%		39.50%	11.80%	46.17%	2.22%	18.76%	39.09%	2.45%	37.48%
1800	2.06%		29.63%	18.87%	49.44%	2.38%		44.39%	5.61%	47.63%
2000	1.47%		17.98%	27.56%	52.98%	1.94%		35.08%	11.76%	51.23%
2250	0.88%		8.45%	34.46%	56.21%	1.47%		23.06%	20.65%	54.81%
2500	0.50%		0.00%	38.80%	60.70%	1.06%		13.56%	27.83%	57.55%

	p3→i2	p3→ $CH+C_6H_6$	p3→p1	p3→ $C_5H_5+C_2H_2$	p3→i2	p3→ $CH+C_6H_6$	p3→p1	p3→ $C_5H_5+C_2H_2$
1000/T, K^{-1}	30 Torr	30 Torr	30 Torr	30 Torr	1 atm	1 atm	1 atm	1 atm
2	3.87E-10	1.75E-19	4.37E-18	3.89E-13	3.87E-10	7.09E-21	3.96E-21	1.22E-14
1.66667	3.89E-10	6.77E-18	1.45E-16	1.50E-12	3.91E-10	2.90E-19	2.04E-19	5.49E-14
1.42857	3.89E-10	1.18E-16	2.50E-15	5.04E-12	3.94E-10	5.72E-18	5.38E-18	2.02E-13
1.25	3.82E-10	1.12E-15	2.32E-14	1.44E-11	3.97E-10	6.74E-17	8.61E-17	6.41E-13
1.11111	3.64E-10	6.58E-15	1.28E-13	3.47E-11	3.98E-10	5.33E-16	9.03E-16	1.81E-12
1	3.29E-10	2.65E-14	4.67E-13	6.95E-11	3.97E-10	3.06E-15	6.49E-15	4.57E-12
0.88889	2.63E-10	1.01E-13	1.52E-12	1.31E-10	3.91E-10	1.85E-14	4.82E-14	1.25E-11
0.8	1.88E-10	2.77E-13	3.43E-12	1.99E-10	3.74E-10	7.78E-14	2.32E-13	2.88E-11
0.72727	1.19E-10	6.02E-13	6.03E-12	2.55E-10	3.42E-10	2.43E-13	7.86E-13	5.61E-11
0.66667	6.83E-11	1.11E-12	8.85E-12	2.89E-10	2.94E-10	5.93E-13	2.00E-12	9.32E-11
0.60606	3.20E-11	1.97E-12	1.20E-11	3.03E-10	2.24E-10	1.34E-12	4.52E-12	1.42E-10
0.55556	1.42E-11	3.08E-12	1.47E-11	2.97E-10	1.55E-10	2.47E-12	8.00E-12	1.83E-10
0.5	4.65E-12	4.89E-12	1.76E-11	2.73E-10	8.47E-11	4.40E-12	1.30E-11	2.11E-10

0.44444		7.46E-12	2.08E-11	2.37E-10	3.56E-11	7.17E-12	1.84E-11	2.12E-10
0.4		1.01E-11	2.34E-11	2.02E-10		1.01E-11	2.26E-11	2.04E-10
Branching Ratios								
	p3→i2	p3→ $CH+C_6H_6$	p3→p1	p3→ $C_5H_5+C_2H_2$	p3→i2	p3→ $CH+C_6H_6$	p3→p1	p3→ $C_5H_5+C_2H_2$
T, K	30 Torr	30 Torr	30 Torr	30 Torr	1 atm	1 atm	1 atm	1 atm
500	99.90%	0.00%	0.00%	0.10%	100.00%	0.00%	0.00%	0.00%
600	99.62%	0.00%	0.00%	0.38%	99.99%	0.00%	0.00%	0.01%
700	98.72%	0.00%	0.00%	1.28%	99.95%	0.00%	0.00%	0.05%
800	96.35%	0.00%	0.01%	3.64%	99.84%	0.00%	0.00%	0.16%
900	91.26%	0.00%	0.03%	8.71%	99.55%	0.00%	0.00%	0.45%
1000	82.44%	0.01%	0.12%	17.44%	98.86%	0.00%	0.00%	1.14%
1125	66.51%	0.03%	0.38%	33.08%	96.89%	0.00%	0.01%	3.10%
1250	48.12%	0.07%	0.88%	50.93%	92.77%	0.02%	0.06%	7.15%
1375	31.29%	0.16%	1.58%	66.97%	85.67%	0.06%	0.20%	14.07%
1500	18.58%	0.30%	2.41%	78.71%	75.44%	0.15%	0.51%	23.90%
1650	9.16%	0.56%	3.44%	86.84%	60.26%	0.36%	1.22%	38.16%
1800	4.31%	0.94%	4.48%	90.27%	44.56%	0.71%	2.30%	52.43%
2000	1.55%	1.63%	5.88%	90.94%	27.03%	1.40%	4.16%	67.40%
2250		2.81%	7.82%	89.37%	13.07%	2.63%	6.75%	77.56%
2500		4.30%	9.92%	85.78%		4.25%	9.57%	86.18%
	p3→i2	p3→ $CH+C_6H_6$	p3→p1	p3→ $C_5H_5+C_2H_2$	p3→i2	p3→ $CH+C_6H_6$	p3→p1	p3→ $C_5H_5+C_2H_2$
1000/T, K^{-1}	10 atm	10 atm	10 atm	10 atm	100 atm	100 atm	100 atm	100 atm
2	3.87E-10	7.10E-22	6.68E-24	4.20E-16	3.87E-10	7.10E-23	1.67E-27	3.13E-18
1.66667	3.91E-10	2.91E-20	7.34E-22	3.09E-15	3.91E-10	2.91E-21	4.84E-25	4.79E-17
1.42857	3.94E-10	5.78E-19	3.10E-20	1.52E-14	3.94E-10	5.79E-20	4.59E-23	4.31E-16
1.25	3.97E-10	6.92E-18	6.74E-19	5.64E-14	3.97E-10	6.94E-19	1.85E-21	2.52E-15
1.11111	4.00E-10	5.68E-17	9.19E-18	1.73E-13	4.00E-10	5.73E-18	3.92E-20	1.06E-14
1	4.02E-10	3.48E-16	8.86E-17	4.64E-13	4.02E-10	3.54E-17	5.16E-19	3.46E-14

0.88889	4.03E-10	2.41E-15	1.01E-15	1.38E-12	4.05E-10	2.51E-16	8.06E-18	1.22E-13
0.8	4.03E-10	1.23E-14	7.81E-15	3.58E-12	4.07E-10	1.35E-15	8.56E-17	3.47E-13
0.72727	3.99E-10	4.87E-14	4.30E-14	8.30E-12	4.08E-10	5.77E-15	6.70E-16	8.62E-13
0.66667	3.89E-10	1.54E-13	1.76E-13	1.70E-11	4.08E-10	2.05E-14	4.01E-15	1.92E-12
0.60606	3.64E-10	4.72E-13	6.74E-13	3.46E-11	4.07E-10	7.62E-14	2.50E-14	4.57E-12
0.55556	3.23E-10	1.14E-12	1.89E-12	5.96E-11	4.00E-10	2.31E-13	1.14E-13	9.48E-12
0.5	2.51E-10	2.71E-12	5.09E-12	9.74E-11	3.79E-10	7.66E-13	5.69E-13	2.09E-11
0.44444	1.58E-10	5.58E-12	1.10E-11	1.34E-10	3.28E-10	2.33E-12	2.46E-12	4.24E-11
0.4	8.93E-11	8.82E-12	1.71E-11	1.48E-10	2.58E-10	5.01E-12	6.40E-12	6.56E-11
Branching Ratios								
	p3→i2	p3→ $CH+C_6H_6$	p3→p1	p3→ $C_5H_5+C_2H_2$	p3→i2	p3→ $CH+C_6H_6$	p3→p1	p3→ $C_5H_5+C_2H_2$
T, K	10 atm	10 atm	10 atm	10 atm	100 atm	100 atm	100 atm	100 atm
500	100.00%	0.00%	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%
600	100.00%	0.00%	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%
700	100.00%	0.00%	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%
800	99.99%	0.00%	0.00%	0.01%	100.00%	0.00%	0.00%	0.00%
900	99.96%	0.00%	0.00%	0.04%	100.00%	0.00%	0.00%	0.00%
1000	99.88%	0.00%	0.00%	0.12%	99.99%	0.00%	0.00%	0.01%
1125	99.66%	0.00%	0.00%	0.34%	99.97%	0.00%	0.00%	0.03%
1250	99.11%	0.00%	0.00%	0.88%	99.91%	0.00%	0.00%	0.09%
1375	97.94%	0.01%	0.01%	2.04%	99.79%	0.00%	0.00%	0.21%
1500	95.72%	0.04%	0.04%	4.20%	99.53%	0.01%	0.00%	0.47%
1650	91.05%	0.12%	0.17%	8.66%	98.86%	0.02%	0.01%	1.11%
1800	83.77%	0.29%	0.49%	15.44%	97.60%	0.06%	0.03%	2.31%
2000	70.46%	0.76%	1.43%	27.35%	94.45%	0.19%	0.14%	5.21%
2250	51.34%	1.81%	3.57%	43.29%	87.42%	0.62%	0.65%	11.30%
2500	33.94%	3.35%	6.50%	56.20%	76.98%	1.50%	1.91%	19.61%

	i2→ $CH+C_6H_6$	i2→p3	i2→p1	i2→ $C_5H_5+C_2H_2$	i2→ $CH+C_6H_6$	i2→p3	i2→p1	i2→ $C_5H_5+C_2H_2$
1000/T, K^{-1}	30 Torr	30 Torr	30 Torr	30 Torr	1 atm	1 atm	1 atm	1 atm
2	1.94E-25	9.56E-21	8.74E-23	2.67E-14	1.96E-25	9.57E-21	7.61E-25	3.57E-15
1.66667	8.87E-19	6.46E-15	1.15E-16	1.59E-09	9.10E-19	6.49E-15	2.09E-18	4.48E-10
1.42857	4.65E-14	9.32E-11	3.27E-12	3.55E-06	4.93E-14	9.44E-11	9.48E-14	1.69E-06
1.25	1.47E-10	1.20E-07	7.94E-09	1.03E-03	1.67E-10	1.24E-07	3.13E-10	6.97E-04
1.11111	7.00E-08	3.01E-05	3.41E-06	7.84E-02	8.94E-08	3.30E-05	1.80E-07	6.44E-02
1	8.59E-06	2.34E-03	4.04E-04	2.34E+00	1.31E-05	2.83E-03	3.01E-05	2.15E+00
0.88889	8.76E-04	1.60E-01	4.05E-02	6.37E+01	1.82E-03	2.38E-01	5.08E-03	6.46E+01
0.8	2.86E-02	3.98E+00	1.30E+00	8.01E+02	8.73E-02	7.93E+00	2.98E-01	9.46E+02
0.72727	4.00E-01	4.58E+01	1.78E+01	5.57E+03	1.89E+00	1.31E+02	7.48E+00	7.75E+03
0.66667	2.97E+00	2.93E+02	1.26E+02	2.44E+04	2.20E+01	1.26E+03	9.73E+01	4.25E+04
0.60606	1.77E+01	1.53E+03	7.03E+02	9.04E+04	2.20E+02	1.06E+04	1.05E+03	2.15E+05
0.55556	6.63E+01	5.13E+03	2.42E+03	2.33E+05	1.27E+03	5.38E+04	6.36E+03	7.50E+05
0.5	2.41E+02	1.66E+04	2.05E+04	5.76E+05	7.01E+03	2.64E+05	3.61E+04	2.55E+06
0.44444					3.07E+04	1.04E+06	1.58E+05	7.29E+06
0.4								
Branching Ratios								
	i2→ $CH+C_6H_6$	i2→p3	i2→p1	i2→ $C_5H_5+C_2H_2$	i2→ $CH+C_6H_6$	i2→p3	i2→p1	i2→ $C_5H_5+C_2H_2$
T, K	30 Torr	30 Torr	30 Torr	30 Torr	1 atm	1 atm	1 atm	1 atm
500	0.00%	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	100.00%
600	0.00%	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	100.00%
700	0.00%	0.00%	0.00%	100.00%	0.00%	0.01%	0.00%	99.99%
800	0.00%	0.01%	0.00%	99.99%	0.00%	0.02%	0.00%	99.98%
900	0.00%	0.04%	0.00%	99.96%	0.00%	0.05%	0.00%	99.95%
1000	0.00%	0.10%	0.02%	99.88%	0.00%	0.13%	0.00%	99.87%
1125	0.00%	0.25%	0.06%	99.68%	0.00%	0.37%	0.01%	99.62%
1250	0.00%	0.49%	0.16%	99.34%	0.01%	0.83%	0.03%	99.13%

1375	0.01%	0.81%	0.32%	98.87%	0.02%	1.67%	0.09%	98.21%
1500	0.01%	1.18%	0.51%	98.30%	0.05%	2.87%	0.22%	96.86%
1650	0.02%	1.65%	0.76%	97.58%	0.10%	4.66%	0.46%	94.78%
1800	0.03%	2.13%	1.00%	96.84%	0.16%	6.63%	0.78%	92.43%
2000	0.04%	2.71%	3.35%	93.90%	0.24%	9.24%	1.26%	89.26%
2250					0.36%	12.24%	1.85%	85.54%
2500								
	i2→ $CH+C_6H_6$	i2→p3	i2→p1	i2→ $C_5H_5+C_2H_2$	i2→ $CH+C_6H_6$	i2→p3	i2→p1	i2→ $C_5H_5+C_2H_2$
1000/T, K^{-1}	10 atm	10 atm	10 atm	10 atm	100 atm	100 atm	100 atm	100 atm
2	1.97E-25	9.57E-21	3.91E-27	2.11E-16	1.97E-25	9.57E-21	3.56E-30	4.04E-18
1.66667	9.11E-19	6.49E-15	2.79E-20	5.14E-11	9.11E-19	6.49E-15	6.25E-23	1.70E-12
1.42857	4.95E-14	9.45E-11	2.58E-15	3.42E-07	4.95E-14	9.45E-11	1.32E-17	2.03E-08
1.25	1.68E-10	1.25E-07	1.44E-11	2.22E-04	1.68E-10	1.25E-07	1.52E-13	2.28E-05
1.11111	9.06E-08	3.31E-05	1.19E-08	3.14E-02	9.07E-08	3.31E-05	2.32E-10	4.91E-03
1	1.35E-05	2.86E-03	2.54E-06	1.35E+00	1.35E-05	2.87E-03	8.14E-08	3.23E-01
0.88889	1.94E-03	2.46E-01	5.45E-04	4.98E+01	1.96E-03	2.46E-01	2.80E-05	2.12E+01
0.8	1.00E-01	8.55E+00	4.07E-02	7.93E+02	1.02E-01	8.63E+00	2.84E-03	4.43E+02
0.72727	2.43E+00	1.53E+02	1.38E+00	8.05E+03	2.53E+00	1.57E+02	1.23E-01	4.78E+03
0.66667	3.32E+01	1.66E+03	2.69E+01	4.61E+04	3.59E+01	1.75E+03	2.87E+00	3.23E+04
0.60606	4.24E+02	1.72E+04	4.55E+02	2.56E+05	4.97E+02	1.92E+04	6.53E+01	2.65E+05
0.55556	3.23E+03	1.12E+05	4.41E+03	1.03E+06	4.29E+03	1.38E+05	1.05E+03	1.11E+06
0.5	2.58E+04	7.70E+05	4.39E+04	4.37E+06	4.31E+04	1.16E+06	1.70E+04	5.23E+06
0.44444	1.63E+05	4.30E+06	3.29E+05	1.61E+07	3.82E+05	8.79E+06	2.63E+05	2.33E+07
0.4	5.85E+05	1.42E+07	1.30E+06	3.98E+07	1.87E+06	3.87E+07	1.77E+06	7.07E+07
Branching Ratios								
	i2→ $CH+C_6H_6$	i2→p3	i2→p1	i2→ $C_5H_5+C_2H_2$	i2→ $CH+C_6H_6$	i2→p3	i2→p1	i2→ $C_5H_5+C_2H_2$
T, K	10 atm	10 atm	10 atm	10 atm	100 atm	100 atm	100 atm	100 atm
500	0.00%	0.00%	0.00%	100.00%	0.00%	0.24%	0.00%	99.76%

600	0.00%	0.01%	0.00%	99.99%	0.00%	0.38%	0.00%	99.62%
700	0.00%	0.03%	0.00%	99.97%	0.00%	0.46%	0.00%	99.54%
800	0.00%	0.06%	0.00%	99.94%	0.00%	0.54%	0.00%	99.45%
900	0.00%	0.11%	0.00%	99.89%	0.00%	0.67%	0.00%	99.33%
1000	0.00%	0.21%	0.00%	99.79%	0.00%	0.88%	0.00%	99.12%
1125	0.00%	0.49%	0.00%	99.50%	0.01%	1.15%	0.00%	98.84%
1250	0.01%	1.07%	0.01%	98.92%	0.02%	1.91%	0.00%	98.07%
1375	0.03%	1.87%	0.02%	98.08%	0.05%	3.18%	0.00%	96.77%
1500	0.07%	3.47%	0.06%	96.40%	0.11%	5.12%	0.01%	94.76%
1650	0.15%	6.25%	0.17%	93.43%	0.17%	6.74%	0.02%	93.06%
1800	0.28%	9.74%	0.38%	89.59%	0.34%	11.01%	0.08%	88.56%
2000	0.49%	14.78%	0.84%	83.88%	0.67%	17.97%	0.26%	81.10%
2250	0.78%	20.60%	1.58%	77.05%	1.17%	26.83%	0.80%	71.20%
2500	1.05%	25.40%	2.33%	71.23%	1.65%	34.27%	1.57%	62.51%

	i8→ $CH+C_6H_6$	i8→p3	i8→p1	i8→ $C_5H_5+C_2H_2$	i8→ $CH+C_6H_6$	i8→p3	i8→p1	i8→ $C_5H_5+C_2H_2$
1000/T, K^{-1}	30 Torr	30 Torr	30 Torr	30 Torr	1 atm	1 atm	1 atm	1 atm
2	1.96E-36	3.47E-33	4.43E-25	1.50E-29	1.83E-38	1.80E-35	2.23E-25	1.19E-30
1.66667	5.52E-28	3.30E-25	3.55E-18	5.15E-22	8.66E-30	3.07E-27	1.17E-18	3.54E-24
1.42857	6.90E-22	1.98E-19	3.41E-13	1.22E-16	1.86E-23	3.50E-21	8.74E-14	1.53E-18
1.25	2.69E-17	4.69E-15	1.81E-09	1.41E-12	1.18E-18	1.43E-16	4.76E-10	3.00E-14
1.11111	9.50E-14	1.19E-11	1.31E-06	2.05E-09	6.84E-15	5.94E-13	4.34E-07	6.98E-11
1	5.85E-11	5.85E-09	2.33E-04	6.66E-07	7.17E-12	4.82E-10	1.04E-04	3.50E-08
0.88889	2.96E-08	2.45E-06	3.69E-02	1.89E-04	7.34E-09	3.90E-07	2.37E-02	1.71E-05
0.8	3.44E-06	2.50E-04	1.86E+00	1.45E-02	1.73E-06	7.78E-05	1.63E+00	2.25E-03
0.72727	1.34E-04	8.86E-03	3.99E+01	4.09E-01	1.33E-04	5.34E-03	4.65E+01	1.10E-01
0.66667	2.32E-03	1.42E-01	4.47E+02	5.40E+00	4.34E-03	1.60E-01	6.83E+02	2.49E+00
0.60606	3.09E-02	1.75E+00	4.01E+03	5.47E+01	1.15E-01	3.93E+00	8.74E+03	4.57E+01
0.55556	2.09E-01	1.11E+01	2.03E+04	2.91E+02	1.44E+00	4.62E+01	6.61E+04	4.22E+02
0.5	1.28E+00	6.33E+01	9.33E+04	1.52E+03	1.68E+01	5.04E+02	4.53E+05	3.52E+03

0.44444	6.54E+00	3.11E+02	3.23E+05	6.32E+03	1.32E+02	3.72E+03	2.29E+06	1.99E+04
0.4					7.97E+02	2.25E+04	6.83E+06	1.17E+05
Branching Ratios								
	i8→ $CH+C_6H_6$	i8→p3	i8→p1	i8→ $C_5H_5+C_2H_2$	i8→ $CH+C_6H_6$	i8→p3	i8→p1	i8→ $C_5H_5+C_2H_2$
T, K	30 Torr	30 Torr	30 Torr	30 Torr	1 atm	1 atm	1 atm	1 atm
500	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	100.00%	0.00%
600	0.00%	0.00%	99.99%	0.01%	0.00%	0.00%	100.00%	0.00%
700	0.00%	0.00%	99.96%	0.04%	0.00%	0.00%	100.00%	0.00%
800	0.00%	0.00%	99.92%	0.08%	0.00%	0.00%	99.99%	0.01%
900	0.00%	0.00%	99.84%	0.16%	0.00%	0.00%	99.98%	0.02%
1000	0.00%	0.00%	99.71%	0.28%	0.00%	0.00%	99.97%	0.03%
1125	0.00%	0.01%	99.48%	0.51%	0.00%	0.00%	99.93%	0.07%
1250	0.00%	0.01%	99.21%	0.77%	0.00%	0.00%	99.86%	0.14%
1375	0.00%	0.02%	98.96%	1.01%	0.00%	0.01%	99.75%	0.23%
1500	0.00%	0.03%	98.77%	1.19%	0.00%	0.02%	99.61%	0.36%
1650	0.00%	0.04%	98.61%	1.34%	0.00%	0.04%	99.43%	0.52%
1800	0.00%	0.05%	98.53%	1.42%	0.00%	0.07%	99.29%	0.63%
2000	0.00%	0.07%	98.33%	1.60%	0.00%	0.11%	99.12%	0.77%
2250	0.00%	0.09%	97.98%	1.92%	0.01%	0.16%	98.98%	0.86%
2500					0.01%	0.32%	97.99%	1.68%
	i8→ $CH+C_6H_6$	i8→p3	i8→p1	i8→ $C_5H_5+C_2H_2$	i8→ $CH+C_6H_6$	i8→p3	i8→p1	i8→ $C_5H_5+C_2H_2$
1000/T, K^{-1}	10 atm	10 atm	10 atm	10 atm	100 atm	100 atm	100 atm	100 atm
2	5.96E-40	4.95E-37	1.35E-25	1.17E-30	4.81E-41	3.61E-38	2.52E-26	1.84E-30
1.66667	2.23E-31	7.25E-29	8.47E-19	2.28E-27	1.15E-32	4.03E-30	2.45E-19	1.25E-26
1.42857	5.87E-25	9.45E-23	6.05E-14	4.06E-20	2.65E-26	4.48E-24	2.54E-14	-7.78E-22
1.25	4.99E-20	5.01E-18	2.71E-10	1.13E-15	2.08E-21	2.11E-19	1.46E-10	2.11E-17
1.11111	3.95E-16	2.85E-14	2.01E-07	3.52E-12	1.65E-17	1.16E-15	1.19E-07	9.79E-14
1	5.61E-13	3.17E-11	4.41E-05	2.28E-09	2.57E-14	1.36E-12	2.47E-05	8.56E-11

0.88889	8.36E-10	3.74E-08	1.06E-02	1.51E-06	4.64E-11	1.91E-09	5.19E-03	7.76E-08
0.8	2.90E-07	1.09E-05	8.69E-01	2.70E-04	2.08E-08	7.06E-07	4.30E-01	1.82E-05
0.72727	3.36E-05	1.10E-03	3.06E+01	1.80E-02	3.21E-06	9.46E-05	1.51E+01	1.54E-03
0.66667	1.66E-03	4.92E-02	5.49E+02	5.64E-01	2.17E-04	5.71E-03	2.97E+02	6.09E-02
0.60606	7.30E-02	1.98E+00	8.83E+03	1.55E+01	1.43E-02	3.40E-01	5.67E+03	2.32E+00
0.55556	1.53E+00	3.89E+01	7.98E+04	2.21E+02	4.45E-01	9.74E+00	6.19E+04	4.68E+01
0.5	3.31E+01	7.85E+02	8.56E+05	3.14E+03	1.71E+01	3.45E+02	7.65E+05	1.04E+03
0.44444	4.87E+02	1.08E+04	6.03E+06	3.04E+04	5.63E+02	1.06E+04	9.95E+06	2.01E+04
0.4	2.97E+03	6.23E+04	2.28E+07	1.37E+05	6.36E+03	1.13E+05	4.96E+07	1.52E+05
Branching Ratios								
	i8→ $CH+C_6H_6$	i8→p3	i8→p1	i8→ $C_5H_5+C_2H_2$	i8→ $CH+C_6H_6$	i8→p3	i8→p1	i8→ $C_5H_5+C_2H_2$
T, K	10 atm	10 atm	10 atm	10 atm	100 atm	100 atm	100 atm	100 atm
500	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	99.99%	0.01%
600	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	100.00%	0.00%
700	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	100.00%	0.00%
800	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	100.00%	0.00%
900	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	100.00%	0.00%
1000	0.00%	0.00%	99.99%	0.01%	0.00%	0.00%	100.00%	0.00%
1125	0.00%	0.00%	99.99%	0.01%	0.00%	0.00%	100.00%	0.00%
1250	0.00%	0.00%	99.97%	0.03%	0.00%	0.00%	100.00%	0.00%
1375	0.00%	0.00%	99.94%	0.06%	0.00%	0.00%	99.99%	0.01%
1500	0.00%	0.01%	99.89%	0.10%	0.00%	0.00%	99.98%	0.02%
1650	0.00%	0.02%	99.80%	0.18%	0.00%	0.01%	99.95%	0.04%
1800	0.00%	0.05%	99.67%	0.28%	0.00%	0.02%	99.91%	0.08%
2000	0.00%	0.09%	99.54%	0.36%	0.00%	0.05%	99.82%	0.14%
2250	0.01%	0.18%	99.31%	0.50%	0.01%	0.11%	99.69%	0.20%
2500	0.01%	0.27%	99.12%	0.59%	0.01%	0.23%	99.46%	0.30%

	i10→p3	i10→p2	i10→p1	i10→ C_5H_5+C_2H_2	i10→p3	i10→p2	i10→p1	i10→ C_5H_5+C_2H_2
1000/T, K^{-1}	30 Torr	30 Torr	30 Torr	30 Torr	1 atm	1 atm	1 atm	1 atm
2	9.65E-24	9.22E-18	1.56E-15	1.49E-15	1.25E-25	1.53E-18	1.56E-15	1.09E-16
1.66667	1.18E-17	1.90E-12	1.34E-10	1.38E-10	2.85E-19	6.13E-13	1.34E-10	2.11E-11
1.42857	3.18E-13	1.14E-08	4.64E-07	4.25E-07	1.10E-14	6.04E-09	4.65E-07	1.24E-07
1.25	7.12E-10	7.46E-06	2.14E-04	1.56E-04	3.24E-11	5.49E-06	2.16E-04	7.40E-05
1.11111	2.75E-07	1.11E-03	2.51E-02	1.41E-02	1.70E-08	1.00E-03	2.60E-02	9.27E-03
1	2.90E-05	5.62E-02	1.09E+00	4.82E-01	2.60E-06	6.02E-02	1.21E+00	3.91E-01
0.88889	2.52E-03	2.48E+00	4.26E+01	1.48E+01	3.89E-04	3.33E+00	5.58E+01	1.46E+01
0.8	7.11E-02	4.23E+01	6.76E+02	1.95E+02	2.00E-02	7.67E+01	1.14E+03	2.58E+02
0.72727	8.68E-01	3.50E+02	5.37E+03	1.35E+03	4.43E-01	8.71E+02	1.25E+04	2.21E+03
0.66667	5.61E+00	1.67E+03	2.50E+04	5.64E+03	5.08E+00	5.80E+03	8.13E+04	1.19E+04
0.60606	2.85E+01	6.49E+03	9.50E+04	1.94E+04	4.79E+01	3.23E+04	4.49E+05	5.53E+04
0.55556	9.05E+01	1.70E+04	2.47E+05	4.64E+04	2.53E+02	1.14E+05	1.58E+06	1.69E+05
0.5					1.21E+03	3.70E+05	5.17E+06	4.83E+05
0.44444					4.45E+03	9.94E+05	1.41E+07	1.15E+06
0.4								
Branching Ratios								
	i10→p3	i10→p2	i10→p1	i10→ C_5H_5+C_2H_2	i10→p3	i10→p2	i10→p1	i10→ C_5H_5+C_2H_2
T, K	30 Torr	30 Torr	30 Torr	30 Torr	1 atm	1 atm	1 atm	1 atm
500	0.00%	0.30%	51.02%	48.68%	0.00%	0.09%	93.39%	6.52%
600	0.00%	0.70%	48.85%	50.45%	0.00%	0.39%	86.00%	13.60%
700	0.00%	1.26%	51.56%	47.17%	0.00%	1.02%	78.14%	20.84%
800	0.00%	1.98%	56.71%	41.31%	0.00%	1.86%	73.08%	25.06%
900	0.00%	2.75%	62.23%	35.01%	0.00%	2.76%	71.69%	25.55%
1000	0.00%	3.45%	66.93%	29.61%	0.00%	3.62%	72.85%	23.53%
1125	0.00%	4.14%	71.09%	24.77%	0.00%	4.52%	75.71%	19.77%
1250	0.01%	4.63%	74.02%	21.35%	0.00%	5.19%	77.35%	17.46%

1375	0.01%	4.95%	75.97%	19.06%	0.00%	5.60%	80.16%	14.23%
1500	0.02%	5.18%	77.35%	17.46%	0.01%	5.86%	82.09%	12.05%
1650	0.02%	5.36%	78.58%	16.04%	0.01%	6.02%	83.67%	10.30%
1800	0.03%	5.49%	79.54%	14.94%	0.01%	6.10%	84.78%	9.11%
2000					0.02%	6.13%	85.84%	8.01%
2250					0.03%	6.12%	86.79%	7.06%
2500								
	i10→p3	i10→p2	i10→p1	i10→ C_5H_5+C_2H_2	i10→p3	i10→p2	i10→p1	i10→ C_5H_5+C_2H_2
1000/T, K^{-1}	10 atm	10 atm	10 atm	10 atm	100 atm	100 atm	100 atm	100 atm
2	9.08E-28	1.87E-19	1.56E-15	6.93E-18	1.01E-30	1.92E-20	1.56E-15	1.70E-19
1.66667	4.91E-21	9.84E-14	1.34E-10	2.04E-12	1.34E-23	1.07E-14	1.34E-10	8.26E-14
1.42857	3.68E-16	1.41E-09	4.65E-07	1.81E-08	2.28E-18	1.75E-10	4.65E-07	1.14E-09
1.25	1.74E-12	1.90E-06	2.16E-04	1.65E-05	2.20E-14	2.93E-07	2.16E-04	1.51E-06
1.11111	1.26E-09	4.95E-04	2.61E-02	3.09E-03	2.89E-11	1.01E-04	2.61E-02	4.02E-04
1	2.42E-07	3.89E-02	1.22E+00	1.81E-01	8.96E-09	1.09E-02	1.22E+00	3.35E-02
0.88889	4.62E-05	2.72E+00	5.77E+01	9.05E+00	2.66E-06	1.11E+00	5.79E+01	2.63E+00
0.8	3.02E-03	7.31E+01	1.26E+03	1.80E+02	2.39E-04	4.02E+01	1.28E+03	7.31E+01
0.72727	8.71E-02	9.91E+02	1.54E+04	1.85E+03	9.02E-03	6.89E+02	1.62E+04	9.82E+02
0.66667	1.49E+00	8.59E+03	1.19E+05	1.47E+04	1.78E-01	6.74E+03	1.33E+05	7.75E+03
0.60606	2.12E+01	6.00E+04	8.36E+05	8.03E+04	2.95E+00	6.00E+04	1.07E+06	5.41E+04
0.55556	1.68E+02	2.66E+05	3.76E+06	2.96E+05	4.43E+01	4.07E+05	5.83E+06	3.79E+05
0.5	1.32E+03	1.13E+06	1.64E+07	1.05E+06	5.39E+02	2.21E+06	3.35E+07	1.62E+06
0.44444	7.65E+03	3.79E+06	5.69E+07	3.01E+06	5.43E+03	9.88E+06	1.60E+08	5.87E+06
0.4	2.54E+04	8.60E+06	1.33E+08	6.08E+06	2.86E+04	2.74E+07	4.68E+08	1.41E+07
Branching Ratios								
	i10→p3	i10→p2	i10→p1	i10→ C_5H_5+C_2H_2	i10→p3	i10→p2	i10→p1	i10→ C_5H_5+C_2H_2
T, K	10 atm	10 atm	10 atm	10 atm	100 atm	100 atm	100 atm	100 atm
500	0.00%	0.01%	99.55%	0.44%	0.00%	0.00%	99.99%	0.01%

600	0.00%	0.07%	98.43%	1.50%	0.00%	0.01%	99.93%	0.06%
700	0.00%	0.29%	95.98%	3.73%	0.00%	0.04%	99.72%	0.24%
800	0.00%	0.81%	92.16%	7.03%	0.00%	0.13%	99.17%	0.69%
900	0.00%	1.67%	87.90%	10.43%	0.00%	0.38%	98.11%	1.51%
1000	0.00%	2.70%	84.75%	12.56%	0.00%	0.86%	96.49%	2.65%
1125	0.00%	3.91%	83.06%	13.03%	0.00%	1.79%	93.93%	4.27%
1250	0.00%	4.83%	83.26%	11.91%	0.00%	2.89%	91.87%	5.24%
1375	0.00%	5.43%	84.40%	10.16%	0.00%	3.86%	90.64%	5.50%
1500	0.00%	6.05%	83.59%	10.36%	0.00%	4.56%	90.20%	5.24%
1650	0.00%	6.15%	85.62%	8.23%	0.00%	5.05%	90.40%	4.55%
1800	0.00%	6.15%	87.01%	6.84%	0.00%	6.15%	88.13%	5.72%
2000	0.01%	6.08%	88.27%	5.64%	0.00%	5.92%	89.74%	4.34%
2250	0.01%	5.96%	89.31%	4.72%	0.00%	5.62%	91.04%	3.34%
2500	0.02%	5.83%	90.03%	4.12%	0.01%	5.39%	91.85%	2.76%

	i13→p3	i13→p2	i13→p1	i13→ C_5H_5+C_2H_2	i13→p3	i13→p2	i13→p1	i13→ C_5H_5+C_2H_2
1000/T, K^{-1}	30 Torr	30 Torr	30 Torr	30 Torr	1 atm	1 atm	1 atm	1 atm
2	1.85E-20	7.20E-17	6.44E-08	1.76E-15	2.22E-23	2.27E-18	6.65E-08	3.17E-17
1.66667	3.89E-15	3.72E-12	2.41E-04	5.75E-11	1.83E-17	3.62E-13	2.71E-04	3.07E-12
1.42857	1.57E-11	7.83E-09	7.73E-02	8.84E-08	4.11E-13	2.07E-09	1.06E-01	1.19E-08
1.25	1.82E-08	2.20E-06	4.86E+00	1.97E-05	7.44E-10	1.30E-06	9.12E+00	5.68E-06
1.11111	2.82E-06	1.62E-04	9.77E+01	1.17E-03	2.67E-07	1.78E-04	2.77E+02	6.08E-04
1	1.44E-04	4.75E-03	8.59E+02	2.92E-02	2.70E-05	8.00E-03	3.84E+03	2.29E-02
0.88889	6.43E-03	1.31E-01	5.81E+03	6.95E-01	2.50E-03	3.04E-01	4.48E+04	7.31E-01
0.8	1.30E-01	1.87E+00	2.22E+04	9.09E+00	8.59E-02	4.84E+00	2.61E+05	1.03E+01
0.72727	1.70E+00	1.89E+01	6.21E+04	8.76E+01	1.50E+00	4.33E+01	9.41E+05	8.46E+01
0.66667					1.72E+01	2.72E+02	2.45E+06	5.17E+02
0.60606					2.46E+02	1.99E+03	6.02E+06	3.99E+03
0.55556								
0.5								

0.44444								
0.4								
Branching Ratios								
	i13→p3	i13→p2	i13→p1	i13→ C_5H_5+C_2H_2	i13→p3	i13→p2	i13→p1	i13→ C_5H_5+C_2H_2
T, K	30 Torr	30 Torr	30 Torr	30 Torr	1 atm	1 atm	1 atm	1 atm
500	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	100.00%	0.00%
600	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	100.00%	0.00%
700	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	100.00%	0.00%
800	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	100.00%	0.00%
900	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	100.00%	0.00%
1000	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	100.00%	0.00%
1125	0.00%	0.00%	99.99%	0.01%	0.00%	0.00%	100.00%	0.00%
1250	0.00%	0.01%	99.95%	0.04%	0.00%	0.00%	99.99%	0.00%
1375	0.00%	0.03%	99.83%	0.14%	0.00%	0.00%	99.99%	0.01%
1500					0.00%	0.01%	99.97%	0.02%
1650					0.00%	0.03%	99.90%	0.07%
1800								
2000								
2250								
2500								
	i13→p3	i13→p2	i13→p1	i13→ C_5H_5+C_2H_2	i13→p3	i13→p2	i13→p1	i13→ C_5H_5+C_2H_2
1000/T, K^{-1}	10 atm	10 atm	10 atm	10 atm	100 atm	100 atm	100 atm	100 atm
2	5.13E-26	4.36E-20	6.65E-08	7.09E-18	1.71E-26	4.79E-22	6.65E-08	1.99E-20
1.66667	8.40E-20	1.33E-14	2.73E-04	8.06E-14	2.48E-22	1.30E-16	2.72E-04	2.86E-15
1.42857	3.55E-15	1.47E-10	1.08E-01	6.15E-10	1.64E-17	2.56E-12	1.08E-01	7.45E-12
1.25	1.36E-11	1.73E-07	9.77E+00	5.35E-07	8.57E-14	5.33E-09	9.81E+00	1.20E-08
1.11111	9.12E-09	4.18E-05	3.26E+02	1.02E-04	8.61E-11	2.23E-06	3.33E+02	4.02E-06
1	1.69E-06	3.16E-03	5.32E+03	6.29E-03	2.52E-08	2.85E-04	5.66E+03	4.23E-04

0.88889	2.96E-04	2.10E-01	8.18E+04	3.42E-01	8.00E-06	3.50E-02	9.60E+04	4.25E-02
0.8	1.71E-02	5.16E+00	6.54E+05	7.15E+00	8.25E-04	1.50E+00	9.09E+05	1.53E+00
0.72727	4.44E-01	6.14E+01	3.15E+06	7.49E+01	3.55E-02	2.90E+01	5.46E+06	2.54E+01
0.66667	6.49E+00	4.40E+02	1.04E+07	5.03E+02	7.84E-01	3.04E+02	2.28E+07	2.35E+02
0.60606	9.82E+01	2.92E+03	3.02E+07	3.09E+03	1.66E+01	2.79E+03	8.59E+07	1.90E+03
0.55556	1.12E+03	1.42E+04	6.77E+07	1.51E+04	2.13E+02	1.66E+04	2.35E+08	1.10E+04
0.5					3.92E+03	1.01E+05	6.37E+08	6.17E+04
0.44444								
0.4								
Branching Ratios								
	i13→p3	i13→p2	i13→p1	i13→ C_5H_5+C_2H_2	i13→p3	i13→p2	i13→p1	i13→ C_5H_5+C_2H_2
T, K	10 atm	10 atm	10 atm	10 atm	100 atm	100 atm	100 atm	100 atm
500	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	100.00%	0.00%
600	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	100.00%	0.00%
700	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	100.00%	0.00%
800	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	100.00%	0.00%
900	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	100.00%	0.00%
1000	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	100.00%	0.00%
1125	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	100.00%	0.00%
1250	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	100.00%	0.00%
1375	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	100.00%	0.00%
1500	0.00%	0.00%	99.99%	0.00%	0.00%	0.00%	100.00%	0.00%
1650	0.00%	0.01%	99.98%	0.01%	0.00%	0.00%	99.99%	0.00%
1800	0.00%	0.02%	99.95%	0.02%	0.00%	0.01%	99.99%	0.00%
2000					0.00%	0.02%	99.97%	0.01%
2250								
2500								

Table S4: Optimized Cartesian coordinates and vibrational frequencies for all intermediates, transition states, reactants and products involved in the reactions of the methylidyne radical (CH) with benzene (C_6H_6).

p0

C_6H_6

C	0.416883	1.330008	0.000087
C	1.360535	0.304227	-0.000056
C	0.943530	-1.026072	-0.000075
C	-0.416737	-1.330068	-0.000064
C	-1.360545	-0.304162	-0.000070
C	-0.943597	1.026041	0.000080
H	0.740547	2.365038	-0.000088
H	2.418891	0.540389	-0.000003
H	1.677805	-1.824080	0.000343
H	-0.741341	-2.364797	0.000477
H	-2.418816	-0.540785	-0.000009
H	-1.677495	1.824389	-0.000128

Frequencies

412.9072	413.7917	623.2855
623.4867	689.0146	723.3252
862.5482	862.8405	981.3337
982.0888	1012.9152	1016.8793
1023.3623	1060.0208	1060.5560
1174.5779	1197.1801	1197.7250
1334.5916	1381.6542	1512.6211
1513.1646	1636.9730	1637.2259
3155.2001	3164.5481	3165.1147
3180.3063	3180.9182	3191.2112

CH

C	0.000000	0.000000	0.161147
H	0.000000	0.000000	-0.966885

Frequencies

2803.8310

p1

C	0.597081	1.180837	0.000003
C	1.874182	0.733846	0.000006
C	1.874223	-0.733783	-0.000006

C	0.597147	-1.180848	-0.000002
H	0.246967	2.201956	-0.000036
H	2.764024	1.348893	0.000027
H	2.764099	-1.348781	-0.000026
H	0.247092	-2.201987	0.000039
C	-0.285538	-0.000031	-0.000001
C	-1.603448	-0.000069	-0.000001
C	-2.901714	0.000021	0.000001
H	-3.466891	0.000039	-0.927939
H	-3.466887	0.000046	0.927942

Frequencies

135.4325	156.0928	369.6242
483.2023	558.0334	564.7589
629.7811	646.3405	728.4586
775.1368	821.8729	868.6236
899.2705	922.5639	936.0807
992.8364	1002.4537	1090.8825
1101.0827	1177.4390	1284.7275
1309.1406	1390.8468	1465.8398
1522.5573	1604.3772	2025.8968
3110.6998	3182.0351	3199.4610
3211.4625	3236.5447	3240.4325

p2

C	-1.905916	-0.616488	-0.000201
C	-1.851780	0.730429	0.000049
C	0.355553	0.074032	-0.000009
C	-0.510286	-1.169520	0.000115
H	-2.796965	-1.229031	-0.000288
C	-0.458350	1.162048	-0.000125
H	-2.698496	1.404414	0.000108
H	-0.309826	-1.796374	-0.877685
H	-0.310093	-1.795882	0.878354
C	1.766874	0.045661	0.000027
C	2.971889	-0.013063	0.000082
H	4.033166	-0.053089	0.000034
H	-0.125690	2.191373	-0.000155

Frequencies

156.3842	165.1169	339.5872

479.7153	525.1075	536.6305
556.4395	612.9124	680.4603
694.5584	825.9235	890.2074
899.9708	917.1360	958.9846
964.2618	1020.7103	1122.3032
1130.3001	1181.3619	1260.7052
1299.0079	1382.7630	1413.7184
1544.1352	1631.5803	2194.4500
3025.1090	3051.1558	3195.8943
3212.4953	3223.3938	3477.3780

p3

C	1.220128	-1.037468	-0.344538
C	1.598189	0.267576	0.183361
C	0.695284	1.289636	0.204786
C	-0.695867	1.289389	-0.204748
C	-1.598278	0.266961	-0.183449
C	-1.219631	-1.037777	0.344695
C	0.000200	-1.421184	-0.000133
H	1.863678	-1.580859	-1.030280
H	2.622822	0.465829	0.491487
H	1.075220	2.264465	0.501565
H	-1.076144	2.264073	-0.501591
H	-2.622910	0.464570	-0.492031
H	-1.862815	-1.580871	1.031003

Frequencies

298.7288	305.9895	377.5428
423.5877	492.9841	604.0727
694.0507	702.1844	801.5146
823.3249	850.0833	894.7300
932.2618	973.8624	993.4599
1036.8310	1041.8478	1124.0121
1214.3541	1238.2189	1305.0497
1385.2816	1409.5982	1453.2450
1564.3995	1616.7493	1889.8722
3117.7957	3122.3499	3135.8283
3139.6866	3142.0659	3151.2855

p4

C	-2.478946	-0.172976	-0.000130

C	-1.046350	-0.039091	0.000042
C	-0.346759	1.197949	0.000073
C	1.037905	1.238711	-0.000007
C	1.761148	0.040876	0.000007
C	1.108483	-1.193979	0.000018
C	-0.278031	-1.230979	-0.000013
H	-2.893191	0.858137	0.000087
H	-0.922383	2.117800	0.000133
H	1.563111	2.187003	-0.000042
H	2.845680	0.072921	-0.000042
H	1.685362	-2.111429	0.000006
H	-0.823283	-2.167502	-0.000078

Frequencies

174.9497	276.0908	391.2768
458.4074	520.8376	541.3388
626.7250	693.0382	783.4044
833.9546	860.8841	975.6042
1005.7054	1015.3582	1027.5907
1039.9347	1076.4831	1145.0940
1184.7631	1190.7062	1280.8552
1337.3363	1349.2540	1473.7226
1502.8145	1596.9993	1624.2457
2905.6304	3162.6450	3170.3363
3181.0955	3188.1729	3198.3443

p5

C	-0.242751	1.405715	-0.168809
C	0.996123	0.729684	-0.370647
C	0.996534	-0.729211	-0.370345
C	-0.242312	-1.405719	-0.168976
C	-1.398906	-0.708061	0.111532
C	-1.399139	0.707623	0.111723
C	1.538222	-0.000042	1.091551
H	-0.258312	2.489076	-0.211550
H	1.834565	1.263458	-0.803132
H	1.834994	-1.262609	-0.803302
H	-0.257511	-2.489079	-0.211908
H	-2.319995	-1.244285	0.306644
H	-2.320369	1.243508	0.307072

Frequencies

50.6090	248.5333	270.7214
372.5175	459.5678	582.6952
605.0259	609.6675	725.4007
836.4247	892.4131	903.2792
959.1596	972.3709	978.3620
993.9231	1019.7364	1040.7150
1161.5883	1184.5527	1186.7752
1345.1024	1357.9312	1458.0785
1487.3024	1545.0897	1585.8982
3156.4972	3163.5089	3171.0447
3177.9540	3187.2434	3197.5189

p6

C_5H_5

C	-0.287303	1.153610	-0.000009
H	-0.521839	2.210352	-0.000004
C	-1.219721	0.099030	0.000058
H	-2.294567	0.197844	0.000120
C	-0.496510	-1.085492	0.000014
H	-0.904584	-2.087637	0.000040
C	1.062038	0.592718	-0.000050
H	1.975601	1.168907	-0.000090
C	0.942189	-0.760171	-0.000019
H	1.741224	-1.487638	-0.000034

Frequencies

14.7449	491.6287	525.1459
679.0370	719.0350	816.8332
847.5814	884.2732	904.7043
921.1475	963.3493	1038.6734
1081.1576	1143.3571	1215.0123
1294.8422	1393.7417	1453.4911
1565.8710	3201.4086	3204.4198
3217.5825	3232.9980	3241.0666

C_2H_2

C	0.000000	0.000000	0.599048
H	0.000000	0.000000	1.661977
C	0.000000	0.000000	-0.599048
H	0.000000	0.000000	-1.661977

Frequencies

642.7437	642.7437	773.3717
773.3717	2069.9740	3420.0953
3523.0840		

p7

C	0	2.145583	0.000100	0.000398
C	0	0.802279	-0.673844	-0.000308
C	0	-0.334177	-1.451664	-0.000218
C	0	-1.526930	-0.700437	0.000138
C	0	-1.527065	0.700325	0.000201
C	0	-0.334382	1.451652	-0.000191
C	0	0.802177	0.673861	-0.000378
H	0	2.745241	0.000118	0.911039
H	0	2.745823	0.000186	-0.909866
H	0	-0.348853	-2.535770	0.000094
H	0	-2.478862	-1.220590	0.000410
H	0	-2.479068	1.220343	0.000470
H	0	-0.349191	2.535755	0.000005

Frequencies

184.7306	348.7235	437.4889
450.9174	585.3848	681.5716
707.2712	749.1137	876.8647
896.1832	928.4085	988.9599
1008.5960	1016.3525	1019.6789
1021.5360	1091.9718	1125.3505
1130.4480	1177.3699	1300.0564
1381.8410	1464.1447	1482.4599
1499.4400	1609.8314	1739.1740
3044.9290	3111.0047	3157.4460
3167.0530	3175.7193	3184.8826

p8

C	0	-1.770813	0.115951	-0.227941
C	0	-1.124686	-1.074950	-0.111641

C	0	1.583501	-0.676399	-0.327848
C	0	1.694738	0.648313	-0.112556
C	0	0.321833	0.707971	0.428436
C	0	-0.868178	1.233868	0.041983
C	0	0.239867	-0.814409	0.443774
H	0	-2.806175	0.235404	-0.527524
H	0	-1.586876	-2.049803	-0.202582
H	0	2.175016	-1.403804	-0.867948
H	0	2.428837	1.398601	-0.373675
H	0	-1.059635	2.256407	-0.257837
H	0	0.391262	-1.278866	1.424324

Frequencies

244.8693	312.1729	460.0553
551.6548	683.8664	730.4890
735.9208	776.4831	850.6176
857.2645	880.9573	920.6109
938.6651	954.6873	1008.8913
1048.5610	1054.0967	1081.1508
1113.2530	1158.6764	1248.7068
1274.7750	1295.1691	1374.2940
1515.3260	1553.9982	1617.1938
3037.2850	3171.9496	3193.9449
3194.4010	3202.5971	3223.8835

i1

C	-1.578003	-0.000064	0.750968
H	-2.596904	-0.000150	1.112464
C	-0.981859	0.821766	-0.299822
C	0.346471	1.432147	-0.156960
C	1.449414	0.722987	0.162487
C	1.449576	-0.722784	0.162415
C	0.346704	-1.432102	-0.156975
C	-0.981667	-0.821947	-0.299664
H	-1.671561	1.338710	-0.966022
H	0.420601	2.495130	-0.363896
H	2.397047	1.235993	0.286304
H	2.397302	-1.235616	0.286179

H	0.421042	-2.495069	-0.363927
H	-1.671343	-1.339013	-0.965797

Frequencies

236.4156	237.1920	307.1289
493.7376	495.7637	619.9006
624.7982	658.7731	764.8271
783.5790	813.7622	921.2324
924.0434	960.7715	981.4585
1008.4595	1033.8900	1044.5211
1058.4606	1094.3656	1198.1203
1212.0304	1220.0789	1337.5204
1398.9266	1401.7669	1459.9280
1593.1288	1679.5009	3088.3543
3092.9046	3149.3041	3154.0739
3168.6326	3180.7390	3198.8774

i2

C	1.514005	0.588421	-0.000585
C	1.386807	-0.820031	0.000073
C	0.257388	-1.602045	0.000453
C	-1.122582	-1.164123	-0.000288
C	-1.613911	0.101314	-0.000244
C	-0.891980	1.355667	0.000492
C	0.470244	1.540784	0.000028
H	2.524468	0.980760	-0.000691
H	2.329304	-1.363306	0.000426
H	0.407095	-2.676472	0.001079
H	-1.856993	-1.964781	-0.000924
H	-2.696260	0.196448	-0.000819
H	-1.506373	2.249603	0.001053
H	0.798929	2.577819	0.000301

Frequencies

22.1104	154.2573	288.8068
420.0112	446.8599	515.7061
564.8645	649.0178	757.0362
764.9281	843.1402	845.0643
904.4157	913.1272	962.8216
966.4986	982.4544	991.8214
1006.2472	1186.9449	1242.7979

1285.8221	1304.8480	1417.0698
1476.5594	1480.6930	1549.2721
1597.7782	1650.7562	3127.9778
3128.4905	3135.2095	3151.9562
3166.8203	3168.9368	3178.2616

i3

C	0.086306	-1.533122	0.203492
C	1.302065	-0.979964	0.239531
C	1.531231	0.366802	-0.279707
C	-1.186421	-1.110679	-0.248349
C	0.616146	1.352541	-0.236052
C	-1.564789	0.188302	-0.168751
C	-0.693696	1.212967	0.513483
H	2.162145	-1.555119	0.576157
H	2.496059	0.558159	-0.743402
H	-1.840525	-1.837504	-0.722003
H	0.820176	2.293944	-0.736917
H	-2.496329	0.505479	-0.629460
H	-0.482914	0.878672	1.538664
H	-1.203666	2.175281	0.575078

Frequencies

226.7651	276.3157	352.1960
403.2039	439.5131	578.8124
654.0079	716.0297	751.5556
823.1160	843.0275	908.8277
931.2463	950.5584	971.3882
979.3556	1029.7044	1059.3706
1190.8868	1210.3921	1263.0555
1302.9362	1325.3851	1394.6767
1406.2139	1474.0281	1567.6152
1603.6810	1674.0159	2988.6183
3091.7076	3118.8626	3134.2302
3137.8069	3157.2756	3163.0738

i4

C	-1.695510	0.000025	-0.361606
C	-0.995553	-1.152492	-0.022277
C	1.516160	-0.667417	-0.381580
C	1.516294	0.667330	-0.381481

C	0.329615	0.792240	0.582893
C	-0.995480	1.152539	-0.022406
H	-2.663455	0.000026	-0.850383
H	-1.331884	2.166121	-0.197291
H	0.546957	1.291465	1.533328
C	0.329601	-0.792223	0.582926
H	0.546955	-1.291419	1.533382
H	2.101445	1.418279	-0.900252
H	-1.331959	-2.166078	-0.197167
H	2.101180	-1.418402	-0.900430

Frequencies

233.8134	261.3722	442.2071
517.0415	640.2670	669.3049
697.2704	735.7049	806.0616
852.3854	875.3371	886.5348
946.6943	950.0453	971.2943
986.4106	1030.4455	1071.7010
1076.3840	1091.0929	1176.8582
1189.5757	1263.0205	1265.9365
1280.0383	1315.9073	1398.1833
1462.4682	1627.0700	3023.2802
3032.6234	3162.7236	3172.6590
3195.3959	3199.4332	3209.3399

i5

C	-0.465412	1.443569	-0.208858
C	-1.462879	0.537921	-0.210550
C	-0.204031	-1.519216	-0.201543
C	1.081557	-1.198508	-0.300790
C	1.603672	0.080366	0.158007
C	0.903601	1.243229	0.218086
H	-0.691587	2.433844	-0.597693
H	-2.403852	0.791568	-0.689722
H	1.789597	-1.905785	-0.727128
H	2.664212	0.112359	0.394781
H	1.454725	2.139875	0.487785
C	-1.350868	-0.827487	0.430900
H	-2.279442	-1.390441	0.307886
H	-1.167490	-0.740660	1.512578

Frequencies

171.9187	304.0875	361.0820
403.3595	422.3546	585.4807
662.4782	707.4805	786.3546
831.2182	886.0419	907.5597
919.6056	945.1219	979.6301
991.1250	997.8059	1064.8265
1203.3139	1234.9059	1246.9869
1291.1589	1307.8310	1399.8594
1456.0394	1458.4342	1565.5707
1661.1757	1679.2713	2967.9309
3064.9248	3121.7252	3127.0556
3136.1339	3153.1903	3160.2185

i6

C	-1.796858	-0.183579	0.550561
C	-0.940527	0.721506	-0.393317
C	0.299241	1.432292	-0.040782
C	1.447961	0.752349	0.184712
C	1.516111	-0.689066	0.077693
C	0.393412	-1.423691	-0.176690
C	-0.849386	-0.768270	-0.406115
H	-1.556549	-0.231098	1.609044
H	-1.569880	1.217862	-1.130735
H	0.301715	2.518107	-0.056738
H	2.357759	1.295018	0.418890
H	2.468956	-1.181896	0.237667
H	0.436580	-2.509545	-0.178076
H	-2.858310	-0.157697	0.323578

Frequencies

141.1263	277.4576	423.7089
522.7553	546.8109	583.0055
673.3906	760.9009	783.5271
823.8412	867.8463	906.4375
947.8587	963.2383	989.2506
996.8207	1020.2599	1036.787
1071.3371	1105.9225	1181.3200
1201.2513	1315.3539	1374.4993
1414.7562	1453.9151	1465.4083
1511.3158	1637.9891	3083.0384

3089.1844	3139.0233	3147.4736
3165.8705	3172.6944	3179.3342

i7

C	-1.787488	-0.479694	-0.427045
C	-0.741378	-1.198206	0.015597
C	1.682416	-0.442886	0.064236
C	2.380250	0.466839	-0.563190
C	-0.343019	1.093972	0.417776
C	-1.540425	0.946767	-0.174954
H	-2.679803	-0.874110	-0.896488
H	-2.226540	1.742355	-0.436041
H	0.127829	2.017592	0.723087
C	0.282759	-0.263100	0.624391
H	0.331669	-0.469367	1.707370
H	3.351461	0.551669	-1.026853
H	-0.619243	-2.271853	-0.028939
H	2.115932	-1.438433	0.217003

Frequencies

94.7108	160.9489	237.0649
407.4353	532.3307	584.4151
631.8030	700.2554	721.4037
803.2944	811.0461	829.8446
867.3479	894.3020	954.5703
957.8011	995.4282	1023.9634
1055.3758	1110.9138	1129.6221
1204.7072	1226.4138	1283.7224
1314.1692	1398.6024	1556.8871
1640.3985	1673.2860	2960.1413
3015.4055	3188.1132	3199.2115
3217.7862	3226.9677	3241.0462

i8

C	2.398347	-0.000071	-0.000724
C	0.993970	-0.000071	0.000166
C	0.251156	-1.216566	0.000239
C	-1.131651	-1.209850	0.000285
C	-1.836220	0.000007	-0.000632
C	-1.131403	1.210042	-0.000029
C	0.251002	1.216615	0.000482

H	2.957302	-0.927503	-0.000885
H	2.957660	0.927148	0.000884
H	0.791155	-2.157498	0.000746
H	-1.674760	-2.148622	0.000679
H	-2.919880	-0.000571	-0.001030
H	-1.674131	2.149064	0.000018
H	0.791445	2.157348	0.000873

Frequencies

199.0149	359.4316	390.3549
478.6789	502.5343	534.1774
628.1880	684.5147	707.1794
773.7172	829.3367	830.7661
898.3914	969.7185	971.6429
989.5136	994.5494	1035.8299
1116.3983	1174.5953	1184.3316
1287.1631	1327.2898	1352.0204
1473.8668	1489.5096	1501.6141
1576.4360	1598.6606	3143.9717
3157.8240	3160.2413	3172.6915
3177.3023	3191.1021	3240.7014

i9

C	-1.799275	-0.804698	0.000031
C	-1.965414	0.532713	-0.000051
C	0.322363	0.242593	-0.000017
C	-0.328497	-1.120292	0.000025
H	-2.578419	-1.554535	0.000038
C	-0.657758	1.182702	0.000066
H	-2.910834	1.059843	-0.000090
H	-0.031197	-1.709008	-0.876643
H	-0.031190	-1.708979	0.876711
C	1.753655	0.483903	-0.000052
H	2.050318	1.540164	-0.000050
C	2.710526	-0.423758	-0.000013
H	3.789455	-0.441049	0.000006
H	-0.501736	2.254584	0.000089

Frequencies

125.4978	204.2332	259.0862
373.4316	481.3968	526.0459

604.1045	630.2828	697.8799
817.4680	823.3621	853.7792
890.5729	900.7841	919.8232
955.9669	960.8683	1021.3048
1122.7332	1129.4842	1206.3277
1233.6123	1276.4116	1334.0776
1390.4303	1415.3379	1546.6752
1616.6670	1648.5174	3012.0908
3025.5013	3049.7696	3188.5312
3199.9763	3221.0031	3247.4036

i10

C	-0.828143	-1.181590	0.000056
C	-2.006903	-0.487260	-0.000120
C	-1.701356	0.952312	-0.000041
C	-0.352564	1.107624	0.000303
C	0.249560	-0.226236	-0.000086
H	-3.003206	-0.908242	-0.000200
H	-2.441255	1.740885	-0.000047
H	0.189553	2.041264	0.000497
H	-0.703262	-2.254926	0.000126
C	1.629623	-0.557543	-0.000133
H	1.866942	-1.618925	-0.000232
C	2.660764	0.328013	-0.000018
H	3.689311	-0.010840	-0.000049
H	2.496028	1.398864	0.000133

Frequencies

127.0842	219.0855	235.0021
469.8776	528.2433	545.4445
620.6839	676.7887	708.0895
721.1842	774.0975	889.2598
895.8211	909.2433	910.5888
987.7263	1002.1914	1027.7319
1063.9322	1098.1959	1172.4807
1286.8600	1292.3323	1313.9723
1408.3051	1456.8463	1477.6342
1549.6984	1577.1846	3136.8827
3147.8418	3201.8550	3211.4418
3225.9666	3233.4518	3237.6898

i11

C	-0.108944	0.780341	0.711092
C	-0.108953	-0.780334	0.711142
C	1.081338	-1.147902	-0.103437
C	1.081345	1.147930	-0.103404
C	1.720707	-0.000055	-0.559521
C	-1.170342	-0.000027	0.032480
C	-2.318411	0.000014	-0.610956
H	-2.809937	-0.927016	-0.890442
H	-2.809772	0.927083	-0.890539
H	-0.377558	-1.358301	1.590851
H	-0.377619	1.358358	1.590743
H	1.365384	-2.167324	-0.325537
H	1.365551	2.167400	-0.325497
H	2.583506	-0.000004	-1.213963

Frequencies

152.8033	238.3436	387.6699
444.1983	552.3069	622.4828
642.2003	686.1313	734.9017
750.7184	803.5166	874.0225
912.1984	915.9539	926.0502
969.1861	997.9890	1028.1455
1065.4881	1069.9436	1106.0585
1109.6716	1256.7799	1267.3872
1310.3022	1391.8375	1448.3518
1462.5873	1801.3805	3113.5387
3127.2200	3133.6602	3188.3865
3191.7579	3208.8795	3219.3132

i12

C	-0.369661	1.096300	0.412905
C	-1.542631	0.944431	-0.225135
C	-1.799956	-0.483940	-0.451974
C	-0.784256	-1.206817	0.047780
H	0.099980	2.019808	0.720378
H	-2.210048	1.741916	-0.527104
H	-2.677883	-0.876615	-0.948655
H	-0.666530	-2.280819	0.029792
C	0.236421	-0.272960	0.672293
C	1.606418	-0.453885	0.145509

C	2.538063	0.192156	-0.507573
H	2.401210	1.222890	-0.845464
H	3.491814	-0.268590	-0.752452
H	0.255063	-0.450304	1.760673

Frequencies

91.5522	148.7416	217.7430
373.4238	479.0280	557.6015
576.6923	703.9765	727.9889
809.9634	829.3399	884.7719
887.5868	954.5827	958.0848
971.4573	999.4142	1016.7751
1038.6872	1108.7282	1124.6283
1194.1015	1235.2913	1302.6821
1390.1833	1411.5235	1552.1692
1641.1181	1736.7799	2965.7473
3042.2862	3142.8997	3188.6366
3201.1424	3224.9820	3230.0374

i13

C	-0.546740	1.186252	0.000010
C	-1.893218	0.754216	-0.000081
C	-1.966640	-0.615020	-0.000155
C	-0.579515	-1.200151	-0.000125
C	0.318458	0.043922	-0.000020
H	-2.745350	1.422480	-0.000075
H	-2.870133	-1.208810	-0.000221
H	-0.391665	-1.827771	0.878856
H	-0.205031	2.211318	0.000093
C	1.646553	0.029491	0.000012
C	2.947407	0.006872	0.000295
H	3.522744	-0.001609	0.925090
H	3.523187	-0.001399	-0.924223
H	-0.391583	-1.827700	-0.879137

Frequencies

124.8278	157.9506	253.9284
403.7759	508.0830	533.5046
563.1531	566.7737	647.0938
752.0397	818.6577	834.1043
883.3276	922.7655	946.3583

958.4502	1000.2671	1044.6981
1105.2837	1144.8355	1186.6851
1202.9347	1280.7181	1324.7900
1389.7428	1445.7641	1462.5394
1503.7569	1961.0357	3019.7680
3043.1992	3073.6658	3133.3519
3191.0447	3215.3858	3226.3092

barrier_i1_i2

C	-1.566033	-0.000458	0.736409
C	-0.986621	0.863255	-0.278803
C	0.345832	1.434366	-0.171598
C	1.444828	0.718541	0.174330
C	1.445504	-0.717370	0.174549
C	0.347223	-1.434220	-0.171537
C	-0.985630	-0.864070	-0.279212
H	-2.592793	-0.001186	1.077709
H	-1.683425	1.386897	-0.932660
H	0.446380	2.481318	-0.441410
H	2.395737	1.229233	0.282472
H	2.396804	-1.227250	0.283195
H	0.448775	-2.481347	-0.440925
H	-1.682090	-1.387930	-0.933214

Frequencies

-284.5590	252.8738	266.5679
465.4391	482.3495	623.0182
630.9998	666.0908	775.4884
784.2054	836.5485	912.3345
920.1354	953.6018	979.9653
984.8143	1033.3115	1042.7688
1072.2815	1132.6781	1201.6972
1219.7582	1225.2930	1340.5916
1406.4303	1409.6136	1471.6583
1569.4550	1663.9347	3090.2745
3093.4036	3146.2519	3150.2886
3165.3969	3178.6840	3188.2865

barrier_i1_i6

C	-1.651370	-0.195639	0.687159
C	-1.096632	0.639371	-0.421997

C	0.103269	1.437661	-0.117018
C	1.301668	0.880074	0.185145
C	1.548082	-0.544586	0.097418
C	0.544970	-1.403879	-0.200080
C	-0.790972	-0.862231	-0.335305
H	-1.448730	-0.195991	1.751146
H	-1.775675	1.041848	-1.170706
H	0.017110	2.517584	-0.186525
H	2.139421	1.528577	0.419133
H	2.562579	-0.908127	0.220716
H	0.725756	-2.459793	-0.364988
H	-1.97455	-1.228725	-0.040707

Frequencies

-1856.8299	230.9801	275.2637
409.5339	527.7428	535.2783
608.6179	662.0405	701.4120
772.1850	798.0311	872.8338
889.5346	932.9848	958.3221
970.1386	986.6763	1021.4419
1031.5940	1083.6141	1146.2489
1179.3304	1212.2658	1332.1943
1361.4913	1417.8840	1453.7777
1559.5236	1649.8028	2298.3139
3093.6643	3150.3399	3160.7917
3173.1007	3173.2998	3183.7835

barrier_i12_p1

C	-0.605568	1.183987	0.041600
C	-1.868359	0.732006	-0.125297
C	-1.868359	-0.732006	-0.125297
C	-0.605568	-1.183988	0.041600
C	0.282708	0.000000	0.148932
C	1.599753	0.000000	-0.057080
C	2.893352	0.000000	-0.148517
H	-0.256529	2.204468	0.078561
H	-2.751523	1.346345	-0.237599
H	-2.751523	-1.346344	-0.237599
H	-0.256529	-2.204468	0.078560
H	0.127348	-0.000003	2.028457

H	3.402323	0.000001	-1.108988
H	3.518671	0.000000	0.742962

Frequencies

-797.3367	140.3530	152.5308
237.9694	331.8147	466.3209
473.2341	546.0069	557.1840
619.3273	646.1758	728.1412
769.1671	819.0564	872.9213
891.0237	926.4612	941.8190
980.6550	1006.8890	1091.0023
1100.5197	1165.5868	1269.7004
1304.1733	1391.9378	1451.7867
1521.9528	1610.2852	1976.6126
3091.2034	3162.4720	3201.3213
3213.4345	3241.0544	3244.5560

barrier_i6_i8

C	-2.041705	-0.134418	0.402057
C	-0.739492	0.877356	-0.353852
C	0.536635	1.406863	0.074443
C	1.605501	0.536384	0.171561
C	1.469948	-0.858899	-0.012527
C	0.177049	-1.407588	-0.126114
C	-0.871375	-0.548201	-0.348729
H	-2.072137	-0.306141	1.471722
H	-2.973998	0.133612	-0.082833
H	-1.377989	1.496542	-0.978959
H	0.674640	2.472807	0.217459
H	2.588554	0.935640	0.401785
H	2.340419	-1.499078	0.064766
H	0.001154	-2.462363	0.065028

Frequencies

-557.9593	219.9567	363.7772
426.1282	556.1659	578.3177
624.2111	697.7042	711.9846
779.3665	801.0489	851.8868
886.2979	902.2318	960.2051
973.0759	991.5363	1020.9687
1075.8552	1140.5933	1146.9072

1182.4158	1277.7556	1351.7034
1421.0678	1445.1927	1460.2806
1523.2039	1632.1983	3104.8861
3112.2506	3145.5468	3153.6187
3172.7687	3187.5447	3214.3804

barrier_i8_i11

C	-1.781826	-0.038977	-0.455804
C	-1.125511	1.153846	-0.045572
C	0.189365	1.010327	0.467797
C	1.116980	-0.021998	-0.030154
C	0.187574	-0.930421	0.592484
C	-1.114410	-1.160635	-0.053380
H	-2.726014	-0.050183	-0.983752
H	-1.629864	2.113047	-0.008372
H	0.587903	1.738402	1.169091
H	0.481447	-1.490427	1.476571
H	-1.482777	-2.171326	-0.189388
C	2.360811	-0.026027	-0.490987
H	2.898974	-0.955664	-0.639552
H	2.872439	0.899465	-0.730902

Frequencies

-696.8130	161.7930	280.1104
381.0760	475.2237	533.4076
593.0058	683.9929	702.1829
726.0034	771.0044	804.2175
856.6736	878.7016	898.2592
927.1799	963.9508	1024.4252
1049.4714	1109.2373	1119.6569
1183.8931	1268.9537	1306.9216
1351.1605	1403.9026	1452.3678
1524.4827	1761.7754	3129.6375
3136.3048	3139.1679	3173.2673
3175.9376	3208.0213	3215.2058

barrier_i11_i12

C	-0.210688	0.354210	0.799274
C	0.305158	-1.045980	0.505819
C	1.444627	-0.945970	-0.273473
C	0.798864	1.226897	0.100739

C	1.732431	0.446323	-0.501651
C	-1.295723	-0.062263	-0.077858
C	-2.532245	0.005017	-0.498381
H	-2.952195	-0.713801	-1.198204
H	-3.200753	0.812753	-0.182887
H	-0.115906	-1.935816	0.947891
H	-0.469428	0.628900	1.828508
H	1.999021	-1.776204	-0.688321
H	0.728961	2.304852	0.069827
H	2.555748	0.809914	-1.103629

Frequencies

-513.5844	121.6815	191.4321
306.9169	392.6726	536.5098
586.5183	712.1896	739.2373
787.7434	819.7989	844.4425
884.6676	911.4560	938.1273
949.7571	987.9866	1010.7522
1040.0135	1100.1551	1107.7506
1161.5382	1239.6219	1296.5783
1376.2964	1410.1140	1428.2994
1555.3706	1757.5560	3009.5042
3022.3391	3129.2200	3192.6076
3212.8926	3225.4001	3240.2578

barrier_i12_i13

C	0.611684	1.176292	0.014265
C	1.907672	0.700384	0.011234
C	1.906799	-0.714624	-0.018501
C	0.587248	-1.160712	-0.042988
C	-0.298237	0.055491	-0.008011
H	2.795766	1.314561	0.080460
H	2.777555	-1.352543	0.026070
H	0.204418	-2.164094	-0.151639
H	0.292665	2.207029	0.049350
C	-1.674405	0.084679	-0.34820
C	-2.894562	-0.019727	0.109969
H	-3.764744	0.030098	-0.539929
H	-3.101887	-0.155129	1.176275
H	-0.080973	-0.610624	1.052804

Frequencies

-1262.2989	106.6028	151.6360
315.8889	370.8757	567.9320
581.6857	600.5276	673.6359
763.7095	769.1041	847.8651
885.9517	903.5298	907.5497
942.1267	1002.7160	1064.1229
1080.5251	1085.9528	1157.8012
1191.5849	1241.1704	1298.6617
1422.8126	1436.8360	1460.6524
1518.9579	1783.9979	1992.8764
3027.6604	3139.1991	3201.1941
3221.3666	3235.3611	3243.6240

barrier_i13_p1

C	0.575575	-1.215228	0.095338
C	1.858399	-0.784081	0.024532
C	1.872244	0.667117	-0.150213
C	0.594272	1.129833	-0.171667
C	-0.297850	-0.037519	-0.032047
C	-1.615749	-0.026879	-0.031769
C	-2.913434	-0.015465	-0.028321
H	0.218826	-2.225610	0.226189
H	2.742187	-1.404296	0.087763
H	2.765888	1.269097	-0.242385
H	0.534050	1.933656	2.082443
H	0.254394	2.140212	-0.336816
H	-3.473565	0.092271	0.896416
H	-3.482522	-0.111998	-0.948730

Frequencies

-129.3993	125.1883	152.5703
163.4245	180.5084	370.6859
484.1916	557.1886	564.8662
634.3425	648.2171	741.6444
775.6879	822.7660	871.0842
899.4285	920.1407	937.3232
991.1450	1009.4420	1090.4174
1099.8348	1178.6887	1284.6350
1310.0532	1391.7998	1459.8095
1503.9563	1590.3219	2026.6646

3112.0094	3183.8781	3203.4851
3215.9073	3239.2169	3246.2082

barrier_i2_i3

C	-0.172001	-1.218917	0.561613
C	1.134285	-1.133203	0.067590
C	1.569957	0.125088	-0.379277
C	-1.346149	-0.915894	-0.258972
C	0.809530	1.257094	-0.099597
C	-1.556967	0.406535	-0.303843
C	-0.508827	1.170924	0.454816
H	1.856538	-1.940309	0.172232
H	2.581697	0.239599	-0.755280
H	-1.875612	-1.672534	-0.825338
H	1.298228	2.226313	-0.146737
H	-2.321214	0.914298	-0.882471
H	-0.264018	0.006332	1.227243
H	-0.854583	2.076531	0.956375

Frequencies

-1383.9430	304.1942	316.5480
516.6499	544.3215	588.9176
629.1702	725.0178	756.9642
792.6994	811.8988	895.7717
917.9765	944.9047	980.2976
987.0851	1032.4570	1060.8847
1122.9273	1129.9891	1200.6712
1255.1371	1331.2159	1375.8302
1397.5889	1429.9316	1488.4178
1541.4926	1549.4665	1616.5623
3083.7904	3123.1469	3145.6472
3166.4615	3167.9237	3196.5639

barrier_i3_i5

C	-0.530150	-1.436282	-0.049058
C	0.708170	-1.144682	0.525558
C	1.565345	-0.250877	-0.330908
C	-1.516954	-0.557148	-0.405199
C	1.131916	1.010188	-0.343291
C	-1.350818	0.781206	-0.000750
C	-0.102112	1.259528	0.472522

H	1.201551	-1.907957	1.128014
H	2.397032	-0.639089	-0.906789
H	-2.468512	-0.896143	-0.800574
H	1.582071	1.815206	-0.914229
H	-2.237834	1.403486	0.092517
H	0.230136	0.033989	1.200113
H	-0.136822	2.218909	0.987704

Frequencies

-1590.1847	323.1887	343.312
494.3594	551.3795	574.1716
611.5257	719.9721	753.5774
767.7843	830.8577	898.7333
920.7766	944.2636	965.9436
987.6046	1032.9405	1039.3060
1086.2316	1135.6598	1188.6441
1280.1104	1322.2799	1366.3965
1379.4797	1420.2228	1468.2512
1515.4352	1559.1673	1656.8923
3094.7871	3105.0832	3137.7727
3164.6791	3167.4643	3195.7327

barrier_i5_i6

C	-0.105939	1.459683	-0.177873
C	1.109236	0.780911	-0.317553
C	0.783964	-1.080186	-0.347789
C	-0.560547	-1.406871	-0.289836
C	-1.522879	-0.505789	0.163150
C	-1.293436	0.875551	0.248202
H	-0.144698	2.483182	-0.541632
H	1.854787	1.175630	-0.999754
H	-0.872745	-2.389316	-0.634225
H	-2.533408	-0.869935	0.321279
H	-2.144132	1.518789	0.447501
C	1.583800	-0.317088	0.594694
H	1.213818	-0.292412	1.622722
H	2.661190	-0.463209	0.546141

Frequencies

-447.6620	247.8671	310.4377
449.2392	457.2042	604.9197

647.2583	719.0926	785.8037
851.0617	867.7416	896.2395
926.6834	949.4312	975.6621
1017.3389	1051.7706	1102.6691
1132.7268	1163.0752	1198.6493
1226.3533	1316.7269	1397.5347
1440.8200	1465.1638	1471.5870
1554.4562	1591.8866	3039.1017
3120.4582	3134.5029	3136.9885
3153.9249	3160.3694	3172.5146

barrier_i2_i5

C	0.149475	-1.661760	0.044966
C	-1.133181	-1.101651	0.162367
C	-1.579191	0.247199	-0.233872
C	-0.803466	1.357090	-0.091389
C	0.591706	1.431375	0.216285
C	1.545983	0.428127	0.045808
C	1.317744	-0.910729	-0.296464
H	-0.394691	-1.324843	1.216976
H	-1.932885	-1.770456	0.486579
H	-2.625555	0.363494	-0.499793
H	-1.298016	2.316956	-0.223326
H	0.969119	2.420971	0.452346
H	2.584427	0.741528	0.145562
H	2.163179	-1.485552	-0.664557

Frequencies

-1497.9796	187.9607	261.7017
380.5243	406.7920	495.2840
551.3553	676.7150	718.2277
767.3051	798.3329	824.7900
883.6886	917.1687	937.9454
958.3463	975.9405	982.6918
1155.5076	1174.1193	1217.0108
1235.2757	1336.9525	1381.4904
1419.4596	1448.8883	1475.0661
1505.7646	1596.5331	1994.2936
3083.4914	3110.3330	3127.9261
3137.9243	3154.9491	3166.3326

barrier_i2_i4

C	1.494066	-0.695881	-0.282032
C	0.351562	-0.959038	0.647358
C	-0.942463	-1.203674	-0.011584
C	-1.034076	1.146585	0.008971
C	0.320908	1.148361	0.418769
C	1.466437	0.625817	-0.402727
H	2.114736	-1.428873	-0.788657
H	0.589366	1.948507	1.113852
H	2.121019	1.271792	-0.984583
H	0.535247	-1.316517	1.660228
C	-1.621618	-0.085642	-0.399868
H	-1.667685	2.006182	0.210622
H	-1.314853	-2.209060	-0.192138
H	-2.586733	-0.131209	-0.892647

Frequencies

-759.0659	215.8127	301.5515
416.4838	480.7311	575.2833
635.0577	698.8546	732.3430
753.0404	818.7736	849.2076
909.9048	940.2161	951.9300
979.5065	989.6466	1041.6440
1058.9048	1107.0322	1132.4546
1178.1873	1271.2579	1334.0357
1364.9784	1389.4235	1438.1108
1533.6160	1673.1178	3060.2788
3104.5077	3121.3699	3135.8494
3141.4367	3162.7430	3177.6926

barrier_i4_i7

C	1.692593	0.211117	-0.464781
C	0.851278	1.192509	-0.055605
C	-1.590076	0.595998	-0.133366
C	-1.782737	-0.629459	-0.579803
C	-0.003621	-0.918397	0.612623
C	1.200860	-1.080739	-0.042413
H	2.600057	0.360997	-1.036999
H	1.695201	-2.023608	-0.234886
H	-0.467968	-1.647368	1.261419
C	-0.314957	0.583271	0.684161

H	-0.421749	0.975453	1.704311
H	-2.497752	-1.133563	-1.220189
H	0.948332	2.250643	-0.257652
H	-2.176165	1.491644	-0.340903

Frequencies

-590.8358	218.7114	247.1242
371.2604	539.9510	649.2556
656.9066	717.7968	751.8945
809.0972	812.7487	840.6764
879.6439	890.9880	911.4156
955.4667	993.9906	1008.7842
1035.6058	1096.5359	1110.8054
1197.0401	1225.7827	1248.5299
1306.5367	1381.4154	1422.8411
1564.0856	1636.5804	3008.4217
3091.4261	3183.874	3185.4944
3201.5686	3214.3805	3221.1698

barrier_i7_p6

C	-0.649350	-1.589670	0.732635
C	-0.649350	-0.300441	1.172340
C	1.443663	1.011415	0.000000
C	1.763078	2.203975	0.000000
C	-0.649350	-0.300441	-1.172340
C	-0.649350	-1.589670	-0.732635
H	-0.655140	-2.478084	1.349987
H	-0.655140	-2.478084	-1.349987
H	-0.650481	0.043543	-2.196063
C	-0.598519	0.568544	0.000000
H	-0.962909	1.586130	0.000000
H	1.734459	3.268989	0.000000
H	-0.650481	0.043543	2.196063
H	1.774760	-0.008311	0.000000

Frequencies

-586.6115	72.7459	132.9124
215.1395	260.6963	502.0536
564.3170	577.0007	636.2861
723.4731	734.1197	758.2962
779.2250	839.7458	870.9308

913.9516	922.3356	945.0774
964.6925	990.5493	1045.9764
1092.9082	1137.7129	1276.9601
1299.2153	1392.2406	1492.8890
1564.1094	1814.9680	3196.7700
3205.6719	3213.1149	3229.4137
3236.9599	3314.1266	3436.8301

barrier_i7_i9

C	1.944435	0.512225	-0.124693
C	0.730947	1.179814	0.003917
C	-1.754836	0.472795	0.028225
C	-2.699318	-0.417977	-0.168992
C	0.360780	-1.115163	0.070063
C	1.733225	-0.877404	-0.079787
H	2.913656	0.989491	-0.185179
H	2.497208	-1.640873	-0.102236
H	-0.176316	-2.051378	0.042516
C	-0.309411	0.217087	0.132383
H	-0.036938	-0.466322	1.185960
H	0.581170	2.249765	0.032060
H	-3.773387	-0.435077	-0.267654
H	-2.040320	1.526134	0.127838

Frequencies

-1196.0183	110.1415	200.5535
279.2652	466.8306	593.4778
596.3785	611.2147	693.4291
760.7085	777.3377	824.3401
843.6822	857.9209	910.5927
924.6322	938.2286	1064.9651
1082.8437	1097.3676	1193.3108
1210.7892	1277.2679	1287.3843
1340.3975	1451.0096	1486.3515
1510.7543	1660.0711	2068.6330
3026.2470	3198.4892	3218.6184
3224.5764	3240.4941	3252.2177

barrier_i9_p2

C	-1.909995	-0.687129	0.000020
C	-1.924259	0.660564	0.000006

C	0.313041	0.118968	-0.000003
C	-0.488076	-1.168445	0.000015
H	-2.768521	-1.344634	0.000033
C	-0.554843	1.162448	-0.000008
H	-2.803579	1.291250	0.000006
H	-0.255747	-1.783493	-0.878116
H	-0.255735	-1.783476	0.878157
C	1.732013	0.119874	-0.000013
H	2.041349	2.066953	-0.000017
C	2.893914	-0.246839	-0.000019
H	3.944206	-0.409555	-0.000025
H	-0.272739	2.206312	-0.000021

Frequencies

-651.0268	89.9975	172.1235
217.7751	342.9555	491.2062
508.1872	528.2280	536.4342
560.7590	609.6337	671.9807
696.2685	825.2655	889.3854
905.7743	918.6421	961.2634
964.6433	1020.9730	1122.5912
1131.4526	1172.5331	1256.8217
1292.7178	1382.8925	1414.2465
1548.6063	1635.9862	2099.0167
3026.4702	3052.9552	3196.6574
3214.4335	3223.6217	3464.7133

barrier_i9_i10

C	1.919357	0.324041	-0.233883
C	0.802862	1.227277	0.004127
C	-1.722309	0.607758	0.132164
C	-2.243183	-0.502290	-0.389068
C	0.120859	-0.975596	0.322900
C	1.516451	-0.978771	-0.098756
H	2.924669	0.647530	-0.475667
C	-0.283037	0.471555	0.319142
H	0.816595	2.291475	-0.190260
H	-3.220432	-0.793020	-0.751845
H	-2.278665	1.517739	0.343209
H	-0.112314	-1.557434	1.217464
H	2.158981	-1.847582	-0.130902

H	-0.954838	-1.302552	-0.351748

Frequencies

-1863.9869	200.0244	285.7871
374.5430	540.4999	591.0774
625.8020	641.1309	695.2323
734.7297	822.4285	843.7374
870.1880	898.6670	906.0871
923.7628	929.1313	1011.1226
1021.7055	1115.0739	1168.4198
1203.7924	1256.4812	1282.8695
1309.9131	1387.2453	1462.9482
1555.3284	1591.4843	1656.6639
3089.3436	3136.8683	3185.5326
3206.5197	3210.8522	3218.6650

barrier_i10_p1

C	-0.629859	-1.180687	-0.012594
C	-1.907487	-0.734734	-0.028049
C	-1.907487	0.734735	-0.028046
C	-0.629859	1.180688	-0.012589
C	0.248852	0.000000	-0.011703
H	-2.797125	-1.349718	-0.042814
H	-2.797125	1.349719	-0.042809
H	-0.278179	2.201062	-0.005963
H	-0.278179	-2.201062	-0.005972
C	1.577274	0.000001	0.019119
H	1.627919	-0.000035	2.169665
C	2.863393	0.000004	-0.178382
H	3.579905	0.000003	0.634494
H	3.253821	-0.000004	-1.193137

Frequencies

-543.5573	92.0809	138.9935
169.9146	382.6761	413.4565
495.2170	557.5805	572.5812
635.5251	652.4564	729.1217
774.0904	814.5457	883.4438
900.3329	921.8976	934.9507
990.3431	1000.1631	1089.7142
1101.4566	1172.0186	1276.3393

1306.2717	1389.7755	1460.1370
1519.2773	1599.3426	1980.6075
3116.9776	3200.5075	3201.4106
3213.2916	3238.7254	3242.4495

barrier_i10_i12

C	-1.963789	-0.591926	-0.156425
C	-1.800407	0.854011	-0.061818
C	-0.487004	1.152435	0.119736
C	0.250719	-0.123997	0.160468
C	-0.752183	-1.190865	-0.019200
H	-2.609653	1.569818	-0.118855
H	-0.028298	2.122933	0.233498
H	-2.908178	-1.097866	-0.303006
C	1.667793	-0.306994	0.170594
C	2.842667	0.118697	-0.239281
H	3.765404	-0.111035	0.283907
H	2.934261	0.685660	-1.169382
H	0.820735	-0.392247	1.269264
H	-0.521049	-2.245444	-0.039868

Frequencies

-1763.7885	130.1318	142.0333
281.5906	389.3783	518.8634
574.9209	603.0663	648.7037
703.9742	758.9183	816.2964
881.7611	889.5643	891.9616
901.5808	923.6897	1008.6021
1014.5579	1086.1202	1096.8853
1170.6208	1229.9775	1301.4920
1395.1006	1438.3748	1496.1717
1581.9196	1735.9964	2109.4168
3046.6713	3164.2233	3199.4584
3212.4247	3234.277	3238.4465

barrier_i6_p7

C	0	-2.103253	-0.117639	0.184961
C	0	-0.808933	0.635742	-0.038660
C	0	0.319699	1.431470	0.116039
C	0	1.529661	0.723155	0.063208

C	0	1.571621	-0.677112	-0.027859
C	0	0.401248	-1.459946	-0.047590
C	0	-0.758873	-0.719209	-0.070938
H	0	-2.528591	-0.175476	1.187196
H	0	-2.848675	-0.105975	-0.607679
H	0	-1.278747	1.315268	-1.918277
H	0	0.298974	2.509670	0.225850
H	0	2.465546	1.269101	0.113154
H	0	2.538528	-1.168310	-0.046381
H	0	0.445943	-2.543047	-0.028833

Frequencies

-489.9030	185.5070	244.2409
355.0152	389.3524	427.0285
475.1835	584.4838	663.3541
714.2162	749.9503	877.2371
893.3849	932.4820	990.9122
1003.7010	1011.4214	1016.5238
1025.1610	1090.9435	1112.4074
1130.1320	1176.6987	1297.6384
1374.5570	1458.1602	1480.7537
1493.0430	1590.2442	1712.1565
3055.7750	3129.5009	3159.6717
3169.0540		

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