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Supporting Information

Unconventional Pathway in the Gas-Phase Synthesis of 9H-Fluorene (C$_{13}$H$_{10}$) via the Radical–Radical Reaction of Benzyl (C$_7$H$_7$) with Phenyl (C$_6$H$_5$)

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Experimental & Computational - Experimental

The experiments were studied at the Chemical Dynamics Beamline (9.0.2.) of the Advanced Light Source (ALS) using a high-temperature chemical reactor consisting of a resistively heated silicon carbide (SiC) tube of 20 mm heating length and 1 mm inner diameter.[1] This device is located inside the source chamber of a molecular beam setup, which is equipped with a Wiley-McLaren reflectron time-of-flight mass spectrometer (Re-TOF-MS).[2] The molecular beam apparatus is designed to study the elementary chemical reactions and ultimately leading to PAH growth in situ via the reactions of aromatic radicals. In detail, phenyl radicals (C_6H_5) were prepared in situ by pyrolysis of the nitrosobenzene precursor (C_6H_5NO; ≥ 97 %; Sigma-Aldrich),[3] whereas a continuous beam of benzyl radicals (C_7H_7) was generated in situ through the pyrolysis of benzylbromide (C_7H_7Br; Sigma Aldrich, 98%).[4] The reactants were seeded in helium carrier gas at total pressures of 200 ± 10 torr at the reactor inlet. The temperature of the SiC tube was determined using a Type-C thermocouple to be 1423 ± 10 K. At this temperature, each precursor dissociates to the corresponding radical in situ followed by the reaction of phenyl (C_6H_5) and benzyl (C_7H_7) radicals. The products formed in the reactor passed through a 2 mm skimmer located 10 mm downstream the reactor and entered the main chamber, which houses the ReTOF-MS. The neutral products within the supersonic molecular beam were then photoionized in the extraction region of the mass spectrometer by utilizing quasi-continuous tunable synchrotron vacuum ultraviolet (VUV) light. VUV single photon ionization represents essentially a fragment-free ionization technique and is admitted as a soft ionization method compared to the harsher conditions of electron impact ionization with latter normally leading to excessive fragmentation of the parent ion.[5] The ions formed via soft photoionization were extracted and ultimately detected by a microchannel plate detector through an ion lens. Under our experimental condition, the residence time in the reactor tube is few tens to hundreds of microseconds.[6] Photoionization efficiency (PIE) curves, which report ion counts as a function of photon energy with a step interval of 0.05 eV at a well-defined mass-to-charge ratio (m/z), were produced by integrating the signal recorded at the specific m/z for the species of interest. Control experiments were also proceeded by expanding neat helium carrier gas with each precursor separately into the resistively-heated silicon carbide tube, but neither 9Hfluorene nor biphenylmethane was detected. Finally, reference PIE curves of helium-seeded diphenylmethane ($C_{13}H_{12}$, Sigma Aldrich, 99%) and 9*H*-fluorene ($C_{13}H_{10}$, Sigma Aldrich, 98%) were recorded in the present work within the same experimental setup, respectively.

Experimental & Computational - Computational

Electronic structure calculations

Geometries of the reactants, products, intermediates, and transition states participating in the reaction of phenyl and benzyl radicals accessing the $C_{13}H_{12}$ and $C_{13}H_{11}$ potential energy surfaces were optimized using the hybrid density functional B3LYP method[7] with the 6-311G(d,p) basis set and vibrational frequencies were computed using the same level of theory. Energies of reactants, products, and various $C_{13}H_x$ (x = 10-12) species were improved via single-point calculations within the composite G3(MP2,CC) model chemistry scheme.[8] Within this scheme, the final energy is obtained as

$$E_0[G3(MP2,CC)] = E[CCSD(T)/6\text{-}311^{**}] + \Delta E_{MP2} + E(ZPE),$$

where ΔE_{MP2} = E[MP2/G3Large] – E[MP2/6-311G**] is the basis set correction and E(ZPE) is the zero-point vibrational energy. Relative energies computed within this scheme are normally accurate within ~4-8 kJ mol^{-1}. The Gaussian 16[9] and MOLPRO 2021[10] program packages were used for the electronic structure calculations.
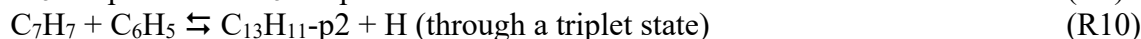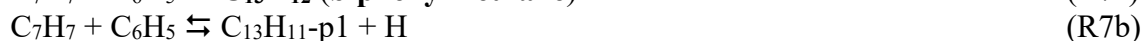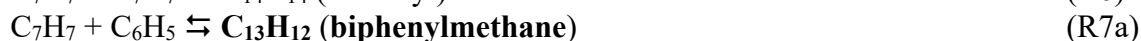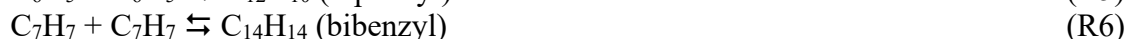
Calculations of temperature- and pressure-dependent rate constants

Temperature- and pressure-dependent rate constants for the C_7H_7 + C_6H_5 reaction and for isomerization and unimolecular decomposition of its $C_{13}H_{11}$ primary radical products were computed within the Rice-Ramsperger-Kassel-Marcus Master Equation (RRKM-ME) theoretical approach solving the one-dimensional master equation using the MESS program package.[11] Densities of states for local minima and numbers of states for transition states and partition functions were assessed within the Rigid-Rotor, Harmonic-Oscillator (RRHO) approximation. Asymmetric Eckart potentials were used to compute tunneling corrections for the rate constants. Collision parameters for RRKM-ME calculations were adopted from our previous studies of the kinetics of the 1- and 2-naphthyl + C_3H_4 reactions[12] and the prototype C_7H_7 + C_2H_2 reaction.[13] In particular, the Lennard-Jones parameters were taken as (ε/cm^{-1}, σ/Å) = (390, 4.46) and the $\alpha(T)$ = $\alpha_{300}(T/300$ K$)^n$ expression with n = 0.62 and α_{300} = 424 cm^{-1} was used for the temperature dependence of the range parameter α for the deactivating wing of the energy transfer function. For the barrierless entrance and exit reaction channels including the initial recombination of benzyl and phenyl radicals and various H losses from $C_{13}H_{12}$ isomers in the singlet electronic state, phase space theory[14] was employed to assess E,J-resolved rate constants of their reverse bimolecular association reactions at the high-pressure limit (HP). Potential power exponents and prefactors in

the phase space theory calculations were fit to match the HP rate constants to those of the closest analogous prototype reactions. For instance, for $C_7H_7 + C_6H_5$ the phase-space rate constants both for phenyl addition to the CH_2 group and to the *ortho* carbon in the ring were matched to one half of the rate constant for the C_3H_5 (allyl) + phenyl reaction computed in our earlier publication[15] using the variable reaction coordinate transition state theory (VRC-TST) method. It was assumed initially that phenyl additions to both CH_2 and *ortho* sites in benzyl occur with identical rate constants. Then, the ratio of these rate constants was used to fit the computed 9*H*-fluorene/diphenylmethane branching ratio to the experimental value (*vide infra*). For the $C_{13}H_{11}$ **p1** $+ H \rightarrow C_{13}H_{12}$ **i1**, $C_{13}H_{11}$ **p3** $+ H \rightarrow C_{13}H_{12}$ **i1**, and biphenylylmethyl $+ H \rightarrow C_{13}H_{12}$ **i3** hydrogen addition reactions, the HP rate constants were fitted to those for i-$C_3H_7 + H$, $C_6H_5 + H$, and $C_5H_5 + H$, respectively, evaluated in the works of Klippenstein and co-workers[16] using state-of-the-art VRC-TST calculations, taking into account the difference in the reaction path degeneracy for the latter. The pressure- and temperature-dependent rate constants for various reaction channels pertinent to the computational fluid dynamics (CFD)/kinetics simulations were fit to a modified Arrhenius expression or a sum of two modified Arrhenius expressions presented in Table S2.

CFD and kinetics simulations of processes in the micro reactor

Modeling of the gas flow and kinetics of the phenyl – benzyl system was carried out employing the COMSOL Multiphysics package[17] using the formalism and physical parameters described in detail in previous publications.[3, 6b] A gas mixture of He (p_{inlet} = 200 Torr), C_6H_5NO (p = 1 Torr), and C_7H_7Br (p = 1.6 Torr) was introduced at the room temperature upstream of the choke orifice. The maximum temperature is 1,373 K at the SiC microreactor surface. We implied the following kinetic mechanism:

$$C_6H_5NO \rightleftarrows C_6H_5 + NO \qquad \text{(R1)}$$
$$C_7H_7Br \rightleftarrows C_7H_7 + Br \qquad \text{(R2)}$$
$$C_6H_5 + Br \rightleftarrows C_6H_5Br \qquad \text{(R3)}$$
$$C_7H_7 + NO \rightleftarrows C_7H_7NO \qquad \text{(R4)}$$
$$C_6H_5 + C_6H_5 \rightarrow C_{12}H_{10} \text{ (biphenyl)} \qquad \text{(R5)}$$
$$C_7H_7 + C_7H_7 \rightleftarrows C_{14}H_{14} \text{ (bibenzyl)} \qquad \text{(R6)}$$
$$C_7H_7 + C_6H_5 \rightleftarrows \textbf{C}_{13}\textbf{H}_{12} \textbf{ (biphenylmethane)} \qquad \text{(R7a)}$$
$$C_7H_7 + C_6H_5 \rightleftarrows C_{13}H_{11}\text{-p1} + H \qquad \text{(R7b)}$$
$$C_7H_7 + C_6H_5 \rightleftarrows C_{13}H_{11}\text{-p3} + H \qquad \text{(R7c)}$$
$$C_{13}H_{12} \rightleftarrows C_{13}H_{11}\text{-p1} + H \qquad \text{(R8a)}$$
$$C_{13}H_{12} \rightleftarrows C_{13}H_{11}\text{-p3} + H \qquad \text{(R8b)}$$
$$C_{13}H_{11}\text{-p1} + H \rightleftarrows C_{13}H_{11}\text{-p3} + H \qquad \text{(R9)}$$
$$C_7H_7 + C_6H_5 \rightleftarrows C_{13}H_{11}\text{-p2} + H \text{ (through a triplet state)} \qquad \text{(R10)}$$

$$C_{13}H_{12} + H \leftrightarrows C_{13}H_{11}\text{-p1} + H_2 \qquad \text{(R11a)}$$
$$C_{13}H_{12} + H \leftrightarrows C_{13}H_{11}\text{-p3} + H_2 \qquad \text{(R11b)}$$
$$C_{13}H_{11}\text{-p1} \leftrightarrows C_{13}H_{11}\text{-p3} \qquad \text{(R12a)}$$
$$C_{13}H_{11}\text{-p1} \rightarrow \mathbf{C_{13}H_{10}}\ (\textbf{9-fluorene},\ \text{p4}) + H \qquad \text{(R12b)}$$
$$C_{13}H_{11}\text{-p2} \rightarrow \mathbf{C_{13}H_{10}}\ (\textbf{9-fluorene},\ \text{p4}) + H \qquad \text{(R13)}$$
$$C_{13}H_{11}\text{-p3} \leftrightarrows \mathbf{C_{13}H_{10}}\ (\textbf{9-fluorene},\ \text{p4}) + H \qquad \text{(R14a)}$$
$$C_{13}H_{11}\text{-p3} \leftrightarrows C_{13}H_{10}\ (\text{p9}) + H \qquad \text{(R14b)}$$
$$C_7H_7 + C_6H_5 \leftrightarrows C_{13}H_{12}\ (\text{i2}) \qquad \text{(R15a)}$$
$$C_7H_7 + C_6H_5 \leftrightarrows C_{13}H_{11}\text{-bpm} + H \qquad \text{(R15b)}$$
$$C_{13}H_{12}\ (\text{i2}) \leftrightarrows C_{13}H_{11}\text{-bpm} + H \qquad \text{(R16)}$$
$$C_{13}H_{11}\text{-bpm} \leftrightarrows \mathbf{C_{13}H_{10}}\ (\textbf{9-fluorene},\ \text{p4}) + H \qquad \text{(R17)}$$
$$C_{13}H_{12}\ (\text{i2}) + H \leftrightarrows C_{13}H_{11}\text{-bpm} + H_2 \qquad \text{(R18)}$$
$$C_{13}H_{10}\ (\text{p9}) + H \rightarrow \mathbf{C_{13}H_{10}}\ (\textbf{9-fluorene},\ \text{p4}) + H \qquad \text{(R19)}$$

Rate constants taken from the literature are shown in Table S1 and those computed in the present work are assembled in Table S2. The rate constants for the primary $C_7H_7 + C_6H_5$ reaction are illustrated in Figure S5.

Supplementary Information Discussion of PIE Curves Figure S1 and S2

The experimental PIE curve of m/z = 154 (Figure S1(a)) can be nicely replicated with the reference curve of the biphenyl (C_6H_5-C_6H_5), whereas the PIE curves at m/z = 154 (Figure S1(a)) and m/z = 155 (Figure S1(b)) depict identical pattern (Figure S1(c)). Hence, signal at m/z = 154 and 155 can be attributed to biphenyl (C_6H_5-C_6H_5) and ^{13}C-biphenyl formed via self-reaction of phenyl radicals. The experimental PIE curves of m/z = 156 (Figure S1(d)) and m/z = 158 (Figure S1(e)) are superimposable (Figure S1(f)) suggesting that signal at m/z = 156 (Figure S1(d)), and 158 (Figure S2(e)) originates from the same species. Considering one of the reactants bromobenzene, ions at m/z = 156 (Figure S1(d)) and 158 (Figure S1(e)) are associated with bromobenzene ($C_6H_5{}^{79}Br^+$/$C_6H_5{}^{81}Br^+$). The ions at m/z = 152 (Figure S1(g)) is presumed to be biphenylene ($C_{12}H_8$) via the recombination of phenyl radicals followed by loss of two hydrogen atoms. The fragmentation by atomic hydrogen loss of 9H-fluorene ($C_{13}H_{10}$, m/z = 166) (Figure 2(a)) yields the dibenzocyclopentadienyl ($C_{13}H_9$, m/z = 165), which is linked with the experimental signals observed at m/z = 165 (Figure S2(a)). The signal detected at m/z = 167 (Figure S2(b)) could originate from two successive atomic hydrogen losses products (**p1** - **p3**), which are predicted via the computational study in the reaction of the benzyl radical ($C_7H_7\bullet$) with the phenyl radical ($C_6H_5\bullet$). Although the reference PIEs of dibenzocyclopentadienyl ($C_{13}H_9$, m/z = 165) and $C_{13}H_{11}$ isomers (**p1** - **p3**, m/z = 167) are not available, the adiabatic ionization energies of accessible isomers of $C_{13}H_9$ and $C_{13}H_{11}$ isomers are calculated to be 6.96 eV (dibenzocyclopentadienyl, $C_{13}H_9$), 7.79 eV (**p1**, $C_{13}H_{11}$), 6.48 eV (**p2**, $C_{13}H_{11}$), and 6.53 eV (**p3**, $C_{13}H_{11}$), respectively, with uncertainties of ± 0.05 eV (Figure S2). The experimental PIE curve of m/z = 168 (Figure 2(b)) and m/z = 169 (Figure S2(c)) are similar (Figure S2(d)), therefore, ions at m/z = 169 are associated with ^{13}C-diphenylmethane ($^{13}CC_{12}H_{12}{}^+$). Further, ion counts are also observable at m/z = 170 (Figure S2(e)) in the benzyl-phenyl system. The recombination of two benzyl radicals,[4] which leads to phenanthrene and anthracene (m/z = 178), are not detected under the current experimental conditions.
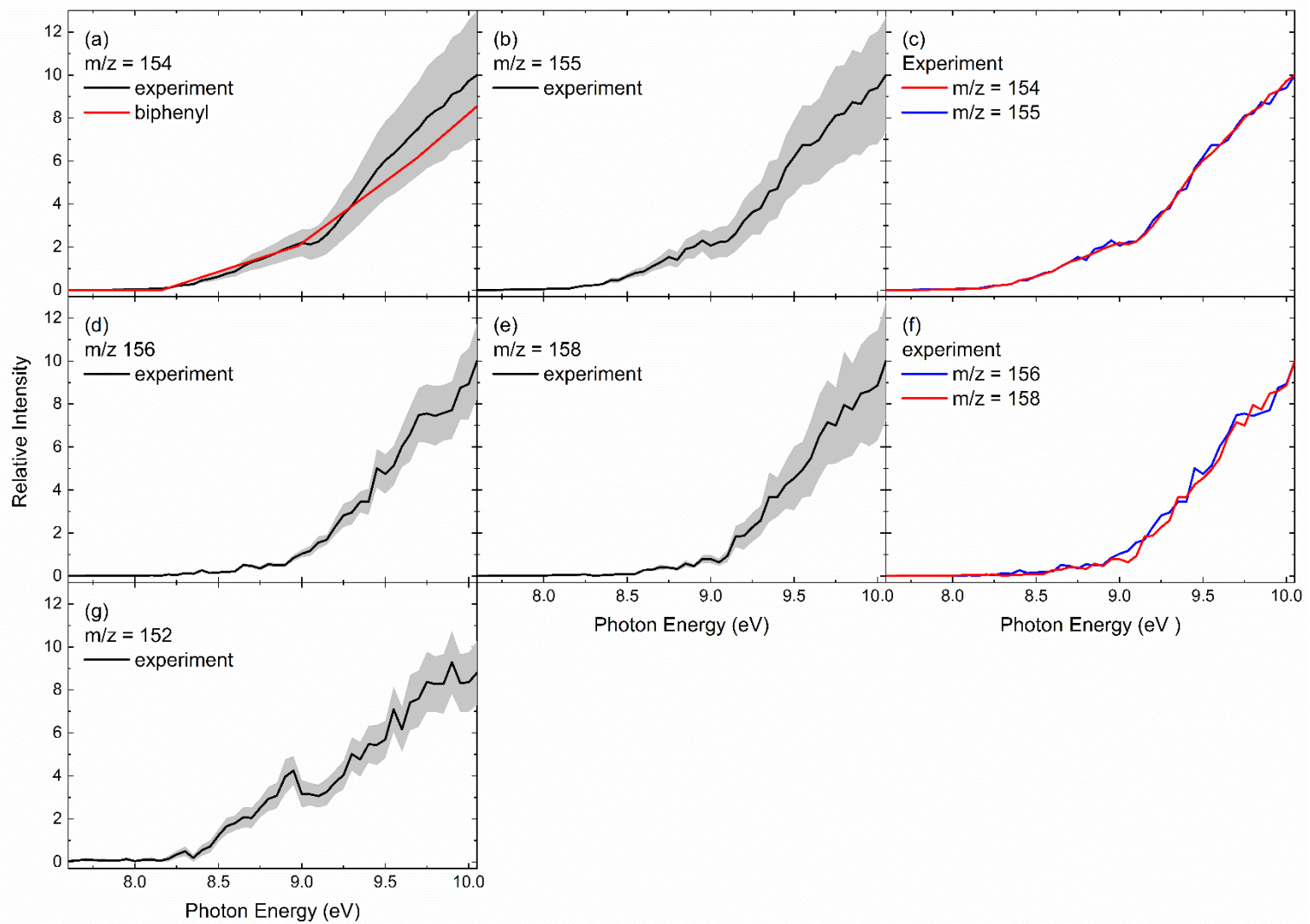
Figure S1. PIE curves ((a)-(g)) and the PIE curves overlap ((c), (f)) for additional species (m/z = 152, 154, 155, 156, 158) in the benzyl $(C_7H_7\bullet)$ + phenyl $(C_6H_5\bullet)$ system.
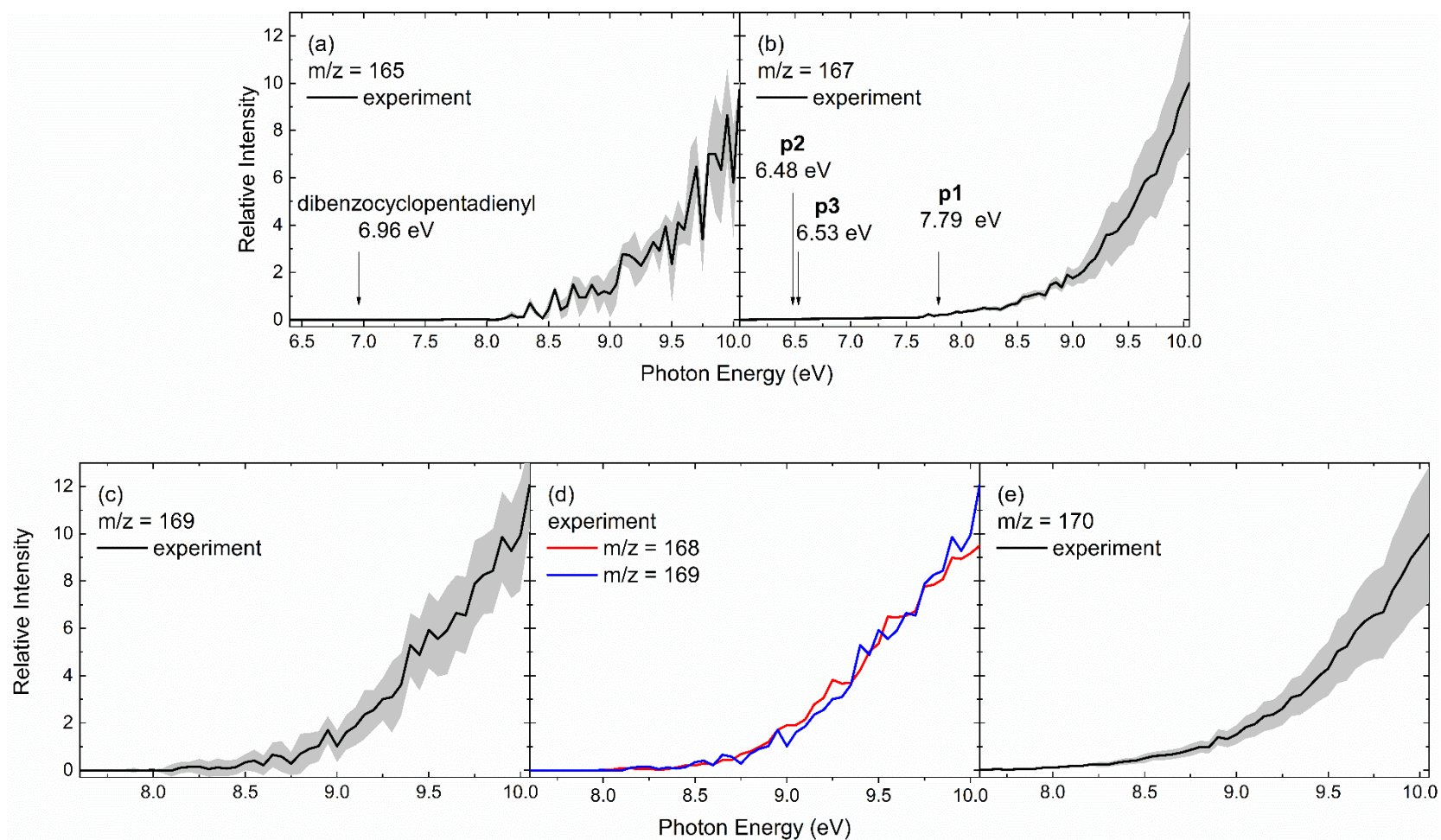
Figure S2. PIE curves ((a)-(e)) and the PIE curves overlap (d) for additional species (m/z = 165, 167, 169, 170) in the benzyl ($C_7H_7\bullet$) + phenyl ($C_6H_5\bullet$) system. The calculated ionization energies for m/z = 165 (a) and 167 (b) species are also included.
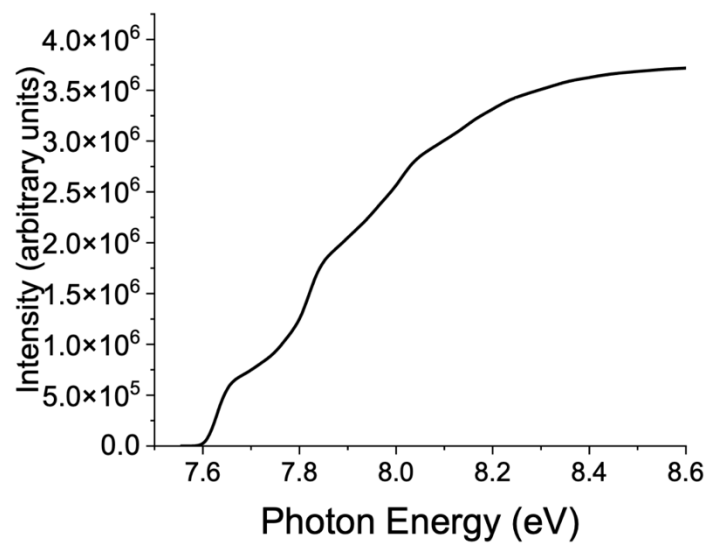
Figure S3. Calculated PIE curve for the $C_{13}H_{12}$ isomer **i3** (only the ground electronic state of the ion is included).
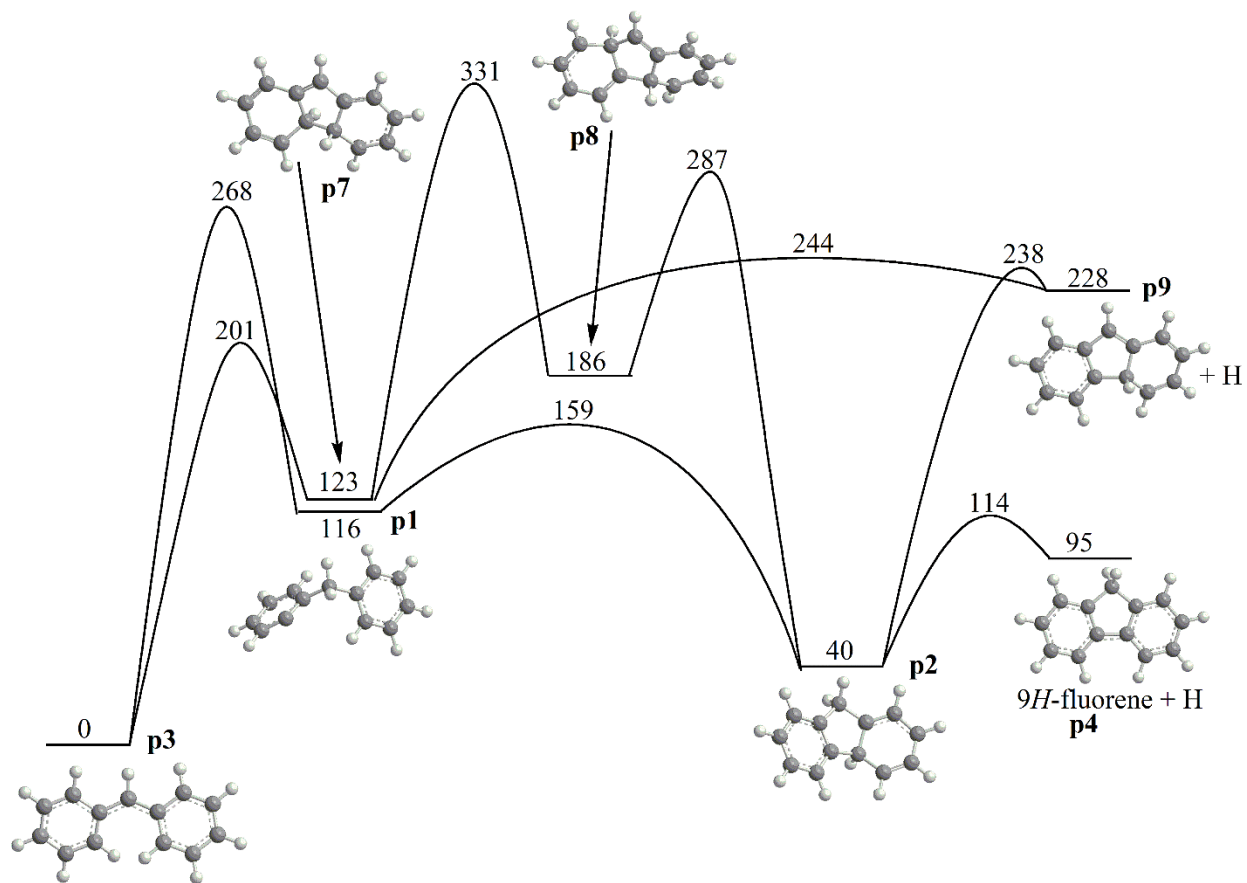
Figure S4. Calculated potential energy diagram for rearrangements and decomposition of $C_{13}H_{11}$ isomers.
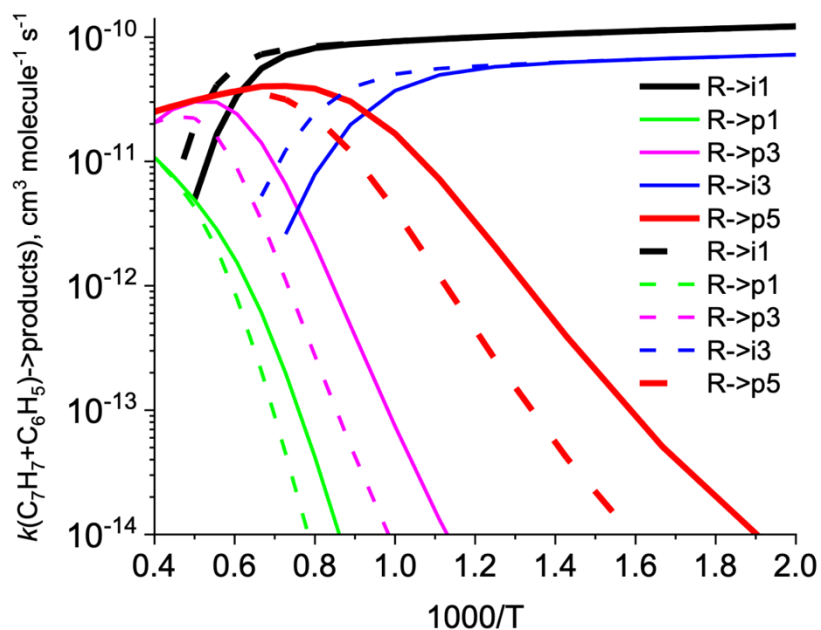
Figure S5. Rate constants for various channels of the $C_7H_7 + C_5H_5$ reaction calculated at the pressures of 0.01 atm (solid lines) and 0.1 atm (dashed lines). The total rate constants for the entrance channel for CH_2 and *ortho* additions of benzyl to phenyl at high pressure limit (HP) were first evaluated using phase-space theory, where each of them was matched to one half of the rate constant for the C_3H_5 (allyl) + phenyl reaction. Then, the total rate constant for CH_2 addition was increased by 30% and that for *ortho* addition was reduced by 30% and the rate constants for individual channels were scaled accordingly.
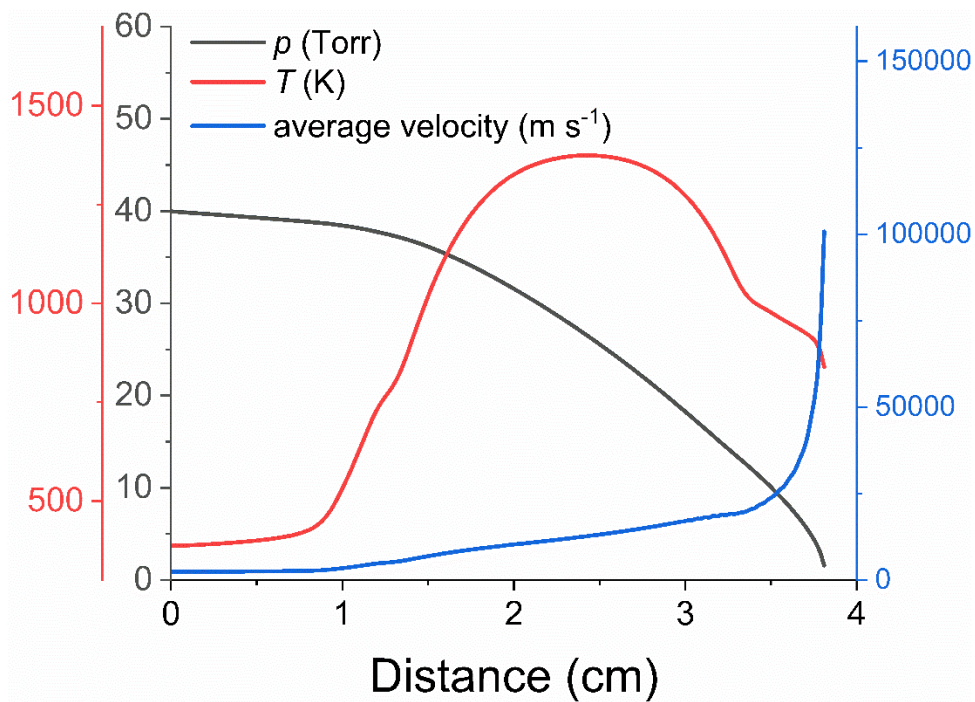
Figure S6. Pressure, temperature, and average axial gas velocity inside the reactor as functions of the distance from the beginning of the micro reactor.

Table S1. Rate constants from the literature.

	Reaction	Rate constant, cm^6 mol^{-2} s^{-1}, cm^3 mol^{-1} s^{-1}, or s^{-1}	1,373 K cm^6 s^{-1}, cm^3 s^{-1}, s^{-1}
k_1[18]	$C_6H_5NO \rightarrow C_6H_5 + NO$	$1.52e17 \times exp(-55200/1.987/T)$	$2.5 \cdot 10^8$
k_{1r}[19]	$C_6H_5 + NO \rightarrow C_6H_5NO$	$1.03e-11 \times exp(1940/8.31/T) \times 6e23$	$8.7 \cdot 10^{-12}$
k_2[20]	$C_7H_7Br \rightarrow C_7H_7 + Br$	1.0×10^{13} [s^{-1}] $e^{-211188 [\pm 8481 \, J/mole]/RT}$ or 7.33×10^{13} [s^{-1}] $e^{-217839 [J/mole]/RT}$	$9.2 \cdot 10^4$ $3.4 \cdot 10^5$
k_{2r}[21]	$C_7H_7 + Br \rightarrow C_7H_7Br$	$(-6.26+0.3949*exp(4542.1/T))*1e-14*p/(1+0.01*p*(-1.453+0.697*exp(2188.62/T)))*6e23$	
k_3[22]	$C_6H_5 + Br \leftrightarrows C_6H_5Br$	$7.0 \cdot 10^{-11}$, T-dependence is assumed to be weak	
k_{3r}[23]	$C_6H_5Br \rightarrow C_6H_5 + Br$	1.50×10^{13} [s^{-1}] $e^{-301000 [J/mole]/RT}$	$5.3 \cdot 10^1$
k_4	$C_7H_7 + NO \rightarrow C_7H_7NO$	taken to be the same as k_{1r}	
k_{4r}	$C_7H_7NO \rightarrow C_7H_7 + NO$	taken to be the same as k_1	
k_5[24]	$C_6H_5 + C_6H_5 \rightarrow C_{12}H_{10}$ The reverse reaction is too slow and is neglected	0.01 atm: $1.66 \cdot 10^{64}$ $T^{-14.68}$ $e^{16740/T}$ 0.1 atm: $6.14 \cdot 10^{37}$ $T^{-7.140}$ $e^{7903/T}$ 1 atm: $7.34 \cdot 10^{20}$ $T^{-2.335}$ $e^{2076/T}$	$1.2 \cdot 10^{-11}$ $1.3 \cdot 10^{-11}$ $1.3 \cdot 10^{-11}$
k_6[25]	$C_7H_7 + C_7H_7 \rightarrow C_{14}H_{14}$	10 Torr: $8.56 \cdot 10^{70}$ $T^{-17.708}$ $e^{-23686.4/1.987/T}$	$6.6 \cdot 10^{-13}$
k_{6r}[25]	$C_{14}H_{14} \rightarrow C_7H_7 + C_7H_7$	10 Torr: $8.86 \cdot 10^{154}$ $T^{-40.625}$ $e^{-143586.3/1.987/T}$	$4.2 \cdot 10^4$

Table S2. Rate constants for the formation of the main observed products. Parameters of fitted modified Arrhenius expressions $k = A\,T^n \exp(-E_a/RT)$ or $k = A_1\,T^{n1} \exp(-E_a^1/RT) + A_2\,T^{n2} \exp(-E_a^2/RT)$ for the considered reactions. Pre-exponential factors A are in cm^3 mol^{-1} s^{-1} for bimolecular reactions and in s^{-1} for unimolecular reactions, E_a are in cal mol^{-1}.

Reaction	p	A_1	n_1	E_a^1	A_2	n_2	E_a^2	T range, K
k_{7a}, $C_7H_7 + C_6H_5$ $\rightarrow C_{13}H_{12}$	0.01 atm	1.71E+117	-29.391	72611	3.29E+41	-8.6251	10367	500-2000
	0.1 atm	1.15E+109	-26.742	73229	4.83E+36	-7.0975	8760.9	500-2250
	1 atm	1.89E+94	-22.353	67400	5.14E+31	-5.5526	6920.6	500-2500
k_{7ar}, $C_{13}H_{12} \rightarrow$ $C_7H_7 + C_6H_5$	0.01 atm	9.06E+122	-30.204	173940	4.48E+51	-10.658	115450	500-2000
	0.1 atm	1.86E+112	-26.882	172000	5.62E+46	-9.1101	113810	500-2250
	1 atm	1.69E+97	-22.451	165280	8.86E+41	-7.6165	112040	500-2500
k_{7b}, $C_7H_7 + C_6H_5$ $\rightarrow C_{13}H_{11}\text{-p1} + H$	0.01 atm	1.72E+05	2.7923	28569	8.58E+78	-17.345	85463	500-2500
	0.1 atm	2.74E-01	4.4231	27750	1.32E+77	-16.579	92881	500-2500
	1 atm	2.32E-12	7.6141	24453	4.92E+63	-12.662	91131	500-2500
k_{7br}, $C_{13}H_{11}\text{-p1} + H$ $\rightarrow C_7H_7 + C_6H_5$	0.01 atm	3.63E+12	0.81156	22627	1.58E+86	-19.315	79413	500-2500
	0.1 atm	6.71E+06	2.4214	21830	1.53E+84	-18.493	86675	500-2500
	1 atm	5.73E-05	5.6115	18536	5.22E+70	-14.565	84890	500-2500
k_{7c}, $C_7H_7 + C_6H_5$ $\rightarrow C_{13}H_{11}\text{-p3} + H$	0.01 atm	1.67E+12	0.49668	17941	7.48E+89	-20.574	80804	500-2500
	0.1 atm	5.51E+02	3.2284	15472	1.30E+84	-18.748	85079	500-2500
	1 atm	1.27E-09	6.5575	11703	8.95E+65	-13.578	78755	500-2500
k_{7cr}, $C_{13}H_{11}\text{-p3} + H$ $\rightarrow C_7H_7 + C_6H_5$	0.01 atm	6.21E+21	-1.5543	39971	1.09E+99	-22.515	102480	500-2500
	0.1 atm	2.20E+12	1.1683	37513	1.70E+93	-20.677	106730	500-2500
	1 atm	4.91E+00	4.5018	33739	1.41E+75	-15.528	100480	500-2500
k_{8a}, $C_{13}H_{12} \rightarrow$ $C_{13}H_{11}\text{-p1} + H$	0.01 atm	2.85E+50	-10.393	124180	3.69E+130	-32.383	188560	500-2000
	0.1 atm	2.69E+119	-28.841	187670	1.17E+44	-8.3717	122080	500-2250
	1 atm	6.24E+103	-24.158	181990	7.97E+37	-6.4488	119850	500-2500
k_{8ar}, $C_{13}H_{11}\text{-p1} + H$ $\rightarrow C_{13}H_{12}$	0.01 atm	7.87E+47	-10.419	13252	6.06E+130	-33.174	80046	500-2000
	0.1 atm	1.05E+122	-30.271	81513	3.24E+41	-8.397	11159	500-2250
	1 atm	4.00E+106	-25.622	76616	1.31E+35	-6.4067	8827.6	500-2500
	0.01 atm	5.40E+07	2.0995	80623	-1.07E+35	-5.0942	113390	500-2000
	0.1 atm	2.26E+93	-21.971	1.46E+05	1.11E+32	-5.3525	90375	500-2250

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k_{8b}, $C_{13}H_{12} \rightarrow$ $C_{13}H_{11}$-p3 + H	1 atm	2.06E+79	-17.877	138570	3.99E+28	-4.2818	89105	500-2500
k_{8br}, $C_{13}H_{11}$-p3 + H $\rightarrow C_{13}H_{12}$	0.01 atm	2.50E+07	2.0064	-2361.3	-5.82E+28	-3.5841	24539	500-2000
	0.1 atm	2.04E+101	-24.319	70394	3.48E+31	-5.3873	7360.1	500-2250
	1 atm	2.08E+87	-20.205	64206	7.14E+27	-4.2427	5989.8	500-2500
k_9, $C_{13}H_{11}$-p1 + H $\rightarrow C_{13}H_{11}$-p3 + H	0.01 atm	6.78E+12	0.50426	16510	1.83E+88	-20.073	75683	500-2500
	0.1 atm	6.68E+05	2.4902	15113	5.92E+84	-18.848	81902	500-2500
	1 atm	2.28E-06	5.7895	11568	1.98E+70	-14.652	79269	500-2500
k_{9r}, $C_{13}H_{11}$-p3 + H $\rightarrow C_{13}H_{11}$-p1 + H	0.01 atm	1.06E+15	0.4509	44466	2.10E+90	-20.09	103530	500-2500
	0.1 atm	1.06E+08	2.4351	43068	6.92E+86	-18.867	109770	500-2500
	1 atm	3.52E-04	5.7374	39519	2.95E+72	-14.699	107240	500-2500
k_{10}, C_7H_7 + C_6H_5 $\rightarrow C_{13}H_{11}$-p2 + H	0.01 atm	4.20E+36	-7.4178	20664	4.29E+15	-1.1163	14550	500-2500
	0.1 atm	6.98E+55	-13.023	31821	2.49E+20	-2.4337	17458	500-2500
	1 atm	1.00E+55	-12.429	36099	5.38E+54	-11.381	62871	500-2500
k_{10r}, $C_{13}H_{11}$-p2 + H $\rightarrow C_7H_7$ + C_6H_5	0.01 atm	5.93E+46	-9.4876	33730	3.07E+25	-3.107	27507	500-2500
	0.1 atm	1.06E+66	-15.102	44900	2.21E+30	-4.4528	30378	500-2500
	1 atm	1.70E+65	-14.525	49185	3.14E+68	-14.411	80176	500-2500
k_{11a}, $C_{13}H_{12}$ + H $\rightarrow$ $C_{13}H_{11}$-p1 + H_2	independent	1.48E+08	1.9026	15151				500-2500
k_{11ar}, $C_{13}H_{11}$-p1 + $H_2 \rightarrow C_{13}H_{12}$ + H	independent	3.88E+03	2.629	4813.9				500-2500
k_{11b}, $C_{13}H_{12}$ + H $\rightarrow$ $C_{13}H_{11}$-p3 + H_2	independent	2.11E+07	1.9536	4724.2				500-2500
k_{11br}, $C_{13}H_{11}$-p3 + $H_2 \rightarrow C_{13}H_{12}$ + H	independent	7.71E+04	2.6396	22302				500-2500
k_{12a}, $C_{13}H_{11}$-p1 $\rightarrow$ $C_{13}H_{11}$-p3	independent	7.84E+09	0.65868	35216	2.06E+02	2.2591	26528	500-2500
k_{12ar}, $C_{13}H_{11}$-p3 $\rightarrow$ $C_{13}H_{11}$-p1	independent	5.17E+11	0.70795	62854	1.42E+04	2.2908	54220	500-2500
k_{12b}, $C_{13}H_{11}$-p1 $\rightarrow$ $C_{13}H_{10}$ + H	independent	1.53E+11	-0.10166	10472				500-2500

k_{13}, $C_{13}H_{11}$-p2 → $C_{13}H_{10}$ + H	independent	6.60E+10	0.80805	17680				500-2500
k_{14af}, $C_{13}H_{11}$-p3 → $C_{13}H_{10}$ (**p4**) + H	0.01 atm	6.01E+91	-22.465	111340	5.01E+29	-5.2161	66106	500-1650
	0.1 atm	5.50E-08	6.3908	53440	-1.183E+17	-0.14561	78770	500-1800
	1 atm	2.04E+64	-14.078	102140	3.96E+35	-6.6392	72560	500-2000
k_{14ar}, $C_{13}H_{10}$ (**p4**) + H → $C_{13}H_{11}$-p3	0.01 atm	3.58E+36	-6.5457	50405				500-1650
	0.1 atm	2.50E-84	26.573	-31505	8.19E+46	-9.2725	60088	500-1800
	1 atm	3.88E+29	-4.2143	50385				500-2000
k_{14bf}, $C_{13}H_{11}$-p3 → $C_{13}H_{10}$ (**p9**) + H	0.01 atm	2.27E+30	-5.1431	66919				500-1650
	0.1 atm	5.51E+85	-20.524	110930	4.87E+31	-5.6612	66768	500-1800
	1 atm	9.58E+85	-20.189	119340	9.65E+33	-6.1534	69782	500-2000
k_{14br}, $C_{13}H_{10}$ (**p9**) + H → $C_{13}H_{11}$-p3	0.01 atm	8.47E+100	-25.153	61324	4.89E+36	-7.3147	13158	500-1650
	0.1 atm	3.24E+95	-23.251	63949	1.08E+30	-5.1521	11475	500-1800
	1 atm	5.02E+90	-21.46	69220	8.44E+32	-5.8394	14639	500-2000
k_{15a}, C_7H_7 + C_6H_5 → $C_{13}H_{12}$ (i2)	0.01 atm	3.89E+132	-35.183	62477	1.57E+63	-15.598	16825	500-1375
	0.1 atm	-1.81E+86	-21.953	30043	1.49E+67	-16.119	21866	500-1500
	1 atm	1.77E+08	1.6283	-2562.9	-1.81E+39	-6.7282	28944	500-1800
k_{15ar}, $C_{13}H_{12}$ (i2) → C_7H_7 + C_6H_5	0.01 atm	1.12E+133	-34.583	1.32E+05	2.55E+77	-19.116	93191	500-1375
	0.1 atm	-7.13E+68	-16.112	89457	6.57E+57	-12.682	85246	500-1500
	1 atm	3.99E+23	-2.1838	74627	-2.85E+75	-16.179	1.27E+05	500-1800
k_{15b}, C_7H_7 + C_6H_5 → $C_{13}H_{11}$-mbp + H	0.01 atm	6.19E+103	-25.596	64222	4.43E+35	-5.9749	23527	500-2500
	0.1 atm	1.28E+73	-16.388	52206	3.84E+131	-30.771	1.59E+05	500-2500
	1 atm	5.89E+62	-13.241	51690				500-2500
k_{15br}, $C_{13}H_{11}$-mbp + H → C_7H_7 + C_6H_5	0.01 atm	5.15E+112	-27.672	83076	1.35E+44	-7.9298	42100	500-2500
	0.1 atm	2.40E+82	-18.568	71260	2.47E+137	-32.032	1.74E+05	500-2500
	1 atm	4.60E+71	-15.311	70503				500-2500
k_{16}, $C_{13}H_{12}$ (i2) → $C_{13}H_{11}$-mbp + H	0.01 atm	2.21E+116	-29.779	1.13E+05	7.83E+48	-10.723	68064	500-1375
	0.1 atm	5.80E+101	-25.195	1.09E+05	1.66E+39	-7.6518	64904	500-1500
	1 atm	1.39E+07	2.3475	53211	-9.89E+35	-5.3873	83769	500-1800
k_{16r}, $C_{13}H_{11}$-mbp + H → $C_{13}H_{12}$ (i2)	0.01 atm	6.69E+114	-29.563	56363	1.14E+53	-12.257	13892	500-1375
	0.1 atm	3.43E+108	-27.346	58228	1.58E+39	-7.8594	9351.3	500-1500
	1 atm	8.72E+06	2.1822	-2503.2	-1.67E+33	-4.8365	26052	500-1800

k_{17}, $C_{13}H_{11}$-mbp $\rightarrow$ $C_{13}H_{10}$ + H	0.03 atm	5.43E+57	-13.74	48326				500-1250
	1 atm	1.01E+57	-13.015	54320	1.32E+73	-16.502	91770	500-1650
k_{17r}, $C_{13}H_{10}$ + H $\rightarrow$ $C_{13}H_{11}$-mbp	0.03 atm	9.05E+55	-12.74	27480				500-1250
	1 atm	6.85E+55	-12.203	33714	7.35E+72	-16.006	70170	500-1650
k_{18}, $C_{13}H_{12}$ (i2) + H $\leftrightarrows$ $C_{13}H_{11}$-mbp+H_2	independent	the same as k_{11b} in both directions						500-2500
k_{19}, $C_{13}H_{10}$(**p9**)+H $\rightarrow$ $C_{13}H_{10}$(**p4**)+H	independent	1.92E+69	-15.04	63863	2.98E+08	1.5828	1651.7	500-2500

Table S3. Coordinates and vibrational frequencies for all species that involved in benzyl + phenyl system.

i0

C	1.4076997065	-0.1034984391	1.3711285266
C	2.5212537047	-0.9281913936	1.4974720515
C	3.4756737849	-0.9771635121	0.4816833888
C	3.3072539068	-0.1946749332	-0.6571324882
C	2.1919678358	0.6334021905	-0.7777220379
C	1.2303051975	0.6916718855	0.2336325467
C	-1.3936747329	0.0151549813	-1.4084276955
C	-2.2964715349	-1.1585328899	-1.3794475599
C	-3.3487825699	-1.1180469944	-0.5271098057
C	-3.4480922982	-0.0662264169	0.4519747897
C	-2.3414172978	0.8120141953	0.6788129853
C	-1.2581339321	0.8054419619	-0.1481617204
C	0.0038936725	1.5836722229	0.1048978247
H	0.6637616975	-0.0765126860	2.1608412645
H	2.6455096722	-1.5335479054	2.3887012826
H	4.3432770746	-1.6200685605	0.5790341656
H	4.0438364448	-0.2259630183	-1.4525121416
H	2.0693916503	1.2448377636	-1.6659780964
H	-1.3943738233	0.6039115681	-2.3334146345
H	-2.1432837301	-1.9887612886	-2.0607940559
H	-4.0892836868	-1.9122581490	-0.5220669031
H	-4.2961960652	-0.0414453766	1.1250853980
H	-2.3421228882	1.4374594229	1.5680814237
H	0.1698421168	2.2868306112	-0.7221837641
H	-0.1164859056	2.1840477606	1.0119902554

Frequencies:

12.5736	47.8804	51.9165
146.6525	208.1619	240.7301
300.6211	358.9983	412.1631
414.6236	423.4169	454.4620
529.9102	550.0569	591.4162
632.5932	637.9540	702.5287
713.4988	735.8042	756.1876
812.2327	827.8433	853.7334
878.7046	907.3289	925.7945
939.1383	956.8854	972.9119
975.5519	999.8057	1007.0589
1018.3018	1050.5634	1074.4990
1102.0881	1162.3833	1171.3170
1181.3240	1201.3294	1202.4912
1210.8679	1290.5982	1308.8257
1338.1809	1342.5363	1358.7365
1363.5651	1399.1737	1474.5695
1485.0258	1526.5064	1541.3469
1592.6650	1626.1775	1644.2849
2994.1634	3006.9341	3055.2024
3135.5461	3146.2570	3153.2739
3156.5776	3166.3852	3166.7341
3174.9541	3186.6176	3189.7445

i1

C	-0.6931514799	-2.5354950177	1.1492852794
C	0.5072590971	-3.2457550295	1.1307489997
C	1.7140557244	-2.5808504563	1.3246605319
C	1.7124556069	-1.2017913519	1.5349502872
C	0.5133078837	-0.4970745623	1.5504210641
C	-0.7081786812	-1.1547221864	1.3601202601
C	-1.9846214000	-0.5023319451	0.9750145036
C	-2.0978829176	1.5347512395	-1.9001978226
C	-2.3446040290	2.8389574724	-1.4707690641
C	-2.4767390853	3.0987725981	-0.1102721353
C	-2.3644093924	2.0600289792	0.8140283909
C	-2.1185763363	0.7498361234	0.3966806153
C	-2.0174088873	-0.3847695335	1.4020997775
H	-1.6306537697	-3.0621659894	1.0006190748
H	0.4964695277	-4.3174049368	0.9645908145
H	2.6489529993	-3.1297045786	1.3109077852
H	2.6484656125	-0.6751007408	1.6857059213
H	0.5222873646	0.5769073383	1.7047884320
H	-1.7831593193	-0.5074102140	-1.3172782603
H	-1.9927117940	1.3230838273	-2.9586676261
H	-2.4312919638	3.6437987480	-2.1920017310
H	-2.6669046838	4.1090067198	0.2353080499
H	-2.4719087305	2.2705673959	1.8735231794
H	-2.1626569111	0.0235973945	2.4078824209
H	-2.8422714350	-1.0861411843	1.2376122590

Frequencies:

192.5380	225.8199	288.8061
341.3179	414.7331	415.4312
461.5491	481.1643	566.0285
623.7253	635.6911	638.2424
713.7286	716.2708	751.7336
751.8686	831.8536	833.5191
856.0820	856.9500	903.5491
933.1894	947.2732	978.0195
978.3792	1001.0019	1001.0675
1017.8577	1018.5130	1050.8278
1051.5505	1097.3186	1107.0823
1180.9713	1181.2615	1197.5082
1202.8167	1203.7251	1210.5422
1220.9671	1302.3109	1341.1569
1345.1871	1362.2145	1366.0644
1478.4712	1482.2827	1491.0125
1526.8655	1528.4643	1623.9397
1628.2552	1643.5652	1648.9583
3021.7697	3054.1958	3152.0301
3152.0950	3157.3278	3157.6759
3167.1568	3167.3753	3175.1531
3175.3508	3186.6852	3186.9654

i2

C	-0.9876109047	-1.0369785524	-0.5113777401
C	0.3546168360	-1.5459142374	-0.9324578934
C	1.2882941309	-1.9111641908	-0.0064561777
C	1.0678774531	-1.7412583835	1.3848300988
C	-0.1040563414	-1.0863726493	1.8394523355
C	-1.0789511505	-0.7160169261	0.9624247982
C	-1.5425712579	0.2887644848	-1.1516820970
C	-1.9746253050	0.2834564290	-2.5838779454
C	-3.1815281840	0.8019056475	-2.9543399545
C	-4.1139411179	1.2823670307	-1.9988996866
C	-3.8447717907	1.1380228385	-0.6148069269
C	-2.6492856658	0.6442575942	-0.1861421787
C	-2.2660433650	0.1915988858	1.2070182714
H	-1.7465802661	-1.8075326361	-0.7561914719
H	0.5456389754	-1.6875647277	-1.9912552608
H	2.2335849586	-2.3295461242	-0.3378570255
H	1.8285852003	-2.0445818393	2.0934800169
H	-0.1940879982	-0.8315024654	2.8919334493
H	-0.7196949035	1.0232264153	-1.0370743378
H	-1.2772277508	-0.0760150517	-3.3335610767
H	-3.4474771404	0.8363394895	-4.0062571300
H	-5.0619593315	1.6905242330	-2.3268238137
H	-4.6247138951	1.3741466843	0.1040223518
H	-1.9940341328	1.0285852159	1.8641134368
H	-3.1011010530	-0.3263891648	1.6975489580

Frequencies:

58.1144	89.1220	187.9645
217.5578	221.5853	369.8029
376.2055	378.8243	458.4420
492.5039	503.9110	518.2635
587.7553	590.5182	616.5066
660.4993	671.3597	687.5000
759.4598	766.5598	782.5083
794.8508	869.0316	887.1256
926.7397	936.9702	959.7368
965.9953	969.1840	995.5961
999.7065	1012.4916	1040.5547
1060.0004	1116.6020	1118.3686
1141.6782	1150.7912	1168.3608
1170.7986	1197.2613	1200.0394
1233.4165	1247.1265	1296.9250
1297.6073	1337.0845	1343.9530
1388.2460	1403.5414	1430.3756
1431.6241	1458.4102	1537.7066
1543.1069	1604.3712	1611.6755
2854.1664	2862.9086	2986.1501
3003.7233	3143.2534	3143.4879
3148.0416	3149.4743	3166.0202
3168.1549	3190.0943	3190.3779

i3

C	-1.7930983918	-1.4638895517	1.3577136236
C	-1.0450202364	-2.5604181258	1.1279786114
C	-0.4542712432	-2.8075158034	-0.1824801406
C	-0.5759881623	-1.9181417715	-1.1754202042
C	-1.2905434767	-0.5935191855	-1.0083055208
C	-2.0561826751	-0.4725338248	0.3216260315
C	-0.2997551695	0.5584336526	-1.2021083578
C	0.8214436107	0.6836722783	-0.3736250877
C	1.7163076387	1.7345723847	-0.5458605900
C	1.5102397277	2.6758935447	-1.5545846745
C	0.4026078471	2.5567456345	-2.3883531342
C	-0.4947948063	1.5037183063	-2.2114808269
C	-2.9383757879	0.5190311432	0.5231959391
H	-2.2484134275	-1.3012995517	2.3295548522
H	-0.8861275902	-3.2881704345	1.9161121053
H	0.0897286018	-3.7326554626	-0.3408489302
H	-0.1263548269	-2.1021519594	-2.1456008673
H	-2.0228300721	-0.5099166915	-1.8192747241
H	0.9905916004	-0.0470707413	0.4094457675
H	2.5783703020	1.8194194805	0.1067478161
H	2.2094177620	3.4935826384	-1.6888630024
H	0.2345440470	3.2810104865	-3.1778873830
H	-1.3561313442	1.4164334047	-2.8662806335
H	-3.1574394348	1.2569959999	-0.2401135467
H	-3.4591654926	0.6210491495	1.4687508773

Frequencies

22.1633	38.2974	93.8748
146.3861	251.8784	264.9912
318.9551	392.2163	414.0003
454.5218	510.9821	514.0802
552.2864	599.6679	635.2364
677.1695	687.1937	714.5069
755.4239	772.1935	796.3823
825.8439	854.6916	864.1743
906.2112	924.1403	942.6002
965.2338	977.8129	981.8436
986.3615	997.2084	1000.2882
1018.1671	1049.9259	1051.5968
1102.0980	1179.6787	1181.3162
1198.8082	1203.9080	1206.6173
1243.2950	1307.6722	1310.9573
1340.9156	1363.4236	1389.9810
1426.1864	1465.8203	1484.2630
1524.2661	1614.9445	1625.8258
1641.5897	1654.2466	1702.8065
3016.6620	3134.1727	3151.0046
3152.1218	3156.2433	3160.3480
3169.9795	3171.7469	3178.6573
3182.1685	3187.4805	3216.9897

p1

C	-0.1907879155	-1.6923463249	0.7008642929
C	1.0468590267	-2.3270483183	0.6961722165
C	1.9083316335	-2.1946345711	1.7854346839
C	1.5200807237	-1.4237424273	2.8767214928
C	0.2772771116	-0.7902326502	2.8784358992
C	-0.5939098340	-0.9158146545	1.7938623297
C	-3.1267363177	0.6133791038	-0.2920172972
C	-3.3863346235	1.4690604919	-1.3366216802
C	-2.5801768795	2.6101227258	-1.4274183278
C	-1.5754876544	2.8234564489	-0.4820356465
C	-1.3640288683	1.9151551905	0.5517402609
C	-2.1581557282	0.7596540848	0.6752989976
C	-1.9543594761	-0.2396169074	1.8021847566
H	-0.8520786520	-1.7938812909	-0.1533856351
H	1.3413330709	-2.9262192225	-0.1584851392
H	2.8733973426	-2.6886743596	1.7810388575
H	2.1818704796	-1.3137715678	3.7288211548
H	-0.0204175256	-0.1946142425	3.7357363306
H	-4.1729781402	1.2790241423	-2.0584773016
H	-2.7385696538	3.3217656631	-2.2307391220
H	-0.9507431928	3.7066818507	-0.5528357355
H	-0.5721007764	2.0906661912	1.2739657347
H	-2.0928517865	0.2703826279	2.7607406284
H	-2.7403293641	-0.9973069838	1.7374322494

Frequencies:

10.2035	22.3326	62.1988
186.8317	225.2602	280.8754
336.6634	414.9156	416.7594
461.6204	485.0586	554.6195
614.9393	631.7603	637.6627
699.2521	716.1932	743.2661
751.2091	821.2313	830.5175
856.4369	857.0617	910.7754
938.6565	946.6597	978.8446
985.3125	991.1837	1001.6328
1018.1329	1043.4614	1051.2055
1098.4716	1120.8067	1170.1853
1181.2475	1187.3749	1203.2316
1206.8061	1217.9560	1273.4469
1315.1428	1330.0131	1342.9235
1363.1753	1448.1019	1477.4720
1481.7127	1488.4290	1527.6258
1574.8945	1625.5531	1634.8420
1646.6709	3032.2645	3069.6524
3150.3666	3152.3826	3157.8887
3159.3746	3167.5181	3172.2272
3175.5511	3184.1582	3187.0762

p2

C	-0.6919815228	-1.3415673097	0.9390533896
C	-0.1067171046	-2.0977773324	-0.1084101519
C	0.3589853058	-1.4441227525	-1.2788982955
C	0.3789653912	-0.0841874778	-1.3837196390
C	0.0344047417	0.7739786919	-0.2018619637
C	-0.6818330972	0.0191208290	0.8992808579
C	-0.8518001312	2.0053881106	-0.3689535916
C	-0.8769325757	2.9449103202	-1.3921344283
C	-1.7573869583	4.0250315086	-1.2997614705
C	-2.5921323062	4.1635799494	-0.1911606661
C	-2.5608461375	3.2221624996	0.8396542383
C	-1.6917408167	2.1413925952	0.7441566312
C	-1.4838371817	0.9975166039	1.7234290897
H	-1.2131128641	-1.8590877049	1.7395581000
H	-0.1065033590	-3.1796749425	-0.0591524243
H	0.6806341957	-2.0488424616	-2.1208912727
H	0.7235830473	0.3964148371	-2.2929601567
H	0.9981954889	1.1498974518	0.2100111798
H	-0.2293955634	2.8442594947	-2.2567568814
H	-1.7937763133	4.7597877072	-2.0964220076
H	-3.2734818182	5.0050397941	-0.1319494169
H	-3.2153036713	3.3320100324	1.6984136517
H	-0.9220074855	1.3472363834	2.6035030199
H	-2.4196432640	0.5697071724	2.0947252080

Frequencies:

66.6269	113.7563	189.8079
234.5266	261.4251	375.1644
414.6820	436.0679	460.1399
499.6617	523.1885	531.6440
599.3132	618.9702	659.6740
694.7568	726.5271	747.0838
760.5556	788.0786	828.6653
838.4535	881.4565	899.1028
936.5936	952.9719	962.8894
977.9175	989.3212	1001.3748
1036.8506	1047.8001	1103.2091
1119.4176	1152.2939	1155.5853
1175.5692	1180.7926	1196.1051
1218.8555	1220.5050	1239.9407
1278.0366	1314.3951	1343.6776
1345.7142	1387.6792	1428.7824
1468.0085	1491.1299	1505.4258
1539.1877	1609.4647	1626.9112
1647.9654	2802.3109	2964.8057
3053.8233	3146.0840	3151.8653
3154.8483	3160.8244	3170.8411
3172.5600	3184.8348	3190.3150

p3

C	1.4966457158	-0.9769913584	-0.1755634679
C	2.6898177011	-1.6345483856	0.0863941856
C	2.9246837744	-2.2198631069	1.3319563768
C	1.9327012210	-2.1573368375	2.3141259782
C	0.7361385965	-1.5091363350	2.0578072233
C	0.4838597443	-0.8767072029	0.8122201071
C	-2.6005553705	0.9334442672	-0.5332343601
C	-3.0873140145	1.8367059552	-1.4632288585
C	-2.2056265814	2.5734689858	-2.2584273584
C	-0.8301758988	2.3988979150	-2.0944509164
C	-0.3348599811	1.4905829590	-1.1702335097
C	-1.2081376661	0.7115753135	-0.3688938413
C	-0.7824579894	-0.2337525604	0.6205540418
H	1.3219255126	-0.5785837676	-1.1654751064
H	3.4411272758	-1.7045018967	-0.6927117962
H	3.8604594262	-2.7295458544	1.5298856228
H	2.0969738192	-2.6201208319	3.2810333751
H	-0.0281221803	-1.4662946059	2.8268300320
H	-3.2932731172	0.3663307675	0.0798419418
H	-4.1577744269	1.9730881771	-1.5708130181
H	-2.5848928865	3.2830608264	-2.9845482379
H	-0.1374779430	2.9885256356	-2.6851189001
H	0.7343991918	1.4143206762	-1.0285372080
H	-1.5453759231	-0.5084447353	1.3441976946

Frequencies:

55.3968	60.4718	110.9993
204.7807	238.4590	298.2518
315.8440	411.6149	423.2506
486.1829	494.7039	578.4475
627.1626	629.9209	652.4739
694.5899	703.6792	718.7562
762.8016	798.9911	817.4151
840.5655	848.6304	890.0081
914.9801	921.3018	976.8319
981.2413	994.5749	997.8103
1002.3211	1007.6202	1044.7449
1046.7926	1098.8498	1119.0803
1179.1891	1179.9598	1190.1323
1203.0503	1227.6398	1232.7808
1328.0179	1332.3600	1349.3459
1362.8018	1429.2975	1477.6360
1496.9845	1506.8138	1515.1288
1589.4045	1591.2519	1608.8934
1621.1403	3138.5446	3157.5924
3158.3079	3164.9213	3165.7276
3174.8597	3175.3571	3188.6030
3189.4749	3201.8861	3215.4241

p4

C	-0.7775947216	-2.4173702899	1.1301353032
C	0.4170543452	-3.1415135829	1.1248697995
C	1.6471512249	-2.4802987206	1.1157827503
C	1.7055894041	-1.0876168843	1.1117304512
C	0.5142702267	-0.3623063018	1.1169244363
C	-0.7251562446	-1.0304050176	1.1260861048
C	0.2659806896	1.0855043795	1.1147119057
C	1.1475639291	2.1662867280	1.1067185891
C	0.6284421886	3.4599261119	1.1065818136
C	-0.7516835858	3.6735313330	1.1143226475
C	-1.6367940250	2.5927392088	1.1223233178
C	-1.1252320973	1.3024911977	1.1224701680
C	-1.8563715793	-0.0236384455	1.1300186469
H	-1.7298865504	-2.9376950689	1.1372164169
H	0.3890612051	-4.2253163921	1.1279338187
H	2.5657412349	-3.0563338087	1.1118283315
H	2.6649912730	-0.5819506690	1.1046417118
H	2.2206316168	2.0091528683	1.1006566606
H	1.3026200919	4.3090933465	1.1004174355
H	-1.1391894710	4.6860820207	1.1141405957
H	-2.7080426649	2.7660607507	1.1283129360
H	-2.4967088442	-0.1321017582	2.0129519147
H	-2.5061326457	-0.1364060057	0.2544902447

Frequencies:

98.2467	136.7022	217.1353
242.4857	276.0305	419.8121
422.9541	437.4612	480.8763
498.8090	553.8100	576.4900
637.0948	645.1440	711.9175
741.2211	754.4592	756.1213
796.3664	813.9210	853.6331
870.8892	879.7876	930.6185
947.8700	972.8917	987.8059
989.8239	1024.6443	1046.1974
1052.2321	1117.4362	1131.0016
1162.4770	1176.1837	1180.1610
1192.1603	1207.3507	1220.5716
1252.7136	1320.1064	1329.5667
1344.5348	1374.7729	1451.2744
1478.6003	1484.8995	1509.4957
1510.8005	1619.7891	1624.1355
1649.0451	1650.1625	3022.6596
3047.4008	3157.5484	3157.9697
3163.6104	3165.3388	3174.7206
3176.0473	3187.4146	3188.1643

p5

C	-0.7875471217	-2.7883036300	0.1441505492
C	0.4052961276	-3.5036701848	0.0553675844
C	1.6102356122	-2.8157279991	-0.0667058994
C	1.6220137064	-1.4236937067	-0.0996977234
C	0.4296975857	-0.6906216111	-0.0165172969
C	-0.7762529114	-1.3969834143	0.1064222885
C	0.4601785521	0.7966921726	-0.0076818813
C	1.2442619795	1.4476739774	0.9428102578
C	1.2941448379	2.8396358305	1.0321059470
C	0.5381799699	3.6166000866	0.1465086027
C	-0.2371420112	3.0035405620	-0.8159674459
C	-0.2973042194	1.5830515766	-0.9468755321
C	-1.0394087256	1.0202973365	-1.9966467686
H	-1.7299102212	-3.3144976264	0.2497914227
H	0.3952932654	-4.5874282737	0.0826031593
H	2.5436985619	-3.3627728608	-0.1404059108
H	2.5621582496	-0.8941237485	-0.2067251242
H	-1.7068996355	-0.8480391061	0.1918742965
H	1.8082397191	0.8482788835	1.6490649808
H	1.9051843064	3.3120381205	1.7923536947
H	0.5636567535	4.6985826758	0.2137192323
H	-0.8105237115	3.6048166145	-1.5135599336
H	-1.5885338136	1.6615315198	-2.6749788253
H	-1.0600478561	-0.0436181949	-2.1815076742

Frequencies

56.6221	85.4892	104.3971
190.0667	272.1221	293.2701
335.5607	414.8131	417.5865
462.0995	496.2387	529.9331
564.6945	572.7694	628.1409
635.2121	716.9757	722.2853
729.2603	747.2491	774.9307
787.7997	851.2822	861.3337
869.4567	935.2312	955.3219
974.5398	981.1994	983.7465
1002.1584	1009.9229	1018.5056
1054.8197	1063.8429	1101.4682
1147.2280	1177.4468	1182.0509
1204.3945	1256.3570	1280.3224
1303.2919	1320.5277	1323.7417
1354.3146	1447.5337	1477.8982
1484.1055	1496.2888	1526.8738
1560.5677	1601.9080	1615.7417
1642.0681	3154.4815	3159.7412
3159.8953	3166.3412	3167.5917
3176.2300	3177.1826	3183.0145
3190.0562	3190.7040	3257.6793

p6

C	-0.8187065052	-2.7827992050	0.1441126131
C	0.3523570990	-3.4760750695	0.1578250989
C	1.6145624937	-2.8236118385	0.0237330514
C	1.6783318523	-1.4520731106	-0.2706972243
C	0.5228248249	-0.7040042811	-0.3144966289
C	-0.8045360692	-1.2852628344	0.1313151489
C	0.2672881512	0.6205127438	-0.8399266887
C	1.1453709752	1.6673091073	-1.1518037735
C	0.6284733154	2.8563348275	-1.6549803005
C	-0.7473801673	3.0088254300	-1.8548043892
C	-1.6273540202	1.9645974889	-1.5571191163
C	-1.1218515040	0.7753924328	-1.0514436788
C	-1.8551568745	-0.5062340036	-0.7099399964
H	-1.7702923652	-3.2969343595	0.2338439448
H	0.3350470468	-4.5577568765	0.2451514989
H	2.5233473307	-3.4127389041	0.0498215806
H	2.6307656777	-1.0072007169	-0.5421832150
H	-0.9558979431	-0.9491166847	1.1782787118
H	2.2122397892	1.5601110708	-0.9892419319
H	1.2974599988	3.6770641326	-1.8890206126
H	-1.1331552045	3.9445065049	-2.2435898332
H	-2.6927363123	2.0861375569	-1.7241022394
H	-2.7930425312	-0.3391001788	-0.1748909094
H	-2.0902080583	-1.0622812323	-1.6261301104

Frequencies

90.0302	102.2500	210.3053
215.9929	263.9787	384.2902
406.5866	448.9328	451.7731
511.6512	524.7107	545.6824
613.5385	618.6836	662.0667
691.7940	728.5141	740.4811
767.6424	782.1282	813.0965
854.6472	874.7150	914.7186
941.9527	967.5705	979.5278
986.1119	994.4567	1003.0528
1044.4735	1054.6634	1072.0606
1114.6339	1125.1750	1160.2152
1177.6420	1181.5146	1196.5057
1223.7562	1247.5675	1275.2178
1309.8899	1326.0491	1327.5636
1353.7965	1392.5447	1425.2538
1478.4549	1491.1549	1494.3911
1536.0986	1594.7974	1608.3764
1635.4039	2842.3241	3011.3698
3075.3245	3150.2543	3154.9774
3157.7109	3164.5896	3169.0037
3175.7802	3187.3314	3189.0093

p7

C	0.9108803453	-0.0527333809	-0.0922011622
C	2.3568613473	0.2936374731	0.0967016195
C	3.1063928653	-0.4112467953	0.9732936265
C	2.5246819782	-1.4045292969	1.8463417101
C	1.1599793987	-1.5652052645	1.9296606851
C	0.3195481867	-0.8084658935	1.0890346347
C	-2.6683844090	0.8900053953	-0.1893372177
C	-2.7567144751	1.6741862674	-1.3173322634
C	-1.5860345064	1.9779164839	-2.1076217641
C	-0.3430488418	1.6380621583	-1.6995404095
C	-0.1410479886	1.0636309505	-0.3299560488
C	-1.4052683988	0.4460290740	0.2500171453
C	-1.0525073539	-0.5583893475	1.1533241925
H	0.8454501570	-0.7275549699	-0.9698376155
H	2.8078431317	1.0477360226	-0.5407160129
H	4.1712704317	-0.2183970490	1.0536218839
H	3.1768310346	-1.9608087531	2.5098062453
H	0.7284047923	-2.2025207952	2.6952085842
H	-3.5680748394	0.5419456506	0.3085682149
H	-3.7268093659	1.9952890801	-1.6789157298
H	-1.7269056597	2.4691090983	-3.0649555456
H	0.5243251524	1.8595314109	-2.3135166663
H	0.1433384515	1.9005530407	0.3398301087
H	-1.7451914340	-1.0708935601	1.8108607850

Frequencies

94.6693	99.6577	201.5188
224.3897	250.1899	378.5865
408.8870	455.7836	463.5482
492.8489	510.5679	546.3381
589.5090	616.8035	668.3481
672.8656	702.1430	706.7866
790.0879	792.1346	811.5573
845.5630	879.6903	902.6986
940.1247	942.6580	945.7001
978.0654	979.4533	981.8387
983.0875	1043.4743	1060.9648
1078.2554	1116.9129	1155.9294
1164.1815	1174.6000	1183.8457
1206.8089	1234.6435	1269.6268
1288.0786	1304.3991	1339.6499
1352.0296	1356.6748	1395.0752
1429.0859	1452.1301	1483.3311
1535.3013	1535.7070	1630.7067
1639.7208	2860.3453	2868.2360
3147.9574	3149.1181	3154.6543
3155.1974	3167.2713	3168.3419
3182.5092	3183.6445	3184.3006

p8

C	0.720969391	-0.1551034489	0.0941226117
C	2.175122472	0.1974686775	0.3290320915
C	2.894722249	-0.5529883299	1.1788521503
C	2.280931613	-1.6210540820	1.9700565028
C	0.937794751	-1.7389476561	2.0665670355
C	0.114420132	-0.7889310876	1.3373397139
C	-2.715430386	1.3157777157	0.3076095022
C	-2.857035236	1.9211783785	-0.9063995670
C	-1.752474887	2.1051494628	-1.7815682014
C	-0.509536979	1.4927815593	-1.4842708135
C	-0.306226395	0.8950522893	-0.2752562548
C	-1.339559034	1.0015246802	0.8262139456
C	-1.058940388	-0.2290562583	1.6698706774
H	0.731469784	-0.9117336271	-0.7129470153
H	2.630385005	0.9863525019	-0.2601968638
H	3.957204100	-0.3715536474	1.3036478476
H	2.928784036	-2.2706939186	2.5484692173
H	0.482505096	-2.4499366554	2.7478817840
H	-3.568820334	1.1568108866	0.9583318099
H	-3.840856011	2.2412501106	-1.2347269422
H	-1.898152472	2.5987076748	-2.7346912160
H	0.243232811	1.4207055816	-2.2648240366
H	-1.074799748	1.8690805868	1.4755259254
H	-1.669919571	-0.5139013944	2.5192720954

Frequencies

73.1116	100.0293	187.6554
209.8289	245.6303	368.6600
386.0915	432.8777	476.5211
493.7903	520.1797	546.0741
593.6842	607.8083	657.3760
673.8518	690.3842	727.3137
760.2781	776.1971	791.0316
850.7570	863.1025	884.5814
908.9052	948.6435	960.7750
964.2961	977.0147	986.9848
996.8273	1023.5325	1045.1264
1067.4788	1118.8439	1153.6314
1162.4295	1172.2700	1187.0680
1201.7943	1225.1241	1238.5336
1272.4779	1280.4870	1318.7769
1335.7754	1382.5671	1389.6223
1421.8368	1434.5665	1532.7578
1585.8628	1597.3466	1651.7303
1688.5487	2775.1252	2897.3109
3141.1389	3150.9448	3151.7692
3160.1786	3169.8480	3173.3341
3176.8995	3182.1432	3188.6072

p9

C	0.4964214166	-0.8786815955	-0.4843768379
C	1.9703409340	-0.6136968250	-0.3435835666
C	2.6987218010	-1.3874091125	0.4799848530
C	2.0817167656	-2.3909127037	1.3405986531
C	0.7352021191	-2.4719855247	1.4807006700
C	-0.0972951873	-1.5677732022	0.7310515727
C	-2.7788868004	0.7919221469	-0.0995868413
C	-2.7750485065	1.7996570696	-1.0628810188
C	-1.6653074216	1.9980896034	-1.8873275482
C	-0.5361336097	1.1801822119	-1.7692346116
C	-0.5265506474	0.1892426565	-0.8019099548
C	-1.6449917581	-0.0121434282	0.0396852096
C	-1.3494032839	-1.0971617756	0.9656327829
H	0.4145469909	-1.6030652916	-1.3207432887
H	2.4377572124	0.1337223167	-0.9756672963
H	3.7750420158	-1.2615894083	0.5329004904
H	2.7290570115	-3.0290467032	1.9318953601
H	0.2899474180	-3.1380572181	2.2124891625
H	-3.6472293458	0.6387327392	0.5322430131
H	-3.6443568016	2.4383382761	-1.1746690105
H	-1.6793638815	2.7923539146	-2.6251550390
H	0.3164079037	1.3323857224	-2.4233664322
H	-2.0204703449	-1.4426888686	1.7423496786

Frequencies

101.4048	110.2342	197.9862
253.7594	291.7947	395.8502
427.5916	441.3721	476.0201
529.7158	542.5243	571.1736
608.7518	643.6297	685.9954
709.2314	740.6619	767.0714
788.9369	826.0027	854.1021
868.1508	877.6894	895.6589
945.5022	963.8292	969.2899
976.3435	985.0557	989.3595
1042.1345	1063.6548	1121.8046
1141.2668	1166.7102	1173.5165
1178.5227	1190.9009	1213.6566
1234.5608	1275.8504	1319.3818
1338.8155	1369.5985	1395.5199
1441.4196	1484.2438	1493.5540
1572.5960	1601.5388	1623.4940
1644.2419	1677.2998	2889.5906
3153.3585	3155.0533	3160.0230
3161.5792	3172.8428	3173.9502
3183.3164	3185.3831	3192.9955

Transition state (TS): reactants to i0

C	1.3549024498	-0.9138689422	-0.0278337415
C	2.5465498308	-1.6474865312	-0.0508331427
C	3.7761668156	-0.9907741703	-0.0277910285
C	3.8270893257	0.4020063889	0.0183429360
C	2.6420642803	1.1455426162	0.0416745468
C	1.4412941073	0.4636618243	0.0178279576
C	-2.0291302026	0.4323000777	-1.2441338965
C	-3.0974735830	-0.4022136141	-1.2556404928
C	-3.6697460110	-0.8878992589	-0.0324634411
C	-3.1001716878	-0.4842455115	1.2214115669
C	-2.0318652098	0.3491227492	1.2674675701
C	-1.4221613383	0.8776926282	0.0284577156
C	-0.2724205321	1.6421407910	0.0550256272
H	0.3948686817	-1.4172628583	-0.0455139806
H	2.5098870532	-2.7317547114	-0.0867464501
H	4.6960151037	-1.5644339346	-0.0457856654
H	4.7849800383	0.9124057479	0.0362551688
H	2.6776154180	2.2309543597	0.0776216710
H	-1.5948624921	0.7939896500	-2.1697118258
H	-3.5326962475	-0.7133889434	-2.1992544275
H	-4.5213620990	-1.5552248660	-0.0554907877
H	-3.5374268801	-0.8571360810	2.1414205404
H	-1.5996421415	0.6487545911	2.2158906832
H	0.0231350225	2.1695401982	-0.8463739645
H	0.0211492979	2.1086988007	0.9899938612

Frequencies:

-769.6639	13.4146	38.6773
49.1662	105.6327	113.1563
169.3899	358.2881	368.1409
393.7224	402.1022	433.2211
504.4884	527.7411	563.7550
573.5320	615.0976	688.0445
690.6430	717.1816	725.5493
738.5657	781.5865	832.6623
844.8450	848.7505	902.4237
942.5551	952.9041	964.0224
965.8346	968.8213	983.6326
994.6018	1006.6876	1029.6257
1033.1654	1059.5917	1081.5529
1147.0865	1176.3807	1184.5857
1199.8955	1276.2732	1319.9922
1325.0893	1343.8976	1348.8820
1382.5629	1443.4969	1464.2342
1476.8087	1521.3509	1564.1518
1585.8043	1624.3265	1668.2230
3108.0679	3136.3256	3151.5596
3158.6081	3158.8485	3159.0935
3173.5594	3177.7433	3178.1950
3182.0764	3192.7127	3200.4390

TS: i0 to i2

C	0.9188570000	-0.4392870000	0.7163460000
C	1.9359280000	-1.4283880000	0.6639050000
C	3.1641510000	-1.1340100000	0.1004060000
C	3.4285750000	0.1512610000	-0.3985740000
C	2.4309460000	1.1347010000	-0.3597410000
C	1.1953090000	0.8696430000	0.2046480000
C	-0.8669100000	-0.4484980000	-0.6884790000
C	-1.8754750000	-1.5033920000	-0.5537570000
C	-3.1315670000	-1.1927260000	-0.1454510000
C	-3.4820920000	0.1551120000	0.2293990000
C	-2.4806600000	1.1523030000	0.2886350000
C	-1.2023720000	0.8906030000	-0.1230530000
C	-0.0031600000	1.7819500000	0.0846560000
H	0.1116470000	-0.5633690000	1.4334920000
H	1.7472690000	-2.4102290000	1.0831830000
H	3.9369520000	-1.8942030000	0.0608200000
H	4.3974380000	0.3787080000	-0.8275170000
H	2.6195240000	2.1098170000	-0.7989500000
H	-0.2764110000	-0.4507430000	-1.6084600000
H	-1.6180800000	-2.5185360000	-0.8368720000
H	-3.8910650000	-1.9657530000	-0.0857370000
H	-4.4945630000	0.3803480000	0.5396890000
H	-2.7216360000	2.1214400000	0.7177980000
H	0.1408560000	2.4656670000	-0.7631430000
H	-0.1411030000	2.4112190000	0.9720640000

Frequencies:

-392.8453	61.3144	90.6384
135.1280	219.6663	250.4868
316.4309	335.1645	402.9791
437.0346	479.8177	511.2574
527.4324	585.4212	606.4753
620.3294	658.7804	705.4819
730.3297	749.1598	762.1711
778.8549	814.0455	840.5488
867.2446	874.9008	913.9074
933.6068	957.2023	964.3137
970.3488	977.1922	1005.5051
1009.6388	1034.7350	1081.1192
1085.8341	1154.2377	1164.6699
1171.0063	1184.2252	1187.7340
1203.8561	1245.0572	1320.4434
1335.2695	1348.9018	1353.1979
1374.3309	1414.9604	1441.7543
1455.7602	1507.9655	1536.5327
1555.1402	1578.6195	1618.1475
2991.5229	3029.0478	3042.3414
3117.6496	3138.9202	3150.1187
3151.1395	3160.2279	3170.2920
3176.6508	3186.9936	3193.3025

TS: i2 to p2

C	0.3903768864	-0.9012801351	0.0751442487
C	1.7822369496	-1.2237032983	-0.3770071676
C	2.7776343329	-1.4158535641	0.5338683709
C	2.5722883873	-1.2080915930	1.9236439009
C	1.3403016793	-0.6813572270	2.3865855867
C	0.3003838100	-0.4921155095	1.5285821926
C	-0.4443238645	0.1897460589	-0.6125039963
C	-0.6979838186	0.3692807688	-1.9843284562
C	-1.7112975976	1.2351764516	-2.3763330837
C	-2.5141252183	1.8693220475	-1.4226395969
C	-2.3306244387	1.6181546980	-0.0594896845
C	-1.3174850103	0.7631464971	0.3441966888
C	-0.9722902802	0.2926523987	1.7453190194
H	-0.2116558979	-1.8265920338	-0.0592081886
H	1.9635148244	-1.3713303737	-1.4361368599
H	3.7643771461	-1.7103818718	0.1910865782
H	3.3869302588	-1.3691523471	2.6187214857
H	1.2532976316	-0.3697461238	3.4236128506
H	0.8951357618	1.4926271553	-0.4828974504
H	-0.0803137920	-0.1249010073	-2.7261291867
H	-1.8875515541	1.4154184034	-3.4309420772
H	-3.3005878749	2.5424316183	-1.7446491479
H	-2.9858802109	2.0816960386	0.6710157562
H	-0.8401382230	1.1169466894	2.4538366811
H	-1.7821608873	-0.3379927414	2.1432235359

Frequencies:

-776.8431	66.4051	116.6571
191.3607	230.4545	245.0702
371.3675	374.6086	415.4818
432.0065	461.6185	497.7099
508.8164	533.5652	537.2387
600.1871	621.2467	657.0193
698.4997	710.0519	744.1148
760.3839	788.5689	828.9691
834.6155	877.6520	898.8758
937.6395	954.9347	963.7646
977.0274	988.0485	999.9896
1037.5245	1044.2923	1101.8512
1118.9400	1154.7130	1157.0228
1176.5943	1177.0261	1192.2611
1211.1432	1220.1266	1235.3713
1279.0607	1308.6495	1336.6587
1344.8525	1390.4699	1429.5191
1462.5443	1479.6427	1492.6704
1541.6191	1597.2058	1612.0575
1627.5752	2822.6797	2965.4763
3040.3756	3146.9677	3152.8576
3156.7252	3163.5344	3171.8185
3175.3584	3186.9828	3191.3952

TS: p1 to p2

C	-2.1785960000	1.1891940000	-0.5555120000
C	-3.1482670000	0.2376420000	-0.9055930000
C	-3.1112230000	-1.0403330000	-0.3416040000
C	-2.1398640000	-1.3632140000	0.5944580000
C	-1.1432850000	-0.4185820000	0.9460640000
C	-1.1942180000	0.8907590000	0.3670850000
C	0.8717120000	-0.5781740000	0.1808160000
C	1.7646560000	-1.5830990000	-0.1185880000
C	3.0798250000	-1.2042180000	-0.4218590000
C	3.4433030000	0.1425110000	-0.4012270000
C	2.5087170000	1.1301240000	-0.0827330000
C	1.1923210000	0.7691650000	0.2149870000
C	0.0512970000	1.7171200000	0.5699440000
H	-2.1815590000	2.1614830000	-1.0380960000
H	-3.9168270000	0.4913600000	-1.6265810000
H	-3.8618310000	-1.7731970000	-0.6167120000
H	-2.1450990000	-2.3360560000	1.0731180000
H	-0.6334180000	-0.5530970000	1.8951410000
H	1.4723780000	-2.6281380000	-0.1312230000
H	3.8148710000	-1.9610690000	-0.6760210000
H	4.4627400000	0.4263330000	-0.6379020000
H	2.8053920000	2.1752160000	-0.0722460000
H	0.1515200000	2.0522170000	1.6112210000
H	0.0535700000	2.6115740000	-0.0581250000

Frequencies:

-388.0030	62.8677	106.3536
179.7128	226.8847	309.3045
328.3923	398.5577	415.2843
481.2647	497.4979	534.0796
583.9297	616.1592	621.7587
702.2191	720.5825	737.5055
745.9274	805.4051	806.5036
836.0899	860.8188	874.3560
921.2182	937.5984	969.0925
978.4648	985.2551	994.3636
1020.4469	1037.8151	1039.8824
1083.5616	1121.7223	1162.8607
1172.9718	1175.7754	1183.8609
1193.8246	1208.0863	1244.3242
1299.8598	1329.5416	1332.3005
1352.4696	1449.8788	1462.4838
1473.4626	1482.8471	1512.8079
1574.9815	1589.4022	1608.7034
1630.0232	2996.1471	3069.8204
3133.6657	3143.9440	3151.5479
3154.6270	3162.4672	3164.4993
3176.4260	3180.0412	3187.1784

TS: p2 to p4

C	-0.5759070953	-1.3735946242	0.9766063120
C	0.1298815354	-2.0916899583	0.0040038381
C	0.5088188449	-1.4811064679	-1.1987072705
C	0.2344071651	-0.1431328060	-1.4341603532
C	-0.3708613427	0.6222423302	-0.4089364549
C	-0.8573403307	-0.0379084380	0.7592179867
C	-1.0129643564	1.9578949635	-0.4695115603
C	-0.9578641265	2.9488588516	-1.4457788676
C	-1.6692917617	4.1307045276	-1.2442261569
C	-2.4174044471	4.3208583379	-0.0805545036
C	-2.4679975301	3.3284716990	0.9004723105
C	-1.7673605594	2.1461113632	0.7005486144
C	-1.6635589007	0.9285816259	1.5956924522
H	-0.9196987766	-1.8726341333	1.8768671867
H	0.3516944328	-3.1403165535	0.1656493810
H	1.0095626298	-2.0683388213	-1.9603446562
H	0.5219677088	0.3235189264	-2.3692696397
H	1.1238971485	1.2452361121	0.2835233183
H	-0.3721029978	2.8106184946	-2.3478739042
H	-1.6406619849	4.9104677280	-1.9970556420
H	-2.9648309857	5.2459783169	0.0608904536
H	-3.0524922572	3.4816052753	1.8018496514
H	-1.1487127745	1.1701168970	2.5353240084
H	-2.6435812381	0.5221783533	1.8675574958

Frequencies:

-953.0092	97.6831	131.8588
210.8386	239.4808	263.3180
398.1024	407.3203	425.8786
457.5170	489.6400	513.2260
520.2351	558.9055	579.5040
638.1012	641.0281	708.4238
736.4983	746.6971	761.6776
800.2051	815.3967	850.3702
865.6402	879.5898	931.5534
948.6260	972.9717	984.4673
989.7943	1021.5539	1042.5334
1050.3065	1115.0756	1128.9203
1162.9705	1174.2339	1179.7897
1189.8192	1204.9870	1220.2167
1246.5574	1313.5911	1323.8111
1343.7154	1363.0793	1448.3606
1469.4459	1478.5298	1501.7687
1510.8660	1588.7142	1623.1846
1630.0341	1650.8130	3004.6989
3046.3938	3157.2378	3158.2644
3164.3673	3166.1961	3175.0421
3179.1658	3186.9154	3189.0704

TS: p1 to p3

C	1.2364398963	-1.0144549442	-0.1643067577
C	2.2699829881	-1.9431866546	-0.1259619773
C	2.5658822131	-2.6215422814	1.0562565496
C	1.8161740356	-2.3627356164	2.2045558226
C	0.7830363540	-1.4355954016	2.1692831908
C	0.4751704896	-0.7388986779	0.9854552973
C	-2.0869057460	0.6404171294	-0.6494913356
C	-2.7781600465	1.1623631816	-1.7296125562
C	-2.1932522623	2.2866704913	-2.3322802113
C	-0.9884911500	2.8247697494	-1.8659787425
C	-0.3119266247	2.2678544542	-0.7746539897
C	-0.8988177880	1.1579400436	-0.1760452917
C	-0.6400226602	0.2167647600	0.9678755884
H	1.0102722606	-0.4937203351	-1.0873802146
H	2.8484377174	-2.1393706993	-1.0220280334
H	3.3728926475	-3.3448264858	1.0833212976
H	2.0409911735	-2.8841577815	3.1284233077
H	0.2036746700	-1.2378032547	3.0654301269
H	-3.7093052362	0.7489838506	-2.0981305574
H	-2.6871204852	2.7509429654	-3.1800594978
H	-0.5736351353	3.6938539114	-2.3647526003
H	0.6242379324	2.6907420155	-0.4266234789
H	-0.9385113644	0.5896702668	1.9487490966
H	-1.8322618793	-0.3148416867	0.4734109667

Frequencies:

-2170.1733	52.2190	62.8715
75.0097	210.1712	216.2339
289.9578	392.2492	410.9845
426.4514	465.2670	503.4565
580.7583	614.9653	635.1189
638.4620	704.7080	715.1070
749.2532	754.5769	802.7810
851.9801	873.1273	882.9381
905.7738	940.7612	948.4246
980.6081	991.1701	991.4667
1001.3972	1012.6428	1023.3689
1047.4844	1104.0829	1120.6804
1153.2228	1173.0556	1180.9461
1191.1544	1202.7327	1215.2841
1264.9856	1306.8610	1327.9768
1350.7846	1377.7057	1454.4721
1481.6840	1484.0583	1520.2600
1586.4538	1609.4394	1630.0272
1632.8603	1759.9567	3089.5203
3153.7552	3156.7324	3164.4600
3167.0074	3174.1229	3180.9525
3183.9911	3187.1289	3191.1506

TS: p5 to p6

C	-0.8686882786	-2.6092987647	-0.0643998104
C	0.2394258267	-3.4282888929	-0.2121876430
C	1.5342111654	-2.9217040075	-0.0415106967
C	1.7221814614	-1.5586171150	0.2317837613
C	0.6355098851	-0.7110320376	0.3626244566
C	-0.7065760188	-1.2219314853	0.2108311316
C	0.6831070690	0.7572646416	0.3313951025
C	1.5417213402	1.6105521282	1.0213382883
C	1.3970600146	2.9906414894	0.8818677602
C	0.3967574507	3.5130196242	0.0625097347
C	-0.4580336430	2.6631673916	-0.6413824345
C	-0.3113143749	1.2798200555	-0.5300018419
C	-1.1066179784	0.2583933898	-1.2486061769
H	-1.8670550576	-3.0277064250	-0.1263485086
H	0.1021592842	-4.4829374431	-0.4263854070
H	2.3918255870	-3.5759414173	-0.1446068714
H	2.7265983227	-1.1515835900	0.2851868544
H	-1.5003430440	-0.7307542635	0.7663309064
H	2.2937062886	1.2032046733	1.6883542859
H	2.0526837698	3.6598900216	1.4276074896
H	0.2830289455	4.5873557432	-0.0313406761
H	-1.2207330927	3.0770023311	-1.2923602056
H	-2.1706852348	0.4343796437	-1.3858700539
H	-0.6269796882	-0.2364866913	-2.0884484454

Frequencies

586.5979i	93.0941	105.9214
177.8774	235.1816	284.5646
364.3257	400.0483	431.8682
456.9222	517.5303	562.5770
570.1120	597.8714	612.5944
627.5484	726.6929	732.2033
744.2282	750.6558	779.3419
813.8782	837.0476	843.0132
881.0256	934.1240	946.3818
951.2860	975.4968	990.3359
1007.8471	1018.0724	1030.8997
1040.9138	1056.6082	1087.3160
1129.2702	1170.7620	1181.6125
1185.3014	1219.0868	1256.9985
1302.4944	1322.3973	1333.0631
1340.8961	1441.4426	1452.5831
1485.7271	1489.4347	1509.2171
1556.7184	1598.9480	1604.1708
1634.9529	3098.6198	3120.9270
3157.9152	3158.8408	3163.8649
3166.7365	3176.0548	3177.0098
3181.9594	3187.4131	3189.1256

TS: p6 to p4

C	-0.8045227783	-2.7846391483	0.0453888375
C	0.3857953505	-3.4696296540	0.2522775403
C	1.6185608849	-2.8164341748	0.1201628596
C	1.6806817948	-1.4756966784	-0.2578550890
C	0.4956826555	-0.7775163530	-0.4704003586
C	-0.7598529035	-1.4079781263	-0.2364412586
C	0.2493114408	0.5885208927	-0.9328026593
C	1.1340249747	1.6301897316	-1.2177012022
C	0.6201234187	2.8533966253	-1.6412172687
C	-0.7581400343	3.0377164766	-1.7786424840
C	-1.6457366875	1.9970929197	-1.4968554842
C	-1.1396777658	0.7744767429	-1.0771109752
C	-1.8773546383	-0.5019916661	-0.7352477344
H	-1.7575513314	-3.2927979966	0.1448039232
H	0.3634878262	-4.5223346892	0.5104519401
H	2.5359762539	-3.3697103981	0.2865409133
H	2.6418524629	-0.9952432599	-0.4044459737
H	-0.9116477263	-0.8456616216	1.5229847159
H	2.2045546881	1.4958957166	-1.1076501423
H	1.2949686788	3.6725606692	-1.8629672350
H	-1.1410624806	3.9977103815	-2.1062308708
H	-2.7147781729	2.1470802989	-1.6068640097
H	-2.6737777672	-0.3503135977	-0.0031048322
H	-2.3374951437	-0.9371750909	-1.6312201521

Frequencies

97.8713	133.2966	
216.0137	239.6740	277.3734
389.8661	416.9473	433.6100
463.3833	492.4703	502.0243
518.2826	567.9760	575.0924
634.2377	648.6942	714.8060
744.9939	751.7015	754.1090
794.0119	813.5845	851.0024
871.1598	880.5362	933.8394
949.5517	972.5071	987.5860
990.6331	1021.8834	1043.5938
1050.0475	1118.2458	1130.0355
1165.6165	1173.6757	1179.2910
1191.2535	1206.0734	1219.4343
1247.2662	1322.1636	1328.7026
1340.0826	1366.5937	1453.2752
1467.2271	1483.2625	1503.1216
1507.3753	1595.4537	1619.7290
1630.7342	1647.9924	3019.2361
3076.5119	3158.6084	3161.3917
3165.1048	3168.0929	3175.7520
3178.0810	3187.9198	3189.4768

TS: p3 to p7

C	1.8968363091	0.4317142592	2.0146535276
C	2.9499148794	-0.4172428361	1.6183762652
C	2.7164884817	-1.4180411632	0.6635920102
C	1.4578841581	-1.6348812533	0.1306977296
C	0.3459535965	-0.8105093225	0.5306968205
C	0.6278752557	0.2649220743	1.4980266372
H	2.0951166381	1.2605273221	2.6866006074
H	3.9413706331	-0.2822111509	2.0329837759
H	3.5339782036	-2.0693010214	0.3706349151
H	1.2864004304	-2.4707921477	-0.5382041974
H	-0.5947003836	-1.3372178404	0.6928076235
C	-2.5001016324	1.7171097378	0.1302292097
C	-3.2260264768	1.2349617839	-0.9136753506
C	-2.6783219640	0.2667438666	-1.8359583310
C	-1.3706916206	-0.1018326137	-1.7642079500
C	-0.5172946860	0.4002542357	-0.7068818270
C	-1.1806284099	1.1937386684	0.3724740408
C	-0.4923506949	1.1865806328	1.5549588343
H	-2.9370463175	2.4113196730	0.8405240218
H	-4.2493530588	1.5650859748	-1.0568115322
H	-3.3103714902	-0.1075001552	-2.6336092050
H	-0.9361860428	-0.7332746397	-2.5332689387
H	0.4274284013	0.8120971403	-1.0598302986
H	-0.7415782095	1.7972567749	2.4147136116

Frequencies

897.1876i	92.7242	105.8955
161.3482	251.5183	279.0436
394.1049	407.8636	418.1816
478.3602	514.1310	554.1464
576.1944	601.3501	620.2430
668.0318	695.4551	710.3869
732.7394	783.7113	802.8527
813.5447	850.6378	853.2210
869.9598	914.4720	961.4630
967.3494	970.5526	981.6446
989.0449	993.5379	1023.5774
1043.9947	1096.6028	1111.0189
1159.9707	1167.5764	1175.0942
1188.1460	1191.2841	1233.7870
1287.8946	1314.0381	1334.5186
1368.0086	1400.0992	1428.5759
1458.4502	1484.1274	1505.2352
1532.9510	1565.0950	1596.1269
1639.5021	3063.4966	3089.3580
3150.2072	3152.5770	3157.0857
3159.0893	3170.9097	3173.2948
3182.3967	3183.6457	3189.7837

TS: p7 to p8

C	0.6787261147	-0.3685172753	0.0191761145
C	2.0772610972	0.14703103 0	0.2447555863
C	2.8476906584	-0.4531820089	1.1787360584
C	2.3281994698	-1.4668657702	2.0694226319
C	0.9765240939	-1.7068287436	2.1497286506
C	0.0917817889	-1.0451059986	1.2655152011
C	-2.9176034867	0.7680754853	-0.0390187986
C	-2.9516530586	1.6307402217	-1.0918668159
C	-1.7780262224	1.9938709495	-1.8358141175
C	-0.5507849297	1.4379288939	-1.5157973127
C	-0.4238348308	0.5642866156	-0.4260330678
C	-1.6399650880	0.2136869484	0.3983654605
C	-1.2633256509	-0.7813629823	1.3622211291
H	0.7359620989	-1.1571026139	-0.7681155696
H	2.4674582345	0.9256361147	-0.4015114544
H	3.8811408131	-0.1445677438	1.3021505456
H	3.0076298538	-1.9511261897	2.7610094494
H	0.5758900839	-2.3370088545	2.9376336522
H	-3.8252988076	0.4728351590	0.4736842627
H	-3.9055323104	2.0461603386	-1.3993264255
H	-1.8654842357	2.6832161757	-2.6653461061
H	0.3243664573	1.6614712908	-2.1173652487
H	-0.9369750060	1.1884779349	0.6941582420
H	-1.9249791373	-1.1532419773	2.1331089326

Frequencies

1847.6158i	96.6435	106.6698
191.0806	237.4641	259.1011
393.2491	405.8282	444.5476
467.1649	500.2723	521.9213
545.9865	594.3065	618.0859
667.4678	677.5892	691.1947
708.8181	748.4664	776.1069
784.951	815.6278	839.5957
859.7293	916.5210	935.1220
949.5798	962.0946	979.8215
981.4357	985.0184	1043.7601
1092.8388	1123.8888	1144.2000
1152.9422	1163.3901	1171.6760
1180.2095	1221.3911	1231.6776
1268.8552	1302.8667	1311.5145
1335.8779	1383.7322	1420.2662
1430.5514	1452.0368	1479.1771
1501.2309	1534.2212	1628.3233
1635.3272	2180.0023	2744.4154
3148.0073	3153.8025	3161.7140
3164.6599	3170.4766	3183.4405
3186.4418	3199.6733	3202.6020

TS: p7 to p9

C	0.6736382347	-0.2977355952	0.0464668342
C	2.0816819807	0.1736421438	0.2659773892
C	2.8402959717	-0.4353085501	1.1950785754
C	2.2944916414	-1.4477479273	2.0895653768
C	0.9639030233	-1.7107910222	2.1373802873
C	0.0801342754	-1.0001989069	1.2542119452
C	-2.8702153102	0.7493730992	-0.0361465261
C	-2.9495250244	1.6320121799	-1.1104192393
C	-1.8135613617	1.9579793982	-1.8633859592
C	-0.5716866687	1.4181498514	-1.5416579199
C	-0.4615186644	0.5981187266	-0.4134996851
C	-1.6279390488	0.2114814557	0.3089990505
C	-1.2536634940	-0.7431968864	1.3331198754
H	0.7424795600	-1.067837061	-0.7490376203
H	2.4938175865	0.9318866754	-0.3906742702
H	3.8827244174	-0.1588328370	1.3113693806
H	2.9697255703	-1.9415373309	2.7795327799
H	0.5547688995	-2.3792160182	2.8876733578
H	-3.7634740863	0.4709051938	0.5124496566
H	-3.9082212505	2.0595851562	-1.3823395474
H	-1.9051151276	2.6339759644	-2.7057846055
H	0.3028773300	-1.6634869443	2.1348554938
H	0.1056271887	2.0551993165	0.8090115778
H	-1.9361196428	-1.1586379699	2.0639867802

Frequencies

593.3700i	105.8238	113.5565
200.3934	248.3482	288.2462
343.8	377.7923	412.5881
428.1975	447.0273	485.0067
530.1402	540.8731	571.2155
608.7379	641.8608	689.4625
707.3846	737.2752	761.9508
790.7711	825.9567	850.2519
867.0874	875.0152	890.7663
948.2569	962.8682	971.2569
975.0233	986.2754	988.6918
1039.7375	1065.0842	1123.8344
1143.2863	1167.7055	1171.1855
1177.3241	1188.8153	1213.2100
1237.2488	1279.2603	1318.5522
1340.6126	1359.7941	1394.7242
1441.7621	1469.1549	1490.9317
1567.9784	1585.9266	1609.7325
1630.2248	1674.8789	2892.2666
3155.6418	3158.7551	3162.0636
3164.7465	3175.4038	3176.2892
3184.8398	3187.5459	3195.1092

TS: p8 to p2

C	0.6691931458	-0.3008382573	0.0966871
C	2.1304258844	0.0628736662	0.16607492
C	2.9212750248	-0.5729765462	1.05593832
C	2.3885826259	-1.4859886508	2.046156
C	1.0351397140	-1.5739016496	2.26104681
C	0.1489180673	-0.8679894221	1.41521988
C	-2.7569924764	1.2135750260	0.2443645
C	-2.7837981749	2.0504329381	-0.8559387
C	-1.6551957581	2.2432528393	-1.668737
C	-0.4669388817	1.5371257738	-1.4027717
C	-0.3885523115	0.7078841278	-0.3095167
C	-1.5150415739	0.5900350779	0.6001535
C	-1.1585191866	-0.4399685471	1.62705885
H	0.6001853212	-1.1260488464	-0.6497328
H	2.5356967770	0.7668406073	-0.5523118
H	3.9880741545	-0.3731508625	1.06739118
H	3.0778865848	-2.0107430366	2.69712611
H	0.6495557953	-2.1178869677	3.11790257
H	-3.6388124406	1.0680068946	0.85765766
H	-3.7093362062	2.5576176549	-1.1071048
H	-1.7124069884	2.9042149507	-2.52468
H	0.3737737867	1.6251742169	-2.084156
H	-1.1248023582	1.0252044322	1.71891054
H	-1.8251985253	-0.7360274192	2.42593259

Frequencies

1547.4983i	97.8786	104.9452
193.5983	245.9914	268.2044
396.5955	411.5468	448.8726
467.7058	514.5867	527.3999
559.4345	600.3280	627.8663
668.4155	694.2779	711.1195
731.9619	768.6055	790.7737
797.7112	837.4669	856.4214
860.6009	931.5661	932.7711
955.2997	963.9152	973.0864
978.0883	1019.0385	1034.8137
1053.963	1117.5759	1157.9347
1159.2152	1166.5314	1172.3241
1185.0908	1203.3835	1215.2897
1258.8457	1297.6644	1313.8164
1342.516	1379.4100	1425.1933
1445.1685	1463.7368	1483.8688
1530.7514	1549.7609	1621.5342
1637.8405	1786.5177	2769.6980
3150.1533	3153.6137	3154.5013
3160.446	3174.1159	3177.9738
3185.135	3191.6774	3209.1696

C₁₃H₁₂ + H TS1 abstraction

C	-0.4577092057	-2.1987033118	1.0408583590
C	0.7612313313	-2.8703296927	0.9608326626
C	1.9128257727	-2.3184807707	1.5178381721
C	1.8395575983	-1.0810762751	2.1660903387
C	0.6137483733	-0.4539338471	2.2156375723
C	-0.5606825108	-0.9510865730	1.6761854923
C	-2.4473730964	0.4446013752	-0.6447796516
C	-2.5934823394	1.3844704277	-1.6611388676
C	-2.3451673563	2.7325916248	-1.4089461992
C	-1.9518325986	3.1304505422	-0.1339191898
C	-1.8068222075	2.1861983800	0.8807730609
C	-2.0508426341	0.8315881629	0.6395738384
C	-1.8813845547	-0.2006331522	1.7436565108
H	-1.3480391900	-2.6477041129	0.6105972899
H	0.8094546734	-3.8333026360	0.4649623400
H	2.8594096101	-2.8443548612	1.4565024186
H	2.7195014285	-0.6348873655	2.6172349738
H	0.5859466450	0.8370689988	2.9750259942
H	-2.6460346575	-0.6021101241	-0.8516633475
H	-2.9049314101	1.0650334301	-2.6496390301
H	-2.4605195742	3.4659403293	-2.1990756396
H	-1.7599093952	4.1773337036	0.0741709047
H	-1.5009775694	2.5055129484	1.8715145774
H	-1.9633160098	0.2949590580	2.7138762254
H	-2.6980539054	-0.9259976837	1.6879251128
H	0.6059537823	1.5540574249	3.4328120814

Frequencies:

-858.4669	10.6981	54.2392
58.0823	162.8686	194.1411
236.0746	262.2341	283.4859
368.3458	412.9366	418.4240
461.4637	488.5433	557.0257
614.9322	622.4896	637.1192
706.2964	716.7047	750.4026
754.6038	827.5968	830.4227
852.9004	865.1595	910.4454
917.5112	931.1835	948.8297
971.6565	976.1895	989.5350
1000.4403	1018.5769	1033.8774
1051.1701	1059.8956	1096.6204
1126.8835	1175.0186	1179.3321
1182.9786	1203.7859	1207.2215
1216.3200	1292.5858	1322.5678
1332.2747	1340.3317	1362.0106
1455.0273	1480.3162	1485.2358
1493.3769	1527.8326	1583.9247
1627.1861	1632.4988	1646.4163
2352.6324	3042.9644	3085.6126
3149.7957	3154.8216	3159.2407
3160.3444	3168.8923	3172.1163
3176.6090	3185.2863	3188.0847

C₁₃H₁₂ + H TS2 abstraction

C	-0.0010047105	-2.0553185976	0.7838621736
C	1.1648546174	-2.8085652539	0.6734323043
C	2.3420756448	-2.3692566731	1.2761587204
C	2.3431472903	-1.1749138519	1.99309 18187
C	1.1751115023	-0.4244706892	2.1037186924
C	-0.0117593069	-0.8491905099	1.4953531394
C	-1.1315053107	0.7022052739	-0.8265506200
C	-1.5633856981	1.5145276296	-1.8732772709
C	-2.5449406256	2.4780994723	-1.6591889097
C	-3.0915934456	2.6282107518	-0.3846013878
C	-2.6583760229	1.8195326531	0.6593670422
C	-1.6726658171	0.8416004912	0.4567344954
C	-1.2638106621	-0.0274281050	1.6154098011
H	-0.9169044257	-2.4102561178	0.3232294592
H	1.1520870925	-3.7424899530	0.1225113923
H	3.2495757322	-2.9565543350	1.1931737496
H	3.2529736469	-0.8279596199	2.4703463676
H	1.1836659141	0.5041918702	2.6650137342
H	-0.3591932417	-0.0354286906	-1.0060625656
H	-1.1266467996	1.3943118700	-2.8586273635
H	-2.8795506347	3.1091463445	-2.4747304593
H	-3.8538108803	3.3783061871	-0.2046524840
H	-3.0886908608	1.9429001873	1.6484143566
H	-1.2581557117	0.5562974103	2.5395651451
H	-2.1634360228	-0.7936204580	1.8079681056
H	-3.0112292637	-1.5478882866	2.0542185629

Frequencies:

-813.2967	23.2795	46.5963
78.0475	166.4291	216.8003
243.9349	284.8060	293.0134
412.8726	413.9937	417.2440
481.6473	503.6938	574.2553
625.4614	635.4749	639.6430
710.9795	715.3747	751.4633
757.9214	824.0884	852.3809
855.1115	857.9769	912.9781
933.5586	975.7611	979.5619
982.5666	1002.2442	1003.2764
1016.5630	1017.6706	1051.0490
1052.0166	1100.9732	1109.0364
1181.8399	1182.0287	1197.7838
1203.6280	1204.6293	1207.5709
1229.6565	1294.4395	1330.4321
1344.6664	1358.6849	1359.7021
1386.5322	1480.5328	1485.1739
1511.4106	1526.8605	1541.7993
1620.3957	1622.7506	1640.8268
1650.2571	3065.4821	3153.8596
3156.4863	3160.6673	3163.7975
3170.2973	3173.8466	3177.8560
3186.2280	3188.8723	3194.5941

Input file for RRKM-ME calculations for the $C_7H_7 + C_6H_5 \rightarrow i1 \rightarrow p1/p3 + H$ reaction

```
TemperatureList[K]                     500. 600. 700. 800. 900. 1000. 1125.
1250. 1375. 1500. 1650. 1800. 2000. 2250. 2500.
PressureList[atm]                      0.01 0.03 0.1 0.3 1. 3. 10. 30. 100.
EnergyStepOverTemperature              0.2          #Ratio of discretization
energy step to T
ExcessEnergyOverTemperature            60
ModelEnergyLimit[kcal/mol]             600
WellCutoff                             10
ChemicalEigenvalueMax                  0.2
ChemicalEigenvalueMin                  1.e-6         #only for direct
diagonalization method
CalculationMethod                      direct
EigenvalueOutput                               eigenvalue.out
Model
EnergyRelaxation
Exponential
Factor[1/cm]              424     ! Jasper calc N2
Power                    0.62
ExponentCutoff            15
End
CollisionFrequency
LennardJones
Epsilons[1/cm]        390. 390.    ! N2
Sigmas[angstrom]      4.46 4.46    ! N2
Masses[amu]           28. 168.
End
OutputTemperatureStep[K]  100
OutputTemperatureSize  24
OutputReferenceEnergy[kcal/mol]  0.

!-------well_i1------------
Well        i1
Species
RRHO
Geometry[angstrom]    25
 C    -0.6931514799    -2.5354950177    1.1492852794
 C     0.5072590971    -3.2457550295    1.1307489997
 C     1.7140557244    -2.5808504563    1.3246605319
 C     1.7124556069    -1.2017913519    1.5349502872
 C     0.5133078837    -0.4970745623    1.5504210641
 C    -0.7081786812    -1.1547221864    1.3601202601
 C    -1.9846214       0.5023319451    -0.9750145036
 C    -2.0978829176    1.5347512395    -1.9001978226
 C    -2.344604029     2.8389574724    -1.4707690641
 C    -2.4767390853    3.0987725981    -0.1102721353
 C    -2.3644093924    2.0600289792    0.8140283909
 C    -2.1185763363    0.7498361234    0.3966806153
 C    -2.0174088873    -0.3847695335    1.4020997775
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 H   -1.6306537697    -3.0621659894    1.0006190748
 H    0.4964695277    -4.3174049368    0.9645908145
 H    2.6489529993    -3.1297045786    1.3109077852
 H    2.6484656125    -0.6751007408    1.6857059213
 H    0.5222873646     0.5769073383    1.704788432
 H   -1.7831593193    -0.507410214    -1.3172782603
 H   -1.992711794     1.3230838273    -2.9586676261
 H   -2.4312919638    3.643798748     -2.192001731
 H   -2.6669046838    4.1090067198    0.2353080499
 H   -2.4719087305    2.2705673959    1.8735231794
 H   -2.1626569111    0.0235973945    2.4078824209
 H   -2.842271435    -1.0861411843    1.237612259
Core   RigidRotor
SymmetryFactor   2.0
End
Frequencies[1/cm]   69
   19.3371               23.2563               64.7858
  192.5380              225.8199              288.8061
  341.3179              414.7331              415.4312
  461.5491              481.1643              566.0285
  623.7253              635.6911              638.2424
  713.7286              716.2708              751.7336
  751.8686              831.8536              833.5191
  856.0820              856.9500              903.5491
  933.1894              947.2732              978.0195
  978.3792             1001.0019             1001.0675
 1017.8577             1018.5130             1050.8278
 1051.5505             1097.3186             1107.0823
 1180.9713             1181.2615             1197.5082
 1202.8167             1203.7251             1210.5422
 1220.9671             1302.3109             1341.1569
 1345.1871             1362.2145             1366.0644
 1478.4712             1482.2827             1491.0125
 1526.8655             1528.4643             1623.9397
 1628.2552             1643.5652             1648.9583
 3021.7697             3054.1958             3152.0301
 3152.0950             3157.3278             3157.6759
 3167.1568             3167.3753             3175.1531
 3175.3508             3186.6852             3186.9654
ZeroEnergy[kcal/mol] -103.6
ElectronicLevels[1/cm]          1
0  1
End
End
!--------------------------------
!-------C13H11_ni1_+_H-----
Bimolecular    p1
Fragment         C13H11_ni1
RRHO
Geometry[angstrom]    24
```

```
C    -0.1907879155   -1.6923463249    0.7008642929
C     1.0468590267   -2.3270483183    0.6961722165
C     1.9083316335   -2.1946345711    1.7854346839
C     1.5200807237   -1.4237424273    2.8767214928
C     0.2772771116   -0.7902326502    2.8784358992
C    -0.593909834    -0.9158146545    1.7938623297
C    -3.1267363177    0.6133791038   -0.2920172972
C    -3.3863346235    1.4690604919   -1.3366216802
C    -2.5801768795    2.6101227258   -1.4274183278
C    -1.5754876544    2.8234564489   -0.4820356465
C    -1.3640288683    1.9151551905    0.5517402609
C    -2.1581557282    0.7596540848    0.6752989976
C    -1.9543594761   -0.2396169074    1.8021847566
H    -0.852078652    -1.7938812909   -0.1533856351
H     1.3413330709   -2.9262192225   -0.1584851392
H     2.8733973426   -2.6886743596    1.7810388575
H     2.1818704796   -1.3137715678    3.7288211548
H    -0.0204175256   -0.1946142425    3.7357363306
H    -4.1729781402    1.2790241423   -2.0584773016
H    -2.7385696538    3.3217656631   -2.230739122
H    -0.9507431928    3.7066818507   -0.5528357355
H    -0.5721007764    2.0906661912    1.2739657347
H    -2.0928517865    0.2703826279    2.7607406284
H    -2.7403293641   -0.9973069838    1.7374322494
Core  RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm]  66
   10.2035              22.3326              62.1988
  186.8317             225.2602             280.8754
  336.6634             414.9156             416.7594
  461.6204             485.0586             554.6195
  614.9393             631.7603             637.6627
  699.2521             716.1932             743.2661
  751.2091             821.2313             830.5175
  856.4369             857.0617             910.7754
  938.6565             946.6597             978.8446
  985.3125             991.1837            1001.6328
 1018.1329            1043.4614            1051.2055
 1098.4716            1120.8067            1170.1853
 1181.2475            1187.3749            1203.2316
 1206.8061            1217.9560            1273.4469
 1315.1428            1330.0131            1342.9235
 1363.1753            1448.1019            1477.4720
 1481.7127            1488.4290            1527.6258
 1574.8945            1625.5531            1634.8420
 1646.6709            3032.2645            3069.6524
 3150.3666            3152.3826            3157.8887
 3159.3746            3167.5181            3172.2272
 3175.5511            3184.1582            3187.0762
```

```
ZeroEnergy[kcal/mol]        0.0
ElectronicLevels[1/cm]          1
0   2
End
Fragment            H
Atom
Mass[amu]    1
ElectronicLevels[1/cm]            1
0    2
End
GroundEnergy[kcal/mol] 6.0
End
!-------C13H11_ni3_+_H-----
Bimolecular    p3
Fragment            C13H11_ni3
RRHO
Geometry[angstrom]    24
  C    1.4966457158    -0.9769913584    -0.1755634679
  C    2.6898177011    -1.6345483856    0.0863941856
  C    2.9246837744    -2.2198631069    1.3319563768
  C    1.932701221    -2.1573368375    2.3141259782
  C    0.7361385965    -1.509136335    2.0578072233
  C    0.4838597443    -0.8767072029    0.8122201071
  C    -2.6005553705    0.9334442672    -0.5332343601
  C    -3.0873140145    1.8367059552    -1.4632288585
  C    -2.2056265814    2.5734689858    -2.2584273584
  C    -0.8301758988    2.398897915    -2.0944509164
  C    -0.3348599811    1.490582959    -1.1702335097
  C    -1.2081376661    0.7115753135    -0.3688938413
  C    -0.7824579894    -0.2337525604    0.6205540418
  H    1.3219255126    -0.5785837676    -1.1654751064
  H    3.4411272758    -1.7045018967    -0.6927117962
  H    3.8604594262    -2.7295458544    1.5298856228
  H    2.0969738192    -2.6201208319    3.2810333751
  H    -0.0281221803    -1.4662946059    2.826830032
  H    -3.2932731172    0.3663307675    0.0798419418
  H    -4.1577744269    1.9730881771    -1.5708130181
  H    -2.5848928865    3.2830608264    -2.9845482379
  H    -0.137477943    2.9885256356    -2.6851189001
  H    0.7343991918    1.4143206762    -1.028537208
  H    -1.5453759231    -0.5084447353    1.3441976946
Core   RigidRotor
SymmetryFactor 2.0
End
Frequencies[1/cm]    66
   55.3968                60.4718                110.9993
  204.7807               238.4590               298.2518
  315.8440               411.6149               423.2506
  486.1829               494.7039               578.4475
  627.1626               629.9209               652.4739
```

```
    694.5899              703.6792              718.7562
    762.8016              798.9911              817.4151
    840.5655              848.6304              890.0081
    914.9801              921.3018              976.8319
    981.2413              994.5749              997.8103
   1002.3211             1007.6202             1044.7449
   1046.7926             1098.8498             1119.0803
   1179.1891             1179.9598             1190.1323
   1203.0503             1227.6398             1232.7808
   1328.0179             1332.3600             1349.3459
   1362.8018             1429.2975             1477.6360
   1496.9845             1506.8138             1515.1288
   1589.4045             1591.2519             1608.8934
   1621.1403             3138.5446             3157.5924
   3158.3079             3164.9213             3165.7276
   3174.8597             3175.3571             3188.6030
   3189.4749             3201.8861             3215.4241
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]          1
0  2
End
Fragment          H
Atom
Mass[amu]    1
ElectronicLevels[1/cm]          1
0    2
End
GroundEnergy[kcal/mol] -21.8
End
!-------c7h7_c6h5_p0------------
Bimolecular    p0
Fragment          c7h7
RRHO
Geometry[angstrom]    14
C   0.2889157829    1.1989076188    0.4411648713
C  -1.0939883347    1.202675661     0.4413513402
C  -1.807524641    -0.00183713     0.4409711028
C  -1.1122846904   -1.2170022185    0.4403700908
C   0.2705184752   -1.2341476129    0.4401674207
C   1.0223144207   -0.0232362299    0.4405761993
C   2.4261644469   -0.0338459674    0.4404154128
H   0.8358147436    2.1357433166    0.4414659983
H  -1.6293443636    2.1457751577    0.4417863345
H  -2.891236489     0.0063579281    0.4411501041
H  -1.661843269    -2.1518968994    0.4400633889
H   0.803184516    -2.1791485564    0.4396957755
H   2.9936507467    0.8883643322    0.4407885382
H   2.9796546555   -0.9645233999    0.4399094226
Core   RigidRotor
SymmetryFactor 2
```

End
Frequencies[1/cm]   36
198.8667   359.1502   390.0539
478.5997   501.2484   534.1703
628.2683   684.5115   708.1095
773.6815   828.7779   831.0629
898.2900   969.2522   971.1917
989.2728   994.6949   1036.0538
1116.2301   1174.6185   1184.2088
1288.0210   1327.3993   1351.7755
1473.5146   1490.2047   1502.2589
1576.9663   1598.0668   3144.6294
3158.6802   3161.3193   3173.1335
3178.3546   3191.1353   3240.2830
ZeroEnergy[kcal/mol]   0.0
ElectronicLevels[1/cm]   1
0 2
End
     Fragment   C6H5
      RRHO
        Geometry[angstrom]   11
C   0.000000   0.000000   1.390346
C   0.000000   1.221722   0.769740
C   0.000000   -1.221722   0.769740
C   0.000000   1.208778   -0.629525
C   0.000000   -1.208778   -0.629525
C   0.000000   0.000000   -1.319309
H   0.000000   2.153977   1.319039
H   0.000000   -2.153977   1.319039
H   0.000000   2.145530   -1.172910
H   0.000000   -2.145530   -1.172910
H   0.000000   0.000000   -2.401057
        Core   RigidRotor
        SymmetryFactor   2
        End
        Frequencies[1/cm]   27
402. 428. 602. 621. 672. 726. 820. 903. 979. 1001. 1009.
1017. 1052. 1073. 1177. 1177. 1303. 1326. 1464. 1473.
1570. 1627. 3154. 3160. 3173. 3175. 3186.
        ZeroEnergy[kcal/mol]   0.
        ElectronicLevels[1/cm]   1
          0   2
    End
GroundEnergy[kcal/mol] 0.0
End
!-------exit_vts1-------
Barrier   vts1 i1 p1
   RRHO
      Stoichiometry C13H12
      Core   PhaseSpaceTheory

```
        FragmentGeometry[angstrom]      24
C    -0.1907879155    -1.6923463249    0.7008642929
C     1.0468590267    -2.3270483183    0.6961722165
C     1.9083316335    -2.1946345711    1.7854346839
C     1.5200807237    -1.4237424273    2.8767214928
C     0.2772771116    -0.7902326502    2.8784358992
C    -0.593909834     -0.9158146545    1.7938623297
C    -3.1267363177     0.6133791038   -0.2920172972
C    -3.3863346235     1.4690604919   -1.3366216802
C    -2.5801768795     2.6101227258   -1.4274183278
C    -1.5754876544     2.8234564489   -0.4820356465
C    -1.3640288683     1.9151551905    0.5517402609
C    -2.1581557282     0.7596540848    0.6752989976
C    -1.9543594761    -0.2396169074    1.8021847566
H    -0.852078652     -1.7938812909   -0.1533856351
H     1.3413330709    -2.9262192225   -0.1584851392
H     2.8733973426    -2.6886743596    1.7810388575
H     2.1818704796    -1.3137715678    3.7288211548
H    -0.0204175256    -0.1946142425    3.7357363306
H    -4.1729781402     1.2790241423   -2.0584773016
H    -2.7385696538     3.3217656631   -2.230739122
H    -0.9507431928     3.7066818507   -0.5528357355
H    -0.5721007764     2.0906661912    1.2739657347
H    -2.0928517865     0.2703826279    2.7607406284
H    -2.7403293641    -0.9973069838    1.7374322494
                FragmentGeometry[angstrom]      1
            H                    0.000000    0.000000   -0.000000
        SymmetryFactor                  0.5
        PotentialPrefactor[au]          3.3E0
        PotentialPowerExponent          6.
      End
        Frequencies[1/cm]               66
   10.2035              22.3326                62.1988
  186.8317             225.2602               280.8754
  336.6634             414.9156               416.7594
  461.6204             485.0586               554.6195
  614.9393             631.7603               637.6627
  699.2521             716.1932               743.2661
  751.2091             821.2313               830.5175
  856.4369             857.0617               910.7754
  938.6565             946.6597               978.8446
  985.3125             991.1837              1001.6328
 1018.1329            1043.4614              1051.2055
 1098.4716            1120.8067              1170.1853
 1181.2475            1187.3749              1203.2316
 1206.8061            1217.9560              1273.4469
 1315.1428            1330.0131              1342.9235
 1363.1753            1448.1019              1477.4720
 1481.7127            1488.4290              1527.6258
 1574.8945            1625.5531              1634.8420
```

```
1646.6709              3032.2645              3069.6524
3150.3666              3152.3826              3157.8887
3159.3746              3167.5181              3172.2272
3175.5511              3184.1582              3187.0762
      ElectronicLevels[1/cm]                     1
              0         1
      ZeroEnergy[kcal/mol]                       6.0
    End
!--------------------------------
!-------exit_vts3------------
Barrier       vts3 i1 p3
   RRHO
      Stoichiometry   C13H12
      Core        PhaseSpaceTheory
        FragmentGeometry[angstrom]     24
  C    1.4966457158    -0.9769913584    -0.1755634679
  C    2.6898177011    -1.6345483856    0.0863941856
  C    2.9246837744    -2.2198631069    1.3319563768
  C    1.932701221     -2.1573368375    2.3141259782
  C    0.7361385965    -1.509136335     2.0578072233
  C    0.4838597443    -0.8767072029    0.8122201071
  C    -2.6005553705   0.9334442672    -0.5332343601
  C    -3.0873140145   1.8367059552    -1.4632288585
  C    -2.2056265814   2.5734689858    -2.2584273584
  C    -0.8301758988   2.398897915     -2.0944509164
  C    -0.3348599811   1.490582959     -1.1702335097
  C    -1.2081376661   0.7115753135    -0.3688938413
  C    -0.7824579894   -0.2337525604   0.6205540418
  H    1.3219255126    -0.5785837676    -1.1654751064
  H    3.4411272758    -1.7045018967    -0.6927117962
  H    3.8604594262    -2.7295458544    1.5298856228
  H    2.0969738192    -2.6201208319    3.2810333751
  H    -0.0281221803   -1.4662946059   2.826830032
  H    -3.2932731172   0.3663307675    0.0798419418
  H    -4.1577744269   1.9730881771    -1.5708130181
  H    -2.5848928865   3.2830608264    -2.9845482379
  H    -0.137477943    2.9885256356    -2.6851189001
  H    0.7343991918    1.4143206762    -1.028537208
  H    -1.5453759231   -0.5084447353   1.3441976946
                   FragmentGeometry[angstrom]     1
              H               0.000000    0.000000   -0.000000
      SymmetryFactor                   2
      PotentialPrefactor[au]           2.0E0
      PotentialPowerExponent           6.7
    End
    Frequencies[1/cm]                 66
  55.3968              60.4718              110.9993
 204.7807             238.4590             298.2518
 315.8440             411.6149             423.2506
 486.1829             494.7039             578.4475
```

627.1626	629.9209	652.4739
694.5899	703.6792	718.7562
762.8016	798.9911	817.4151
840.5655	848.6304	890.0081
914.9801	921.3018	976.8319
981.2413	994.5749	997.8103
1002.3211	1007.6202	1044.7449
1046.7926	1098.8498	1119.0803
1179.1891	1179.9598	1190.1323
1203.0503	1227.6398	1232.7808
1328.0179	1332.3600	1349.3459
1362.8018	1429.2975	1477.6360
1496.9845	1506.8138	1515.1288
1589.4045	1591.2519	1608.8934
1621.1403	3138.5446	3157.5924
3158.3079	3164.9213	3165.7276
3174.8597	3175.3571	3188.6030
3189.4749	3201.8861	3215.4241

```
      ElectronicLevels[1/cm]                   1
                0        1
      ZeroEnergy[kcal/mol]                    -21.8
    End
!--------------------------------
!-------entrance_vts0------------
Barrier      vts0 p0 i1
   RRHO
      Stoichiometry   C13H12
      Core        PhaseSpaceTheory
        FragmentGeometry[angstrom]     14
C  0.2889157829    1.1989076188    0.4411648713
C  -1.0939883347   1.202675661     0.4413513402
C  -1.807524641   -0.00183713      0.4409711028
C  -1.1122846904   -1.2170022185    0.4403700908
C  0.2705184752    -1.2341476129    0.4401674207
C  1.0223144207    -0.0232362299    0.4405761993
C  2.4261644469    -0.0338459674    0.4404154128
H  0.8358147436    2.1357433166     0.4414659983
H  -1.6293443636   2.1457751577     0.4417863345
H  -2.891236489    0.0063579281     0.4411501041
H  -1.661843269    -2.1518968994    0.4400633889
H  0.803184516    -2.1791485564     0.4396957755
H  2.9936507467    0.8883643322     0.4407885382
H  2.9796546555    -0.9645233999    0.4399094226
                    FragmentGeometry[angstrom]     11
C      0.000000     0.000000     1.390346
C      0.000000     1.221722     0.769740
C      0.000000    -1.221722     0.769740
C      0.000000     1.208778    -0.629525
C      0.000000    -1.208778    -0.629525
C      0.000000     0.000000    -1.319309
```

```
H     0.000000     2.153977     1.319039
H     0.000000    -2.153977     1.319039
H     0.000000     2.145530    -1.172910
H     0.000000    -2.145530     -1.172910
H     0.000000     0.000000    -2.401057
       SymmetryFactor                    4
       PotentialPrefactor[au]            8.300E-2
       PotentialPowerExponent            2.22
    End
     Frequencies[1/cm]                  63
198.8667             359.1502             390.0539
478.5997             501.2484             534.1703
628.2683             684.5115             708.1095
773.6815             828.7779             831.0629
898.2900             969.2522             971.1917
989.2728             994.6949            1036.0538
1116.2301            1174.6185            1184.2088
1288.0210            1327.3993            1351.7755
1473.5146            1490.2047            1502.2589
1576.9663            1598.0668            3144.6294
3158.6802            3161.3193            3173.1335
3178.3546            3191.1353            3240.2830
402. 428. 602. 621. 672. 726. 820. 903. 979. 1001. 1009.
1017. 1052. 1073. 1177. 1177. 1303. 1326. 1464. 1473.
1570. 1627. 3154. 3160. 3173. 3175. 3186.
       ElectronicLevels[1/cm]               1
                0       1
       ZeroEnergy[kcal/mol]                 0.0
    End
!----------------------------------------------------------------
End
```

Input file for RRKM-ME calculations for the $C_7H_7 + C_6H_5 \rightarrow i3 \rightarrow p5 + H$ reaction

```
TemperatureList[K]                          500. 600. 700. 800. 900. 1000. 1125.
1250. 1375. 1500. 1650. 1800. 2000. 2250. 2500.
PressureList[atm]                           0.01 0.03 0.1 0.3 1. 3. 10. 30. 100.
EnergyStepOverTemperature                   0.2            #Ratio of discretization
energy step to T
ExcessEnergyOverTemperature                 60
ModelEnergyLimit[kcal/mol]                   600
WellCutoff                                   10
ChemicalEigenvalueMax                        0.2
ChemicalEigenvalueMin                        1.e-6          #only for direct
diagonalization method
CalculationMethod                           direct
EigenvalueOutput                                      eigenvalue.out
Model
EnergyRelaxation
Exponential
Factor[1/cm]                    424      ! Jasper calc N2
Power                        0.62
ExponentCutoff               15
End
CollisionFrequency
LennardJones
Epsilons[1/cm]          390. 390.     ! N2
Sigmas[angstrom]        4.46 4.46     ! N2
Masses[amu]             28. 168.
End
OutputTemperatureStep[K]  100
OutputTemperatureSize  24
OutputReferenceEnergy[kcal/mol]  0.

!-------well_i2------------
Well        i2
Species
RRHO
Geometry[angstrom]    25
 C   -1.7930983918    -1.4638895517    1.3577136236
 C   -1.0450202364    -2.5604181258    1.1279786114
 C   -0.4542712432    -2.8075158034    -0.1824801406
 C   -0.5759881623    -1.9181417715    -1.1754202042
 C   -1.2905434767    -0.5935191855    -1.0083055208
 C   -2.0561826751    -0.4725338248    0.3216260315
 C   -0.2997551695    0.5584336526    -1.2021083578
 C   0.8214436107    0.6836722783    -0.3736250877
 C   1.7163076387    1.7345723847    -0.54586059
 C   1.5102397277    2.6758935447    -1.5545846745
 C   0.4026078471    2.5567456345    -2.3883531342
 C   -0.4947948063    1.5037183063    -2.2114808269
 C   -2.9383757879    0.5190311432    0.5231959391
```

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```
  H    -2.2484134275    -1.3012995517    2.3295548522
  H    -0.8861275902    -3.2881704345    1.9161121053
  H     0.0897286018    -3.7326554626    -0.3408489302
  H    -0.1263548269    -2.1021519594    -2.1456008673
  H    -2.0228300721    -0.5099166915    -1.8192747241
  H     0.9905916004    -0.0470707413    0.4094457675
  H     2.578370302     1.8194194805    0.1067478161
  H     2.209417762     3.4935826384    -1.6888630024
  H     0.234544047     3.2810104865    -3.177887383
  H    -1.3561313442    1.4164334047    -2.8662806335
  H    -3.1574394348    1.2569959999    -0.2401135467
  H    -3.4591654926    0.6210491495    1.4687508773
Core  RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  69
    22.1633              38.2974              93.8748
   146.3861             251.8784             264.9912
   318.9551             392.2163             414.0003
   454.5218             510.9821             514.0802
   552.2864             599.6679             635.2364
   677.1695             687.1937             714.5069
   755.4239             772.1935             796.3823
   825.8439             854.6916             864.1743
   906.2112             924.1403             942.6002
   965.2338             977.8129             981.8436
   986.3615             997.2084            1000.2882
  1018.1671            1049.9259            1051.5968
  1102.0980            1179.6787            1181.3162
  1198.8082            1203.9080            1206.6173
  1243.2950            1307.6722            1310.9573
  1340.9156            1363.4236            1389.9810
  1426.1864            1465.8203            1484.2630
  1524.2661            1614.9445            1625.8258
  1641.5897            1654.2466            1702.8065
  3016.6620            3134.1727            3151.0046
  3152.1218            3156.2433            3160.3480
  3169.9795            3171.7469            3178.6573
  3182.1685            3187.4805            3216.9897
ZeroEnergy[kcal/mol] -73.9
ElectronicLevels[1/cm]          1
0  1
End
End
!--------------------------------
!-------C13H11_methylbiphenylyl_+_H-----
Bimolecular    p1
Fragment          C13H11_methylbiphenylyl
RRHO
Geometry[angstrom]    24
```

```
C  -0.7875471217  -2.78830363   0.1441505492
 C   0.4052961276  -3.5036701848  0.0553675844
 C   1.6102356122  -2.8157279991  -0.0667058994
 C   1.6220137064  -1.4236937067  -0.0996977234
 C   0.4296975857  -0.6906216111  -0.0165172969
 C  -0.7762529114  -1.3969834143  0.1064222885
 C   0.4601785521   0.7966921726  -0.0076818813
 C   1.2442619795   1.4476739774  0.9428102578
 C   1.2941448379   2.8396358305  1.032105947
 C   0.5381799699   3.6166000866  0.1465086027
 C  -0.2371420112   3.003540562   -0.8159674459
 C  -0.2973042194   1.5830515766  -0.9468755321
 C  -1.0394087256   1.0202973365  -1.9966467686
 H  -1.7299102212  -3.3144976264  0.2497914227
 H   0.3952932654  -4.5874282737  0.0826031593
 H   2.5436985619  -3.3627728608  -0.1404059108
 H   2.5621582496  -0.8941237485  -0.2067251242
 H  -1.7068996355  -0.8480391061  0.1918742965
 H   1.8082397191   0.8482788835  1.6490649808
 H   1.9051843064   3.3120381205  1.7923536947
 H   0.5636567535   4.6985826758  0.2137192323
 H  -0.8105237115   3.6048166145  -1.5135599336
 H  -1.5885338136   1.6615315198  -2.6749788253
 H  -1.0600478561  -0.0436181949  -2.1815076742
Core  RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm]  66
  56.6221              85.4892              104.3971
 190.0667             272.1221             293.2701
 335.5607             414.8131             417.5865
 462.0995             496.2387             529.9331
 564.6945             572.7694             628.1409
 635.2121             716.9757             722.2853
 729.2603             747.2491             774.9307
 787.7997             851.2822             861.3337
 869.4567             935.2312             955.3219
 974.5398             981.1994             983.7465
1002.1584            1009.9229            1018.5056
1054.8197            1063.8429            1101.4682
1147.2280            1177.4468            1182.0509
1204.3945            1256.3570            1280.3224
1303.2919            1320.5277            1323.7417
1354.3146            1447.5337            1477.8982
1484.1055            1496.2888            1526.8738
1560.5677            1601.9080            1615.7417
1642.0681            3154.4815            3159.7412
3159.8953            3166.3412            3167.5917
3176.2300            3177.1826            3183.0145
3190.0562            3190.7040            3257.6793
```

```
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]        1
0  2
End
Fragment          H
Atom
Mass[amu]    1
ElectronicLevels[1/cm]        1
0    2
End
GroundEnergy[kcal/mol] -19.16
End
!-------c7h7_c6h5_p0------------
Bimolecular    p0
Fragment          c7h7
RRHO
Geometry[angstrom]    14
C   0.2889157829    1.1989076188    0.4411648713
C  -1.0939883347    1.202675661    0.4413513402
C  -1.807524641    -0.00183713    0.4409711028
C  -1.1122846904    -1.2170022185    0.4403700908
C   0.2705184752    -1.2341476129    0.4401674207
C   1.0223144207    -0.0232362299    0.4405761993
C   2.4261644469    -0.0338459674    0.4404154128
H   0.8358147436    2.1357433166    0.4414659983
H  -1.6293443636    2.1457751577    0.4417863345
H  -2.891236489    0.0063579281    0.4411501041
H  -1.661843269    -2.1518968994    0.4400633889
H   0.803184516    -2.1791485564    0.4396957755
H   2.9936507467    0.8883643322    0.4407885382
H   2.9796546555    -0.9645233999    0.4399094226
Core   RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm]   36
198.8667               359.1502               390.0539
478.5997               501.2484               534.1703
628.2683               684.5115               708.1095
773.6815               828.7779               831.0629
898.2900               969.2522               971.1917
989.2728               994.6949               1036.0538
1116.2301              1174.6185              1184.2088
1288.0210              1327.3993              1351.7755
1473.5146              1490.2047              1502.2589
1576.9663              1598.0668              3144.6294
3158.6802              3161.3193              3173.1335
3178.3546              3191.1353              3240.2830
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]        1
0  2
```

```
End
     Fragment          C6H5
       RRHO
         Geometry[angstrom]       11
C     0.000000      0.000000      1.390346
C     0.000000      1.221722      0.769740
C     0.000000     -1.221722      0.769740
C     0.000000      1.208778     -0.629525
C     0.000000     -1.208778      -0.629525
C     0.000000      0.000000     -1.319309
H     0.000000      2.153977      1.319039
H     0.000000     -2.153977      1.319039
H     0.000000      2.145530     -1.172910
H     0.000000     -2.145530      -1.172910
H     0.000000      0.000000     -2.401057
         Core      RigidRotor
         SymmetryFactor        2
         End
         Frequencies[1/cm]       27
402. 428. 602. 621. 672. 726. 820. 903. 979. 1001. 1009.
1017. 1052. 1073. 1177. 1177. 1303. 1326. 1464. 1473.
1570. 1627. 3154. 3160. 3173. 3175. 3186.
         ZeroEnergy[kcal/mol]        0.
         ElectronicLevels[1/cm]        1
             0    2
     End
GroundEnergy[kcal/mol] 0.0
End
!-------exit_vts1-------
Barrier      vts1  i2 p1
   RRHO
     Stoichiometry   C13H12
     Core        PhaseSpaceTheory
       FragmentGeometry[angstrom]     24
C  -0.7875471217  -2.78830363  0.1441505492
 C  0.4052961276  -3.5036701848  0.0553675844
 C  1.6102356122  -2.8157279991  -0.0667058994
 C  1.6220137064  -1.4236937067  -0.0996977234
 C  0.4296975857  -0.6906216111  -0.0165172969
 C  -0.7762529114  -1.3969834143  0.1064222885
 C  0.4601785521  0.7966921726  -0.0076818813
 C  1.2442619795  1.4476739774  0.9428102578
 C  1.2941448379  2.8396358305  1.032105947
 C  0.5381799699  3.6166000866  0.1465086027
 C  -0.2371420112  3.003540562  -0.8159674459
 C  -0.2973042194  1.5830515766  -0.9468755321
 C  -1.0394087256  1.0202973365  -1.9966467686
 H  -1.7299102212  -3.3144976264  0.2497914227
 H  0.3952932654  -4.5874282737  0.0826031593
 H  2.5436985619  -3.3627728608  -0.1404059108
```

```
 H   2.5621582496   -0.8941237485   -0.2067251242
 H  -1.7068996355   -0.8480391061    0.1918742965
 H   1.8082397191    0.8482788835    1.6490649808
 H   1.9051843064    3.3120381205    1.7923536947
 H   0.5636567535    4.6985826758    0.2137192323
 H  -0.8105237115    3.6048166145   -1.5135599336
 H  -1.5885338136    1.6615315198   -2.6749788253
 H  -1.0600478561   -0.0436181949   -2.1815076742
                     FragmentGeometry[angstrom]      1
              H                    0.000000    0.000000   -0.000000
        SymmetryFactor                    0.5
        PotentialPrefactor[au]            3.90E0
        PotentialPowerExponent            6.70
     End
      Frequencies[1/cm]                 66
  56.6221            85.4892                104.3971
 190.0667           272.1221                293.2701
 335.5607           414.8131                417.5865
 462.0995           496.2387                529.9331
 564.6945           572.7694                628.1409
 635.2121           716.9757                722.2853
 729.2603           747.2491                774.9307
 787.7997           851.2822                861.3337
 869.4567           935.2312                955.3219
 974.5398           981.1994                983.7465
1002.1584          1009.9229               1018.5056
1054.8197          1063.8429               1101.4682
1147.2280          1177.4468               1182.0509
1204.3945          1256.3570               1280.3224
1303.2919          1320.5277               1323.7417
1354.3146          1447.5337               1477.8982
1484.1055          1496.2888               1526.8738
1560.5677          1601.9080               1615.7417
1642.0681          3154.4815               3159.7412
3159.8953          3166.3412               3167.5917
3176.2300          3177.1826               3183.0145
3190.0562          3190.7040               3257.6793
      ElectronicLevels[1/cm]               1
              0        1
      ZeroEnergy[kcal/mol]                -19.16
    End
!--------------------------------
!-------entrance_vts0------------
Barrier       vts0 p0 i2
   RRHO
      Stoichiometry  C13H12
      Core       PhaseSpaceTheory
      FragmentGeometry[angstrom]     14
C  0.2889157829   1.1989076188   0.4411648713
C  -1.0939883347   1.202675661    0.4413513402
```

```
C  -1.807524641   -0.00183713    0.4409711028
C  -1.1122846904  -1.2170022185   0.4403700908
C  0.2705184752   -1.2341476129   0.4401674207
C  1.0223144207   -0.0232362299   0.4405761993
C  2.4261644469   -0.0338459674   0.4404154128
H  0.8358147436    2.1357433166   0.4414659983
H  -1.6293443636   2.1457751577   0.4417863345
H  -2.891236489    0.0063579281   0.4411501041
H  -1.661843269   -2.1518968994   0.4400633889
H  0.803184516    -2.1791485564   0.4396957755
H  2.9936507467    0.8883643322   0.4407885382
H  2.9796546555   -0.9645233999   0.4399094226
                    FragmentGeometry[angstrom]     11
C      0.000000     0.000000     1.390346
C      0.000000     1.221722     0.769740
C      0.000000    -1.221722     0.769740
C      0.000000     1.208778    -0.629525
C      0.000000    -1.208778    -0.629525
C      0.000000     0.000000    -1.319309
H      0.000000     2.153977     1.319039
H      0.000000    -2.153977     1.319039
H      0.000000     2.145530    -1.172910
H      0.000000    -2.145530    -1.172910
H      0.000000     0.000000    -2.401057
      SymmetryFactor                  4
      PotentialPrefactor[au]          8.300E-2
      PotentialPowerExponent          2.22
   End
   Frequencies[1/cm]                  63
198.8667            359.1502            390.0539
478.5997            501.2484            534.1703
628.2683            684.5115            708.1095
773.6815            828.7779            831.0629
898.2900            969.2522            971.1917
989.2728            994.6949            1036.0538
1116.2301           1174.6185           1184.2088
1288.0210           1327.3993           1351.7755
1473.5146           1490.2047           1502.2589
1576.9663           1598.0668           3144.6294
3158.6802           3161.3193           3173.1335
3178.3546           3191.1353           3240.2830
402. 428. 602. 621. 672. 726. 820. 903. 979. 1001. 1009.
1017. 1052. 1073. 1177. 1177. 1303. 1326. 1464. 1473.
1570. 1627. 3154. 3160. 3173. 3175. 3186.
   ElectronicLevels[1/cm]                    1
              0         1
   ZeroEnergy[kcal/mol]                    0.0
   End
!-------------------------------------------------------------
End
```

Input file for RRKM-ME calculations for the $C_7H_7 + C_6H_5 \rightarrow i0 \rightarrow i2 \rightarrow p2 + H$ reaction

```
TemperatureList[K]                       500. 600. 700. 800. 900. 1000. 1125.
1250. 1375. 1500. 1650. 1800. 2000. 2250. 2500.
PressureList[atm]                        0.01 0.03 0.1 0.3 1. 3. 10. 30. 100.
EnergyStepOverTemperature        0.2          #Ratio of discretization
energy step to T
ExcessEnergyOverTemperature      60
ModelEnergyLimit[kcal/mol]        600
WellCutoff                       10
ChemicalEigenvalueMax            0.2
ChemicalEigenvalueMin            1.e-6        #only for direct
diagonalization method
CalculationMethod                direct
Model
EnergyRelaxation
Exponential
Factor[1/cm]                424     ! Jasper calc N2
Power                       0.62
ExponentCutoff              15
End
CollisionFrequency
LennardJones
Epsilons[1/cm]         390. 390.    ! N2
Sigmas[angstrom]       4.46 4.46    ! N2
Masses[amu]            28. 168.
End
OutputTemperatureStep[K]  100
OutputTemperatureSize  24
OutputReferenceEnergy[kcal/mol]  0.

!-------well_i1t-----------
Well        i1t
Species
RRHO
Geometry[angstrom]    25
 C   -0.9876109047   -1.0369785524   -0.5113777401
 C    0.354616836   -1.5459142374   -0.9324578934
 C    1.2882941309   -1.9111641908   -0.0064561777
 C    1.0678774531   -1.7412583835    1.3848300988
 C   -0.1040563414   -1.0863726493    1.8394523355
 C   -1.0789511505   -0.7160169261    0.9624247982
 C   -1.5425712579    0.2887644848   -1.151682097
 C   -1.974625305    0.283456429    -2.5838779454
 C   -3.181528184    0.8019056475   -2.9543399545
 C   -4.1139411179    1.2823670307   -1.9988996866
 C   -3.8447717907    1.1380228385   -0.6148069269
 C   -2.6492856658    0.6442575942   -0.1861421787
 C   -2.266043365    0.1915988858    1.2070182714
 H   -1.7465802661   -1.8075326361   -0.7561914719
```

```
 H    0.5456389754   -1.6875647277   -1.9912552608
 H    2.2335849586   -2.3295461242   -0.3378570255
 H    1.8285852003   -2.0445818393    2.0934800169
 H   -0.1940879982   -0.8315024654    2.8919334493
 H   -0.7196949035    1.0232264153   -1.0370743378
 H   -1.2772277508   -0.0760150517   -3.3335610767
 H   -3.4474771404    0.8363394895   -4.00625713
 H   -5.0619593315    1.690524233    -2.3268238137
 H   -4.6247138951    1.3741466843    0.1040223518
 H   -1.9940341328    1.0285852159    1.8641134368
 H   -3.101101053    -0.3263891648    1.697548958
Core  RigidRotor
SymmetryFactor  2.0
End
Frequencies[1/cm]  69
   58.1144              89.1220             187.9645
  217.5578             221.5853            369.8029
  376.2055             378.8243            458.4420
  492.5039             503.9110            518.2635
  587.7553             590.5182            616.5066
  660.4993             671.3597            687.5000
  759.4598             766.5598            782.5083
  794.8508             869.0316            887.1256
  926.7397             936.9702            959.7368
  965.9953             969.1840            995.5961
  999.7065            1012.4916           1040.5547
 1060.0004            1116.6020           1118.3686
 1141.6782            1150.7912           1168.3608
 1170.7986            1197.2613           1200.0394
 1233.4165            1247.1265           1296.9250
 1297.6073            1337.0845           1343.9530
 1388.2460            1403.5414           1430.3756
 1431.6241            1458.4102           1537.7066
 1543.1069            1604.3712           1611.6755
 2854.1664            2862.9086           2986.1501
 3003.7233            3143.2534           3143.4879
 3148.0416            3149.4743           3166.0202
 3168.1549            3190.0943           3190.3779
ZeroEnergy[kcal/mol] -31.7
ElectronicLevels[1/cm]          1
0  3
End
End
!--------------------------------
!-------well_i0t-----------
Well        i0t
Species
RRHO
Geometry[angstrom]   25
 C   1.4076997065   -0.1034984391    1.3711285266
```

```
C    2.5212537047    -0.9281913936    1.4974720515
C    3.4756737849    -0.9771635121    0.4816833888
C    3.3072539068    -0.1946749332    -0.6571324882
C    2.1919678358    0.6334021905    -0.7777220379
C    1.2303051975    0.6916718855    0.2336325467
C    -1.3936747329    0.0151549813    -1.4084276955
C    -2.2964715349    -1.1585328899    -1.3794475599
C    -3.3487825699    -1.1180469944    -0.5271098057
C    -3.4480922982    -0.0662264169    0.4519747897
C    -2.3414172978    0.8120141953    0.6788129853
C    -1.2581339321    0.8054419619    -0.1481617204
C    0.0038936725    1.5836722229    0.1048978247
H    0.6637616975    -0.076512686    2.1608412645
H    2.6455096722    -1.5335479054    2.3887012826
H    4.3432770746    -1.6200685605    0.5790341656
H    4.0438364448    -0.2259630183    -1.4525121416
H    2.0693916503    1.2448377636    -1.6659780964
H    -1.3943738233    0.6039115681    -2.3334146345
H    -2.1432837301    -1.9887612886    -2.0607940559
H    -4.0892836868    -1.912258149    -0.5220669031
H    -4.2961960652    -0.0414453766    1.125085398
H    -2.3421228882    1.4374594229    1.5680814237
H    0.1698421168    2.2868306112    -0.7221837641
H    -0.1164859056    2.1840477606    1.0119902554
Core   RigidRotor
SymmetryFactor   0.5
End
Frequencies[1/cm]   69
   12.5736              47.8804              51.9165
  146.6525             208.1619             240.7301
  300.6211             358.9983             412.1631
  414.6236             423.4169             454.4620
  529.9102             550.0569             591.4162
  632.5932             637.9540             702.5287
  713.4988             735.8042             756.1876
  812.2327             827.8433             853.7334
  878.7046             907.3289             925.7945
  939.1383             956.8854             972.9119
  975.5519             999.8057            1007.0589
 1018.3018            1050.5634            1074.4990
 1102.0881            1162.3833            1171.3170
 1181.3240            1201.3294            1202.4912
 1210.8679            1290.5982            1308.8257
 1338.1809            1342.5363            1358.7365
 1363.5651            1399.1737            1474.5695
 1485.0258            1526.5064            1541.3469
 1592.6650            1626.1775            1644.2849
 2994.1634            3006.9341            3055.2024
 3135.5461            3146.2570            3153.2739
 3156.5776            3166.3852            3166.7341
```

```
3174.9541              3186.6176                  3189.7445
ZeroEnergy[kcal/mol] -18.3
ElectronicLevels[1/cm]        1
0   3
End
End
!-------------------------------
!-------C13H11_ni2_+_H-----
Bimolecular    p2
Fragment          C13H11_ni2
RRHO
Geometry[angstrom]    24
 C    -0.6919815228    -1.3415673097    0.9390533896
 C    -0.1067171046    -2.0977773324    -0.1084101519
 C     0.3589853058    -1.4441227525    -1.2788982955
 C     0.3789653912    -0.0841874778    -1.383719639
 C     0.0344047417     0.7739786919    -0.2018619637
 C    -0.6818330972     0.019120829      0.8992808579
 C    -0.8518001312     2.0053881106    -0.3689535916
 C    -0.8769325757     2.9449103202    -1.3921344283
 C    -1.7573869583     4.0250315086    -1.2997614705
 C    -2.5921323062     4.1635799494    -0.1911606661
 C    -2.5608461375     3.2221624996     0.8396542383
 C    -1.6917408167     2.1413925952     0.7441566312
 C    -1.4838371817     0.9975166039     1.7234290897
 H    -1.2131128641    -1.8590877049     1.7395581
 H    -0.106503359     -3.1796749425    -0.0591524243
 H     0.6806341957    -2.0488424616    -2.1208912727
 H     0.7235830473     0.3964148371    -2.2929601567
 H     0.9981954889     1.1498974518     0.2100111798
 H    -0.2293955634     2.8442594947    -2.2567568814
 H    -1.7937763133     4.7597877072    -2.0964220076
 H    -3.2734818182     5.0050397941    -0.1319494169
 H    -3.2153036713     3.3320100324     1.6984136517
 H    -0.9220074855     1.3472363834     2.6035030199
 H    -2.419643264      0.5697071724     2.094725208
Core   RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm]   66
  66.6269              113.7563                   189.8079
 234.5266              261.4251                   375.1644
 414.6820              436.0679                   460.1399
 499.6617              523.1885                   531.6440
 599.3132              618.9702                   659.6740
 694.7568              726.5271                   747.0838
 760.5556              788.0786                   828.6653
 838.4535              881.4565                   899.1028
 936.5936              952.9719                   962.8894
 977.9175              989.3212                  1001.3748
```

1036.8506	1047.8001	1103.2091
1119.4176	1152.2939	1155.5853
1175.5692	1180.7926	1196.1051
1218.8555	1220.5050	1239.9407
1278.0366	1314.3951	1343.6776
1345.7142	1387.6792	1428.7824
1468.0085	1491.1299	1505.4258
1539.1877	1609.4647	1626.9112
1647.9654	2802.3109	2964.8057
3053.8233	3146.0840	3151.8653
3154.8483	3160.8244	3170.8411
3172.5600	3184.8348	3190.3150

```
ZeroEnergy[kcal/mol]     0.0
ElectronicLevels[1/cm]        1
0  2
End
Fragment        H
Atom
Mass[amu]   1
ElectronicLevels[1/cm]        1
0    2
End
GroundEnergy[kcal/mol] -12.2
End
!-------c7h7_c6h5_p0------------
Bimolecular    p0
Fragment        c7h7
RRHO
Geometry[angstrom]   14
C   0.2889157829    1.1989076188    0.4411648713
C  -1.0939883347    1.202675661     0.4413513402
C  -1.807524641    -0.00183713     0.4409711028
C  -1.1122846904   -1.2170022185    0.4403700908
C   0.2705184752   -1.2341476129    0.4401674207
C   1.0223144207   -0.0232362299    0.4405761993
C   2.4261644469   -0.0338459674    0.4404154128
H   0.8358147436    2.1357433166    0.4414659983
H  -1.6293443636    2.1457751577    0.4417863345
H  -2.891236489     0.0063579281    0.4411501041
H  -1.661843269    -2.1518968994    0.4400633889
H   0.803184516    -2.1791485564    0.4396957755
H   2.9936507467    0.8883643322    0.4407885382
H   2.9796546555   -0.9645233999    0.4399094226
Core  RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm]   36
```

198.8667	359.1502	390.0539
478.5997	501.2484	534.1703
628.2683	684.5115	708.1095

```
773.6815              828.7779              831.0629
898.2900              969.2522              971.1917
989.2728              994.6949             1036.0538
1116.2301            1174.6185             1184.2088
1288.0210            1327.3993             1351.7755
1473.5146            1490.2047             1502.2589
1576.9663            1598.0668             3144.6294
3158.6802            3161.3193             3173.1335
3178.3546            3191.1353             3240.2830
ZeroEnergy[kcal/mol]     0.0
ElectronicLevels[1/cm]         1
0  2
End
      Fragment          C6H5
       RRHO
         Geometry[angstrom]      11
C     0.000000     0.000000     1.390346
C     0.000000     1.221722     0.769740
C     0.000000    -1.221722      0.769740
C     0.000000     1.208778    -0.629525
C     0.000000    -1.208778     -0.629525
C     0.000000     0.000000    -1.319309
H     0.000000     2.153977     1.319039
H     0.000000    -2.153977      1.319039
H     0.000000     2.145530    -1.172910
H     0.000000    -2.145530     -1.172910
H     0.000000     0.000000    -2.401057
         Core      RigidRotor
         SymmetryFactor         2
         End
         Frequencies[1/cm]       27
402. 428. 602. 621. 672. 726. 820. 903. 979. 1001. 1009.
1017. 1052. 1073. 1177. 1177. 1303. 1326. 1464. 1473.
1570. 1627. 3154. 3160. 3173. 3175. 3186.
         ZeroEnergy[kcal/mol]        0.
         ElectronicLevels[1/cm]       1
            0   2
     End
GroundEnergy[kcal/mol] 0.0
End
   Barrier      ts2t   p0   i0t    #  ts2t
     RRHO
         Geometry[angstrom]      25        #
 C   1.3549024498   -0.9138689422    -0.0278337415
 C   2.5465498308   -1.6474865312    -0.0508331427
 C   3.7761668156   -0.9907741703    -0.0277910285
 C   3.8270893257    0.4020063889    0.018342936
 C   2.6420642803    1.1455426162    0.0416745468
 C   1.4412941073    0.4636618243    0.0178279576
 C   -2.0291302026    0.4323000777    -1.2441338965
```

```
C    -3.097473583    -0.4022136141    -1.2556404928
C    -3.669746011    -0.8878992589    -0.0324634411
C    -3.1001716878   -0.4842455115     1.2214115669
C    -2.0318652098    0.3491227492     1.2674675701
C    -1.4221613383    0.8776926282     0.0284577156
C    -0.2724205321    1.642140791      0.0550256272
H     0.3948686817   -1.4172628583    -0.0455139806
H     2.5098870532   -2.7317547114    -0.0867464501
H     4.6960151037   -1.5644339346    -0.0457856654
H     4.7849800383    0.9124057479     0.0362551688
H     2.677615418     2.2309543597     0.077621671
H    -1.5948624921    0.79398965      -2.1697118258
H    -3.5326962475   -0.7133889434    -2.1992544275
H    -4.521362099    -1.555224866     -0.0554907877
H    -3.5374268801   -0.857136081      2.1414205404
H    -1.5996421415    0.6487545911     2.2158906832
H     0.0231350225    2.1695401982    -0.8463739645
H     0.0211492979    2.1086988007     0.9899938612
      Core      RigidRotor
        SymmetryFactor     1.0
      End
      Tunneling        Eckart
        ImaginaryFrequency[1/cm]     769.6639
        WellDepth[kcal/mol]          6.8
        WellDepth[kcal/mol]          25.1
      End
      Frequencies[1/cm]      68
   13.4146                38.6773
   49.1662               105.6327                113.1563
  169.3899               358.2881                368.1409
  393.7224               402.1022                433.2211
  504.4884               527.7411                563.7550
  573.5320               615.0976                688.0445
  690.6430               717.1816                725.5493
  738.5657               781.5865                832.6623
  844.8450               848.7505                902.4237
  942.5551               952.9041                964.0224
  965.8346               968.8213                983.6326
  994.6018              1006.6876               1029.6257
 1033.1654              1059.5917               1081.5529
 1147.0865              1176.3807               1184.5857
 1199.8955              1276.2732               1319.9922
 1325.0893              1343.8976               1348.8820
 1382.5629              1443.4969               1464.2342
 1476.8087              1521.3509               1564.1518
 1585.8043              1624.3265               1668.2230
 3108.0679              3136.3256               3151.5596
 3158.6081              3158.8485               3159.0935
 3173.5594              3177.7433               3178.1950
 3182.0764              3192.7127               3200.4390
```

```
        ZeroEnergy[kcal/mol]           6.8
        ElectronicLevels[1/cm]         1
            0    3
    End
    Barrier        tts1    i0t    i1t    #   t-ts1
      RRHO
        Geometry[angstrom]        25          #
C                 0.918857   -0.439287    0.716346
C                 1.935928   -1.428388    0.663905
C                 3.164151   -1.134010    0.100406
C                 3.428575    0.151261   -0.398574
C                 2.430946    1.134701   -0.359741
C                 1.195309    0.869643    0.204648
C                -0.866910   -0.448498   -0.688479
C                -1.875475   -1.503392   -0.553757
C                -3.131567   -1.192726   -0.145451
C                -3.482092    0.155112    0.229399
C                -2.480660    1.152303    0.288635
C                -1.202372    0.890603   -0.123053
C                -0.003160    1.781950    0.084656
H                 0.111647   -0.563369    1.433492
H                 1.747269   -2.410229    1.083183
H                 3.936952   -1.894203    0.060820
H                 4.397438    0.378708   -0.827517
H                 2.619524    2.109817   -0.798950
H                -0.276411   -0.450743   -1.608460
H                -1.618080   -2.518536   -0.836872
H                -3.891065   -1.965753   -0.085737
H                -4.494563    0.380348    0.539689
H                -2.721636    2.121440    0.717798
H                 0.140856    2.465667   -0.763143
H                -0.141103    2.411219    0.972064
        Core       RigidRotor
          SymmetryFactor      0.5
        End
        Tunneling       Eckart
          ImaginaryFrequency[1/cm]     392.8453
          WellDepth[kcal/mol]          9.4
          WellDepth[kcal/mol]          22.8
        End
        Frequencies[1/cm]       68
   61.3144              90.6384
  135.1280             219.6663                250.4868
  316.4309             335.1645                402.9791
  437.0346             479.8177                511.2574
  527.4324             585.4212                606.4753
  620.3294             658.7804                705.4819
  730.3297             749.1598                762.1711
  778.8549             814.0455                840.5488
  867.2446             874.9008                913.9074
```

```
  933.6068                957.2023                964.3137
  970.3488                977.1922               1005.5051
 1009.6388               1034.7350               1081.1192
 1085.8341               1154.2377               1164.6699
 1171.0063               1184.2252               1187.7340
 1203.8561               1245.0572               1320.4434
 1335.2695               1348.9018               1353.1979
 1374.3309               1414.9604               1441.7543
 1455.7602               1507.9655               1536.5327
 1555.1402               1578.6195               1618.1475
 2991.5229               3029.0478               3042.3414
 3117.6496               3138.9202               3150.1187
 3151.1395               3160.2279               3170.2920
 3176.6508               3186.9936               3193.3025
         ZeroEnergy[kcal/mol]            -8.9
         ElectronicLevels[1/cm]           1
           0    3
   End
   Barrier        tts2   i1t   p2    #  t-ts2
     RRHO
       Geometry[angstrom]       25          #
C                 -0.737173   -0.463807   -0.579912
C                 -1.698233   -1.527040   -0.142224
C                 -2.969063   -1.200576    0.226346
C                 -3.397997    0.149784    0.323055
C                 -2.466739    1.203320    0.143121
C                 -1.189967    0.941242   -0.250046
C                  0.719618   -0.448892   -0.092614
C                  1.658769   -1.496014   -0.095876
C                  3.000411   -1.200853    0.111790
C                  3.423620    0.124488    0.255214
C                  2.507768    1.176733    0.160702
C                  1.165579    0.894447   -0.037531
C                  0.010243    1.858742   -0.235012
H                 -0.651108   -0.546375   -1.685566
H                 -1.384812   -2.564106   -0.193922
H                 -3.669935   -1.989513    0.479850
H                 -4.415260    0.372059    0.620518
H                 -2.763833    2.220207    0.383479
H                  0.262532   -0.593600    1.718071
H                  1.334195   -2.524228   -0.211748
H                  3.727926   -2.003722    0.155099
H                  4.474050    0.338315    0.416971
H                  2.851625    2.203735    0.230685
H                 -0.053355    2.618159    0.551222
H                  0.126959    2.399621   -1.186726
        Core      RigidRotor
          SymmetryFactor     0.5
        End
        Tunneling       Eckart
```

```
        ImaginaryFrequency[1/cm]      776.8431
        WellDepth[kcal/mol]           26.0
        WellDepth[kcal/mol]           6.7
      End
      Frequencies[1/cm]      68
  66.4051              116.6571
 191.3607              230.4545                 245.0702
 371.3675              374.6086                 415.4818
 432.0065              461.6185                 497.7099
 508.8164              533.5652                 537.2387
 600.1871              621.2467                 657.0193
 698.4997              710.0519                 744.1148
 760.3839              788.5689                 828.9691
 834.6155              877.6520                 898.8758
 937.6395              954.9347                 963.7646
 977.0274              988.0485                 999.9896
1037.5245             1044.2923                1101.8512
1118.9400             1154.7130                1157.0228
1176.5943             1177.0261                1192.2611
1211.1432             1220.1266                1235.3713
1279.0607             1308.6495                1336.6587
1344.8525             1390.4699                1429.5191
1462.5443             1479.6427                1492.6704
1541.6191             1597.2058                1612.0575
1627.5752             2822.6797                2965.4763
3040.3756             3146.9677                3152.8576
3156.7252             3163.5344                3171.8185
3175.3584             3186.9828                3191.3952
        ZeroEnergy[kcal/mol]          -5.7
        ElectronicLevels[1/cm]        1
            0    3
    End
End
```

Input file for RRKM-ME calculations on the C$_{13}$H$_{11}$ PES

```
TemperatureList[K]                            500. 600. 700. 800. 900. 1000. 1125.
1250. 1375. 1500. 1650. 1800. 2000. 2250. 2500.
PressureList[atm]                             0.01 0.03 0.1 0.3 1. 3. 10. 30. 100.
EnergyStepOverTemperature         0.2          #Ratio of discretization
energy step to T
ExcessEnergyOverTemperature       60
ModelEnergyLimit[kcal/mol]         600
WellCutoff                         10
ChemicalEigenvalueMax              0.2
ChemicalEigenvalueMin              1.e-6        #only for direct
diagonalization method
CalculationMethod                  direct
EigenvalueOutput                               eigenvalue.out
Model
EnergyRelaxation
Exponential
Factor[1/cm]                       424    ! Jasper calc N2
Power                      0.62
ExponentCutoff             15
End
CollisionFrequency
LennardJones
Epsilons[1/cm]          390. 390.    ! N2
Sigmas[angstrom]        4.46 4.46    ! N2
Masses[amu]             28. 167.
End
OutputTemperatureStep[K]  100
OutputTemperatureSize  24
OutputReferenceEnergy[kcal/mol]  0.

!-------well_ni1-----------
Well        ni1
Species
RRHO
Geometry[angstrom]    24
 C   -0.1907879155   -1.6923463249   0.7008642929
 C    1.0468590267   -2.3270483183   0.6961722165
 C    1.9083316335   -2.1946345711   1.7854346839
 C    1.5200807237   -1.4237424273   2.8767214928
 C    0.2772771116   -0.7902326502   2.8784358992
 C   -0.593909834    -0.9158146545   1.7938623297
 C   -3.1267363177    0.6133791038   -0.2920172972
 C   -3.3863346235    1.4690604919   -1.3366216802
 C   -2.5801768795    2.6101227258   -1.4274183278
 C   -1.5754876544    2.8234564489   -0.4820356465
 C   -1.3640288683    1.9151551905   0.5517402609
 C   -2.1581557282    0.7596540848   0.6752989976
 C   -1.9543594761   -0.2396169074   1.8021847566
```

```
 H    -0.852078652    -1.7938812909    -0.1533856351
 H     1.3413330709   -2.9262192225    -0.1584851392
 H     2.8733973426   -2.6886743596     1.7810388575
 H     2.1818704796   -1.3137715678     3.7288211548
 H    -0.0204175256   -0.1946142425     3.7357363306
 H    -4.1729781402    1.2790241423    -2.0584773016
 H    -2.7385696538    3.3217656631    -2.230739122
 H    -0.9507431928    3.7066818507    -0.5528357355
 H    -0.5721007764    2.0906661912     1.2739657347
 H    -2.0928517865    0.2703826279     2.7607406284
 H    -2.7403293641   -0.9973069838     1.7374322494
Core   RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm]   66
   10.2035              22.3326              62.1988
  186.8317             225.2602             280.8754
  336.6634             414.9156             416.7594
  461.6204             485.0586             554.6195
  614.9393             631.7603             637.6627
  699.2521             716.1932             743.2661
  751.2091             821.2313             830.5175
  856.4369             857.0617             910.7754
  938.6565             946.6597             978.8446
  985.3125             991.1837            1001.6328
 1018.1329            1043.4614            1051.2055
 1098.4716            1120.8067            1170.1853
 1181.2475            1187.3749            1203.2316
 1206.8061            1217.9560            1273.4469
 1315.1428            1330.0131            1342.9235
 1363.1753            1448.1019            1477.4720
 1481.7127            1488.4290            1527.6258
 1574.8945            1625.5531            1634.8420
 1646.6709            3032.2645            3069.6524
 3150.3666            3152.3826            3157.8887
 3159.3746            3167.5181            3172.2272
 3175.5511            3184.1582            3187.0762
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm]          1
0  2
End
End
!--------------------------------
!-------well_ni2-----------
Well         ni2
Species
RRHO
Geometry[angstrom]    24
 C    -0.6919815228    -1.3415673097     0.9390533896
 C    -0.1067171046    -2.0977773324    -0.1084101519
```

```
C    0.3589853058    -1.4441227525    -1.2788982955
C    0.3789653912    -0.0841874778    -1.383719639
C    0.0344047417    0.7739786919    -0.2018619637
C    -0.6818330972    0.019120829    0.8992808579
C    -0.8518001312    2.0053881106    -0.3689535916
C    -0.8769325757    2.9449103202    -1.3921344283
C    -1.7573869583    4.0250315086    -1.2997614705
C    -2.5921323062    4.1635799494    -0.1911606661
C    -2.5608461375    3.2221624996    0.8396542383
C    -1.6917408167    2.1413925952    0.7441566312
C    -1.4838371817    0.9975166039    1.7234290897
H    -1.2131128641    -1.8590877049    1.7395581
H    -0.106503359    -3.1796749425    -0.0591524243
H    0.6806341957    -2.0488424616    -2.1208912727
H    0.7235830473    0.3964148371    -2.2929601567
H    0.9981954889    1.1498974518    0.2100111798
H    -0.2293955634    2.8442594947    -2.2567568814
H    -1.7937763133    4.7597877072    -2.0964220076
H    -3.2734818182    5.0050397941    -0.1319494169
H    -3.2153036713    3.3320100324    1.6984136517
H    -0.9220074855    1.3472363834    2.6035030199
H    -2.419643264    0.5697071724    2.094725208
Core   RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm]   66
   66.6269              113.7563              189.8079
  234.5266              261.4251              375.1644
  414.6820              436.0679              460.1399
  499.6617              523.1885              531.6440
  599.3132              618.9702              659.6740
  694.7568              726.5271              747.0838
  760.5556              788.0786              828.6653
  838.4535              881.4565              899.1028
  936.5936              952.9719              962.8894
  977.9175              989.3212             1001.3748
 1036.8506             1047.8001             1103.2091
 1119.4176             1152.2939             1155.5853
 1175.5692             1180.7926             1196.1051
 1218.8555             1220.5050             1239.9407
 1278.0366             1314.3951             1343.6776
 1345.7142             1387.6792             1428.7824
 1468.0085             1491.1299             1505.4258
 1539.1877             1609.4647             1626.9112
 1647.9654             2802.3109             2964.8057
 3053.8233             3146.0840             3151.8653
 3154.8483             3160.8244             3170.8411
 3172.5600             3184.8348             3190.3150
ZeroEnergy[kcal/mol] -18.2
ElectronicLevels[1/cm]          1
```

```
0  2
End
End
!----------------------------------
!-------well_ni3-----------
Well          ni3
Species
RRHO
Geometry[angstrom]    24
  C    1.4966457158   -0.9769913584   -0.1755634679
  C    2.6898177011   -1.6345483856    0.0863941856
  C    2.9246837744   -2.2198631069    1.3319563768
  C    1.932701221    -2.1573368375    2.3141259782
  C    0.7361385965   -1.509136335     2.0578072233
  C    0.4838597443   -0.8767072029    0.8122201071
  C   -2.6005553705    0.9334442672   -0.5332343601
  C   -3.0873140145    1.8367059552   -1.4632288585
  C   -2.2056265814    2.5734689858   -2.2584273584
  C   -0.8301758988    2.398897915    -2.0944509164
  C   -0.3348599811    1.490582959    -1.1702335097
  C   -1.2081376661    0.7115753135   -0.3688938413
  C   -0.7824579894   -0.2337525604    0.6205540418
  H    1.3219255126   -0.5785837676   -1.1654751064
  H    3.4411272758   -1.7045018967   -0.6927117962
  H    3.8604594262   -2.7295458544    1.5298856228
  H    2.0969738192   -2.6201208319    3.2810333751
  H   -0.0281221803   -1.4662946059    2.826830032
  H   -3.2932731172    0.3663307675    0.0798419418
  H   -4.1577744269    1.9730881771   -1.5708130181
  H   -2.5848928865    3.2830608264   -2.9845482379
  H   -0.137477943     2.9885256356   -2.6851189001
  H    0.7343991918    1.4143206762   -1.028537208
  H   -1.5453759231   -0.5084447353    1.3441976946
Core  RigidRotor
SymmetryFactor 2.0
End
Frequencies[1/cm]   66
    55.3968              60.4718              110.9993
   204.7807             238.4590             298.2518
   315.8440             411.6149             423.2506
   486.1829             494.7039             578.4475
   627.1626             629.9209             652.4739
   694.5899             703.6792             718.7562
   762.8016             798.9911             817.4151
   840.5655             848.6304             890.0081
   914.9801             921.3018             976.8319
   981.2413             994.5749             997.8103
  1002.3211            1007.6202            1044.7449
  1046.7926            1098.8498            1119.0803
  1179.1891            1179.9598            1190.1323
```

```
1203.0503            1227.6398            1232.7808
1328.0179            1332.3600            1349.3459
1362.8018            1429.2975            1477.6360
1496.9845            1506.8138            1515.1288
1589.4045            1591.2519            1608.8934
1621.1403            3138.5446            3157.5924
3158.3079            3164.9213            3165.7276
3174.8597            3175.3571            3188.6030
3189.4749            3201.8861            3215.4241
ZeroEnergy[kcal/mol] -27.8
ElectronicLevels[1/cm]          1
0  2
End
End
!--------------------------------
!------well_i4-----------
Well          i4
Species
RRHO
Geometry[angstrom]    24
  C    0.9108803453   -0.0527333809   -0.0922011622
  C    2.3568613473    0.2936374731    0.0967016195
  C    3.1063928653   -0.4112467953    0.9732936265
  C    2.5246819782   -1.4045292969    1.8463417101
  C    1.1599793987   -1.5652052645    1.9296606851
  C    0.3195481867   -0.8084658935    1.0890346347
  C   -2.668384409     0.8900053953   -0.1893372177
  C   -2.7567144751    1.6741862674   -1.3173322634
  C   -1.5860345064    1.9779164839   -2.1076217641
  C   -0.3430488418    1.6380621583   -1.6995404095
  C   -0.1410479886    1.0636309505   -0.3299560488
  C   -1.4052683988    0.446029074    0.2500171453
  C   -1.0525073539   -0.5583893475    1.1533241925
  H    0.845450157    -0.7275549699   -0.9698376155
  H    2.8078431317    1.0477360226   -0.5407160129
  H    4.1712704317   -0.218397049    1.0536218839
  H    3.1768310346   -1.9608087531    2.5098062453
  H    0.7284047923   -2.2025207952    2.6952085842
  H   -3.5680748394    0.5419456506    0.3085682149
  H   -3.7268093659    1.9952890801   -1.6789157298
  H   -1.7269056597    2.4691090983   -3.0649555456
  H    0.5243251524    1.8595314109   -2.3135166663
  H    0.1433384515    1.9005530407    0.3398301087
  H   -1.745191434    -1.0708935601    1.810860785
Core  RigidRotor
SymmetryFactor 2.0
End
Frequencies[1/cm]  66
   94.6693             99.6577            201.5188
  224.3897            250.1899            378.5865
```

408.8870	455.7836	463.5482
492.8489	510.5679	546.3381
589.5090	616.8035	668.3481
672.8656	702.1430	706.7866
790.0879	792.1346	811.5573
845.5630	879.6903	902.6986
940.1247	942.6580	945.7001
978.0654	979.4533	981.8387
983.0875	1043.4743	1060.9648
1078.2554	1116.9129	1155.9294
1164.1815	1174.6000	1183.8457
1206.8089	1234.6435	1269.6268
1288.0786	1304.3991	1339.6499
1352.0296	1356.6748	1395.0752
1429.0859	1452.1301	1483.3311
1535.3013	1535.7070	1630.7067
1639.7208	2860.3453	2868.2360
3147.9574	3149.1181	3154.6543
3155.1974	3167.2713	3168.3419
3182.5092	3183.6445	3184.3006

ZeroEnergy[kcal/mol] 1.656
ElectronicLevels[1/cm]   1
0 2
End
End
!--------------------------------
!-------well_i5-----------
Well   i5
Species
RRHO
Geometry[angstrom]   24
  C   0.7209693918   -0.1551034489   0.0941226117
  C   2.1751224724   0.1974686775   0.3290320915
  C   2.8947222492   -0.5529883299   1.1788521503
  C   2.280931613   -1.621054082   1.9700565028
  C   0.937794751   -1.7389476561   2.0665670355
  C   0.1144201329   -0.7889310876   1.3373397139
  C   -2.7154303862   1.3157777157   0.3076095022
  C   -2.8570352364   1.9211783785   -0.906399567
  C   -1.7524748872   2.1051494628   -1.7815682014
  C   -0.5095369794   1.4927815593   -1.4842708135
  C   -0.306226395   0.8950522893   -0.2752562548
  C   -1.339559034   1.0015246802   0.8262139456
  C   -1.0589403882   -0.2290562583   1.6698706774
  H   0.7314697845   -0.9117336271   -0.7129470153
  H   2.6303850052   0.9863525019   -0.2601968638
  H   3.9572041006   -0.3715536474   1.3036478476
  H   2.9287840361   -2.2706939186   2.5484692173
  H   0.4825050965   -2.4499366554   2.747881784
  H   -3.5688203343   1.1568108866   0.9583318099

```
   H    -3.8408560115    2.2412501106    -1.2347269422
   H    -1.898152472     2.5987076748    -2.734691216
   H     0.2432328113    1.4207055816    -2.2648240366
   H    -1.0747997485    1.8690805868     1.4755259254
   H    -1.6699195718   -0.5139013944     2.5192720954
Core   RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm]   66
   73.1116              100.0293               187.6554
  209.8289              245.6303               368.6600
  386.0915              432.8777               476.5211
  493.7903              520.1797               546.0741
  593.6842              607.8083               657.3760
  673.8518              690.3842               727.3137
  760.2781              776.1971               791.0316
  850.7570              863.1025               884.5814
  908.9052              948.6435               960.7750
  964.2961              977.0147               986.9848
  996.8273             1023.5325              1045.1264
 1067.4788             1118.8439              1153.6314
 1162.4295             1172.2700              1187.0680
 1201.7943             1225.1241              1238.5336
 1272.4779             1280.4870              1318.7769
 1335.7754             1382.5671              1389.6223
 1421.8368             1434.5665              1532.7578
 1585.8628             1597.3466              1651.7303
 1688.5487             2775.1252              2897.3109
 3141.1389             3150.9448              3151.7692
 3160.1786             3169.8480              3173.3341
 3176.8995             3182.1432              3188.6072
ZeroEnergy[kcal/mol] 16.52
ElectronicLevels[1/cm]          1
0  2
End
End
!-------fluorene----------------
Bimolecular    fluorene
Fragment          c13h10
RRHO
Geometry[angstrom]    23
  C    -0.7775947216   -2.4173702899     1.1301353032
  C     0.4170543452   -3.1415135829     1.1248697995
  C     1.6471512249   -2.4802987206     1.1157827503
  C     1.7055894041   -1.0876168843     1.1117304512
  C     0.5142702267   -0.3623063018     1.1169244363
  C    -0.7251562446   -1.0304050176     1.1260861048
  C     0.2659806896    1.0855043795     1.1147119057
  C     1.1475639291    2.166286728      1.1067185891
  C     0.6284421886    3.4599261119     1.1065818136
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  C    -0.7516835858     3.673531333     1.1143226475
  C    -1.636794025      2.5927392088    1.1223233178
  C    -1.1252320973     1.3024911977    1.122470168
  C    -1.8563715793    -0.0236384455    1.1300186469
  H    -1.7298865504    -2.9376950689    1.1372164169
  H     0.3890612051    -4.2253163921    1.1279338187
  H     2.5657412349    -3.0563338087    1.1118283315
  H     2.664991273     -0.581950669     1.1046417118
  H     2.2206316168     2.0091528683    1.1006566606
  H     1.3026200919     4.3090933465    1.1004174355
  H    -1.139189471      4.6860820207    1.1141405957
  H    -2.7080426649     2.7660607507    1.128312936
  H    -2.4967088442    -0.1321017582    2.0129519147
  H    -2.5061326457    -0.1364060057    0.2544902447
Core  RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm]   63
   98.2467             136.7023             217.1353
  242.4856             276.0305             419.8121
  422.9541             437.4613             480.8764
  498.8089             553.8100             576.4901
  637.0948             645.1439             711.9176
  741.2213             754.4593             756.1212
  796.3666             813.9211             853.6331
  870.8892             879.7877             930.6185
  947.8700             972.8919             987.8059
  989.8239            1024.6443            1046.1974
 1052.2321            1117.4362            1131.0016
 1162.4774            1176.1838            1180.1610
 1192.1604            1207.3507            1220.5716
 1252.7137            1320.1064            1329.5667
 1344.5349            1374.7729            1451.2749
 1478.6003            1484.8995            1509.4957
 1510.8004            1619.7890            1624.1355
 1649.0451            1650.1625            3022.6596
 3047.4009            3157.5485            3157.9697
 3163.6104            3165.3387            3174.7206
 3176.0473            3187.4146            3188.1642
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]        1
0  1
End
Fragment          H
Atom
Mass[amu]    1
ElectronicLevels[1/cm]        1
0    2
End
GroundEnergy[kcal/mol] -5.2
```

End
!-------C13H10_p1----------------
Bimolecular   p1
Fragment   c13h10
RRHO
Geometry[angstrom]   23
  C   0.4964214166   -0.8786815955   -0.4843768379
  C   1.970340934   -0.613696825   -0.3435835666
  C   2.698721801   -1.3874091125   0.479984853
  C   2.0817167656   -2.3909127037   1.3405986531
  C   0.7352021191   -2.4719855247   1.48070067
  C   -0.0972951873   -1.5677732022   0.7310515727
  C   -2.7788868004   0.7919221469   -0.0995868413
  C   -2.7750485065   1.7996570696   -1.0628810188
  C   -1.6653074216   1.9980896034   -1.8873275482
  C   -0.5361336097   1.1801822119   -1.7692346116
  C   -0.5265506474   0.1892426565   -0.8019099548
  C   -1.6449917581   -0.0121434282   0.0396852096
  C   -1.3494032839   -1.0971617756   0.9656327829
  H   0.4145469909   -1.6030652916   -1.3207432887
  H   2.4377572124   0.1337223167   -0.9756672963
  H   3.7750420158   -1.2615894083   0.5329004904
  H   2.7290570115   -3.0290467032   1.9318953601
  H   0.289947418   -3.1380572181   2.2124891625
  H   -3.6472293458   0.6387327392   0.5322430131
  H   -3.6443568016   2.4383382761   -1.1746690105
  H   -1.6793638815   2.7923539146   -2.625155039
  H   0.3164079037   1.3323857224   -2.4233664322
  H   -2.0204703449   -1.4426888686   1.7423496786
Core   RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm]   63
 101.4048   110.2342   197.9862
 253.7594   291.7947   395.8502
 427.5916   441.3721   476.0201
 529.7158   542.5243   571.1736
 608.7518   643.6297   685.9954
 709.2314   740.6619   767.0714
 788.9369   826.0027   854.1021
 868.1508   877.6894   895.6589
 945.5022   963.8292   969.2899
 976.3435   985.0557   989.3595
1042.1345   1063.6548   1121.8046
1141.2668   1166.7102   1173.5165
1178.5227   1190.9009   1213.6566
1234.5608   1275.8504   1319.3818
1338.8155   1369.5985   1395.5199
1441.4196   1484.2438   1493.5540
1572.5960   1601.5388   1623.4940

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1644.2419                1677.2998                2889.5906
3153.3585                3155.0533                3160.0230
3161.5792                3172.8428                3173.9502
3183.3164                3185.3831                3192.9955
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]        1
0  1
End
Fragment          H
Atom
Mass[amu]    1
ElectronicLevels[1/cm]          1
0   2
End
GroundEnergy[kcal/mol] 26.69
End
   Barrier        nts1   ni1   ni2    #  nts1
     RRHO
        Geometry[angstrom]        24          #
C                 -2.178596    1.189194   -0.555512
C                 -3.148267    0.237642   -0.905593
C                 -3.111223   -1.040333   -0.341604
C                 -2.139864   -1.363214    0.594458
C                 -1.143285   -0.418582    0.946064
C                 -1.194218    0.890759    0.367085
C                  0.871712   -0.578174    0.180816
C                  1.764656   -1.583099   -0.118588
C                  3.079825   -1.204218   -0.421859
C                  3.443303    0.142511   -0.401227
C                  2.508717    1.130124   -0.082733
C                  1.192321    0.769165    0.214987
C                  0.051297    1.717120    0.569944
H                 -2.181559    2.161483   -1.038096
H                 -3.916827    0.491360   -1.626581
H                 -3.861831   -1.773197   -0.616712
H                 -2.145099   -2.336056    1.073118
H                 -0.633418   -0.553097    1.895141
H                  1.472378   -2.628138   -0.131223
H                  3.814871   -1.961069   -0.676021
H                  4.462740    0.426333   -0.637902
H                  2.805392    2.175216   -0.072246
H                  0.151520    2.052217    1.611221
H                  0.053570    2.611574   -0.058125
        Core      RigidRotor
          SymmetryFactor    0.5
        End
        Tunneling      Eckart
          ImaginaryFrequency[1/cm]     388.0030
          WellDepth[kcal/mol]          10.3
          WellDepth[kcal/mol]          28.5
```

```
        End
        Frequencies[1/cm]        65
  62.8677                106.3536
 179.7128                226.8847                        309.3045
 328.3923                398.5577                        415.2843
 481.2647                497.4979                        534.0796
 583.9297                616.1592                        621.7587
 702.2191                720.5825                        737.5055
 745.9274                805.4051                        806.5036
 836.0899                860.8188                        874.3560
 921.2182                937.5984                        969.0925
 978.4648                985.2551                        994.3636
1020.4469               1037.8151                       1039.8824
1083.5616               1121.7223                       1162.8607
1172.9718               1175.7754                       1183.8609
1193.8246               1208.0863                       1244.3242
1299.8598               1329.5416                       1332.3005
1352.4696               1449.8788                       1462.4838
1473.4626               1482.8471                       1512.8079
1574.9815               1589.4022                       1608.7034
1630.0232               2996.1471                       3069.8204
3133.6657               3143.9440                       3151.5479
3154.6270               3162.4672                       3164.4993
3176.4260               3180.0412                       3187.1784
        ZeroEnergy[kcal/mol]            10.3
        ElectronicLevels[1/cm]          1
            0    2
    End
    Barrier        nts2    ni2    fluorene    #   nts2
      RRHO
        Geometry[angstrom]        24          #
 C    -0.5759070953    -1.3735946242    0.976606312
 C     0.1298815354    -2.0916899583    0.0040038381
 C     0.5088188449    -1.4811064679   -1.1987072705
 C     0.2344071651    -0.143132806    -1.4341603532
 C    -0.3708613427     0.6222423302   -0.4089364549
 C    -0.8573403307    -0.037908438     0.7592179867
 C    -1.0129643564     1.9578949635   -0.4695115603
 C    -0.9578641265     2.9488588516   -1.4457788676
 C    -1.6692917617     4.1307045276   -1.2442261569
 C    -2.4174044471     4.3208583379   -0.0805545036
 C    -2.4679975301     3.328471699     0.9004723105
 C    -1.7673605594     2.1461113632    0.7005486144
 C    -1.6635589007     0.9285816259    1.5956924522
 H    -0.9196987766    -1.8726341333    1.8768671867
 H     0.3516944328    -3.1403165535    0.165649381
 H     1.0095626298    -2.0683388213   -1.9603446562
 H     0.5219677088     0.3235189264   -2.3692696397
 H     1.1238971485     1.2452361121    0.2835233183
 H    -0.3721029978     2.8106184946   -2.3478739042
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H    -1.6406619849    4.910467728    -1.997055642
H    -2.9648309857    5.2459783169   0.0608904536
H    -3.0524922572    3.4816052753   1.8018496514
H    -1.1487127745    1.170116897    2.5353240084
H    -2.6435812381    0.5221783533   1.8675574958
      Core      RigidRotor
        SymmetryFactor      0.5
      End
      Tunneling        Eckart
        ImaginaryFrequency[1/cm]     953.0092
        WellDepth[kcal/mol]          17.6
        WellDepth[kcal/mol]          4.6
      End
      Frequencies[1/cm]      65
  97.6831               131.8588
 210.8386               239.4808                263.3180
 398.1024               407.3203                425.8786
 457.5170               489.6400                513.2260
 520.2351               558.9055                579.5040
 638.1012               641.0281                708.4238
 736.4983               746.6971                761.6776
 800.2051               815.3967                850.3702
 865.6402               879.5898                931.5534
 948.6260               972.9717                984.4673
 989.7943              1021.5539               1042.5334
1050.3065              1115.0756               1128.9203
1162.9705              1174.2339               1179.7897
1189.8192              1204.9870               1220.2167
1246.5574              1313.5911               1323.8111
1343.7154              1363.0793               1448.3606
1469.4459              1478.5298               1501.7687
1510.8660              1588.7142               1623.1846
1630.0341              1650.8130               3004.6989
3046.3938              3157.2378               3158.2644
3164.3673              3166.1961               3175.0421
3179.1658              3186.9154               3189.0704
      ZeroEnergy[kcal/mol]         -0.6
      ElectronicLevels[1/cm]        1
          0    2
    End
    Barrier        nts3   ni1   ni3   #  nts3
      RRHO
        Geometry[angstrom]      24         #
C    1.2364398963   -1.0144549442   -0.1643067577
C    2.2699829881   -1.9431866546   -0.1259619773
C    2.5658822131   -2.6215422814   1.0562565496
C    1.8161740356   -2.3627356164   2.2045558226
C    0.783036354    -1.4355954016   2.1692831908
C    0.4751704896   -0.7388986779   0.9854552973
C    -2.086905746    0.6404171294   -0.6494913356
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C   -2.7781600465    1.1623631816   -1.7296125562
C   -2.1932522623    2.2866704913   -2.3322802113
C   -0.98849115      2.8247697494   -1.8659787425
C   -0.3119266247    2.2678544542   -0.7746539897
C   -0.898817788     1.1579400436   -0.1760452917
C   -0.6400226602    0.21676476      0.9678755884
H    1.0102722606   -0.4937203351   -1.0873802146
H    2.8484377174   -2.1393706993   -1.0220280334
H    3.3728926475   -3.3448264858    1.0833212976
H    2.0409911735   -2.8841577815    3.1284233077
H    0.20367467     -1.2378032547    3.0654301269
H   -3.7093052362    0.7489838506   -2.0981305574
H   -2.6871204852    2.7509429654   -3.1800594978
H   -0.5736351353    3.6938539114   -2.3647526003
H    0.6242379324    2.6907420155   -0.4266234789
H   -0.9385113644    0.5896702668    1.9487490966
H   -1.8322618793   -0.3148416867    0.4734109667
        Core      RigidRotor
          SymmetryFactor     0.5
        End
        Tunneling        Eckart
          ImaginaryFrequency[1/cm]     2170.1733
          WellDepth[kcal/mol]          36.2
          WellDepth[kcal/mol]          64.0
        End
        Frequencies[1/cm]       65
   52.2190              62.8715
   75.0097             210.1712              216.2339
  289.9578             392.2492              410.9845
  426.4514             465.2670              503.4565
  580.7583             614.9653              635.1189
  638.4620             704.7080              715.1070
  749.2532             754.5769              802.7810
  851.9801             873.1273              882.9381
  905.7738             940.7612              948.4246
  980.6081             991.1701              991.4667
 1001.3972            1012.6428             1023.3689
 1047.4844            1104.0829             1120.6804
 1153.2228            1173.0556             1180.9461
 1191.1544            1202.7327             1215.2841
 1264.9856            1306.8610             1327.9768
 1350.7846            1377.7057             1454.4721
 1481.6840            1484.0583             1520.2600
 1586.4538            1609.4394             1630.0272
 1632.8603            1759.9567             3089.5203
 3153.7552            3156.7324             3164.4600
 3167.0074            3174.1229             3180.9525
 3183.9911            3187.1289             3191.1506
        ZeroEnergy[kcal/mol]            36.2
        ElectronicLevels[1/cm]           1
```

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         0    2
  End
  Barrier        ts3    ni3    i4     #  ts3
     RRHO
        Geometry[angstrom]       24           #
C   1.8968363091    0.4317142592    2.0146535276
C   2.9499148794   -0.4172428361    1.6183762652
C   2.7164884817   -1.4180411632    0.6635920102
C   1.4578841581   -1.6348812533    0.1306977296
C   0.3459535965   -0.8105093225    0.5306968205
C   0.6278752557    0.2649220743    1.4980266372
H   2.0951166381    1.2605273221    2.6866006074
H   3.9413706331   -0.2822111509    2.0329837759
H   3.5339782036   -2.0693010214    0.3706349151
H   1.2864004304   -2.4707921477   -0.5382041974
H  -0.5947003836   -1.3372178404    0.6928076235
C  -2.5001016324    1.7171097378    0.1302292097
C  -3.2260264768    1.2349617839   -0.9136753506
C  -2.678321964     0.2667438666   -1.835958331
C  -1.3706916206   -0.1018326137   -1.76420795
C  -0.517294686     0.4002542357   -0.706881827
C  -1.1806284099    1.1937386684    0.3724740408
C  -0.4923506949    1.1865806328    1.5549588343
H  -2.9370463175    2.411319673     0.8405240218
H  -4.2493530588    1.5650859748   -1.0568115322
H  -3.3103714902   -0.1075001552   -2.633609205
H  -0.9361860428   -0.7332746397   -2.5332689387
H   0.4274284013    0.8120971403   -1.0598302986
H  -0.7415782095    1.7972567749    2.4147136116
        Core       RigidRotor
          SymmetryFactor     0.5
        End
        Tunneling       Eckart
          ImaginaryFrequency[1/cm]     897.1876
          WellDepth[kcal/mol]          47.95
          WellDepth[kcal/mol]          18.46
        End
        Frequencies[1/cm]        65
  92.7242              105.8955
 161.3482              251.5183                 279.0436
 394.1049              407.8636                 418.1816
 478.3602              514.1310                 554.1464
 576.1944              601.3501                 620.2430
 668.0318              695.4551                 710.3869
 732.7394              783.7113                 802.8527
 813.5447              850.6378                 853.2210
 869.9598              914.4720                 961.4630
 967.3494              970.5526                 981.6446
 989.0449              993.5379                1023.5774
1043.9947             1096.6028                1111.0189
```

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1159.9707              1167.5764              1175.0942
1188.1460              1191.2841              1233.7870
1287.8946              1314.0381              1334.5186
1368.0086              1400.0992              1428.5759
1458.4502              1484.1274              1505.2352
1532.9510              1565.0950              1596.1269
1639.5021              3063.4966              3089.3580
3150.2072              3152.5770              3157.0857
3159.0893              3170.9097              3173.2948
3182.3967              3183.6457              3189.7837
        ZeroEnergy[kcal/mol]           20.116
        ElectronicLevels[1/cm]           1
           0    2
   End
   Barrier        ts4    i4    p1     #   ts4
      RRHO
         Geometry[angstrom]       24          #
   C    0.6736382347    -0.2977355952    0.0464668342
   C    2.0816819807    0.1736421438    0.2659773892
   C    2.8402959717    -0.4353085501    1.1950785754
   C    2.2944916414    -1.4477479273    2.0895653768
   C    0.9639030233    -1.7107910222    2.1373802873
   C    0.0801342754    -1.0001989069    1.2542119452
   C    -2.8702153102    0.7493730992    -0.0361465261
   C    -2.9495250244    1.6320121799    -1.1104192393
   C    -1.8135613617    1.9579793982    -1.8633859592
   C    -0.5716866687    1.4181498514    -1.5416579199
   C    -0.4615186644    0.5981187266    -0.4134996851
   C    -1.6279390488    0.2114814557    0.3089990505
   C    -1.253663494    -0.7431968864    1.3331198754
   H    0.74247956    -1.067837061    -0.7490376203
   H    2.4938175865    0.9318866754    -0.3906742702
   H    3.8827244174    -0.158832837    1.3113693806
   H    2.9697255703    -1.9415373309    2.7795327799
   H    0.5547688995    -2.3792160182    2.8876733578
   H    -3.7634740863    0.4709051938    0.5124496566
   H    -3.9082212505    2.0595851562    -1.3823395474
   H    -1.9051151276    2.6339759644    -2.7057846055
   H    0.30287733    1.6634869443    -2.1348554938
   H    0.1056271887    2.0551993165    0.8090115778
   H    -1.9361196428    -1.1586379699    2.06398678015
        Core        RigidRotor
          SymmetryFactor      0.5
        End
        Tunneling       Eckart
          ImaginaryFrequency[1/cm]     593.3700
          WellDepth[kcal/mol]          28.8
          WellDepth[kcal/mol]          3.8
        End
        Frequencies[1/cm]        65
```

105.8238	113.5565	
200.3934	248.3482	288.2462
343.8000	377.7923	412.5881
428.1975	447.0273	485.0067
530.1402	540.8731	571.2155
608.7379	641.8608	689.4625
707.3846	737.2752	761.9508
790.7711	825.9567	850.2519
867.0874	875.0152	890.7663
948.2569	962.8682	971.2569
975.0233	986.2754	988.6918
1039.7375	1065.0842	1123.8344
1143.2863	1167.7055	1171.1855
1177.3241	1188.8153	1213.2100
1237.2488	1279.2603	1318.5522
1340.6126	1359.7941	1394.7242
1441.7621	1469.1549	1490.9317
1567.9784	1585.9266	1609.7325
1630.2248	1674.8789	2892.2666
3155.6418	3158.7551	3162.0636
3164.7465	3175.4038	3176.2892
3184.8398	3187.5459	3195.1092

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        ZeroEnergy[kcal/mol]           30.48
        ElectronicLevels[1/cm]          1
              0    2
    End
    Barrier        ts5    i4    i5      #   ts5
      RRHO
          Geometry[angstrom]       24           #
C     0.6787261147    -0.3685172753     0.0191761145
C     2.0772610972     0.14703103      0.2447555863
C     2.8476906584    -0.4531820089     1.1787360584
C     2.3281994698    -1.4668657702     2.0694226319
C     0.9765240939    -1.7068287436     2.1497286506
C     0.0917817889    -1.0451059986     1.2655152011
C    -2.9176034867     0.7680754853    -0.0390187986
C    -2.9516530586     1.6307402217    -1.0918668159
C    -1.7780262224     1.9938709495    -1.8358141175
C    -0.5507849297     1.4379288939    -1.5157973127
C    -0.4238348308     0.5642866156    -0.4260330678
C    -1.639965088      0.2136869484     0.3983654605
C    -1.2633256509    -0.7813629823     1.3622211291
H     0.7359620989    -1.1571026139    -0.7681155696
H     2.4674582345     0.9256361147    -0.4015114544
H     3.8811408131    -0.1445677438     1.3021505456
H     3.0076298538    -1.9511261897     2.7610094494
H     0.5758900839    -2.3370088545     2.9376336522
H    -3.8252988076     0.472835159      0.4736842627
H    -3.9055323104     2.0461603386    -1.3993264255
H    -1.8654842357     2.6832161757    -2.6653461061
```

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H    0.3243664573    1.6614712908   -2.1173652487
H   -0.936975006     1.1884779349    0.694158242
H   -1.9249791373   -1.1532419773    2.1331089326
        Core      RigidRotor
          SymmetryFactor      0.5
        End
        Tunneling        Eckart
          ImaginaryFrequency[1/cm]     1847.6158
          WellDepth[kcal/mol]          49.6
          WellDepth[kcal/mol]          34.7
        End
        Frequencies[1/cm]        65
  96.6435                 106.6698
 191.0806                 237.4641                  259.1011
 393.2491                 405.8282                  444.5476
 467.1649                 500.2723                  521.9213
 545.9865                 594.3065                  618.0859
 667.4678                 677.5892                  691.1947
 708.8181                 748.4664                  776.1069
 784.9510                 815.6278                  839.5957
 859.7293                 916.5210                  935.1220
 949.5798                 962.0946                  979.8215
 981.4357                 985.0184                 1043.7601
1092.8388                1123.8888                 1144.2000
1152.9422                1163.3901                 1171.6760
1180.2095                1221.3911                 1231.6776
1268.8552                1302.8667                 1311.5145
1335.8779                1383.7322                 1420.2662
1430.5514                1452.0368                 1479.1771
1501.2309                1534.2212                 1628.3233
1635.3272                2180.0023                 2744.4154
3148.0073                3153.8025                 3161.7140
3164.6599                3170.4766                 3183.4405
3186.4418                3199.6733                 3202.6020
        ZeroEnergy[kcal/mol]            51.26
        ElectronicLevels[1/cm]          1
            0    2
    End
    Barrier       ts6   i5   ni2   #   ts6
      RRHO
        Geometry[angstrom]      24          #
C    0.6691931458   -0.3008382573    0.0966870994
C    2.1304258844    0.0628736662    0.1660749239
C    2.9212750248   -0.5729765462    1.0559383208
C    2.3885826259   -1.4859886508    2.0461559988
C    1.035139714    -1.5739016496    2.2610468056
C    0.1489180673   -0.8679894221    1.4152198798
C   -2.7569924764    1.213575026     0.2443645012
C   -2.7837981749    2.0504329381   -0.8559387412
C   -1.6551957581    2.2432528393   -1.6687370475
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C    -0.4669388817     1.5371257738    -1.4027717059
C    -0.3885523115     0.7078841278    -0.309516699
C    -1.5150415739     0.5900350779     0.6001534962
C    -1.1585191866    -0.4399685471     1.6270588478
H     0.6001853212    -1.1260488464    -0.6497327554
H     2.535696777      0.7668406073    -0.5523118232
H     3.9880741545    -0.3731508625     1.0673911843
H     3.0778865848    -2.0107430366     2.6971261121
H     0.6495557953    -2.1178869677     3.1179025663
H    -3.6388124406     1.0680068946     0.857657661
H    -3.7093362062     2.5576176549    -1.1071047655
H    -1.7124069884     2.9042149507    -2.5246799589
H     0.3737737867     1.6251742169    -2.0841560344
H    -1.1248023582     1.0252044322     1.7189105396
H    -1.8251985253    -0.7360274192     2.4259325939
      Core       RigidRotor
        SymmetryFactor     0.5
      End
      Tunneling       Eckart
        ImaginaryFrequency[1/cm]     1547.4983
        WellDepth[kcal/mol]          24.2
        WellDepth[kcal/mol]          58.9
      End
      Frequencies[1/cm]     65
  97.8786            104.9452
 193.5983            245.9914                268.2044
 396.5955            411.5468                448.8726
 467.7058            514.5867                527.3999
 559.4345            600.3280                627.8663
 668.4155            694.2779                711.1195
 731.9619            768.6055                790.7737
 797.7112            837.4669                856.4214
 860.6009            931.5661                932.7711
 955.2997            963.9152                973.0864
 978.0883           1019.0385               1034.8137
1053.9630           1117.5759               1157.9347
1159.2152           1166.5314               1172.3241
1185.0908           1203.3835               1215.2897
1258.8457           1297.6644               1313.8164
1342.5160           1379.4100               1425.1933
1445.1685           1463.7368               1483.8688
1530.7514           1549.7609               1621.5342
1637.8405           1786.5177               2769.6980
3150.1533           3153.6137               3154.5013
3160.4460           3174.1159               3177.9738
3185.1350           3191.6774               3209.1696
      ZeroEnergy[kcal/mol]          40.69
      ElectronicLevels[1/cm]         1
          0    2
   End
```

```
   Barrier        ts8    ni2  p1     #  ts8
      RRHO
        Geometry[angstrom]      24           #
C   0.6847337581   -0.1531946935   0.1330044347
C   2.1147579098    0.15525861    0.4752145014
C   2.7987684338   -0.7059862544   1.2502046211
C   2.1549725019   -1.8540111131   1.8740642714
C   0.8054990676   -2.0144903613   1.8484085677
C   0.0077565608   -1.0484833904   1.1519063908
C   -2.7276149065   1.2563654966   0.3097015567
C   -2.6839054062   2.3852769751   -0.5065383183
C   -1.4990463286   2.7634073073   -1.1424334733
C   -0.3336303626   2.0069140154   -0.9830616724
C   -0.3680959185   0.8917347268   -0.1615615421
C   -1.5610115552   0.5114347075   0.4908998331
C   -1.2995050163   -0.6719135271   1.3074360923
H   0.7432219677   -0.7560517318   -0.7976490542
H   2.5983928283    1.0120316113   0.018811077
H   3.8536309026   -0.5436767619   1.4439204842
H   2.77163589    -2.5457008667   2.4370928214
H   0.3277974125   -2.7965871409   2.4289609698
H   -3.6505235429   0.9680665692   0.8009164314
H   -3.5796719576   2.9795739195   -0.6487050999
H   -1.4834795978   3.6500542219   -1.7660595875
H   0.5785294625   2.2986609764   -1.4934427007
H   -1.1778965579   0.2905018902   3.2594755419
H   -2.0534685454   -1.2174751861   1.8591058535
      Core      RigidRotor
        SymmetryFactor     0.5
      End
      Tunneling      Eckart
        ImaginaryFrequency[1/cm]     389.6422
        WellDepth[kcal/mol]       47.4
        WellDepth[kcal/mol]       2.5
      End
      Frequencies[1/cm]     65
 101.9471            109.4219
 195.8888            205.5462            237.4731
 281.5840            322.0272            397.1098
 427.2085            447.9804            477.0917
 527.9859            542.2799            576.4937
 609.1819            643.4132            689.6549
 710.2046            740.1718            770.3878
 790.0780            825.0854            854.1237
 872.6694            875.1624            894.9740
 946.4970            963.7845            971.7526
 976.0217            986.8694            989.5032
1042.6783           1065.5900           1121.8247
1141.4804           1165.1926           1171.8868
1178.3246           1190.0617           1212.8939
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1232.6788              1273.4674              1317.0644
1337.8082              1364.3156              1394.0190
1440.3928              1486.4313              1493.0258
1550.0042              1569.2997              1619.5352
1644.8992              1667.4370              2878.8622
3156.0013              3156.6670              3162.7342
3163.8701              3174.9440              3176.2634
3185.2677              3186.8505              3203.1194
        ZeroEnergy[kcal/mol]           29.17
        ElectronicLevels[1/cm]         1
            0    2
    End
End
```

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