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Authors

Zhao, Long

Kaiser, Ralf I

Lu, Wenchao

et al.

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Gas Phase Formation of Phenalene via 10π -Aromatic, Resonantly Stabilized Free Radical Intermediates

Long Zhao¹, Ralf I. Kaiser^{1*}

¹*Department of Chemistry, University of Hawaii at Manoa, Honolulu, Hawaii, 96822*
(USA)

Wenchao Lu², Musahid Ahmed^{2*}

²*Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720*
(USA)

Artem D. Oleinikov^{3,4}, Valeriy N. Azyazov^{3,4}

³*Department of Physics, Samara National Research University, Samara 443086*
(Russian Federation)

⁴*Lebedev Physical Institute, Samara 443011*
(Russian Federation)

Alexander M. Mebel^{3,5*}, A. Hasan Howlader,⁵ Stanislaw F. Wnuk⁵

⁵*Department of Chemistry and Biochemistry, Florida International University, Miami, FL 33199*
(USA)

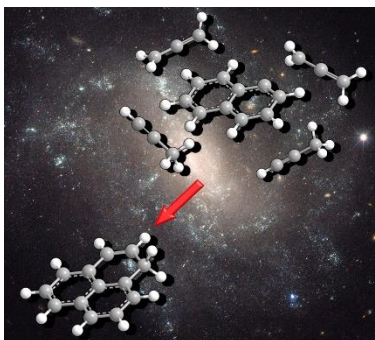
* Corresponding author:

Ralf I. Kaiser <ralfk@hawaii.edu>

Musahid Ahmed <mahmed@lbl.gov>

Alexander M. Mebel <mebela@fiu.edu>

Abstract: For the last decades, the Hydrogen-Abstraction/aCetylene-Addition (HACA) mechanism has been fundamental in aiding our understanding of the source of polycyclic aromatic hydrocarbons (PAHs) in combustion processes and in circumstellar envelopes of carbon rich stars. However, the reaction mechanisms driving high temperature molecular mass growth beyond triphenylene ($C_{18}H_{12}$) along with the link between PAHs and graphene-type nanostructures as identified in carbonaceous meteorites such as in Murchison and Allende has remained elusive. By exploring the reaction of the 1-naphthyl radical ($[C_{10}H_7]^*$) with methylacetylene (CH_3CCH) and allene (H_2CCCH_2) under conditions prevalent in carbon-rich circumstellar environments and combustion systems, we provide compelling evidence on a facile formation of 1H-phenalene ($C_{13}H_{10}$) – the central molecular building block of graphene-type nanostructures. Beyond PAHs, molecular mass growth processes from 1H-phenalene via ring-annulation through C3 molecular building blocks may ultimately lead to two-dimensional structures such as graphene nano flakes and after condensation of multiple layers to graphitized carbon. These fundamental reaction mechanisms are of crucial significance to facilitate an understanding of the origin and chemical evolution of carbon in our Galaxy.



1H-phenalene can be synthesized via the reaction of the 1-naphthyl radical with methylacetylene and allene under high temperature conditions prevalent in carbon-rich circumstellar environments and combustion systems.

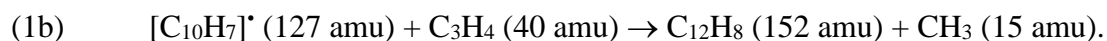
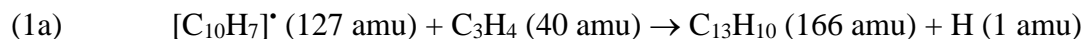
1. INTRODUCTION

Since the groundbreaking isolation of 1H-phenalene ($C_{13}H_{10}$) (**1**) 75 years ago by Lock and Gergely,¹ 1H-phenalene (**1**) together with the phenalenyl radical ($C_{13}H_9\cdot$) (**2**)^{2, 3} have attracted extensive interest from the (physical)organic,⁴ theoretical,² combustion,⁵ and astrochemical communities. This stems from their electronic structure and chemical bonding acting as prototypes of non-benzoid polycyclic aromatic hydrocarbons (PAHs) and resonantly stabilized free radicals (RSFRs), respectively (Schemes 1 and 2).⁶ The planar 1H-phenalene molecule (**1**) is best characterized as a cyclohexene ring ortho- and peri-fused to naphthalene and belongs to the C_s point group with a $^1A'$ electronic ground state. 1H-phenalene possesses a very weak carbon-hydrogen bond at the CH_2 moiety of only 260 kJ mol^{-1} ,⁷ one of the weakest existing C-H bonds on record, compared to a bond energy of 415 kJ mol^{-1} in methane (CH_4).⁸ Hence one of the methylene hydrogen atoms can be easily abstracted or eliminated via unimolecular decomposition of 1H-phenalene (**1**) yielding the highly symmetric D_{3h} resonantly stabilized phenalenyl radical (**2**) holding a $^2A''_1$ electronic ground state. That is to say the presence of an sp^3 hybridized saturated carbon in 1H-phenalene (**1**) prevents the molecule from exhibiting a complete π delocalization over the carbon periphery, with the loss of a hydrogen atom resulting in an energetically favored, delocalized π -system in (**2**) with phenalenyl (**2**) affected by Jahn–Teller distortion in its lowest excited $^2E''$ state.^{9, 10} Due to this extremely high stabilization, the C-H bond at the CH_2 moiety of 1H-phenalene is much weaker than the analogous bond at the CH_2 group in indene (327 kJ mol^{-1})¹¹ and the benzylic bond in the methyl group of toluene (373 kJ mol^{-1}).¹²

The high stability and amphoteric redox nature of this odd-alternant radical (**2**), which can be oxidized or reduced to a 12π -electron cation $C_{13}H_9^+$ and 14π -electron anion $C_{13}H_9^-$,¹³ prompted the synthesis of exotic organometallic species involving, for instance, iron, chromium, and manganese, in which the phenalenyl moiety bonds in via η^1 -, an η^3 -allylic mode, or via η^6 -bonding.¹⁴⁻²¹ Competing σ -to- σ and π -to- π dimerization can be modulated by directing the bonding and molecular overlap through functionalization involving bulky side groups such as phenyl ($C_6H_5\cdot$) and tertiary butyl ($C(CH_3)_3\cdot$) with sterically hindering substituents favoring σ -bonding;^{2, 3, 22-26} the formation of stacked π -dimers of phenalenyl is promoted by removing one electron from the singly occupied molecular orbital (SOMO) of one phenalenyl reactant.² The inherent σ -radical character of the resonance structure of the phenalenyl radical (**2**) has been recognized as a critical

prerequisite of the phenalenyl radical (**2**) self-association in combustion flames and in deep space potentially leading to benzenoid aromatic structures such as peropyrene (C₂₆H₁₄).²⁷ The identification of the 1H-phenalene (**1**) moiety and the phenalenyl radical (**2**)^{28, 29} in pyrolyzed hydrocarbon samples^{5, 28, 30-32} suggests that phenalenyl (**2**) and its higher homologues play a critical role in the formation of complex, benzenoid PAHs through reactions with C₂–C₄ alkenes and recombination of phenalenyl (**2**) with arylmethyl radicals such as naphthylmethyl (C₁₁H₉[•]) or phenanthrenylmethyl (C₁₄H₁₁[•]). Phenalenyl-type radicals were also speculated to play a fundamental role in soot nucleation processes – a kinetic bottleneck in the formation of carbonaceous nanostructures (soot, grains).³³ However, the underlying synthetic routes to 1H-phenalene (**1**) itself have remained largely elusive to date with only one pathway to 1H-phenalene (**1**), via the recombination of the 1-acenaphthyl and methyl radicals, being explored theoretically.⁷

In this study, we untangle synthetic routes to 1H-phenalene (**1**) via a gas phase synthesis under simulated combustion conditions involving low-barrier reactions through directed ring expansion reactions involving 10π aromatic and resonantly stabilized free radical intermediates. Exploiting 1H-phenalene (**1**) as a benchmark, we expose the hitherto unknown gas phase chemistry synthesizing 1H-phenalene (**1**) (C₁₃H₁₀; 166 amu) – together with its 1-methylacenaphthylene and 3H-cyclopenta(a)naphthalene isomers – plus atomic hydrogen (1 amu) via the elementary reaction of the 1-naphthyl radical (C₁₀H₇[•]; 127 amu) with allene and methylacetylene (C₃H₄; 40 amu) (reaction (1a)). Our combined experimental and ab initio study discloses archetypes of low-barrier reaction pathways guiding the facile formation of 1H-phenalene (**1**) via molecular mass growth in a reaction of 1-naphthyl with a single allene or methylacetylene molecule. Briefly, 1H-phenalene (**1**) was synthesized in a high temperature chemical reactor through a directed synthesis via the reaction of the 1-naphthyl radical (C₁₀H₇[•]) with allene (H₂CCCH₂) and methylacetylene (CH₃CCH) at 1350 K and 300 Torr.³⁴⁻³⁶ The products were probed isomer-selectively by exploiting fragment-free photoionization of the products utilizing tunable vacuum ultraviolet (VUV) light in tandem with the detection of the ionized molecules by a high resolution reflectron time-of-flight mass spectrometer (Re-TOF-MS) with mass spectra being collected at intervals of 0.05 eV between 7.30 and 10.00 eV (Supporting Information).



2. METHODS

2.1. Experimental method

By studying the reactions of the 1-naphthyl radical ($C_{10}H_7^{\bullet}$) with methylacetylene (CH_3CCH ; Organic Technologies; 99%) and allene (H_2CCCH_2 ; Organic Technologies; 98%) under simulated combustion conditions, we deliver experimental and computational evidence of the molecular growth processes to 1H-phenalene along with its isomers. Briefly, a continuous beam of 1-naphthyl radicals ($C_{10}H_7^{\bullet}$) was prepared *in situ* through pyrolysis of the 1-iodonaphthalene ($C_{10}H_7I$) precursor (TCI America, > 97%). In three separate experiments, the precursor was kept in a bubbler at room temperature and seeded in pure helium (blank experiment) and in the hydrocarbon gases (methylacetylene and allene) at pressures of 300 Torr. Each gas mixture was then expanded into a resistively heated silicon carbide (SiC) tube (“pyrolytic reactor”) held at 1350 ± 10 K as monitored by a Type-C thermocouple. The hydrocarbon gases do not only serve as seeding gases, but also as reactants with the pyrolytically generated 1-naphthyl radicals. The products formed in the reactor were expanded supersonically, passed through a 2 mm diameter skimmer located 10 mm downstream of the pyrolytic reactor, and entered into the photoionization chamber, which houses the Wiley–McLaren reflectron time-of-flight mass spectrometer (ReTOF-MS). The quasi-continuous tunable synchrotron vacuum ultraviolet (VUV) light from the Advanced Light Source (ALS) intercepted the neutral molecular beam perpendicularly in the extraction region of the ReTOF-MS. VUV single photon ionization is essentially a fragment-free ionization technique and is compared soft to electron impact ionization.³⁷ The ions formed via photoionization are extracted and detected by a multichannel plate (MCP) detector. 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 from 7.30 eV to 10.00 eV. It shall be noted that under these experimental conditions, methylacetylene and allene do not isomerize to each other in the pyrolysis tube.^{38, 39} Detailed computational fluid dynamics (CFD) simulations of the gas flow in the microreactor suggest residence times of the reactants of a few 100 μs .^{36, 40, 41} Typically, at the reaction center, this would give rise to a few tens collisions between the 1-naphthyl radical and the allene/methylacetylene molecules and/or between reaction products. PIE calibration curves for helium-seeded $C_{13}H_{10}$ isomers were also collected (Fig. S1), to identify the products of interest

observed in this work. Synthesis and characterization of 1*H*-phenalene and 1-methylacenaphthylene are described in the Supporting Information.

2.2. Computational methods

Geometries of the reactants and products of the reactions of 1-naphthyl with allene and methylacetylene and various intermediates and transition states on the C₁₃H₁₁ PES were optimized at the density functional B3LYP/6-311G(d,p) level of theory and their vibrational frequencies were computed using the same theoretical method. Single-point energies were then refined at the G3(MP2,CC) level using a series of coupled clusters CCSD(T) and second-order Møller-Plesset perturbation theory MP2 calculations, where the final energy was computed as

$$E[\text{G3(MP2,CC)}] = E[\text{CCSD(T)/6-311G(d,p)}] + E[\text{MP2/G3Large}] - E[\text{MP2/6-311G(d,p)}] + \text{ZPE}[\text{B3LYP/6-311G(d,p)}]^{42-44}$$

The G3(MP2,CC) model chemistry approach normally provides chemical accuracy of 0.01–0.02 Å for bond lengths, 1–2° for bond angles, and 3–6 kJ mol⁻¹ for relative energies of hydrocarbons, their radicals, reaction energies, and barrier heights in terms of average absolute deviations.⁴³ The GAUSSIAN 09⁴⁵ and MOLPRO 2010⁴⁶ program packages were used for the ab initio calculations. Pressure- and temperature-dependent rate constants for the 1-naphthyl + C₃H₄ reactions at different temperatures and pressures were evaluated using the Rice-Ramsperger-Kassel-Marcus Master Equation (RRKM-ME) theoretical approach utilizing the MESS software package.^{47, 48} Here, densities of states and partition functions for local minima and numbers of states for transition states were computed within the Rigid-Rotor, Harmonic-Oscillator (RRHO) model. For critical entrance transition states of allene/methylacetylene addition to 1-naphthyl, low-frequency normal modes corresponding to internal rotations were treated as one-dimensional hindered rotors in partition function calculations, where the corresponding vibrational frequencies were removed. Corresponding one-dimensional torsional potentials were calculated by scanning PESs at the B3LYP/6-311G(d,p) level of theory. Tunneling corrections using asymmetric Eckart potentials were included in rate constant calculations. We employed collision parameters used by us earlier for RRKM-ME calculations of the prototype C₆H₅ + C₃H₄⁴⁹ and 1-naphthyl + C₃H₄ reactions;³⁸ the Lennard-Jones parameters were taken as (ϵ/cm^{-1} , $\sigma/\text{\AA}$) = (390, 4.46) and the temperature dependence of the range parameter α for the deactivating wing of the energy transfer function was expressed as $\alpha(T) = \alpha_{300}(T/300 \text{ K})^n$, with $n = 0.62$ and $\alpha_{300} = 424 \text{ cm}^{-1}$. Calculations

at $p = 10^{-10}$ atm emulating the zero-pressure limit took into account radiational stabilization of $C_{13}H_{11}$ intermediates. Additional details of RRKM-ME calculations can be found in our previous publications⁴⁹ and in the input file for the MESS package given as Note S1.

3. EXPERIMENTAL RESULTS

We analyzed first the mass spectra of the 1-naphthyl–allene and 1-naphthyl–methylacetylene systems qualitatively and extract the molecular formulae of the reaction products related to the formation of 1H-phenalene (**1**). Illustrative mass spectra recorded at a photoionization energy of 9.50 eV are presented in Figure 1 for the reactions of 1-naphthyl with allene and methylacetylene (Figs. 1a-b) to reveal the molecular formula of reaction 1a and 1b. Replacing the hydrocarbon reactant (allene, methylacetylene) with non-reactive helium carrier gas (Figs. 1c) confirmed that the products (Figs. 1a-b) are synthesized as a result of the reaction of the 1-naphthyl radical with allene and methylacetylene, but not from decomposition of the 1-naphthyl radicals. An analysis of these mass spectra discloses the formation of molecules with the molecular formulae $C_{13}H_{10}$ (166 amu) and $C_{12}H_8$ (152 amu) along with the ^{13}C isotopologues at $m/z = 167$ and 153 in both systems. Further, signal is observable for $C_{13}H_9$ (165 amu). These ion counts are clearly absent in the control experiments suggesting that molecules detected via $m/z = 152, 153, 165, 166,$ and 167 signify reaction products in both $C_{10}H_7 - C_3H_4$ systems. Considering the molecular weight of the reactants and the products, the $C_{13}H_{10}$ isomer(s) along with atomic hydrogen are the result of the reaction of the 1-naphthyl radical with allene/methylacetylene via channel(1a). Signal at $C_{12}H_8$ (152 amu) can be linked with the methyl (CH_3) loss channel in reaction (1b). Reaction channel(s) attributed to $C_{13}H_9$ (165 amu) are revealed below. The ion counts at mass-to-charge ratios (m/z) of 254 ($C_{10}H_7I^+$), 128 ($C_{10}H_8^+$), and 129 ($C_9^{13}CH_8^+$) are detectable in the control experiments as well and hence cannot be linked to the reaction of 1-naphthyl radicals with allene/methylacetylene. These species are associated with the 1-iodonaphthalene precursor (254 amu) and naphthalene ($C_{10}H_8$) with the latter likely formed through recombination of 1-naphthyl with a hydrogen atom.

The investigation of the mass spectra delivered convincing evidence on the formation of $C_{13}H_{10}$ (166 amu) and $C_{12}H_8$ (152 amu) isomer(s) along with their ^{13}C analogous species $C_{12}^{13}CH_{10}$ (167 amu) and $C_{11}^{13}CH_8$ (153 amu) through the reaction of 1-naphthyl with allene and methylacetylene (reactions (1a)/(1b)); also, contributions of $C_{13}H_9$ (165 amu) isomer(s) are likely. The primary interest is, however, to elucidate which isomer(s) is/are formed. This necessitates an in-

depth analysis of the underlying photoionization efficiency (PIE) curves of the mass-to-charge ratios of interest (Fig. 2) to reveal the isomers formed. Each PIE curve reports the ion counts at a well-defined m/z ratio such as $m/z = 166$ as a function of the photon energy from 7.30 eV to 10.00 eV (Figure 2). The shapes of the PIE curves of $C_{13}H_{10}$ isomers- 1H-phenalene, 3H-cyclopenta(a)naphthalene, 1-methylacenaphthylene are very different and therefore unique as recorded in separate calibration experiments within the same experimental setup under identical experimental conditions (Figure S1)³⁸. A linear combination of these are used to fit the experimental PIE curves, shown for $m/z = 165$, 166, and 167 (Fig. 2). Even after scaling, these PIE curves are not superimposable suggesting that $m/z = 165$ does not represent a fragment of $m/z = 166$, but rather distinct isomer(s) of $C_{13}H_9$ (165 amu). Since no reference curves of any $C_{13}H_9$ isomer exists, we conclude that although $C_{13}H_9$ isomer(s) are formed, it is not feasible to elucidate the actual structure(s) at the present stage. However, considering a 1.1% natural abundance of ^{13}C , 14.3% of the ion signal of $m/z = 165$ ($C_{13}H_9^+$) has to contribute to ion counts of $m/z = 166$ ($C_{12}^{13}CH_9^+$) (Fig. 2). Fitting of the PIE curves at $m/z = 166$ ($C_{12}^{13}CH_9^+/C_{13}H_{10}^+$) reveals the formation of three $C_{13}H_{10}$ isomers: 1H-phenalene (**p1**), 1-methylacenaphthalene (**p8**), and 3H-cyclopenta(a)naphthalene (**p2**) (Figure 2). Branching ratios of the ion counts of these isomers were derived at 10.0 eV for the 1-naphthyl – allene and 1-naphthyl - methylacetylene system to be 32 ± 3 % (**p1**), 38 ± 4 % (**p8**), and 30 ± 3 % (**p2**) as well as 28 ± 3 % (**p1**), 61 ± 6 % (**p8**), and 11 ± 1 % (**p2**), respectively. 1H-phenalene is more abundant in the 1-naphthyl-allene system at the expense of 1-methylacenaphthalene, which dominates the ion counts in the 1-naphthyl-methylacetylene system. We emphasize that the aforementioned contributions to the fit of the experimental PIE curve do not represent the product branching ratios since absolute ionization cross sections are not available for any of the $C_{13}H_{10}$ isomers. However, the experiments provide explicit evidence and the proof-of-concept that the reaction of 1-naphthyl with allene and methylacetylene leads to the formation of three distinct $C_{13}H_{10}$ isomers: 1H-phenalene (**p1**), 1-methylacenaphthalene (**p8**), and 3H-cyclopenta(a)naphthalene (**p2**). The corresponding PIE curves of $m/z = 167$ ($C_{11}^{13}C_2H_9^+/C_{12}^{13}CH_{10}^+$) match these findings and reveal that ion signal at $m/z = 167$ originate predominantly from the aforementioned ^{13}C -isotopologue PAHs ($C_{13}H_{10}$) and to a minor amount from doubly ^{13}C substituted $C_{13}H_9$ radicals.

4. DISCUSSION

The experimental data provide explicit evidence on the detection of 1H-phenalene (C₁₃H₁₀) (**p1**) along with two of its isomers (1-methylacenaphthylene (**p8**), 3H-cyclopenta(a)naphthalene (**p2**)) and acenaphthylene (C₁₂H₈) (**p9**) formed via the elementary reactions of 1-naphthyl with allene and methylacetylene in the gas phase. Coupling these experimental finding with electronic structure calculations allows us to untangle the synthetic routes (Figs. 3 and S3) for these complex processes. Our computations disclose that the 1-naphthyl radical adds to the π -electron density of the terminal (C1) or central carbon atom (C2) of the methylacetylene or allene reactants yielding intermediates **i1** and **i5** or **i8** and **i10**, respectively. These processes involve small barriers to addition of only 5 to 11 kJ mol⁻¹. These doublet intermediates can isomerize via the low energy reaction sequence **i1** → **i2** → **i3** → **i4** → **i5** → **i7** → **i8** involving cis-trans isomerization, a shift of the naphthyl group from the terminal to the central carbon in the side chain via three-member ring cyclization followed by the three-member ring opening, and consecutive hydrogen shifts from the naphthyl moiety to the side chain (**i5** → **i7**) and vice versa (**i7** → **i8**). Further, the **i8** intermediate is connected to the complex **i10** of the 1-naphthyl - allene system via a similar shift of the naphthyl group from the central to the terminal carbon atom of allene occurring via intermediate **i9** featuring a three-member ring. It is important to highlight that both the 1-naphthyl – methylacetylene and 1-naphthyl – allene surfaces are connected via intermediate **i8**. The doublet radical intermediate **i8** is central to rationalize that in both systems, the same reaction channels leading to 1H-phenalene (C₁₃H₁₀) (**p1**, via **i8**, **i9**, **i10**, **i13**, and **i14**) and 3H-cyclopenta(a)naphthalene (C₁₃H₁₀) (**p2**, via **i8**, **i9**, **i10**, **i11**, and **i12**) are open, whereas 1-methylacenaphthylene (C₁₃H₁₀) (**p8**), and acenaphthylene (C₁₂H₈) (**p9**) are produced via the intermediates **i2**, **i21**, and **i22**. Here, **i2** can be formed in one step in the 1-naphthyl - methylacetylene system or via the reaction sequence **i8** → **i7** → **i5** → **i4** → **i3** → **i2** in the 1-naphthyl - allene system. Interestingly, **i8** together with the less important **i15** and **i16** intermediates represent resonantly stabilized allylic radicals also containing a 10 π aromatic naphthalene moiety. Due to this resonance stabilization, **i8**, **i15**, and **i16** reside 100 or more kJ mol⁻¹ lower in energy than similar two-ring-side-chain intermediates **i1**, **i2**, **i4**, **i5**, **i7**, **i10**, **i11**, and **i13**. The calculated potential energy diagram also suggests that isomerization of **i2** to **i15**, **i16**, and then **i19** or **i17**, followed by formation of 1H-phenalene(**p1**) or 3H-cyclopenta(s)naphthalene (**p2**) along with atomic hydrogen are unfavorable due to inherent barrier height of 179 kJ mol⁻¹ involved in the hydrogen migration **i2** → **i15** compared to the more facile cyclization of **i2** to **i3** and five-member ring closure **i2** → **i21**. The existence of intermediate **i10** is central to understand the

underlying reaction mechanism(s). The facile reaction sequence via **i13** and **i14** through ring expansion leads via hydrogen elimination to 1H-phenalene ($C_{13}H_{10}$) (**p1**); likewise, intermediate **i10** can undergo unimolecular decomposition to form 3H-cyclopenta(a)naphthalene (**p2**) and 1H-cyclopenta(a)naphthalene (**p3**).

The latter two products are predicted by our RRKM-Master Equation calculations to have very similar branching ratios of 4 % as compared to ~40 % for **p1** at the experimental temperature of 1350 ± 10 K (see Table S1; the computed **p1** branching ratios are 42.2 % at 1300 K and 37.6 % at 1400 K). Since the reaction pathways leading to **p1** and **p2/p3** both proceed via the common intermediate **i10** (Figs. 3 and S3), the larger yield of **p1** as compared to **p2** and **p3** can be attributed to the higher barrier for isomerization of **i10** to **i11** (1,4-hydrogen shift) compared to **i13** (1,5-hydrogen shift), where the production of **i11** is unavoidable to form **i12**, which then fragments to **p2** or **p3** (Fig. S3), whereas **p1** is produced via **i13** and **i14**. The failed detection of **p3** might be explained by its small photoionization cross section; interestingly, 1H-cyclopenta(a)naphthalene (**p3**) could not be detected in our earlier study of the 2-naphthyl - allene/methylacetylene systems, where its computed branching ratio is also similar to that of 3H-cyclopenta(a) naphthalene (**p2**).³⁸ As noted above, the alternative channel to form **p2** via **i17** is hindered by the high barrier for the **i2** \rightarrow **i15** step. Besides **i10**, which is central to rationalize the formation of **p1** and **p2**, intermediate **i2** is of fundamental importance to understand the detection of acenaphthylene ($C_{12}H_8$) (**p9**) and 1-methylacenaphthalene ($C_{13}H_{10}$) (**p8**). Intermediate **i2** can undergo a facile five-member ring closure to **i21** which then either ejects a hydrogen atom to form 1-methylacenaphthylene ($C_{13}H_{10}$) (**p8**) or isomerizes to **i22** prior to emission of a methyl group along with formation of acenaphthylene ($C_{12}H_8$) (**p9**). The overall reactions are exoergic and all transition states involved for the isomerization processes lie below the energy of the separated reactants. 1-ethynynaphthalene ($C_{12}H_8$) (**p7**) can be produced by the CH_3 group loss from **i4**. No substituted naphthalene species (**p4-p6**) which can be formed via 1-naphthyl addition – hydrogen atom elimination (Fig. S3) were detected. This finding is supported by statistical calculations revealing that the thermodynamically more favorable 1H-phenalene ($C_{13}H_{10}$) (**p1**) formation along with the tricyclic aromatic systems **p2**, **p8**, and **p9** is preferred, and that under our experimental conditions, multi-step reaction sequences via addition – hydrogen shifts – cyclization – hydrogen/methyl elimination are favorable compared to ‘simple’ addition – hydrogen elimination steps (Table S1). It should be noted however that the statistical calculations predict a rapid growth of the entropically

favorable products **p4** and **p7** (methylacetylene) and **p5** and **p6** (allene) with the temperature increase beyond 1500 K. Under real combustion conditions, **p4-p6** can be converted to the thermodynamically preferable phenalene, cyclopenta(a)naphthalenes, and 1-methylacenaphthalene via hydrogen-assisted isomerization. At very low pressures, the formation of 1H-phenalene (**p1**) is clearly preferable for the 1-naphthyl - allene system up to 1500 K (Fig. S5 and Table S1), whereas the 1-naphthyl - methylacetylene system is dominated by the production of **p9** plus methyl and **p8** plus atomic hydrogen also up to 1500 K (Fig. S5 and Table S2).

5. CONCLUSION

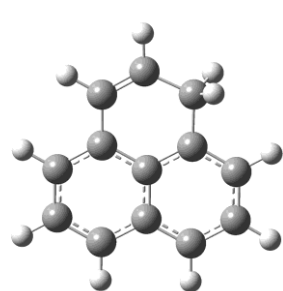
To conclude, our joint experimental and computational investigation delivers explicit proof on the formation of 1H-phenalene through molecular mass growth processes in a reaction of 1-naphthyl with allene and methylacetylene in the gas phase. Rather than traditional bay closures in aromatic radicals involving the hydrogen abstraction – acetylene addition (HACA) mechanism such as the formation of phenanthrene ($C_{14}H_{10}$) and pyrene ($C_{16}H_{10}$) via the reactions of biphenyl ($C_{12}H_9^*$)⁵⁰ and 4-phenanthryl ($C_{14}H_9^*$)³⁵ with the C2 building block acetylene (C_2H_2) [C4-C2 annulation], the present study reveals a hitherto unfamiliar bay closure pathway through ring annulation involving an aromatic radical (1-naphthyl) plus a C3 hydrocarbon (methylacetylene, allene) [C3-C3 annulation]. This mechanism might be fundamental in aiding our understanding of molecular mass growth processes of graphene nano flakes and graphene sheets starting from 1H-phenalene via peripheral expansion of the 1H-phenalene moiety to triangular graphene-type molecules 1,5-dihydrodibenzo[*cd,mn*]pyrene ($C_{22}H_{14}$) and 6,11-dihydro-1H-tribenzo[*bc,hi,no*] coronene ($C_{33}H_{18}$) (Scheme 3).⁶ This pathway could also explain the detection of graphitized carbon with grain sizes of up to 80 nm as probed in carbonaceous chondrites like Allende and Murchison, which are likely formed via condensation of multiple layers to graphene-like nanostructures.³⁵ In circumstellar envelopes of carbon-rich stars with temperatures of up to a few 1,000 K and even in combustion flames, the entrance barriers to addition can be overcome easily thus providing a versatile, hitherto overlooked pathways to two dimensional nanostructures in oxygen poor combustion systems and in deep space with aryl radicals and methylacetylene and allene centered molecular building blocks.

Conflicts of interest

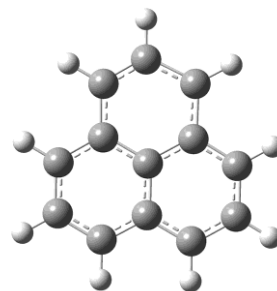
There are no conflicts to declare.

Acknowledgments

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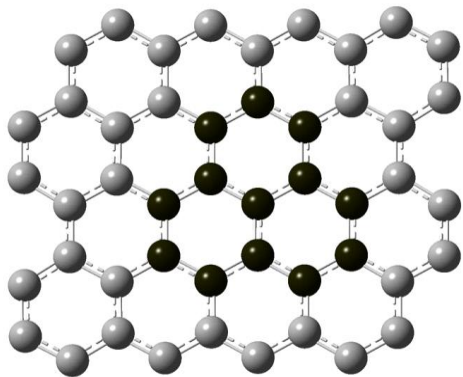


(1)

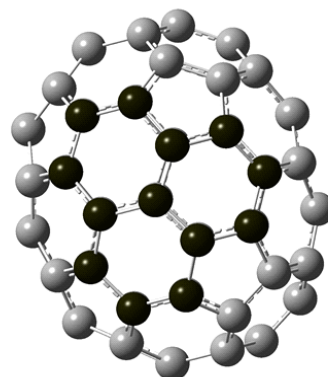


(2)

Scheme 1. Molecular structures of the 1H-phenalene molecule (1) and the phenalenyl radical (2).



(3)



(4)

Scheme 2. Molecular building blocks of the 1H-phenalene carbon skeleton (black) in graphene (3)⁵¹ and C₇₀-fullerene (4).⁵²⁻⁵⁴

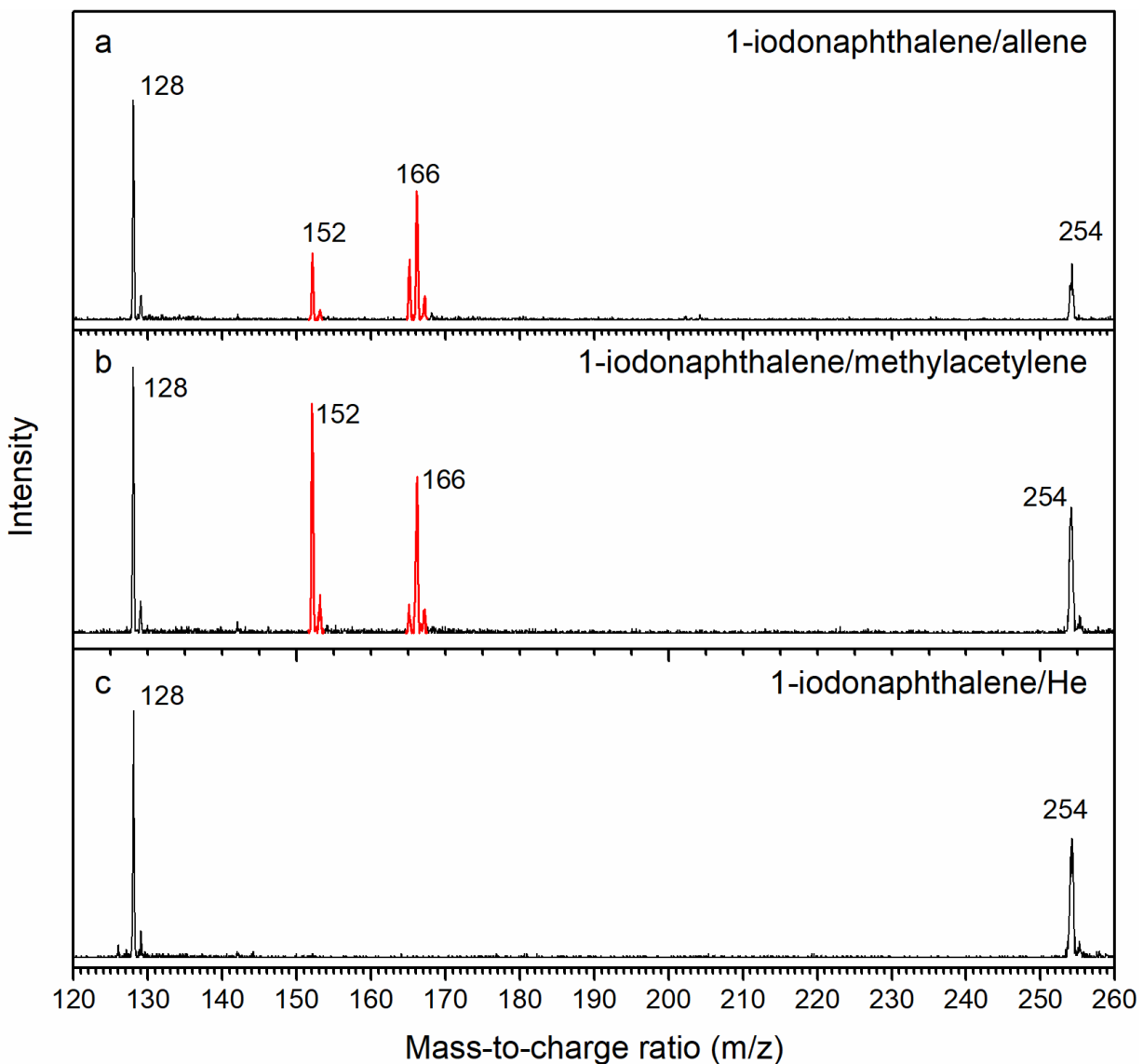


Figure 1. Comparison of photoionization mass spectra recorded at a photon energy of 9.50 eV. (a) 1-iodonaphthalene ($C_{10}H_7I$) - allene (C_3H_4) system; (b) 1-iodonaphthalene ($C_{10}H_7I$) - methylacetylene (C_3H_4) system; and (c) 1-iodonaphthalene ($C_{10}H_7I$) - helium (He) system. The mass peaks of the newly formed species along with the ^{13}C -counterparts are highlighted in red.

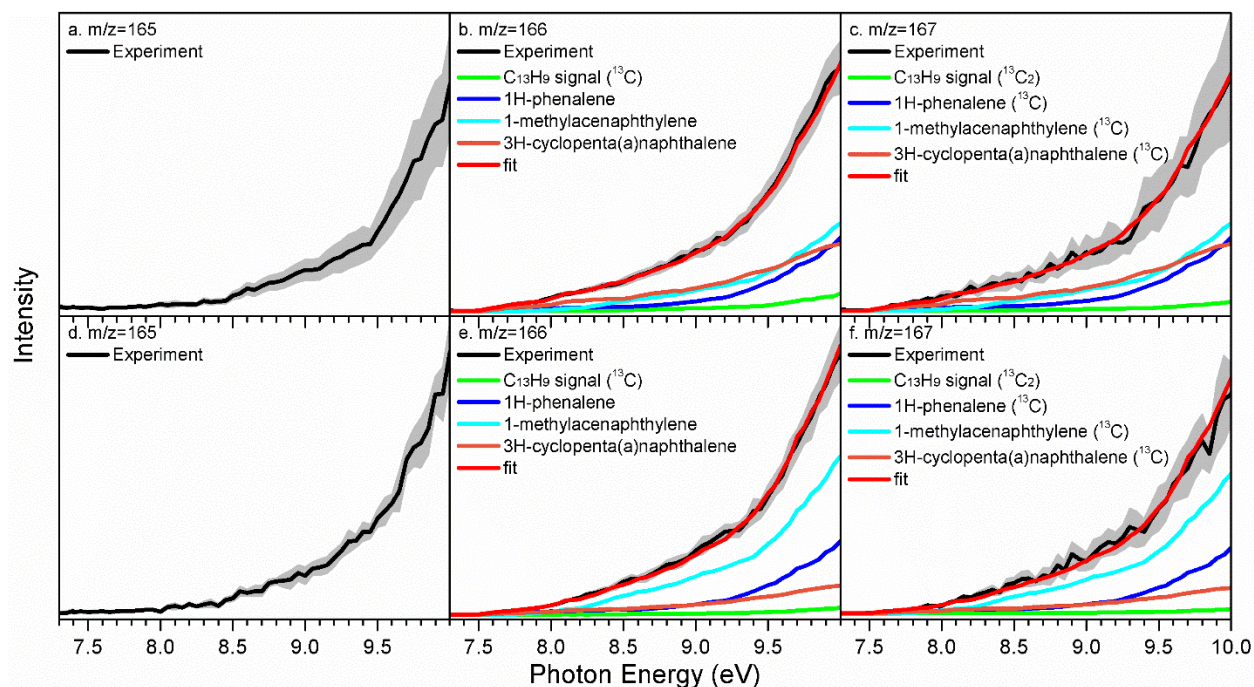


Figure 2. Photoionization efficiency (PIE) curves for signal at $m/z = 165$ to 167 in the systems of (a), (b) and (c): 1-iodonaphthalene ($C_{10}H_7I$) + allene (C_3H_4); (d), (e) and (f): 1-iodonaphthalene ($C_{10}H_7I$) + methylacetylene (C_3H_4). Black: experimentally derived PIE curves; colored lines (green, blue, cyan and brown): reference PIE curves; red lines: overall fit. The overall error bars consist of two parts: $\pm 10\%$ based on the accuracy of the photodiode and a 1σ error of the PIE curve averaged over the individual scans.

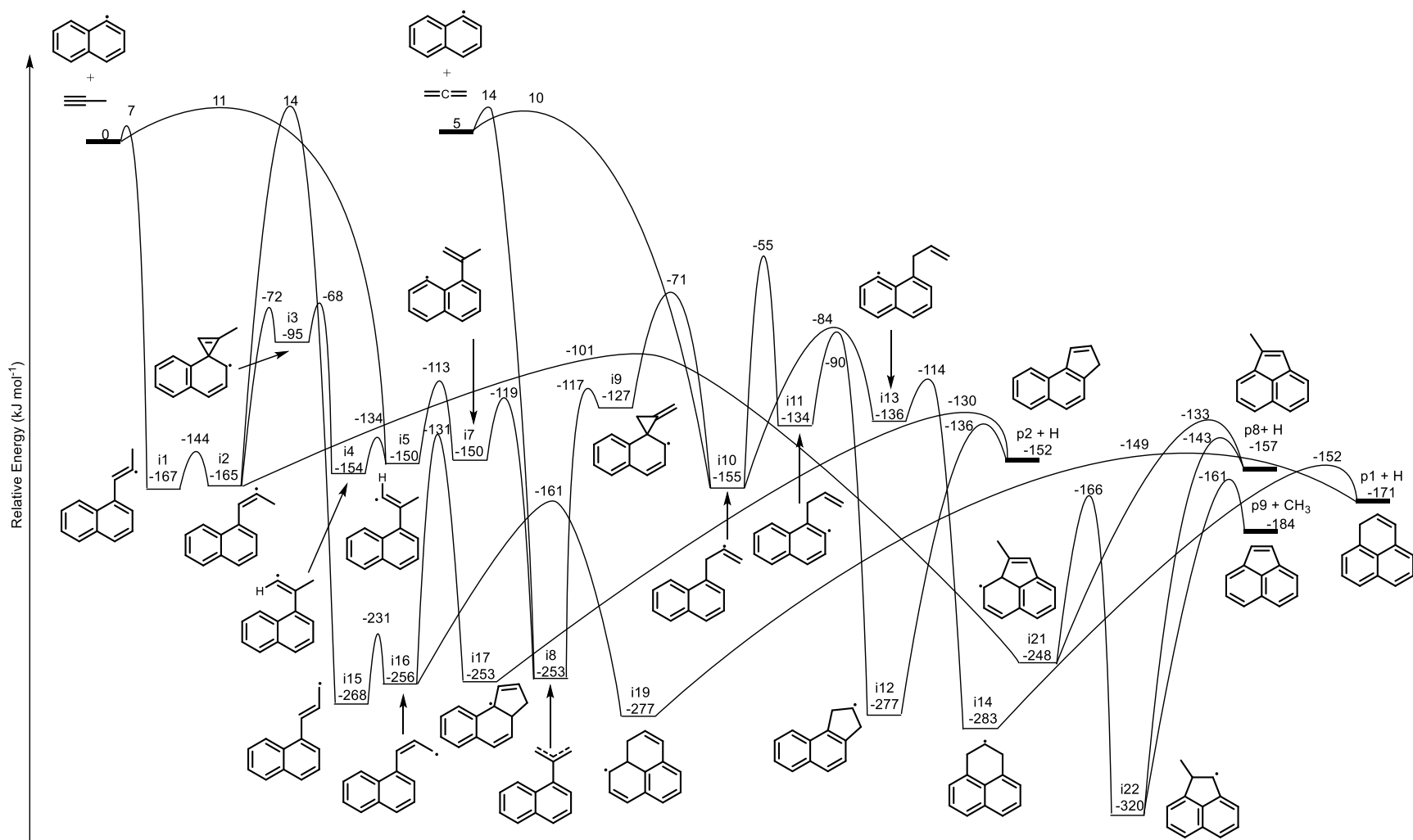
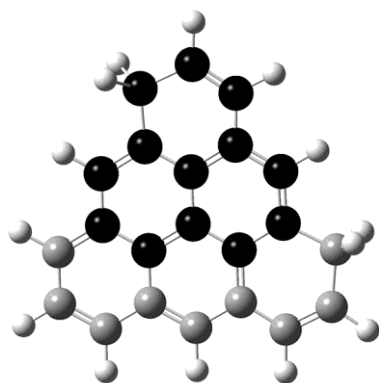
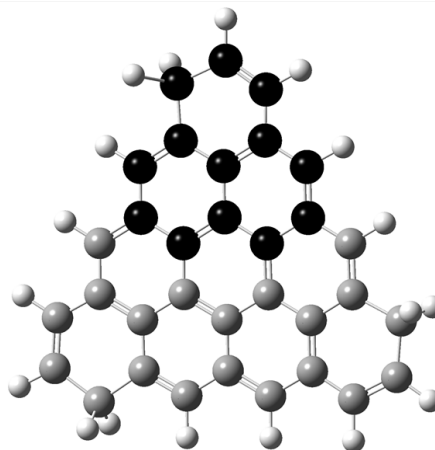


Figure 3. Potential energy surface (PES) for the 1-naphthyl ($\text{C}_{10}\text{H}_7^{\bullet}$) reaction with allene/methylacetylene (C_3H_4). This PES was calculated at the G3(MP2,CC)//B3LYP/6-311G(d,p) level of theory for the channels leading to 1H-phenalene (**p1**), 3H-cyclopenta(a)naphthalene (**p2**), 1-methylacenaphthylene (**p8**), and acenaphthylene (**p9**). The relative energies are given in kJ mol^{-1} . The complete PES is provided in the Supporting Information.



(5)



(6)

Scheme 3. Molecular mass growth processes involving the 1H-phenalene molecule (1) via peripheral expansion of the 1H-phenalene moiety to triangular graphene-type molecules 1,5-dihydrodibenzo[*cd,mn*]pyrene (5) and 6,11-dihydro-1H-tribenzo[*bc,hi,no*]coronene (6).

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Supporting Information

Gas Phase Formation of 1H-Phenalene via 10 π -Aromatic, Resonantly Stabilized Free Radical Intermediates

Long Zhao¹, Ralf I. Kaiser^{1*}

¹ *Department of Chemistry, University of Hawaii at Manoa, Honolulu, Hawaii, 96822*

(USA)

Wenchao Lu, Musahid Ahmed^{2*}

² *Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 (USA)*

Artem D. Oleinikov^{3,4}, Valeriy N. Azyazov^{3,4}

³ *Department of Physics, Samara National Research University, Samara 443086*

(Russian Federation)

⁴ *Lebedev Physical Institute, Samara 443011*

(Russian Federation)

Alexander M. Mebel^{3,5*}, A. Hasan Howlader,⁵ Stanislaw F. Wnuk⁵

⁵ *Department of Chemistry and Biochemistry, Florida International University, Miami, FL 33199*

(USA)

* Corresponding author:

Ralf I. Kaiser <ralfk@hawaii.edu>

Musahid Ahmed <mahmed@lbl.gov>

Alexander M. Mebel <mebela@fiu.edu>

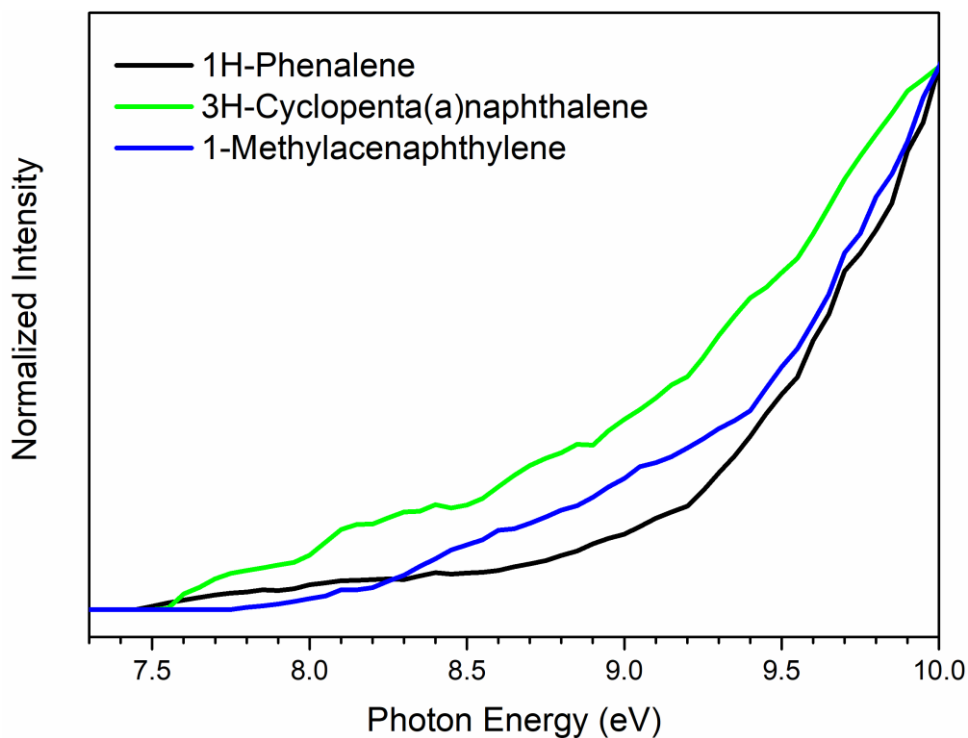


Figure S1. PIE calibration curves for distinct $C_{13}H_{10}$ isomers along with their adiabatic ionization energies: 1H-phenalene (**p1**; 7.45 ± 0.05 eV), 3H-cyclopenta(a)naphthalene (**p2**; 7.55 ± 0.05 eV), 1-methylacenaphthylene (**p8**; 7.75 ± 0.05 eV). The measured ionization energy of 1H-phenalene agrees well with the reference data of 7.449 eV.² Error bars of the calibration curves are given within $\pm 1\sigma$ and are extracted from averaging multiple calibration scans. Please note that these are normalized PIE curves, and the accurate photoionization cross sections are unknown.

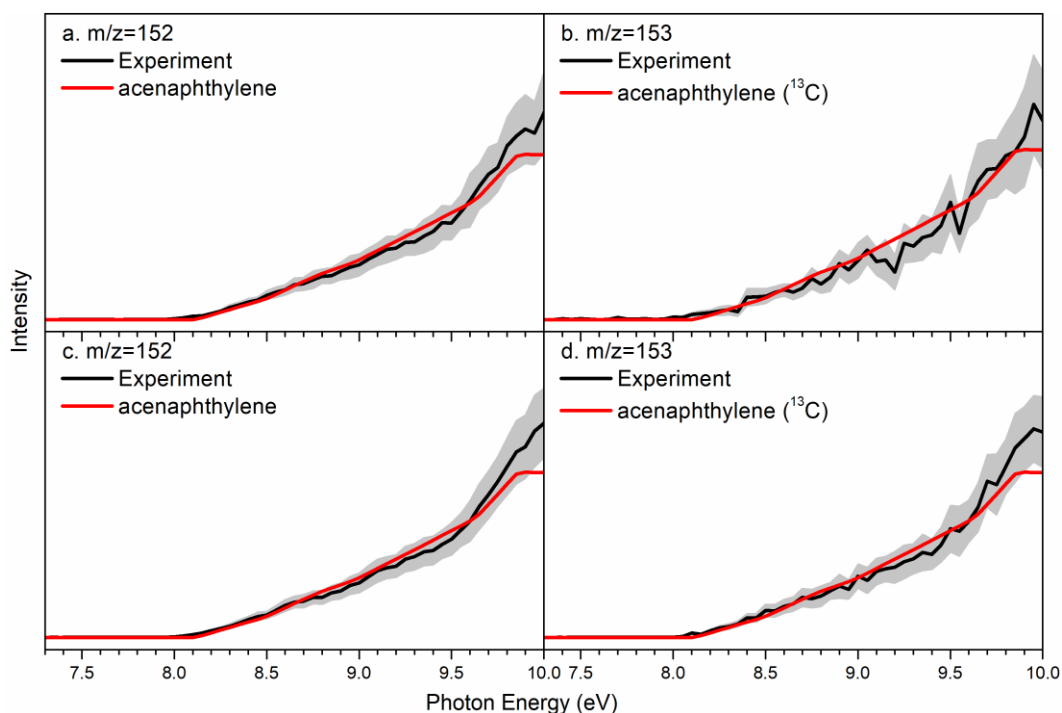


Figure S2. Photoionization efficiency (PIE) curves for signal at $m/z = 152$ and 153 in the reaction systems of (a) and (b): 1-iodonaphthalene ($C_{10}H_7I$) + allene (C_3H_4); (c) and (d): 1-iodonaphthalene ($C_{10}H_7I$) + methylacetylene (C_3H_4). Black: experimentally derived PIE curves; red: reference PIE curves. The overall error bars consist of two parts: $\pm 10\%$ based on the accuracy of the photodiode and a 1σ error of the PIE curve averaged over the individual scans. It is noticeable that there is a small discrepancy between the measured PIE curves and the references when the energy is over 9.5 eV, possibly due to the photodissociation of large molecule(s) leading to the fragments at $m/z = 152$ and 153 .

The PIE curve at $m/z = 152$ ($C_{12}H_8^+$) can be replicated in both systems solely by the reference curve of acenaphthylene formed via the methyl loss channel (reaction (1b) in the manuscript). The onset of the ion signal at 8.05 ± 0.05 eV agrees nicely with the adiabatic ionization energy of acenaphthylene of 8.02 ± 0.01 eV.⁴ These graphs are - after scaling - superimposable with the PIE curves of 153 ($C_{11}^{13}CH_8^+$) with signal at $m/z = 153$ accounting for about 11% of signal at $m/z = 152$. These findings suggest that ion counts at $m/z = 153$ arise from ^{13}C substituted acenaphthylene ($C_{12}H_8$) accounting for its natural abundance.

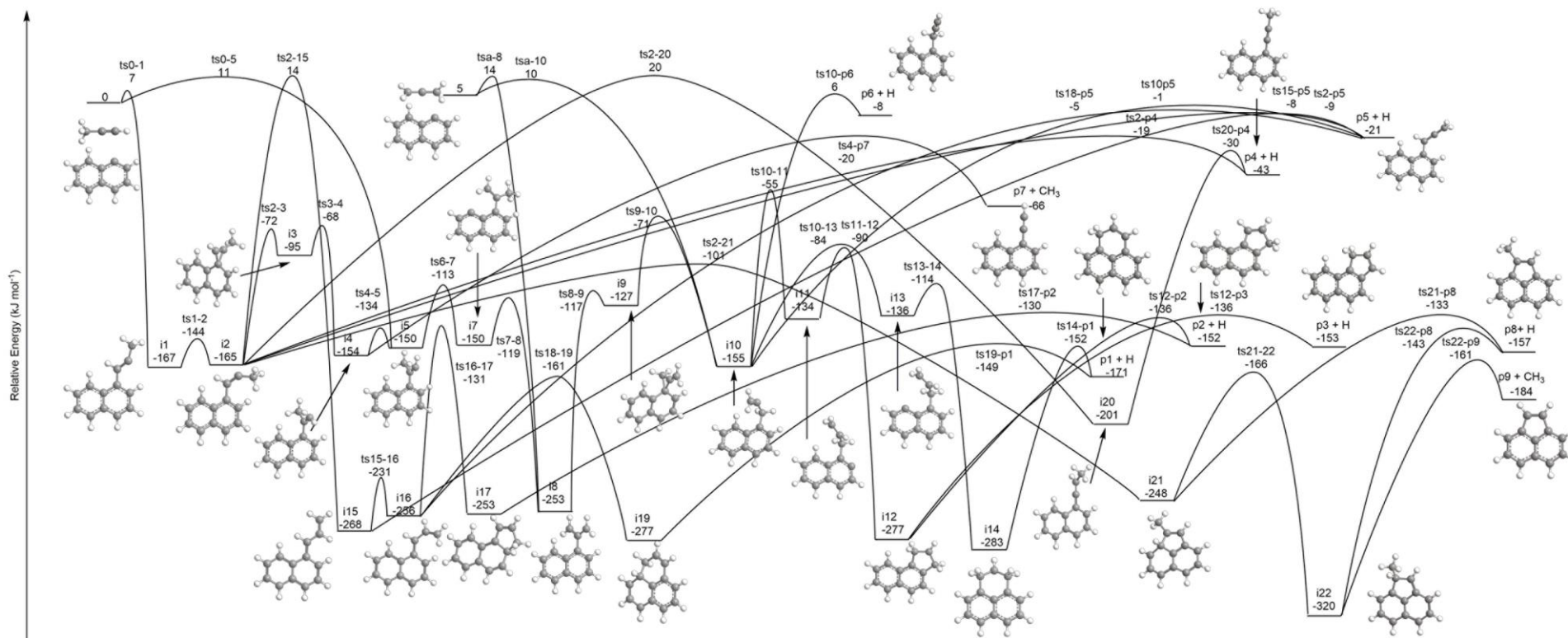
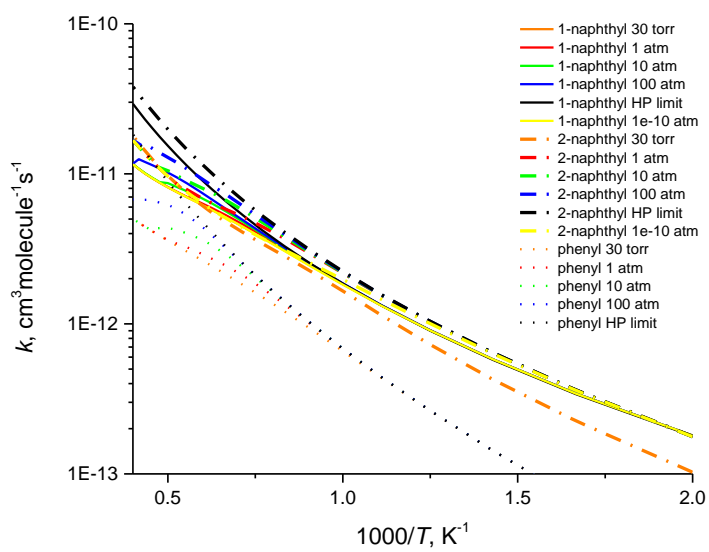
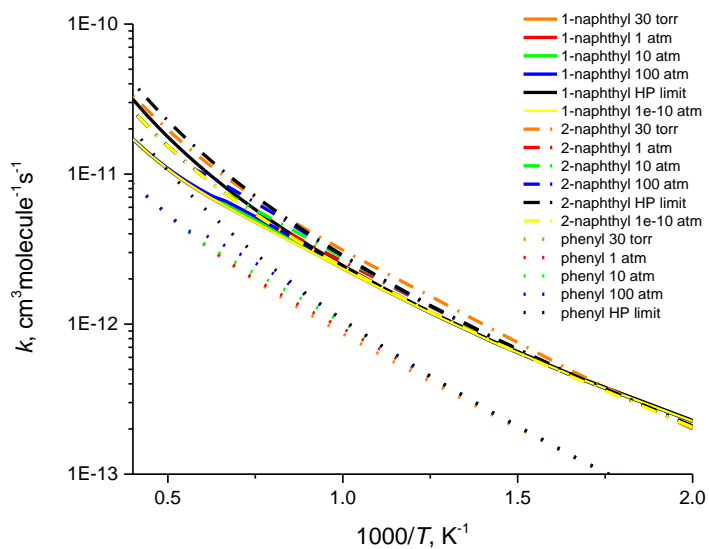


Figure S3. Complete potential energy surface (PES) for the 1-naphthyl ($\text{C}_{10}\text{H}_7^\bullet$) reaction with allene/methylacetylene (C_3H_4) calculated at the G3(MP2,CC)//B3LYP/6-311G(d,p) level. The relative energies are given in kJ mol^{-1} .



(a)



(b)

Figure S4. Total rate constants for the 1-naphthyl + allene (a) and 1-naphthyl + methylacetylene (b) reactions calculated at various pressures in comparison with total rate constants for 2-naphthyl + allene/methylacetylene¹ and phenyl + allene/methylacetylene.³

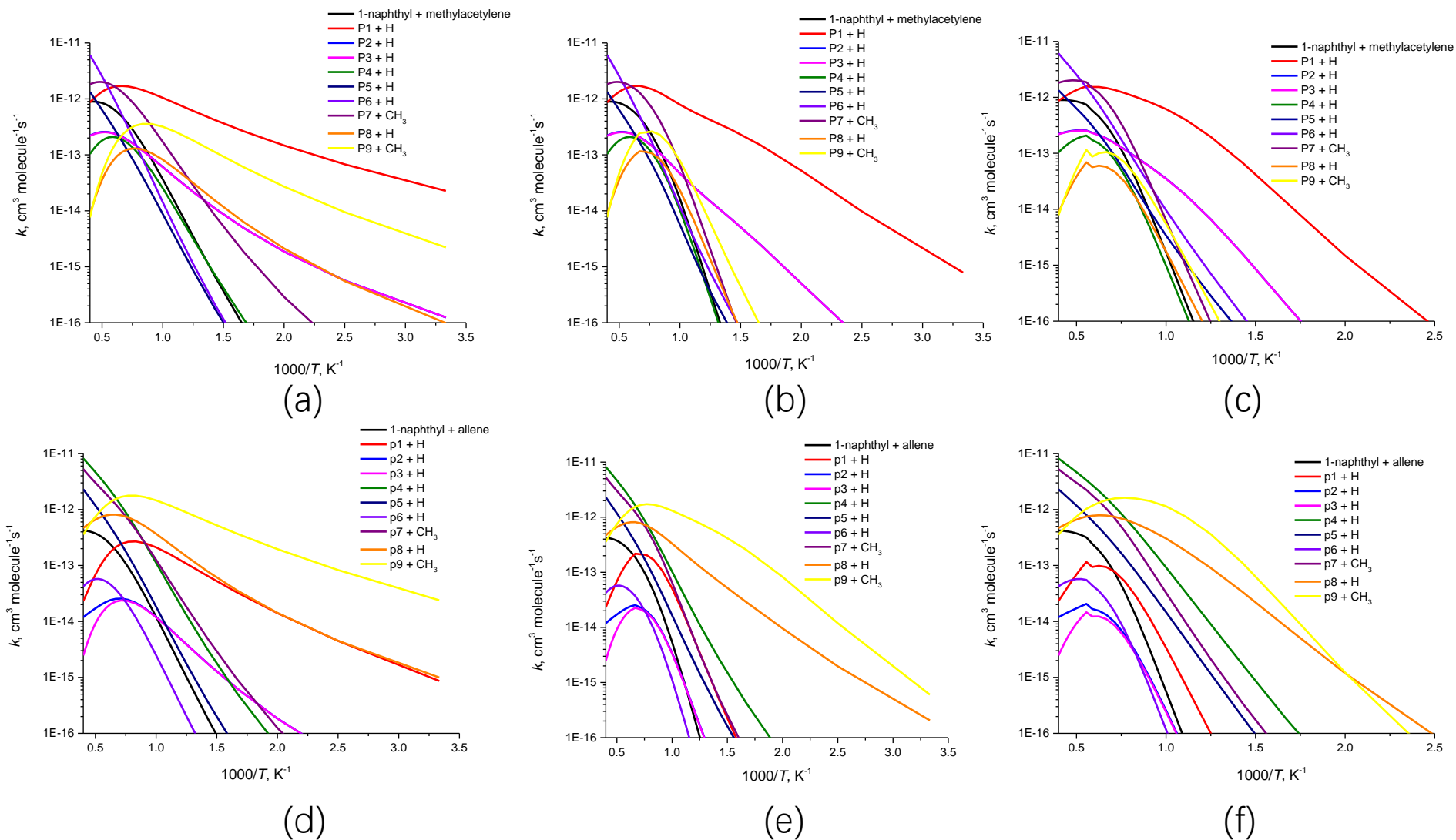


Figure S5. Calculated rate constants for individual reaction channels leading to various bimolecular products: (a) 1-naphthyl + allene at zero-pressure limit; (b) 1-naphthyl + allene at 30 Torr; (c) 1-naphthyl + allene at 1 atm; (d) 1-naphthyl + methylacetylene at zero-pressure limit; (e) 1-naphthyl + methylacetylene at 30 Torr; (f) 1-naphthyl + methylacetylene at 1 atm.

Table S1. Calculated rate constants and branching ratios of the 1-naphthyl + allene reaction at various pressures and temperatures.

a) Total and individual channel rate constants for 1-naphthyl + allene ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$), zero-pressure limit (calculated at 10^{-10} atm taking into account radiational relaxation).

T(K)	R-ma ^a	p1	p2	p3	p4	p5	p6	p7	p8	p9	total	total-HP ^b
300	3.07E-21	2.27E-14	1.24E-16	1.24E-16	2.37E-20	3.39E-21	1.76E-21	1.62E-18	9.84E-17	2.22E-15	2.54E-14	2.52E-14
400	2.37E-19	6.78E-14	5.65E-16	5.64E-16	7.50E-19	1.32E-19	9.94E-20	2.90E-17	5.53E-16	9.44E-15	7.90E-14	7.84E-14
500	6.48E-18	1.47E-13	1.86E-15	1.86E-15	1.22E-17	2.47E-18	2.30E-18	2.88E-16	2.12E-15	2.70E-14	1.80E-13	1.79E-13
600	8.64E-17	2.64E-13	4.94E-15	4.92E-15	1.16E-16	2.62E-17	2.80E-17	1.84E-15	6.30E-15	6.03E-14	3.43E-13	3.40E-13
700	6.77E-16	4.20E-13	1.11E-14	1.10E-14	7.23E-16	1.79E-16	2.13E-16	8.32E-15	1.53E-14	1.12E-13	5.80E-13	5.76E-13
800	3.50E-15	6.10E-13	2.18E-14	2.16E-14	3.15E-15	8.62E-16	1.12E-15	2.84E-14	3.13E-14	1.81E-13	9.03E-13	8.99E-13
900	1.30E-14	8.25E-13	3.82E-14	3.79E-14	1.01E-14	3.09E-15	4.48E-15	7.67E-14	5.46E-14	2.55E-13	1.32E-12	1.32E-12
1000	3.65E-14	1.05E-12	6.07E-14	6.02E-14	2.53E-14	8.74E-15	1.42E-14	1.71E-13	8.19E-14	3.18E-13	1.82E-12	1.85E-12
1100	8.21E-14	1.26E-12	8.86E-14	8.78E-14	5.08E-14	2.03E-14	3.76E-14	3.22E-13	1.07E-13	3.55E-13	2.41E-12	2.51E-12
1200	1.54E-13	1.44E-12	1.20E-13	1.19E-13	8.54E-14	4.06E-14	8.51E-14	5.31E-13	1.25E-13	3.58E-13	3.06E-12	3.29E-12
1300	2.49E-13	1.58E-12	1.53E-13	1.51E-13	1.24E-13	7.16E-14	1.70E-13	7.82E-13	1.31E-13	3.31E-13	3.74E-12	4.22E-12
1400	3.60E-13	1.67E-12	1.83E-13	1.81E-13	1.60E-13	1.15E-13	3.06E-13	1.05E-12	1.26E-13	2.84E-13	4.43E-12	5.29E-12
1500	4.73E-13	1.70E-12	2.10E-13	2.07E-13	1.87E-13	1.71E-13	5.03E-13	1.31E-12	1.13E-13	2.29E-13	5.11E-12	6.53E-12
1600	5.80E-13	1.68E-12	2.31E-13	2.28E-13	2.04E-13	2.41E-13	7.70E-13	1.55E-12	9.59E-14	1.76E-13	5.76E-12	7.93E-12
1700	6.73E-13	1.63E-12	2.46E-13	2.42E-13	2.09E-13	3.22E-13	1.11E-12	1.73E-12	7.80E-14	1.31E-13	6.37E-12	9.51E-12
1800	7.48E-13	1.55E-12	2.54E-13	2.51E-13	2.06E-13	4.15E-13	1.52E-12	1.87E-12	6.15E-14	9.43E-14	6.97E-12	1.13E-11
1900	8.05E-13	1.45E-12	2.57E-13	2.54E-13	1.95E-13	5.19E-13	1.99E-12	1.96E-12	4.73E-14	6.67E-14	7.55E-12	1.32E-11
2000	8.45E-13	1.34E-12	2.56E-13	2.53E-13	1.81E-13	6.33E-13	2.53E-12	2.00E-12	3.59E-14	4.66E-14	8.13E-12	1.54E-11
2100	8.71E-13	1.24E-12	2.52E-13	2.49E-13	1.64E-13	7.56E-13	3.13E-12	2.01E-12	2.69E-14	3.23E-14	8.73E-12	1.77E-11
2200	8.87E-13	1.13E-12	2.46E-13	2.42E-13	1.48E-13	8.88E-13	3.79E-12	1.99E-12	2.01E-14	2.24E-14	9.37E-12	2.03E-11
2300	8.95E-13	1.03E-12	2.38E-13	2.35E-13	1.32E-13	1.03E-12	4.50E-12	1.95E-12	1.50E-14	1.55E-14	1.00E-11	2.30E-11
2400	8.97E-13	9.46E-13	2.30E-13	2.27E-13	1.17E-13	1.18E-12	5.27E-12	1.89E-12	1.13E-14	1.08E-14	1.08E-11	2.60E-11
2500	8.96E-13	8.66E-13	2.22E-13	2.19E-13	1.04E-13	1.33E-12	6.10E-12	1.83E-12	8.50E-15	7.62E-15	1.16E-11	2.93E-11

b) Branching ratios for 1-naphthyl + allene, zero-pressure limit (calculated at 10^{-10} atm taking into account radiational relaxation).

T(K)	R-ma ^a	p1	p2	p3	p4	p5	p6	p7	p8	p9
300	0.00%	89.32%	0.49%	0.49%	0.00%	0.00%	0.00%	0.01%	0.39%	8.74%
400	0.00%	85.77%	0.71%	0.71%	0.00%	0.00%	0.00%	0.04%	0.70%	11.95%
500	0.00%	81.58%	1.03%	1.03%	0.01%	0.00%	0.00%	0.16%	1.18%	14.99%
600	0.03%	77.09%	1.44%	1.43%	0.03%	0.01%	0.01%	0.54%	1.84%	17.59%
700	0.12%	72.42%	1.91%	1.90%	0.12%	0.03%	0.04%	1.43%	2.64%	19.38%
800	0.39%	67.59%	2.41%	2.40%	0.35%	0.10%	0.12%	3.14%	3.47%	20.04%
900	0.98%	62.58%	2.90%	2.87%	0.77%	0.23%	0.34%	5.82%	4.14%	19.36%
1000	2.00%	57.43%	3.33%	3.30%	1.39%	0.48%	0.78%	9.35%	4.49%	17.46%
1100	3.40%	52.23%	3.67%	3.64%	2.11%	0.84%	1.56%	13.36%	4.45%	14.74%
1200	5.03%	47.12%	3.92%	3.88%	2.79%	1.33%	2.78%	17.35%	4.07%	11.71%
1300	6.66%	42.21%	4.08%	4.03%	3.31%	1.91%	4.55%	20.91%	3.49%	8.85%
1400	8.12%	37.58%	4.14%	4.09%	3.61%	2.59%	6.90%	23.74%	2.84%	6.41%
1500	9.27%	33.26%	4.11%	4.06%	3.67%	3.35%	9.85%	25.72%	2.21%	4.49%
1600	10.08%	29.27%	4.01%	3.96%	3.54%	4.18%	13.37%	26.86%	1.67%	3.07%
1700	10.56%	25.59%	3.85%	3.80%	3.29%	5.05%	17.38%	27.20%	1.22%	2.05%
1800	10.73%	22.24%	3.65%	3.60%	2.95%	5.96%	21.77%	26.86%	0.88%	1.35%
1900	10.66%	19.22%	3.41%	3.36%	2.58%	6.88%	26.41%	25.97%	0.63%	0.88%
2000	10.39%	16.53%	3.15%	3.11%	2.22%	7.79%	31.15%	24.65%	0.44%	0.57%
2100	9.98%	14.15%	2.89%	2.85%	1.88%	8.66%	35.88%	23.04%	0.31%	0.37%
2200	9.47%	12.08%	2.62%	2.59%	1.58%	9.48%	40.48%	21.25%	0.21%	0.24%
2300	8.91%	10.30%	2.37%	2.34%	1.31%	10.23%	44.84%	19.40%	0.15%	0.15%
2400	8.32%	8.77%	2.13%	2.10%	1.09%	10.91%	48.91%	17.55%	0.10%	0.10%
2500	7.74%	7.48%	1.92%	1.89%	0.90%	11.52%	52.65%	15.77%	0.07%	0.07%

c) Total and individual channel rate constants for 1-naphthyl + allene ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$), 30 Torr.

T(K)	i8	i10	i12	i14	i15	i21	R-ma ^a	p1	p2	p3	p4	p5	p6	p7	p8	p9	total	total-HP ^b
300	4.14E-15	9.78E-15	1.03E-16	1.06E-14		3.66E-23	2.58E-26	7.86E-16	1.83E-18	1.83E-18	6.28E-26	1.05E-21	7.86E-22	6.45E-24	7.16E-23	3.19E-22	2.54E-14	2.52E-14
400	2.02E-14	1.04E-14	6.22E-16	3.79E-14	4.99E-16	1.12E-15	2.81E-23	9.76E-15	4.81E-17	4.81E-17	4.93E-23	5.53E-20	6.32E-20	1.67E-21	1.03E-20	8.10E-20	7.90E-14	7.84E-14
500	6.06E-14	4.77E-15	1.67E-15	5.97E-14	6.63E-17		6.93E-21	5.23E-14	5.02E-16	5.01E-16	9.05E-21	1.04E-18	1.59E-18	1.60E-19	5.11E-19	4.30E-18	1.80E-13	1.79E-13
600	1.37E-13	1.32E-15	2.23E-15	4.92E-14			5.84E-19	1.48E-13	2.44E-15	2.43E-15	6.05E-19	1.04E-17	1.93E-17	7.06E-18	1.20E-17	8.43E-17	3.43E-13	3.40E-13
700	2.61E-13	3.14E-16	1.67E-15	2.44E-14			2.10E-17	2.78E-13	6.98E-15	6.95E-15	1.83E-17	6.87E-17	1.46E-16	1.62E-16	1.63E-16	9.02E-16	5.81E-13	5.76E-13
800	4.34E-13		7.87E-16	8.33E-15			3.61E-16	4.21E-13	1.48E-14	1.47E-14	2.77E-16	3.57E-16	7.90E-16	2.06E-15	1.35E-15	6.11E-15	9.05E-13	8.99E-13
900	6.22E-13		2.71E-16	2.23E-15			3.21E-15	5.85E-13	2.72E-14	2.70E-14	2.23E-15	1.57E-15	3.38E-15	1.50E-14	7.01E-15	2.69E-14	1.32E-12	1.32E-12
1000	7.40E-13		8.24E-17	5.81E-16			1.63E-14	7.90E-13	4.66E-14	4.62E-14	1.04E-14	5.65E-15	1.18E-14	6.61E-14	2.32E-14	7.85E-14	1.84E-12	1.85E-12
1100	7.07E-13		2.83E-17				5.33E-14	1.04E-12	7.45E-14	7.38E-14	3.11E-14	1.60E-14	3.38E-14	1.93E-13	5.20E-14	1.57E-13	2.43E-12	2.51E-12
1200	5.46E-13						1.24E-13	1.29E-12	1.09E-13	1.08E-13	6.62E-14	3.60E-14	8.09E-14	4.10E-13	8.42E-14	2.29E-13	3.08E-12	3.29E-12
1300	3.56E-13						2.24E-13	1.49E-12	1.45E-13	1.44E-13	1.09E-13	6.78E-14	1.66E-13	6.91E-13	1.07E-13	2.61E-13	3.76E-12	4.22E-12
1400	2.06E-13						3.42E-13	1.62E-12	1.79E-13	1.77E-13	1.50E-13	1.12E-13	3.03E-13	9.93E-13	1.14E-13	2.52E-13	4.45E-12	5.29E-12
1500							4.67E-13	1.71E-12	2.10E-13	2.07E-13	1.85E-13	1.70E-13	5.02E-13	1.30E-12	1.16E-13	2.45E-13	5.12E-12	6.53E-12
1600							5.77E-13	1.69E-12	2.31E-13	2.28E-13	2.03E-13	2.40E-13	7.69E-13	1.54E-12	9.79E-14	1.85E-13	5.76E-12	7.93E-12
1700							6.71E-13	1.64E-12	2.46E-13	2.42E-13	2.09E-13	3.22E-13	1.11E-12	1.73E-12	7.92E-14	1.35E-13	6.38E-12	9.51E-12
1800							7.47E-13	1.55E-12	2.54E-13	2.51E-13	2.06E-13	4.15E-13	1.52E-12	1.87E-12	6.22E-14	9.66E-14	6.97E-12	1.13E-11
1900							8.04E-13	1.45E-12	2.57E-13	2.54E-13	1.95E-13	5.19E-13	1.99E-12	1.96E-12	4.77E-14	6.78E-14	7.55E-12	1.32E-11
2000							8.45E-13	1.34E-12	2.56E-13	2.53E-13	1.81E-13	6.33E-13	2.53E-12	2.00E-12	3.61E-14	4.71E-14	8.13E-12	1.54E-11
2100							8.71E-13	1.24E-12	2.52E-13	2.49E-13	1.64E-13	7.56E-13	3.13E-12	2.01E-12	2.70E-14	3.26E-14	8.73E-12	1.77E-11
2200							8.87E-13	1.13E-12	2.46E-13	2.42E-13	1.48E-13	8.88E-13	3.79E-12	1.99E-12	2.02E-14	2.25E-14	9.37E-12	2.03E-11
2300							8.95E-13	1.03E-12	2.38E-13	2.35E-13	1.32E-13	1.03E-12	4.50E-12	1.95E-12	1.51E-14	1.56E-14	1.00E-11	2.30E-11
2400							8.97E-13	9.46E-13	2.30E-13	2.27E-13	1.17E-13	1.18E-12	5.27E-12	1.89E-12	1.13E-14	1.09E-14	1.08E-11	2.60E-11
2500							8.96E-13	8.66E-13	2.22E-13	2.19E-13	1.04E-13	1.33E-12	6.10E-12	1.83E-12	8.50E-15	7.64E-15	1.16E-11	2.93E-11

d) Branching ratios for 1-naphthyl + allene, 30 Torr.

T(K)	i8	i10	i12	i14	i15	i21	R-ma ^a	p1	p2	p3	p4	p5	p6	p7	p8	p9
300	16.33%	38.57%	0.41%	41.62%	0.00%	0.00%	0.00%	3.10%	0.01%	0.01%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
400	25.60%	13.20%	0.79%	47.93%	0.63%	1.42%	0.00%	12.35%	0.06%	0.06%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
500	33.65%	2.65%	0.93%	33.15%	0.04%	0.00%	0.00%	29.06%	0.28%	0.28%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
600	39.96%	0.39%	0.65%	14.35%	0.00%	0.00%	0.00%	43.19%	0.71%	0.71%	0.00%	0.00%	0.01%	0.00%	0.00%	0.02%
700	44.92%	0.05%	0.29%	4.21%	0.00%	0.00%	0.00%	47.88%	1.20%	1.20%	0.00%	0.01%	0.03%	0.03%	0.03%	0.16%
800	47.93%		0.09%	0.92%	0.00%		0.04%	46.56%	1.63%	1.62%	0.03%	0.04%	0.09%	0.23%	0.15%	0.68%
900	47.03%		0.02%	0.17%	0.00%		0.24%	44.21%	2.05%	2.04%	0.17%	0.12%	0.26%	1.13%	0.53%	2.03%
1000	40.32%		0.00%	0.03%	0.00%		0.89%	43.04%	2.54%	2.52%	0.57%	0.31%	0.64%	3.60%	1.27%	4.28%
1100	29.09%		0.00%		0.00%		2.19%	42.71%	3.07%	3.04%	1.28%	0.66%	1.39%	7.95%	2.14%	6.47%
1200	17.72%				0.00%		4.01%	41.79%	3.54%	3.50%	2.15%	1.17%	2.63%	13.32%	2.74%	7.43%
1300	9.47%				0.00%		5.96%	39.61%	3.86%	3.82%	2.90%	1.80%	4.42%	18.37%	2.84%	6.95%
1400	4.63%						7.69%	36.42%	4.03%	3.98%	3.38%	2.53%	6.81%	22.33%	2.55%	5.66%
1500							9.14%	33.45%	4.11%	4.06%	3.62%	3.33%	9.81%	25.43%	2.26%	4.79%
1600							10.01%	29.36%	4.01%	3.96%	3.52%	4.16%	13.34%	26.72%	1.70%	3.21%
1700							10.52%	25.64%	3.85%	3.80%	3.28%	5.05%	17.36%	27.14%	1.24%	2.12%
1800							10.72%	22.27%	3.65%	3.60%	2.95%	5.96%	21.75%	26.83%	0.89%	1.39%
1900							10.65%	19.23%	3.41%	3.36%	2.58%	6.88%	26.40%	25.95%	0.63%	0.90%
2000							10.39%	16.53%	3.15%	3.11%	2.22%	7.79%	31.15%	24.64%	0.44%	0.58%
2100							9.98%	14.15%	2.89%	2.85%	1.88%	8.66%	35.88%	23.04%	0.31%	0.37%
2200							9.47%	12.08%	2.62%	2.59%	1.58%	9.48%	40.47%	21.26%	0.22%	0.24%
2300							8.91%	10.30%	2.37%	2.34%	1.31%	10.23%	44.84%	19.40%	0.15%	0.16%
2400							8.32%	8.77%	2.13%	2.10%	1.09%	10.91%	48.91%	17.55%	0.10%	0.10%
2500							7.74%	7.48%	1.92%	1.89%	0.90%	11.52%	52.65%	15.77%	0.07%	0.07%

e) Total and individual channel rate constants for 1-naphthyl + allene ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$), 1 atm.

T(K)	i8	i10	i14	i15	i19	R-ma ^a	p1	p2	p3	p4	p5	p6	p7	p8	p9	total	total-HP ^b
300	2.63E-15	2.19E-14	8.26E-16	2.64E-12	1.76E-16	2.06E-28	2.29E-18	2.58E-21	2.58E-21	4.48E-29	9.12E-23	7.28E-23	5.72E-26	1.81E-26	4.17E-27	2.54E-14	2.52E-14
400	1.23E-14	5.93E-14	7.14E-15	9.55E-17	2.93E-17	3.59E-25	7.89E-17	2.97E-19	2.96E-19	1.40E-25	1.14E-20	1.40E-20	2.54E-23	1.46E-23	1.18E-23	7.90E-14	7.84E-14
500	4.11E-14	9.94E-14	3.73E-14	1.35E-18		1.36E-22	1.48E-15	1.25E-17	1.24E-17	8.30E-23	4.56E-19	7.26E-19	3.79E-21	3.00E-21	5.86E-21	1.80E-13	1.79E-13
600	1.11E-13	1.04E-13	1.11E-13	2.68E-19		1.59E-20	1.37E-14	2.06E-16	2.05E-16	1.16E-20	7.06E-18	1.35E-17	2.20E-19	1.83E-19	5.82E-19	3.43E-13	3.40E-13
700	2.40E-13	7.10E-14	1.90E-13	1.72E-20		7.38E-19	6.71E-14	1.57E-15	1.57E-15	5.46E-19	5.58E-17	1.23E-16	6.07E-18	4.32E-18	1.65E-17	5.81E-13	5.76E-13
800	4.35E-13	3.71E-14	2.07E-13	4.23E-20		1.67E-17	1.97E-13	6.63E-15	6.58E-15	1.16E-17	2.83E-16	7.03E-16	9.50E-17	5.09E-17	1.95E-16	9.05E-13	8.99E-13
900	6.99E-13	1.69E-14	1.57E-13	3.04E-19		2.14E-16	3.96E-13	1.79E-14	1.77E-14	1.36E-16	1.08E-15	2.91E-15	9.45E-16	3.63E-16	1.27E-15	1.33E-12	1.32E-12
1000	1.03E-12		9.33E-14	2.19E-18		1.71E-15	6.17E-13	3.54E-14	3.52E-14	9.84E-16	3.40E-15	9.62E-15	6.36E-15	1.77E-15	5.50E-15	1.85E-12	1.85E-12
1100	1.37E-12		4.34E-14	9.59E-18		9.03E-15	8.22E-13	5.81E-14	5.76E-14	4.76E-15	9.30E-15	2.69E-14	3.02E-14	6.16E-15	1.70E-14	2.46E-12	2.51E-12
1200	1.65E-12		1.85E-14	2.81E-17		3.34E-14	1.01E-12	8.55E-14	8.47E-14	1.61E-14	2.25E-14	6.54E-14	1.03E-13	1.59E-14	3.93E-14	3.15E-12	3.29E-12
1300	1.76E-12		7.88E-15	5.81E-17		9.06E-14	1.19E-12	1.17E-13	1.16E-13	4.01E-14	4.78E-14	1.41E-13	2.65E-13	3.09E-14	6.89E-14	3.88E-12	4.22E-12
1400	1.65E-12			9.09E-17		1.88E-13	1.36E-12	1.52E-13	1.51E-13	7.60E-14	8.91E-14	2.70E-13	5.26E-13	4.66E-14	9.41E-14	4.60E-12	5.29E-12
1500	1.38E-12			1.15E-16		3.16E-13	1.47E-12	1.85E-13	1.83E-13	1.16E-13	1.47E-13	4.67E-13	8.53E-13	5.72E-14	1.05E-13	5.29E-12	6.53E-12
1600	1.05E-12			1.22E-16		4.53E-13	1.53E-12	2.13E-13	2.10E-13	1.50E-13	2.21E-13	7.37E-13	1.19E-12	6.00E-14	1.01E-13	5.92E-12	7.93E-12
1700	7.45E-13			1.15E-16		5.80E-13	1.53E-12	2.34E-13	2.31E-13	1.73E-13	3.08E-13	1.08E-12	1.48E-12	5.64E-14	8.73E-14	6.51E-12	9.51E-12
1800						7.42E-13	1.57E-12	2.56E-13	2.52E-13	2.08E-13	4.14E-13	1.51E-12	1.87E-12	6.90E-14	1.15E-13	7.01E-12	1.13E-11
1900						8.02E-13	1.47E-12	2.58E-13	2.55E-13	1.98E-13	5.19E-13	1.99E-12	1.96E-12	5.18E-14	7.77E-14	7.58E-12	1.32E-11
2000						8.45E-13	1.35E-12	2.57E-13	2.53E-13	1.83E-13	6.33E-13	2.53E-12	2.01E-12	3.85E-14	5.24E-14	8.15E-12	1.54E-11
2100						8.72E-13	1.24E-12	2.53E-13	2.49E-13	1.66E-13	7.56E-13	3.13E-12	2.02E-12	2.84E-14	3.53E-14	8.75E-12	1.77E-11
2200						8.88E-13	1.13E-12	2.46E-13	2.43E-13	1.49E-13	8.88E-13	3.79E-12	1.99E-12	2.09E-14	2.39E-14	9.38E-12	2.03E-11
2300						8.96E-13	1.04E-12	2.38E-13	2.35E-13	1.32E-13	1.03E-12	4.50E-12	1.95E-12	1.55E-14	1.63E-14	1.01E-11	2.30E-11
2400						8.98E-13	9.47E-13	2.30E-13	2.27E-13	1.17E-13	1.18E-12	5.27E-12	1.89E-12	1.15E-14	1.12E-14	1.08E-11	2.60E-11
2500						8.97E-13	8.67E-13	2.22E-13	2.19E-13	1.04E-13	1.33E-12	6.10E-12	1.83E-12	8.62E-15	7.83E-15	1.16E-11	2.93E-11

f) Branching ratios for 1-naphthyl + allene, 1 atm.

T(K)	i8	i10	i12	i14	i15	i19	R-ma ^a	p1	p2	p3	p4	p5	p6	p7	p8	p9
300	10.36%	86.34%	0.02%	3.26%	0.00%	0.69%	0.00%	0.01%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
400	15.62%	75.07%	0.12%	9.03%	0.12%	0.04%	0.00%	0.10%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
500	22.80%	55.16%	0.47%	20.71%	0.00%		0.00%	0.82%	0.01%	0.01%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
600	32.25%	30.25%	1.13%	32.22%	0.00%		0.00%	4.00%	0.06%	0.06%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
700	41.34%	12.22%	1.66%	32.64%	0.00%		0.00%	11.56%	0.27%	0.27%	0.00%	0.01%	0.02%	0.00%	0.00%	0.00%
800	48.09%	4.10%	1.59%	22.83%	0.00%		0.00%	21.77%	0.73%	0.73%	0.00%	0.03%	0.08%	0.01%	0.01%	0.02%
900	52.72%	1.27%	1.07%	11.87%	0.00%		0.02%	29.85%	1.35%	1.34%	0.01%	0.08%	0.22%	0.07%	0.03%	0.10%
1000	55.53%		0.55%	5.05%	0.00%		0.09%	33.44%	1.92%	1.90%	0.05%	0.18%	0.52%	0.34%	0.10%	0.30%
1100	55.71%		0.23%	1.76%	0.00%		0.37%	33.39%	2.36%	2.34%	0.19%	0.38%	1.09%	1.22%	0.25%	0.69%
1200	52.42%		0.09%	0.59%	0.00%		1.06%	32.11%	2.71%	2.68%	0.51%	0.71%	2.07%	3.28%	0.50%	1.25%
1300	45.36%		0.03%	0.20%	0.00%		2.33%	30.75%	3.03%	2.99%	1.03%	1.23%	3.63%	6.82%	0.79%	1.77%
1400	35.88%				0.00%		4.09%	29.47%	3.31%	3.27%	1.65%	1.93%	5.87%	11.43%	1.01%	2.04%
1500	26.15%				0.00%		5.98%	27.84%	3.50%	3.46%	2.20%	2.79%	8.83%	16.14%	1.08%	1.99%
1600	17.81%				0.00%		7.66%	25.86%	3.60%	3.55%	2.54%	3.73%	12.45%	20.04%	1.01%	1.70%
1700	11.45%				0.00%		8.91%	23.57%	3.59%	3.54%	2.65%	4.73%	16.61%	22.69%	0.87%	1.34%
1800							10.59%	22.46%	3.65%	3.60%	2.97%	5.91%	21.55%	26.66%	0.99%	1.63%
1900							10.59%	19.34%	3.41%	3.36%	2.61%	6.85%	26.24%	25.89%	0.68%	1.03%
2000							10.36%	16.59%	3.15%	3.11%	2.24%	7.76%	31.04%	24.63%	0.47%	0.64%
2100							9.97%	14.19%	2.89%	2.85%	1.89%	8.64%	35.80%	23.04%	0.32%	0.40%
2200							9.47%	12.10%	2.63%	2.59%	1.59%	9.47%	40.42%	21.27%	0.22%	0.26%
2300							8.91%	10.31%	2.37%	2.34%	1.32%	10.23%	44.80%	19.41%	0.15%	0.16%
2400							8.33%	8.78%	2.14%	2.10%	1.09%	10.91%	48.89%	17.56%	0.11%	0.10%
2500							7.74%	7.48%	1.92%	1.89%	0.90%	11.52%	52.64%	15.78%	0.07%	0.07%

g) Total and individual channel rate constants for 1-naphthyl + allene (cm³ molecule⁻¹ s⁻¹), 10 atm.

T(K)	i8	i10	i11	i12	i13	i14	R-ma ^a	p1	p2	p3	p4	p5	p6	p7	p8	p9	total	total-HP ^b
300	2.52E-15	2.28E-14	7.39E-19	2.78E-20	1.69E-17	6.96E-17	1.85E-30	1.38E-20	4.34E-24	4.34E-24	4.13E-32	9.61E-24	7.71E-24	4.93E-28	2.46E-30	6.04E-32	2.54E-14	2.52E-14
400	1.11E-14	6.71E-14	9.97E-18	2.92E-18	6.98E-17	7.55E-16	4.92E-27	6.94E-19	9.95E-22	9.94E-22	2.40E-28	1.41E-21	1.75E-21	3.62E-25	6.23E-27	5.95E-28	7.90E-14	7.84E-14
500	3.24E-14	1.42E-13	7.61E-17	6.36E-17	3.40E-16	5.25E-15	2.55E-24	2.10E-17	1.03E-19	1.03E-19	2.84E-25	7.94E-20	1.31E-19	8.16E-23	4.08E-24	1.21E-24	1.80E-13	1.79E-13
600	7.80E-14	2.37E-13	3.29E-16	6.87E-16		2.71E-14	4.15E-22	3.74E-16	4.39E-18	4.37E-18	9.13E-23	1.99E-18	3.96E-18	7.21E-21	7.71E-22	5.39E-22	3.43E-13	3.40E-13
700	1.71E-13	3.11E-13	9.18E-16	3.86E-15		9.02E-14	2.77E-20	3.85E-15	8.24E-17	8.19E-17	9.58E-21	2.51E-17	5.72E-17	2.93E-19	4.99E-20	6.24E-20	5.81E-13	5.76E-13
800	3.43E-13	3.21E-13	1.95E-15	1.25E-14		2.02E-13	8.75E-19	2.35E-14	7.71E-16	7.65E-16	3.87E-19	1.79E-16	4.54E-16	6.14E-18	1.31E-18	2.33E-18	9.06E-13	8.99E-13
900	6.11E-13	2.70E-13		2.91E-14		3.15E-13	1.48E-17	9.01E-14	4.12E-15	4.08E-15	7.19E-18	8.28E-16	2.29E-15	7.53E-17	1.64E-17	3.56E-17	1.33E-12	1.32E-12
1000	9.73E-13	1.97E-13		4.13E-14		3.64E-13	1.49E-16	2.35E-13	1.39E-14	1.38E-14	7.30E-17	2.80E-15	8.31E-15	6.04E-16	1.16E-16	2.73E-16	1.85E-12	1.85E-12
1100	1.41E-12	1.30E-13		4.42E-14		3.34E-13	9.91E-16	4.48E-13	3.28E-14	3.25E-14	4.62E-16	7.59E-15	2.39E-14	3.43E-15	5.23E-16	1.22E-15	2.47E-12	2.51E-12
1200	1.93E-12			3.89E-14		2.76E-13	4.69E-15	7.18E-13	6.10E-14	6.04E-14	2.02E-15	1.76E-14	5.76E-14	1.47E-14	1.55E-15	3.16E-15	3.19E-12	3.29E-12
1300	2.41E-12			2.72E-14		1.72E-13	1.69E-14	9.36E-13	9.24E-14	9.15E-14	6.81E-15	3.60E-14	1.22E-13	4.88E-14	4.77E-15	9.85E-15	3.97E-12	4.22E-12
1400	2.80E-12			1.72E-14		9.97E-14	4.71E-14	1.11E-12	1.24E-13	1.23E-13	1.73E-14	6.68E-14	2.31E-13	1.29E-13	9.28E-15	1.74E-14	4.79E-12	5.29E-12
1500	3.03E-12			1.04E-14			1.05E-13	1.28E-12	1.55E-13	1.53E-13	3.49E-14	1.14E-13	4.04E-13	2.79E-13	1.46E-14	2.45E-14	5.61E-12	6.53E-12
1600	3.03E-12						1.95E-13	1.33E-12	1.85E-13	1.83E-13	5.80E-14	1.79E-13	6.52E-13	4.99E-13	1.91E-14	2.88E-14	6.37E-12	7.93E-12
1700	2.83E-12						3.07E-13	1.35E-12	2.06E-13	2.04E-13	8.20E-14	2.63E-13	9.83E-13	7.67E-13	2.15E-14	2.92E-14	7.04E-12	9.51E-12
1800	2.47E-12						4.28E-13	1.33E-12	2.23E-13	2.20E-13	1.02E-13	3.63E-13	1.40E-12	1.04E-12	2.18E-14	2.69E-14	7.64E-12	1.13E-11
1900	2.04E-12						5.42E-13	1.29E-12	2.33E-13	2.30E-13	1.16E-13	4.75E-13	1.89E-12	1.29E-12	2.05E-14	2.32E-14	8.17E-12	1.32E-11
2000	1.61E-12						6.41E-13	1.23E-12	2.39E-13	2.35E-13	1.23E-13	5.98E-13	2.44E-12	1.49E-12	1.82E-14	1.92E-14	8.67E-12	1.54E-11
2100							8.79E-13	1.25E-12	2.53E-13	2.51E-13	1.73E-13	7.55E-13	3.13E-12	2.04E-12	3.21E-14	4.18E-14	8.81E-12	1.77E-11
2200							8.94E-13	1.15E-12	2.48E-13	2.44E-13	1.53E-13	8.88E-13	3.79E-12	2.02E-12	2.32E-14	2.76E-14	9.43E-12	2.03E-11
2300							9.01E-13	1.04E-12	2.39E-13	2.36E-13	1.36E-13	1.03E-12	4.50E-12	1.97E-12	1.68E-14	1.83E-14	1.01E-11	2.30E-11
2400							9.02E-13	9.51E-13	2.31E-13	2.28E-13	1.20E-13	1.18E-12	5.27E-12	1.91E-12	1.23E-14	1.23E-14	1.08E-11	2.60E-11
2500							9.00E-13	8.70E-13	2.22E-13	2.19E-13	1.06E-13	1.33E-12	6.10E-12	1.84E-12	9.06E-15	8.43E-15	1.16E-11	2.93E-11

h) Branching ratios for 1-naphthyl + allene, 10 atm.

T(K)	i8	i10	i11	i12	i13	i14	R-ma ^a	p1	p2	p3	p4	p5	p6	p7	p8	p9
300	9.95%	89.71%	0.00%	0.00%	0.07%	0.27%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
400	14.03%	84.91%	0.01%	0.00%	0.09%	0.96%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
500	17.97%	78.84%	0.04%	0.04%	0.19%	2.91%	0.00%	0.01%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
600	22.73%	68.96%	0.10%	0.20%		7.90%	0.00%	0.11%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
700	29.45%	53.49%	0.16%	0.66%		15.53%	0.00%	0.66%	0.01%	0.01%	0.00%	0.00%	0.01%	0.00%	0.00%	0.00%
800	37.86%	35.39%	0.22%	1.38%		22.30%	0.00%	2.59%	0.09%	0.08%	0.00%	0.02%	0.05%	0.00%	0.00%	0.00%
900	46.01%	20.34%		2.19%		23.74%	0.00%	6.79%	0.31%	0.31%	0.00%	0.06%	0.17%	0.01%	0.00%	0.00%
1000	52.58%	10.64%		2.23%		19.66%	0.01%	12.71%	0.75%	0.75%	0.00%	0.15%	0.45%	0.03%	0.01%	0.01%
1100	57.09%	5.27%		1.79%		13.51%	0.04%	18.11%	1.33%	1.32%	0.02%	0.31%	0.96%	0.14%	0.02%	0.05%
1200	60.49%			1.22%		8.66%	0.15%	22.53%	1.92%	1.90%	0.06%	0.55%	1.81%	0.46%	0.05%	0.10%
1300	60.56%			0.69%		4.33%	0.43%	23.58%	2.33%	2.30%	0.17%	0.91%	3.06%	1.23%	0.12%	0.25%
1400	58.46%			0.36%		2.08%	0.98%	23.07%	2.59%	2.57%	0.36%	1.39%	4.83%	2.70%	0.19%	0.36%
1500	54.02%			0.19%			1.88%	22.80%	2.76%	2.73%	0.62%	2.03%	7.20%	4.97%	0.26%	0.44%
1600	47.64%						3.06%	20.85%	2.90%	2.87%	0.91%	2.82%	10.24%	7.84%	0.30%	0.45%
1700	40.13%						4.36%	19.10%	2.93%	2.89%	1.16%	3.73%	13.96%	10.88%	0.31%	0.42%
1800	32.28%						5.60%	17.45%	2.91%	2.88%	1.34%	4.75%	18.29%	13.65%	0.29%	0.35%
1900	24.98%						6.64%	15.83%	2.86%	2.82%	1.42%	5.82%	23.10%	15.82%	0.25%	0.28%
2000	18.57%						7.39%	14.22%	2.75%	2.72%	1.42%	6.90%	28.21%	17.22%	0.21%	0.22%
2100							9.98%	14.24%	2.86%	2.85%	1.96%	8.57%	35.46%	23.17%	0.36%	0.47%
2200							9.49%	12.16%	2.63%	2.59%	1.63%	9.42%	40.16%	21.39%	0.25%	0.29%
2300							8.93%	10.34%	2.37%	2.34%	1.34%	10.19%	44.62%	19.51%	0.17%	0.18%
2400							8.34%	8.80%	2.14%	2.10%	1.11%	10.89%	48.76%	17.64%	0.11%	0.11%
2500							7.76%	7.50%	1.92%	1.89%	0.91%	11.50%	52.55%	15.83%	0.08%	0.07%

i) Total and individual channel rate constants for 1-naphthyl + allene ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$), 100 atm.

T(K)	i5	i8	i10	i11	i12	i13	i14	R-ma ^a	p1	p2	p3	p4	p5	p6	p7	p8	p9	total	total-HP ^b
300	2.40E-21	2.51E-15	2.28E-14	8.05E-20	1.14E-21	7.20E-18	1.63E-18	4.67E-33	2.55E-23	4.65E-27	4.66E-27	7.72E-36	9.66E-25	7.76E-25	1.01E-30	4.61E-35		2.54E-14	2.52E-14
400	4.89E-21	1.09E-14	6.80E-14	1.28E-18	3.81E-20	5.88E-17	2.71E-17	2.05E-29	1.93E-21	1.25E-24	1.25E-24	9.35E-32	1.44E-22	1.80E-22	1.36E-27	2.83E-31	2.97E-33	7.90E-14	7.84E-14
500	6.01E-20	3.10E-14	1.48E-13	1.40E-17	5.01E-17	3.34E-16	3.37E-16	1.60E-26	9.12E-20	1.83E-22	1.82E-22	1.90E-28	8.69E-21	1.44E-20	5.00E-25	4.25E-28	1.47E-29	1.80E-13	1.79E-13
600	6.28E-19	6.96E-14	2.70E-13	1.06E-16	1.83E-17	1.51E-15	1.80E-15	3.47E-24	2.56E-18	1.35E-20	1.35E-20	9.69E-26	2.53E-19	5.11E-19	6.41E-23	1.85E-25	1.74E-26	3.43E-13	3.40E-13
700	4.43E-18	1.36E-13	4.30E-13	5.62E-16	1.99E-16	6.39E-15	7.49E-15	2.96E-22	4.35E-17	5.16E-19	5.13E-19	1.74E-23	4.14E-18	9.65E-18	3.67E-21	2.91E-23	6.17E-24	5.81E-13	5.76E-13
800	1.83E-17	2.45E-13	6.11E-13	2.14E-15	1.29E-15	3.79E-14	7.87E-15	1.26E-20	4.43E-16	1.06E-17	1.05E-17	1.35E-21	4.21E-17	1.09E-16	1.12E-19	1.93E-21	7.70E-22	9.07E-13	8.99E-13
900	1.25E-16	4.24E-13	7.80E-13	6.14E-15	5.32E-15		1.11E-13	3.03E-19	3.41E-15	1.24E-16	1.23E-16	5.10E-20	2.83E-16	8.00E-16	2.03E-18	6.10E-20	3.89E-20	1.33E-12	1.32E-12
1000	4.95E-16	7.02E-13	8.90E-13	1.39E-14	1.49E-14		2.16E-13	4.47E-18	1.65E-14	8.63E-16	8.56E-16	1.01E-18	1.32E-15	4.02E-15	2.34E-17	9.81E-19	8.90E-19	1.86E-12	1.85E-12
1100	1.74E-15	1.10E-12	9.18E-13	2.60E-14	2.98E-14		3.40E-13	4.23E-17	5.63E-14	3.76E-15	3.73E-15	1.14E-17	4.58E-15	1.47E-14	1.78E-16	8.63E-18	1.01E-17	2.49E-12	2.51E-12
1200	5.81E-15	1.60E-12	8.73E-13		8.05E-14		4.41E-13	2.68E-16	1.41E-13	1.29E-14	1.27E-14	7.74E-17	1.24E-14	4.19E-14	9.47E-16	4.44E-17	5.99E-17	3.23E-12	3.29E-12
1300	2.49E-14	2.19E-12	7.72E-13		1.01E-13		4.95E-13	1.16E-15	2.69E-13	2.93E-14	2.90E-14	3.31E-16	2.76E-14	9.75E-14	3.49E-15	1.34E-16	1.70E-16	4.04E-12	4.22E-12
1400		2.86E-12	6.48E-13		1.14E-13		5.17E-13	4.33E-15	4.01E-13	5.11E-14	5.05E-14	1.11E-15	5.33E-14	1.95E-13	1.29E-14	4.46E-16	6.26E-16	4.91E-12	5.29E-12
1500		3.74E-12			1.11E-13		5.52E-13	1.29E-14	7.14E-13	9.50E-14	9.39E-14	2.83E-15	9.47E-14	3.56E-13	3.74E-14			5.82E-12	6.53E-12
1600		4.29E-12			8.83E-14		4.08E-13	3.28E-14	8.64E-13	1.27E-13	1.25E-13	8.47E-15	1.49E-13	5.74E-13	8.44E-14	2.40E-15	2.39E-15	6.76E-12	7.93E-12
1700		4.74E-12			6.60E-14		2.88E-13	6.56E-14	9.67E-13	1.55E-13	1.53E-13	1.50E-14	2.19E-13	8.65E-13	1.63E-13	3.18E-15	2.71E-15	7.71E-12	9.51E-12
1800		5.01E-12					1.98E-13	1.15E-13	1.02E-12	1.97E-13	1.94E-13	2.31E-14	3.05E-13	1.24E-12	2.77E-13	3.73E-15	3.08E-15	8.62E-12	1.13E-11
1900		5.10E-12						1.80E-13	1.16E-12	2.08E-13	2.06E-13	3.18E-14	4.08E-13	1.69E-12	4.21E-13	3.97E-15	2.88E-15	9.45E-12	1.32E-11
2000		4.99E-12						2.57E-13	1.11E-12	2.14E-13	2.11E-13	4.03E-14	5.26E-13	2.22E-12	5.83E-13	3.98E-15	2.56E-15	1.02E-11	1.54E-11
2100		4.71E-12						3.40E-13	1.04E-12	2.17E-13	2.14E-13	4.76E-14	6.57E-13	2.83E-12	7.51E-13	3.86E-15	2.27E-15	1.09E-11	1.77E-11
2200		4.29E-12						4.25E-13	9.81E-13	2.17E-13	2.14E-13	5.34E-14	7.99E-13	3.51E-12	9.09E-13	3.69E-15	2.07E-15	1.14E-11	2.03E-11
2300		3.78E-12						5.05E-13	9.19E-13	2.15E-13	2.12E-13	5.76E-14	9.52E-13	4.25E-12	1.05E-12	3.49E-15	1.94E-15	1.20E-11	2.30E-11
2400		3.23E-12						5.78E-13	8.59E-13	2.12E-13	2.09E-13	6.01E-14	1.11E-12	5.06E-12	1.17E-12	3.27E-15	1.84E-15	1.25E-11	2.60E-11
2500								9.14E-13	8.79E-13	2.24E-13	2.21E-13	1.10E-13	1.34E-12	6.10E-12	1.88E-12	9.87E-15	9.30E-15	1.17E-11	2.93E-11

j) Branching ratios for 1-naphthyl + allene, 100 atm.

T(K)	i5	i8	i10	i11	i12	i13	i14	R-ma ^a	p1	p2	p3	p4	p5	p6	p7	p8	p9
300	0.00%	9.91%	90.06%	0.00%	0.00%	0.03%	0.01%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
400	0.00%	13.85%	86.04%	0.00%	0.00%	0.07%	0.03%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
500	0.00%	17.23%	82.42%	0.01%	0.03%	0.19%	0.19%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
600	0.00%	20.28%	78.72%	0.03%	0.01%	0.44%	0.52%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
700	0.00%	23.37%	74.10%	0.10%	0.03%	1.10%	1.29%	0.00%	0.01%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
800	0.00%	27.07%	67.43%	0.24%	0.14%	4.18%	0.87%	0.00%	0.05%	0.00%	0.00%	0.00%	0.00%	0.01%	0.00%	0.00%	0.00%
900	0.01%	31.87%	58.60%	0.46%	0.40%		8.31%	0.00%	0.26%	0.01%	0.01%	0.00%	0.02%	0.06%	0.00%	0.00%	0.00%
1000	0.03%	37.71%	47.82%	0.75%	0.80%		11.63%	0.00%	0.89%	0.05%	0.05%	0.00%	0.07%	0.22%	0.00%	0.00%	0.00%
1100	0.07%	43.93%	36.81%	1.04%	1.19%		13.61%	0.00%	2.26%	0.15%	0.15%	0.00%	0.18%	0.59%	0.01%	0.00%	0.00%
1200	0.18%	49.69%	27.07%		2.49%		13.67%	0.01%	4.36%	0.40%	0.39%	0.00%	0.38%	1.30%	0.03%	0.00%	0.00%
1300	0.62%	54.18%	19.11%		2.50%		12.27%	0.03%	6.65%	0.73%	0.72%	0.01%	0.68%	2.41%	0.09%	0.00%	0.00%
1400		58.27%	13.18%		2.31%		10.51%	0.09%	8.16%	1.04%	1.03%	0.02%	1.08%	3.96%	0.26%	0.01%	0.01%
1500		64.22%			1.91%		9.49%	0.22%	12.27%	1.63%	1.62%	0.05%	1.63%	6.12%	0.64%	0.00%	0.00%
1600		63.45%			1.31%		6.03%	0.48%	12.78%	1.87%	1.85%	0.13%	2.20%	8.48%	1.25%	0.04%	0.04%
1700		61.46%			0.86%		3.74%	0.85%	12.55%	2.00%	1.98%	0.19%	2.84%	11.22%	2.11%	0.04%	0.04%
1800		58.14%					2.30%	1.33%	11.86%	2.28%	2.25%	0.27%	3.54%	14.34%	3.21%	0.04%	0.04%
1900		53.96%						1.91%	12.31%	2.21%	2.18%	0.34%	4.32%	17.85%	4.45%	0.04%	0.03%
2000		48.96%						2.52%	10.85%	2.10%	2.07%	0.39%	5.15%	21.77%	5.72%	0.04%	0.03%
2100		43.39%						3.13%	9.62%	1.99%	1.97%	0.44%	6.05%	26.06%	6.91%	0.04%	0.02%
2200		37.44%						3.71%	8.57%	1.89%	1.87%	0.47%	6.98%	30.66%	7.94%	0.03%	0.02%
2300		31.51%						4.21%	7.66%	1.79%	1.77%	0.48%	7.93%	35.46%	8.76%	0.03%	0.02%
2400		25.80%						4.61%	6.85%	1.69%	1.67%	0.48%	8.88%	40.35%	9.31%	0.03%	0.01%
2500								7.83%	7.53%	1.92%	1.89%	0.94%	11.44%	52.22%	16.06%	0.08%	0.08%

^aR-ma indicates formation of 1-naphthyl + methylacetylene as the product of the 1-naphthyl + allene reaction.

^bTotal reaction rate constant at the high-pressure limit.

Table S2. Calculated rate constants and branching ratios of the 1-naphthyl + methylacetylene reaction at various pressures and temperatures.

a) Total and individual channel rate constants for 1-naphthyl + methylacetylene ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$), zero-pressure limit (calculated at 10^{-10} atm taking into account radiational relaxation).

T(K)	R•a ^a	p1	p2	p3	p4	p5	p6	p7	p8	p9	total	total-HP ^b
300	3.07E-22	8.64E-16	4.82E-18	4.81E-18	1.54E-19	5.66E-21	7.67E-23	4.05E-19	9.96E-16	2.39E-14	2.58E-14	2.62E-14
400	3.64E-20	4.49E-15	3.84E-17	3.83E-17	4.24E-18	2.41E-19	7.64E-21	1.01E-17	4.51E-15	8.31E-14	9.22E-14	9.36E-14
500	1.28E-18	1.41E-14	1.84E-16	1.83E-16	6.05E-17	4.70E-18	2.53E-19	1.25E-16	1.42E-14	1.96E-13	2.25E-13	2.28E-13
600	2.02E-17	3.30E-14	6.36E-16	6.33E-16	5.22E-16	5.12E-17	3.94E-18	9.32E-16	3.59E-14	3.71E-13	4.43E-13	4.49E-13
700	1.79E-16	6.42E-14	1.74E-15	1.73E-15	3.05E-15	3.57E-16	3.52E-17	4.79E-15	7.73E-14	6.06E-13	7.60E-13	7.71E-13
800	1.01E-15	1.08E-13	3.91E-15	3.88E-15	1.30E-14	1.75E-15	2.03E-16	1.81E-14	1.46E-13	8.89E-13	1.18E-12	1.21E-12
900	4.04E-15	1.60E-13	7.42E-15	7.34E-15	4.25E-14	6.38E-15	8.23E-16	5.34E-14	2.45E-13	1.19E-12	1.72E-12	1.76E-12
1000	1.21E-14	2.11E-13	1.20E-14	1.19E-14	1.12E-13	1.83E-14	2.49E-15	1.27E-13	3.68E-13	1.46E-12	2.34E-12	2.46E-12
1100	2.86E-14	2.50E-13	1.70E-14	1.67E-14	2.45E-13	4.32E-14	5.95E-15	2.52E-13	5.02E-13	1.67E-12	3.03E-12	3.28E-12
1200	5.59E-14	2.69E-13	2.14E-14	2.08E-14	4.62E-13	8.63E-14	1.16E-14	4.34E-13	6.26E-13	1.77E-12	3.76E-12	4.26E-12
1300	9.40E-14	2.66E-13	2.44E-14	2.32E-14	7.70E-13	1.52E-13	1.94E-14	6.66E-13	7.23E-13	1.77E-12	4.51E-12	5.38E-12
1400	1.40E-13	2.45E-13	2.56E-14	2.38E-14	1.17E-12	2.40E-13	2.85E-14	9.38E-13	7.85E-13	1.69E-12	5.28E-12	6.66E-12
1500	1.90E-13	2.13E-13	2.54E-14	2.27E-14	1.64E-12	3.52E-13	3.76E-14	1.24E-12	8.12E-13	1.54E-12	6.07E-12	8.09E-12
1600	2.38E-13	1.77E-13	2.41E-14	2.04E-14	2.17E-12	4.83E-13	4.57E-14	1.56E-12	8.10E-13	1.37E-12	6.90E-12	9.68E-12
1700	2.83E-13	1.42E-13	2.24E-14	1.75E-14	2.75E-12	6.33E-13	5.18E-14	1.90E-12	7.86E-13	1.19E-12	7.77E-12	1.14E-11
1800	3.20E-13	1.13E-13	2.05E-14	1.45E-14	3.36E-12	8.00E-13	5.57E-14	2.25E-12	7.50E-13	1.03E-12	8.71E-12	1.33E-11
1900	3.51E-13	8.79E-14	1.87E-14	1.17E-14	4.00E-12	9.81E-13	5.74E-14	2.62E-12	7.07E-13	8.77E-13	9.72E-12	1.54E-11
2000	3.75E-13	6.86E-14	1.71E-14	9.20E-15	4.66E-12	1.18E-12	5.71E-14	3.01E-12	6.62E-13	7.49E-13	1.08E-11	1.77E-11
2100	3.92E-13	5.38E-14	1.58E-14	7.15E-15	5.35E-12	1.38E-12	5.55E-14	3.43E-12	6.18E-13	6.40E-13	1.19E-11	2.01E-11
2200	4.05E-13	4.27E-14	1.46E-14	5.51E-15	6.04E-12	1.60E-12	5.28E-14	3.86E-12	5.76E-13	5.49E-13	1.31E-11	2.27E-11
2300	4.14E-13	3.43E-14	1.36E-14	4.22E-15	6.75E-12	1.83E-12	4.95E-14	4.31E-12	5.37E-13	4.73E-13	1.44E-11	2.54E-11
2400	4.20E-13	2.80E-14	1.27E-14	3.23E-15	7.46E-12	2.06E-12	4.60E-14	4.79E-12	5.01E-13	4.10E-13	1.57E-11	2.84E-11
2500	4.24E-13	2.32E-14	1.19E-14	2.47E-15	8.17E-12	2.30E-12	4.24E-14	5.28E-12	4.69E-13	3.58E-13	1.71E-11	3.15E-11

b) Branching ratios for 1-naphthyl + methylacetylene, zero-pressure limit (calculated at 10^{-10} atm taking into account radiational relaxation).

T(K)	R-a ^a	p1	p2	p3	p4	p5	p6	p7	p8	p9
300	0.00%	3.35%	0.02%	0.02%	0.00%	0.00%	0.00%	0.00%	3.86%	92.58%
400	0.00%	4.87%	0.04%	0.04%	0.00%	0.00%	0.00%	0.01%	4.89%	90.09%
500	0.00%	6.24%	0.08%	0.08%	0.03%	0.00%	0.00%	0.06%	6.32%	87.18%
600	0.00%	7.45%	0.14%	0.14%	0.12%	0.01%	0.00%	0.21%	8.12%	83.80%
700	0.02%	8.45%	0.23%	0.23%	0.40%	0.05%	0.00%	0.63%	10.18%	79.81%
800	0.09%	9.12%	0.33%	0.33%	1.10%	0.15%	0.02%	1.53%	12.32%	75.03%
900	0.24%	9.34%	0.43%	0.43%	2.48%	0.37%	0.05%	3.11%	14.27%	69.29%
1000	0.52%	9.04%	0.52%	0.51%	4.79%	0.78%	0.11%	5.42%	15.76%	62.57%
1100	0.94%	8.26%	0.56%	0.55%	8.09%	1.43%	0.20%	8.32%	16.58%	55.06%
1200	1.49%	7.16%	0.57%	0.55%	12.28%	2.30%	0.31%	11.54%	16.65%	47.16%
1300	2.08%	5.89%	0.54%	0.51%	17.07%	3.36%	0.43%	14.77%	16.03%	39.31%
1400	2.65%	4.63%	0.49%	0.45%	22.09%	4.55%	0.54%	17.77%	14.87%	31.96%
1500	3.12%	3.50%	0.42%	0.37%	26.97%	5.79%	0.62%	20.40%	13.38%	25.42%
1600	3.45%	2.56%	0.35%	0.30%	31.45%	7.01%	0.66%	22.60%	11.74%	19.87%
1700	3.63%	1.83%	0.29%	0.23%	35.34%	8.15%	0.67%	24.39%	10.11%	15.36%
1800	3.68%	1.29%	0.24%	0.17%	38.58%	9.18%	0.64%	25.83%	8.61%	11.79%
1900	3.61%	0.90%	0.19%	0.12%	41.19%	10.09%	0.59%	26.99%	7.28%	9.03%
2000	3.47%	0.64%	0.16%	0.09%	43.23%	10.89%	0.53%	27.93%	6.13%	6.94%
2100	3.29%	0.45%	0.13%	0.06%	44.79%	11.58%	0.46%	28.71%	5.18%	5.36%
2200	3.08%	0.32%	0.11%	0.04%	45.96%	12.16%	0.40%	29.36%	4.38%	4.18%
2300	2.87%	0.24%	0.09%	0.03%	46.81%	12.67%	0.34%	29.93%	3.73%	3.28%
2400	2.67%	0.18%	0.08%	0.02%	47.42%	13.10%	0.29%	30.44%	3.19%	2.61%
2500	2.48%	0.14%	0.07%	0.01%	47.84%	13.47%	0.25%	30.89%	2.74%	2.10%

c) Total and individual channel rate constants for 1-naphthyl + methylacetylene ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$), 30 Torr.

T(K)	i1	i8	i21	i22	R-a ^a	p1	p2	p3	p4	p5	p6	p7	p8	p9	total	total-HP ^b
300	1.43E-14	1.33E-15	2.56E-16	9.09E-15	2.58E-27	1.26E-22	4.54E-25	4.52E-25	4.91E-20	1.85E-21	4.64E-28	2.93E-21	2.05E-16	6.01E-16	2.58E-14	2.62E-14
400	2.48E-14	7.61E-15		4.73E-14	4.31E-24	3.08E-20	2.66E-22	2.63E-22	2.54E-18	1.44E-19	8.17E-25	1.64E-19	1.97E-15	1.19E-14	9.22E-14	9.36E-14
500	1.82E-14	2.61E-14	3.15E-16	8.81E-14	1.37E-21	1.83E-18	3.09E-20	3.05E-20	4.68E-17	3.54E-18	2.63E-22	4.04E-18	9.59E-15	8.27E-14	2.25E-13	2.28E-13
600	7.41E-15	6.66E-14	1.08E-16	7.85E-14	1.36E-19	4.05E-17	1.11E-18	1.09E-18	4.38E-16	4.14E-17	2.67E-20	5.51E-17	2.93E-14	2.60E-13	4.43E-13	4.49E-13
700	2.33E-15	1.39E-13	5.01E-17	3.92E-14	5.54E-18	4.78E-16	1.83E-17	1.79E-17	2.61E-15	2.93E-16	1.11E-18	5.02E-16	6.67E-14	5.08E-13	7.60E-13	7.71E-13
800		2.48E-13		1.35E-14	1.04E-16	3.49E-15	1.71E-16	1.67E-16	1.12E-14	1.45E-15	2.13E-17	3.42E-15	1.27E-13	7.77E-13	1.19E-12	1.21E-12
900		3.73E-13		3.39E-15	1.00E-15	1.65E-14	9.65E-16	9.42E-16	3.77E-14	5.50E-15	2.07E-16	1.75E-14	2.15E-13	1.05E-12	1.72E-12	1.76E-12
1000		4.55E-13		7.55E-16	5.41E-15	5.11E-14	3.45E-15	3.36E-15	1.03E-13	1.65E-14	1.13E-15	6.50E-14	3.32E-13	1.31E-12	2.35E-12	2.46E-12
1100		4.41E-13		1.75E-16	1.85E-14	1.09E-13	8.30E-15	8.04E-15	2.33E-13	4.06E-14	3.87E-15	1.75E-13	4.67E-13	1.54E-12	3.05E-12	3.28E-12
1200		3.42E-13			4.49E-14	1.68E-13	1.45E-14	1.39E-14	4.50E-13	8.37E-14	9.35E-15	3.62E-13	6.00E-13	1.69E-12	3.78E-12	4.26E-12
1300		2.24E-13			8.45E-14	2.05E-13	1.98E-14	1.87E-14	7.61E-13	1.50E-13	1.75E-14	6.13E-13	7.07E-13	1.72E-12	4.53E-12	5.38E-12
1400		1.29E-13			1.33E-13	2.12E-13	2.30E-14	2.12E-14	1.16E-12	2.39E-13	2.71E-14	9.04E-13	7.77E-13	1.66E-12	5.29E-12	6.66E-12
1500					1.87E-13	2.18E-13	2.54E-14	2.27E-14	1.64E-12	3.51E-13	3.71E-14	1.23E-12	8.13E-13	1.55E-12	6.07E-12	8.09E-12
1600					2.37E-13	1.79E-13	2.41E-14	2.04E-14	2.17E-12	4.83E-13	4.54E-14	1.56E-12	8.10E-13	1.37E-12	6.90E-12	9.68E-12
1700					2.82E-13	1.44E-13	2.24E-14	1.75E-14	2.75E-12	6.33E-13	5.17E-14	1.89E-12	7.87E-13	1.20E-12	7.77E-12	1.14E-11
1800					3.20E-13	1.13E-13	2.05E-14	1.45E-14	3.36E-12	8.00E-13	5.56E-14	2.25E-12	7.50E-13	1.03E-12	8.71E-12	1.33E-11
1900					3.51E-13	8.82E-14	1.87E-14	1.17E-14	4.00E-12	9.81E-13	5.73E-14	2.62E-12	7.07E-13	8.78E-13	9.72E-12	1.54E-11
2000					3.75E-13	6.87E-14	1.71E-14	9.20E-15	4.66E-12	1.18E-12	5.71E-14	3.01E-12	6.62E-13	7.49E-13	1.08E-11	1.77E-11
2100					3.92E-13	5.39E-14	1.58E-14	7.15E-15	5.35E-12	1.38E-12	5.55E-14	3.43E-12	6.18E-13	6.40E-13	1.19E-11	2.01E-11
2200					4.05E-13	4.27E-14	1.46E-14	5.51E-15	6.04E-12	1.60E-12	5.28E-14	3.86E-12	5.76E-13	5.49E-13	1.31E-11	2.27E-11
2300					4.14E-13	3.43E-14	1.36E-14	4.22E-15	6.75E-12	1.83E-12	4.95E-14	4.31E-12	5.37E-13	4.73E-13	1.44E-11	2.54E-11
2400					4.20E-13	2.80E-14	1.27E-14	3.23E-15	7.46E-12	2.06E-12	4.60E-14	4.79E-12	5.01E-13	4.10E-13	1.57E-11	2.84E-11
2500					4.24E-13	2.32E-14	1.19E-14	2.47E-15	8.17E-12	2.30E-12	4.24E-14	5.28E-12	4.69E-13	3.58E-13	1.71E-11	3.15E-11

d) Branching ratios for 1-naphthyl + methylacetylene, 30 Torr.

T(K)	i1	i8	i21	i22	R-a ^a	p1	p2	p3	p4	p5	p6	p7	p8	p9
300	55.45%	5.17%	0.99%	35.25%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.79%	2.33%
400	26.88%	8.26%		51.25%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	2.13%	12.92%
500	8.08%	11.61%	0.14%	39.15%	0.00%	0.00%	0.00%	0.00%	0.02%	0.00%	0.00%	0.00%	4.26%	36.74%
600	1.67%	15.05%	0.02%	17.73%	0.00%	0.01%	0.00%	0.00%	0.10%	0.01%	0.00%	0.01%	6.62%	58.78%
700	0.31%	18.34%	0.01%	5.16%	0.00%	0.06%	0.00%	0.00%	0.34%	0.04%	0.00%	0.07%	8.78%	66.89%
800		20.94%		1.14%	0.01%	0.29%	0.01%	0.01%	0.95%	0.12%	0.00%	0.29%	10.73%	65.50%
900		21.66%		0.20%	0.06%	0.96%	0.06%	0.05%	2.19%	0.32%	0.01%	1.02%	12.52%	60.94%
1000		19.37%		0.03%	0.23%	2.17%	0.15%	0.14%	4.38%	0.70%	0.05%	2.76%	14.12%	55.88%
1100		14.47%		0.01%	0.61%	3.57%	0.27%	0.26%	7.66%	1.33%	0.13%	5.76%	15.34%	50.59%
1200		9.07%			1.19%	4.46%	0.38%	0.37%	11.92%	2.22%	0.25%	9.59%	15.88%	44.67%
1300		4.94%			1.87%	4.54%	0.44%	0.41%	16.82%	3.30%	0.39%	13.54%	15.62%	38.12%
1400		2.44%			2.52%	4.02%	0.43%	0.40%	21.94%	4.52%	0.51%	17.10%	14.68%	31.44%
1500					3.08%	3.58%	0.42%	0.37%	26.94%	5.78%	0.61%	20.29%	13.39%	25.52%
1600					3.43%	2.60%	0.35%	0.30%	31.44%	7.00%	0.66%	22.56%	11.75%	19.92%
1700					3.62%	1.85%	0.29%	0.23%	35.33%	8.15%	0.66%	24.38%	10.12%	15.37%
1800					3.67%	1.30%	0.24%	0.17%	38.58%	9.18%	0.64%	25.83%	8.61%	11.79%
1900					3.61%	0.91%	0.19%	0.12%	41.18%	10.09%	0.59%	26.99%	7.28%	9.03%
2000					3.47%	0.64%	0.16%	0.09%	43.22%	10.89%	0.53%	27.93%	6.13%	6.94%
2100					3.29%	0.45%	0.13%	0.06%	44.79%	11.58%	0.46%	28.71%	5.18%	5.36%
2200					3.08%	0.32%	0.11%	0.04%	45.95%	12.16%	0.40%	29.36%	4.38%	4.18%
2300					2.87%	0.24%	0.09%	0.03%	46.81%	12.67%	0.34%	29.93%	3.73%	3.28%
2400					2.67%	0.18%	0.08%	0.02%	47.42%	13.10%	0.29%	30.44%	3.19%	2.61%
2500					2.48%	0.14%	0.07%	0.01%	47.84%	13.47%	0.25%	30.89%	2.74%	2.10%

e) Total and individual channel rate constants for 1-naphthyl + methylacetylene ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$), 1 atm.

T(K)	i1	i2	i4	i5	i8	i21	i22	R-a ^a	p1	p2	p3	p4	p5	p6	p7	p8	p9	total	total-HP ^b
300	2.83E-15	2.11E-14	4.97E-16		7.33E-16	3.89E-16	1.91E-16	2.06E-29	6.27E-27	1.46E-29	1.42E-29	2.97E-21	1.15E-22	7.52E-31	8.82E-22	3.43E-18	4.33E-19	2.58E-14	2.62E-14
400	7.98E-14			1.28E-15	5.34E-15	2.42E-15	3.22E-15	5.51E-26	9.85E-24	7.24E-26	7.05E-26	2.85E-19	1.70E-20	5.16E-27	7.46E-20	9.16E-17	3.56E-17	9.22E-14	9.36E-14
500	1.68E-13			1.52E-15	2.02E-14	7.43E-15	2.60E-14	2.68E-23	3.19E-21	4.92E-23	4.76E-23	1.10E-17	8.72E-19	3.96E-24	2.32E-18	1.18E-15	1.22E-15	2.25E-13	2.28E-13
600	2.42E-13			1.30E-15	5.39E-14	1.20E-14	1.08E-13	3.71E-21	2.68E-19	6.98E-21	6.72E-21	1.89E-16	1.85E-17	6.59E-22	3.63E-17	8.17E-15	1.73E-14	4.43E-13	4.49E-13
700	2.46E-13				1.22E-13	1.01E-14	2.37E-13	1.95E-19	7.73E-18	2.96E-19	2.84E-19	1.67E-15	1.91E-16	3.75E-20	3.40E-16	3.34E-14	1.10E-13	7.61E-13	7.71E-13
800	1.89E-13				2.37E-13	6.12E-15	2.90E-13	4.85E-18	1.00E-16	5.12E-18	4.88E-18	8.90E-15	1.16E-15	9.74E-19	2.12E-15	9.04E-14	3.63E-13	1.19E-12	1.21E-12
900	1.21E-13				4.02E-13	4.23E-15	2.21E-13	6.68E-17	7.22E-16	4.61E-17	4.36E-17	3.28E-14	4.75E-15	1.37E-17	9.47E-15	1.82E-13	7.45E-13	1.72E-12	1.76E-12
1000					6.03E-13		1.60E-13	5.65E-16	3.41E-15	2.58E-16	2.42E-16	9.27E-14	1.47E-14	1.17E-16	3.26E-14	3.05E-13	1.15E-12	2.36E-12	2.46E-12
1100					7.91E-13		6.54E-14	3.14E-15	1.13E-14	9.93E-16	9.21E-16	2.13E-13	3.64E-14	6.53E-16	9.07E-14	4.33E-13	1.42E-12	3.07E-12	3.28E-12
1200					9.10E-13		2.39E-14	1.22E-14	2.79E-14	2.78E-15	2.54E-15	4.19E-13	7.64E-14	2.51E-15	2.10E-13	5.58E-13	1.58E-12	3.82E-12	4.26E-12
1300					9.12E-13		8.31E-15	3.42E-14	5.23E-14	5.85E-15	5.24E-15	7.23E-13	1.40E-13	6.95E-15	4.11E-13	6.65E-13	1.62E-12	4.59E-12	5.38E-12
1400					8.01E-13			7.33E-14	7.72E-14	9.66E-15	8.42E-15	1.12E-12	2.28E-13	1.46E-14	6.95E-13	7.41E-13	1.59E-12	5.36E-12	6.66E-12
1500					6.28E-13			1.27E-13	9.37E-14	1.31E-14	1.10E-14	1.60E-12	3.41E-13	2.46E-14	1.04E-12	7.82E-13	1.48E-12	6.14E-12	8.09E-12
1600					4.50E-13			1.86E-13	9.86E-14	1.55E-14	1.23E-14	2.14E-12	4.75E-13	3.50E-14	1.41E-12	7.91E-13	1.33E-12	6.95E-12	9.68E-12
1700					3.00E-13			2.44E-13	9.40E-14	1.67E-14	1.22E-14	2.73E-12	6.28E-13	4.38E-14	1.79E-12	7.75E-13	1.17E-12	7.81E-12	1.14E-11
1800								3.18E-13	1.16E-13	2.06E-14	1.46E-14	3.36E-12	7.99E-13	5.52E-14	2.25E-12	7.51E-13	1.03E-12	8.71E-12	1.33E-11
1900								3.50E-13	8.94E-14	1.88E-14	1.17E-14	4.00E-12	9.80E-13	5.71E-14	2.62E-12	7.08E-13	8.79E-13	9.72E-12	1.54E-11
2000								3.75E-13	6.93E-14	1.72E-14	9.21E-15	4.66E-12	1.17E-12	5.71E-14	3.01E-12	6.62E-13	7.50E-13	1.08E-11	1.77E-11
2100								3.93E-13	5.41E-14	1.58E-14	7.15E-15	5.35E-12	1.38E-12	5.54E-14	3.43E-12	6.18E-13	6.40E-13	1.19E-11	2.01E-11
2200								4.05E-13	4.28E-14	1.47E-14	5.50E-15	6.04E-12	1.60E-12	5.28E-14	3.86E-12	5.76E-13	5.49E-13	1.31E-11	2.27E-11
2300								4.14E-13	3.44E-14	1.36E-14	4.22E-15	6.75E-12	1.83E-12	4.95E-14	4.31E-12	5.37E-13	4.73E-13	1.44E-11	2.54E-11
2400								4.20E-13	2.80E-14	1.27E-14	3.22E-15	7.46E-12	2.06E-12	4.60E-14	4.79E-12	5.01E-13	4.10E-13	1.57E-11	2.84E-11
2500								4.24E-13	2.32E-14	1.19E-14	2.47E-15	8.17E-12	2.30E-12	4.24E-14	5.28E-12	4.69E-13	3.58E-13	1.71E-11	3.15E-11

f) Branching ratios for 1-naphthyl + methylacetylene, 1 atm.

T(K)	i1	i2	i4	i5	i8	i21	i22	R-a ^a	p1	p2	p3	p4	p5	p6	p7	p8	p9
300	10.96%	81.94%	1.93%		2.84%	1.51%	0.74%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.01%	0.00%
400	86.51%			1.39%	5.79%	2.63%	3.49%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.10%	0.04%
500	74.44%			0.67%	8.97%	3.30%	11.54%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.53%	0.54%
600	54.62%			0.29%	12.18%	2.71%	24.40%	0.00%	0.00%	0.00%	0.00%	0.04%	0.00%	0.00%	0.01%	1.84%	3.91%
700	32.31%				16.05%	1.32%	31.19%	0.00%	0.00%	0.00%	0.00%	0.22%	0.03%	0.00%	0.04%	4.39%	14.44%
800	15.89%				19.94%	0.52%	24.44%	0.00%	0.01%	0.00%	0.00%	0.75%	0.10%	0.00%	0.18%	7.62%	30.55%
900	7.01%				23.31%	0.25%	12.84%	0.00%	0.04%	0.00%	0.00%	1.90%	0.28%	0.00%	0.55%	10.56%	43.23%
1000					25.56%		6.77%	0.02%	0.14%	0.01%	0.01%	3.93%	0.62%	0.00%	1.38%	12.90%	48.60%
1100					25.77%		2.13%	0.10%	0.37%	0.03%	0.03%	6.95%	1.19%	0.02%	2.95%	14.10%	46.29%
1200					23.80%		0.62%	0.32%	0.73%	0.07%	0.07%	10.96%	2.00%	0.07%	5.49%	14.60%	41.20%
1300					19.87%		0.18%	0.74%	1.14%	0.13%	0.11%	15.74%	3.04%	0.15%	8.96%	14.49%	35.37%
1400					14.95%			1.37%	1.44%	0.18%	0.16%	20.94%	4.26%	0.27%	12.96%	13.83%	29.58%
1500					10.23%			2.06%	1.53%	0.21%	0.18%	26.11%	5.56%	0.40%	16.89%	12.74%	24.06%
1600					6.47%			2.68%	1.42%	0.22%	0.18%	30.85%	6.84%	0.50%	20.27%	11.38%	19.15%
1700					3.84%			3.12%	1.20%	0.21%	0.16%	34.96%	8.04%	0.56%	22.97%	9.92%	14.99%
1800								3.65%	1.33%	0.24%	0.17%	38.56%	9.17%	0.63%	25.80%	8.62%	11.83%
1900								3.60%	0.92%	0.19%	0.12%	41.18%	10.09%	0.59%	26.98%	7.28%	9.05%
2000								3.47%	0.64%	0.16%	0.09%	43.22%	10.89%	0.53%	27.92%	6.14%	6.95%
2100								3.29%	0.45%	0.13%	0.06%	44.78%	11.57%	0.46%	28.70%	5.18%	5.36%
2200								3.08%	0.33%	0.11%	0.04%	45.95%	12.16%	0.40%	29.36%	4.38%	4.18%
2300								2.87%	0.24%	0.09%	0.03%	46.81%	12.67%	0.34%	29.93%	3.73%	3.28%
2400								2.67%	0.18%	0.08%	0.02%	47.42%	13.10%	0.29%	30.43%	3.19%	2.61%
2500								2.48%	0.14%	0.07%	0.01%	47.84%	13.47%	0.25%	30.89%	2.74%	2.10%

g) Total and individual channel rate constants for 1-naphthyl + methylacetylene ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$), 10 atm.

T(K)	i1	i2	i5	i7	i8	i21	i22	R-a ^a	p1	p2	p3	p4	p5	p6	p7	p8	p9	total	total-HP ^b
300	1.56E-14	8.85E-15	1.29E-15	4.86E-17	8.86E-17	5.62E-17	2.59E-18	1.85E-31	3.06E-31	6.38E-34	3.10E-34	2.99E-22	1.16E-23	8.52E-34	1.20E-22	4.51E-20	5.76E-22	2.58E-14	2.62E-14
400	8.50E-14		5.30E-15	2.62E-16	1.05E-15	5.40E-16	6.42E-17	7.54E-28	1.90E-27	9.07E-30	6.79E-30	3.06E-20	1.84E-21	1.38E-29	1.39E-20	1.81E-18	7.64E-20	9.22E-14	9.36E-14
500	2.00E-13		1.38E-14	8.29E-16	6.23E-15	3.19E-15	9.79E-16	5.03E-25	1.89E-24	2.35E-26	2.00E-26	1.38E-18	1.12E-19	2.62E-26	6.16E-19	4.27E-17	5.49E-18	2.25E-13	2.28E-13
600	3.72E-13		2.41E-14	3.13E-15	2.24E-14	1.20E-14	8.91E-15	9.70E-23	4.88E-22	1.19E-23	1.06E-23	3.17E-17	3.18E-18	9.80E-24	1.29E-17	5.75E-16	1.92E-16	4.43E-13	4.49E-13
700	5.76E-13		3.44E-14		6.62E-14	2.77E-14	4.79E-14	7.30E-21	4.04E-20	1.56E-21	1.41E-21	4.15E-16	4.89E-17	1.06E-21	1.51E-16	4.53E-15	3.24E-15	7.61E-13	7.71E-13
800	7.56E-13		4.29E-14		1.44E-13	3.92E-14	1.52E-13	2.53E-19	1.31E-18	6.99E-20	6.33E-20	3.33E-15	4.45E-16	4.41E-20	1.14E-15	2.22E-14	2.81E-14	1.19E-12	1.21E-12
900	8.47E-13		5.47E-14		2.71E-13	3.76E-14	2.91E-13	4.61E-18	1.95E-17	1.33E-18	1.21E-18	1.74E-14	2.57E-15	8.77E-19	5.97E-15	7.21E-14	1.34E-13	1.73E-12	1.76E-12
1000	8.26E-13				5.20E-13	3.01E-14	3.55E-13	4.94E-17	1.58E-16	1.29E-17	1.17E-17	6.28E-14	1.01E-14	9.81E-18	2.30E-14	1.68E-13	3.84E-13	2.38E-12	2.46E-12
1100	7.17E-13				7.49E-13	2.38E-14	3.09E-13	3.45E-16	7.40E-16	7.35E-17	6.56E-17	1.69E-13	2.91E-14	6.95E-17	6.74E-14	3.01E-13	7.37E-13	3.11E-12	3.28E-12
1200	5.66E-13				9.65E-13		2.65E-13	1.71E-15	2.70E-15	2.92E-16	2.57E-16	3.63E-13	6.65E-14	3.43E-16	1.59E-13	4.43E-13	1.04E-12	3.88E-12	4.26E-12
1300					1.17E-12		2.51E-13	6.37E-15	6.90E-15	8.46E-16	7.26E-16	6.72E-13	1.29E-13	1.26E-15	3.17E-13	6.35E-13	1.45E-12	4.65E-12	5.38E-12
1400					1.21E-12		1.23E-13	1.83E-14	1.34E-14	1.87E-15	1.55E-15	1.07E-12	2.15E-13	3.54E-15	5.47E-13	7.19E-13	1.50E-12	5.43E-12	6.66E-12
1500					1.15E-12			4.22E-14	2.13E-14	3.36E-15	2.64E-15	1.55E-12	3.27E-13	7.87E-15	8.48E-13	7.67E-13	1.49E-12	6.22E-12	8.09E-12
1600					1.02E-12			8.00E-14	2.84E-14	5.15E-15	3.77E-15	2.10E-12	4.60E-13	1.43E-14	1.21E-12	7.79E-13	1.33E-12	7.04E-12	9.68E-12
1700					8.40E-13			1.29E-13	3.31E-14	6.88E-15	4.59E-15	2.70E-12	6.13E-13	2.20E-14	1.60E-12	7.66E-13	1.17E-12	7.89E-12	1.14E-11
1800					6.55E-13			1.83E-13	3.51E-14	8.39E-15	4.98E-15	3.32E-12	7.83E-13	2.96E-14	2.02E-12	7.37E-13	1.01E-12	8.80E-12	1.33E-11
1900					4.89E-13			2.36E-13	3.49E-14	9.58E-15	4.96E-15	3.98E-12	9.67E-13	3.60E-14	2.45E-12	6.99E-13	8.67E-13	9.78E-12	1.54E-11
2000					3.52E-13			2.84E-13	3.32E-14	1.04E-14	4.64E-15	4.65E-12	1.16E-12	4.06E-14	2.89E-12	6.57E-13	7.42E-13	1.08E-11	1.77E-11
2100								3.96E-13	4.97E-14	1.36E-14	7.08E-15	5.34E-12	1.38E-12	5.57E-14	3.42E-12	6.18E-13	6.41E-13	1.19E-11	2.01E-11
2200								4.08E-13	4.31E-14	1.48E-14	5.44E-15	6.04E-12	1.60E-12	5.30E-14	3.86E-12	5.76E-13	5.50E-13	1.31E-11	2.27E-11
2300								4.17E-13	3.46E-14	1.38E-14	4.16E-15	6.74E-12	1.82E-12	4.96E-14	4.31E-12	5.37E-13	4.73E-13	1.44E-11	2.54E-11
2400								4.22E-13	2.82E-14	1.29E-14	3.18E-15	7.46E-12	2.06E-12	4.60E-14	4.78E-12	5.01E-13	4.10E-13	1.57E-11	2.84E-11
2500								4.25E-13	2.33E-14	1.20E-14	2.44E-15	8.17E-12	2.30E-12	4.24E-14	5.27E-12	4.69E-13	3.58E-13	1.71E-11	3.15E-11

h) Branching ratios for 1-naphthyl + methylacetylene, 10 atm.

T(K)	i1	i2	i5	i7	i8	i21	i22	R-a ^a	p1	p2	p3	p4	p5	p6	p7	p8	p9
300	60.62%	34.33%	5.01%	0.19%	0.34%	0.22%	0.01%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
400	92.17%		5.74%	0.28%	1.14%	0.59%	0.07%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
500	88.86%		6.13%	0.37%	2.77%	1.42%	0.43%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.02%	0.00%
600	83.90%		5.43%	0.71%	5.06%	2.70%	2.01%	0.00%	0.00%	0.00%	0.00%	0.01%	0.00%	0.00%	0.00%	0.13%	0.04%
700	75.73%		4.53%		8.70%	3.64%	6.30%	0.00%	0.00%	0.00%	0.00%	0.05%	0.01%	0.00%	0.02%	0.60%	0.43%
800	63.56%		3.60%		12.12%	3.29%	12.78%	0.00%	0.00%	0.00%	0.00%	0.28%	0.04%	0.00%	0.10%	1.86%	2.36%
900	48.88%		3.15%		15.64%	2.17%	16.77%	0.00%	0.00%	0.00%	0.00%	1.00%	0.15%	0.00%	0.34%	4.16%	7.72%
1000	34.69%				21.85%	1.26%	14.93%	0.00%	0.01%	0.00%	0.00%	2.64%	0.42%	0.00%	0.96%	7.04%	16.15%
1100	23.08%				24.11%	0.77%	9.93%	0.01%	0.02%	0.00%	0.00%	5.44%	0.94%	0.00%	2.17%	9.70%	23.73%
1200	14.62%				24.90%		6.83%	0.04%	0.07%	0.01%	0.01%	9.37%	1.71%	0.01%	4.10%	11.44%	26.75%
1300					25.10%		5.39%	0.14%	0.15%	0.02%	0.02%	14.45%	2.77%	0.03%	6.81%	13.66%	31.26%
1400					22.28%		2.27%	0.34%	0.25%	0.03%	0.03%	19.66%	3.97%	0.07%	10.07%	13.24%	27.58%
1500					18.52%			0.68%	0.34%	0.05%	0.04%	24.90%	5.25%	0.13%	13.62%	12.33%	23.90%
1600					14.44%			1.14%	0.40%	0.07%	0.05%	29.80%	6.54%	0.20%	17.14%	11.06%	18.92%
1700					10.64%			1.63%	0.42%	0.09%	0.06%	34.18%	7.77%	0.28%	20.30%	9.70%	14.79%
1800					7.44%			2.08%	0.40%	0.10%	0.06%	37.76%	8.90%	0.34%	22.95%	8.37%	11.47%
1900					5.00%			2.42%	0.36%	0.10%	0.05%	40.64%	9.89%	0.37%	25.06%	7.14%	8.86%
2000					3.25%			2.62%	0.31%	0.10%	0.04%	42.87%	10.74%	0.37%	26.68%	6.06%	6.85%
2100								3.32%	0.42%	0.11%	0.06%	44.77%	11.55%	0.47%	28.69%	5.18%	5.37%
2200								3.11%	0.33%	0.11%	0.04%	45.95%	12.15%	0.40%	29.35%	4.38%	4.18%
2300								2.89%	0.24%	0.10%	0.03%	46.81%	12.66%	0.34%	29.92%	3.73%	3.29%
2400								2.68%	0.18%	0.08%	0.02%	47.42%	13.10%	0.29%	30.43%	3.19%	2.61%
2500								2.49%	0.14%	0.07%	0.01%	47.84%	13.47%	0.25%	30.89%	2.74%	2.10%

i) Total and individual channel rate constants for 1-naphthyl + methylacetylene ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$), 100 atm.

T(K)	i1	i2	i4	i5	i8	i21	i22	R-a ^a	p1	p2	p3	p4	p5	p6	p7	p8	p9	total	total-HP ^b
300	1.63E-14	8.23E-15	4.17E-16	8.09E-16	2.34E-18	5.36E-18	2.33E-20	4.67E-34				2.59E-23	1.01E-24	2.13E-37	1.11E-23	4.10E-22	5.19E-25	2.58E-14	2.62E-14
400	5.20E-14	3.35E-14		6.80E-15	4.47E-17	5.74E-17	6.42E-19	3.14E-30	5.81E-32	1.87E-33	2.12E-34	2.89E-21	1.73E-22	6.59E-33	1.46E-21	1.88E-20	8.06E-23	9.22E-14	9.36E-14
500	2.04E-13			1.96E-14	4.25E-16	4.06E-16	1.20E-17	3.15E-27	1.11E-28	3.67E-30	3.95E-31	1.37E-19	1.11E-20	2.36E-29	7.40E-20	5.43E-19	7.45E-21	2.25E-13	2.28E-13
600	3.92E-13			4.43E-14	2.37E-15	2.08E-15	1.57E-16	8.10E-25	6.36E-26	2.29E-27	6.01E-28	3.36E-18	3.38E-19	1.69E-26	1.83E-18	1.02E-17	3.97E-19	4.43E-13	4.49E-13
700	6.55E-13			8.22E-14	8.79E-15	7.90E-15	1.38E-15	7.81E-23	1.25E-23	5.66E-25	2.51E-25	4.92E-17	5.85E-18	3.57E-24	2.63E-17	1.26E-16	1.22E-17	7.61E-13	7.71E-13
800	9.90E-13			1.31E-13	2.23E-14	2.19E-14	8.31E-15	3.64E-21	9.48E-22	5.97E-23	3.46E-23	4.75E-16	6.45E-17	2.91E-22	2.45E-16	1.04E-15	2.19E-16	1.19E-12	1.21E-12
900	1.38E-12			1.99E-13	7.46E-14	4.44E-14	3.37E-14	9.46E-20	3.74E-20	2.86E-21	1.90E-21	3.24E-15	4.90E-16	1.09E-20	1.60E-15	5.89E-15	2.35E-15	1.74E-12	1.76E-12
1000	1.77E-12			2.75E-13	1.42E-13	6.66E-14	9.15E-14	1.48E-18	7.06E-19	6.65E-20	4.72E-20	1.62E-14	2.67E-15	2.14E-19	7.72E-15	2.31E-14	1.54E-14	2.42E-12	2.46E-12
1100	2.11E-12			3.61E-13	2.41E-13	7.83E-14	1.69E-13	1.47E-17	7.31E-18	7.85E-19	5.65E-19	6.02E-14	1.07E-14	2.40E-18	2.85E-14	6.57E-14	6.39E-14	3.20E-12	3.28E-12
1200	2.32E-12			4.51E-13	3.66E-13	7.68E-14	2.25E-13	9.74E-17	4.31E-17	5.96E-18	4.39E-18	1.72E-13	3.24E-14	1.68E-17	8.22E-14	1.41E-13	1.74E-13	4.04E-12	4.26E-12
1300	2.34E-12			5.66E-13	4.61E-13	6.67E-14	2.33E-13	4.39E-16	1.25E-16	2.29E-17	1.53E-17	3.89E-13	7.72E-14	7.64E-17	1.91E-13	2.44E-13	3.35E-13	4.91E-12	5.38E-12
1400	2.23E-12				1.11E-12		3.27E-13	1.69E-15		2.69E-17	3.21E-19	7.34E-13	1.52E-13	2.71E-16	3.98E-13	3.26E-13	4.63E-13	5.76E-12	6.66E-12
1500	1.93E-12				1.19E-12		2.94E-13	5.16E-15	1.28E-15	2.48E-16	1.72E-16	1.20E-12	2.59E-13	8.91E-16	6.65E-13	4.30E-13	5.72E-13	6.58E-12	8.09E-12
1600					1.35E-12		4.92E-13	1.35E-14	2.67E-15	5.69E-16	3.74E-16	2.00E-12	4.39E-13	2.24E-15	1.07E-12	7.64E-13	9.84E-13	7.16E-12	9.68E-12
1700					1.24E-12		2.96E-13	2.76E-14	3.90E-15	9.80E-16	5.78E-16	2.61E-12	5.94E-13	4.33E-15	1.46E-12	7.59E-13	9.60E-13	8.00E-12	1.14E-11
1800					1.09E-12			4.93E-14	5.14E-15	1.52E-15	7.84E-16	3.26E-12	7.65E-13	7.24E-15	1.87E-12	7.43E-13	1.05E-12	8.90E-12	1.33E-11
1900					9.36E-13			7.86E-14	6.11E-15	2.16E-15	9.54E-16	3.92E-12	9.49E-13	1.07E-14	2.31E-12	7.02E-13	8.91E-13	9.86E-12	1.54E-11
2000					7.86E-13			1.14E-13	7.16E-15	2.88E-15	1.07E-15	4.63E-12	1.15E-12	1.44E-14	2.76E-12	6.59E-13	7.55E-13	1.09E-11	1.77E-11
2100					6.45E-13			1.53E-13	8.01E-15	3.64E-15	1.12E-15	5.32E-12	1.35E-12	1.80E-14	3.23E-12	6.16E-13	6.43E-13	1.20E-11	2.01E-11
2200					5.19E-13			1.94E-13	8.68E-15	4.39E-15	1.12E-15	6.02E-12	1.57E-12	2.11E-14	3.71E-12	5.75E-13	5.50E-13	1.32E-11	2.27E-11
2300					4.10E-13			2.33E-13	9.18E-15	5.11E-15	1.08E-15	6.73E-12	1.80E-12	2.35E-14	4.20E-12	5.36E-13	4.74E-13	1.45E-11	2.54E-11
2400					3.18E-13			2.70E-13	9.51E-15	5.74E-15	1.02E-15	7.45E-12	2.04E-12	2.53E-14	4.70E-12	5.01E-13	4.10E-13	1.58E-11	2.84E-11
2500								4.32E-13	1.65E-14	7.64E-15	2.32E-15	8.17E-12	2.29E-12	4.24E-14	5.27E-12	4.69E-13	3.59E-13	1.71E-11	3.15E-11

j) Branching ratios for 1-naphthyl + methylacetylene, 100 atm.

T(K)	i1	i2	i4	i5	i8	i21	i22	R-a ^a	p1	p2	p3	p4	p5	p6	p7	p8	p9
300	63.26%	31.89%	1.62%	3.13%	0.01%	0.02%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
400	56.42%	36.36%		7.37%	0.05%	0.06%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
500	90.59%			8.71%	0.19%	0.18%	0.01%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
600	88.45%			10.00%	0.53%	0.47%	0.04%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
700	86.09%			10.80%	1.15%	1.04%	0.18%	0.00%	0.00%	0.00%	0.00%	0.01%	0.00%	0.00%	0.00%	0.02%	0.00%
800	83.11%			11.02%	1.87%	1.84%	0.70%	0.00%	0.00%	0.00%	0.00%	0.04%	0.01%	0.00%	0.02%	0.09%	0.02%
900	79.06%			11.40%	4.28%	2.55%	1.93%	0.00%	0.00%	0.00%	0.00%	0.19%	0.03%	0.00%	0.09%	0.34%	0.13%
1000	73.48%			11.38%	5.88%	2.76%	3.79%	0.00%	0.00%	0.00%	0.00%	0.67%	0.11%	0.00%	0.32%	0.96%	0.64%
1100	66.19%			11.31%	7.55%	2.45%	5.30%	0.00%	0.00%	0.00%	0.00%	1.89%	0.33%	0.00%	0.89%	2.06%	2.00%
1200	57.38%			11.14%	9.05%	1.90%	5.55%	0.00%	0.00%	0.00%	0.00%	4.25%	0.80%	0.00%	2.03%	3.50%	4.31%
1300	47.68%			11.51%	9.38%	1.36%	4.74%	0.01%	0.00%	0.00%	0.00%	7.91%	1.57%	0.00%	3.88%	4.96%	6.82%
1400	38.69%				19.30%		5.67%	0.03%	0.00%	0.00%	0.00%	12.74%	2.64%	0.00%	6.90%	5.66%	8.04%
1500	29.41%				18.12%		4.47%	0.08%	0.02%	0.00%	0.00%	18.22%	3.93%	0.01%	10.10%	6.54%	8.70%
1600					18.89%		6.88%	0.19%	0.04%	0.01%	0.01%	27.93%	6.12%	0.03%	14.95%	10.67%	13.74%
1700					15.47%		3.70%	0.34%	0.05%	0.01%	0.01%	32.66%	7.42%	0.05%	18.20%	9.49%	12.01%
1800					12.25%			0.55%	0.06%	0.02%	0.01%	36.60%	8.60%	0.08%	21.04%	8.35%	11.83%
1900					9.49%			0.80%	0.06%	0.02%	0.01%	39.75%	9.62%	0.11%	23.41%	7.12%	9.03%
2000					7.20%			1.05%	0.07%	0.03%	0.01%	42.43%	10.51%	0.13%	25.33%	6.04%	6.93%
2100					5.37%			1.27%	0.07%	0.03%	0.01%	44.24%	11.27%	0.15%	26.86%	5.12%	5.35%
2200					3.93%			1.47%	0.07%	0.03%	0.01%	45.59%	11.91%	0.16%	28.07%	4.35%	4.16%
2300					2.84%			1.61%	0.06%	0.04%	0.01%	46.57%	12.47%	0.16%	29.05%	3.71%	3.28%
2400					2.02%			1.71%	0.06%	0.04%	0.01%	47.26%	12.94%	0.16%	29.84%	3.18%	2.60%
2500								2.53%	0.10%	0.04%	0.01%	47.83%	13.39%	0.25%	30.86%	2.75%	2.10%

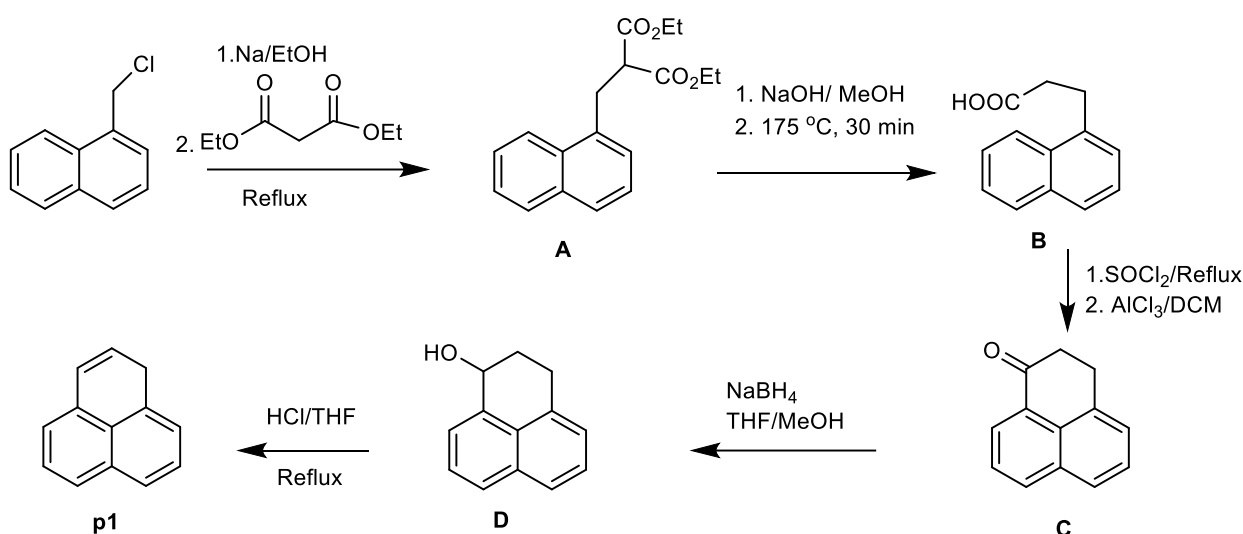
^aR-a indicates formation of 1-naphthyl + allene as the product of the 1-naphthyl + methylacetylene reaction.

^bTotal reaction rate constant at the high-pressure limit.

Synthesis and characterization of 1*H*-phenalene **p1** and 1-methylacenaphthylene **p8**

Synthesis of 1*H*-Phenalene **p1**

The 1*H*-phenalene **p1** was synthesized from commercially available 1-chloromethylnaphthalene by modifying reported protocols.^{5, 6} Shortly, treatment of 1-chloromethylnaphthalene with sodium ethoxide and malonic ester under reflux afforded diethyl 2-(naphthalene-1-ylmethyl)malonate **A** (Scheme 1). Hydrolysis and subsequent decarboxylation of **A** gave 3-(naphthalene-1-yl)propanoic acid **B**.⁷ Acylation of **B** with SOCl₂ and cyclization with AlCl₃ provided perinaphthanone-7 **C** in 75% yield. Reduction of ketone **C** with NaBH₄ and dehydration of the resulting **D** with HCl gave 1*H*-Phenalene **p1** in high overall yields (67%). Described here method uses SOCl₂/AlCl₃ instead of HF for the cyclization of **B** to **C**.



Scheme S1. Synthesis of 1*H*-phenalene **p1**

Diethyl 2-(naphthalen-1-ylmethyl)malonate; **A**.

Sodium (1.1 g, 47.9 mmol) was added to a stirred absolute EtOH (22 mL) at rt for 20 min and the resulting solution was cooled to 0 °C. Then malonic ester (12.8 g, 80 mmol) was then added slowly, followed by 1-chloromethylnaphthalene (5.0 g, 28.3 mmol). After 4 h of refluxing at 90 °C, the mixture was diluted with 20 mL water and neutralized with dilute HCl and extracted with EtOAc. The organic layer was washed with NaHCO₃ and brine. The EtOAc layer was separated, dried over anhydrous Na₂SO₄, filtered, and evaporated. The residue was column chromatographed (0 → 5 % EtOAc/hexane) to give **A**⁸ (6.8 g, 80%) as a clear liquid: ¹H NMR (400 MHz, Chloroform-*d*) δ 8.06 (dq, *J* = 8.6, 0.9 Hz, 1H), 7.87 (dt, *J* = 8.0, 0.8 Hz, 1H), 7.77-7.73 (m, 1H), 7.55 (ddd, *J* = 8.5, 6.8, 1.5 Hz, 1H), 7.50 (ddd, *J* = 8.1, 6.8, 1.3 Hz, 1H), 7.40-7.36 (m, 2H), 4.22 – 4.12 (m, 4H), 3.86 (dd, *J* = 8.1, 7.0 Hz, 1H), 3.73 (d, *J* = 7.5 Hz, 2H), 1.20 (t, *J* = 7.1 Hz, 6H); ¹³C NMR (101 MHz, CDCl₃) δ 169.13, 134.00, 133.92, 131.68, 129.06, 127.76, 127.26, 126.37, 125.74, 125.49, 123.31, 61.60, 52.97, 31.90, 14.09.

3-(Naphthalen-1-yl)propanoic acid; B.

A mixture of ester **A** (5 g, 16.6 mmol) in the solution of MeOH (5 mL) and NaOH (20 mL; 4 g, 0.1 mol) was refluxed at 110 °C for 3 h. After adding another 10 mL of hot water, the pH of the solution was made below 2.0 with 4 M HCl (10 mL). The precipitated solid was filtered and washed with cold water and dried in piston under the reduced pressure. The white powder was placed in round-bottom flask and was heated at 175 °C (oil bath) while evolution of carbon dioxide was observed. After 30 min, the heating was stopped and the flask was cooled to rt. Recrystallization from mixture of MeOH/benzene gave **B**⁵ (3.0 g, 90%) as a white powder: ¹H NMR (400 MHz, Chloroform-*d*) δ 8.04 (dq, *J* = 8.8, 1.0 Hz, 1H), 7.87 (dt, *J* = 8.0, 0.8 Hz, 1H), 7.75 (dt, *J* = 8.0, 1.2 Hz, 1H), 7.52 (dddd, *J* = 19.2, 8.1, 6.8, 1.4 Hz, 2H), 7.44 – 7.36 (m, 2H), 3.49 – 3.42 (m, 2H), 2.88 – 2.81 (m, 2H); ¹³C NMR (101 MHz, CDCl₃) δ 178.48, 136.24, 134.04, 131.69, 129.09, 127.43, 126.33, 126.07, 125.81, 125.73, 123.42, 34.88, 27.95.

2,3-Dihydro-1H-phenalen-1-one; C.

Compound **B** (2.8 g, 13.98 mmol) was dissolved in SOCl₂ (40 mL) and the solution was refluxed at 85 °C for 1 h. The SOCl₂ was distilled off under reduced pressure. The resulted acid chloride was dissolved in 10 mL of dry dichloromethane and then added dropwise to a cold (-10 °C) solution of 4.47 g (33.5 mmol) of aluminum chloride in 100 mL of dry dichloromethane. After stirring for 30 min at 0 °C, the mixture was poured into 100 mL of ice/water and the resulting solution was extracted with dichloromethane. The organic layer was separated, dried over anhydrous Na₂SO₄, filtered, and evaporated. The residue was column chromatographed (5 → 10 % EtOAc/hexane) to give **C**⁵ (1.91 g, 75%) as off-white solid: ¹H NMR (600 MHz, Chloroform-*d*) δ 8.20 (dd, *J* = 7.2, 1.3 Hz, 1H), 8.09 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.80 (d, *J* = 8.1 Hz, 1H), 7.60 (t, *J* = 7.7 Hz, 1H), 7.50 (t, *J* = 7.5 Hz, 1H), 7.48 – 7.45 (m, 1H), 3.44 (t, *J* = 7.2 Hz, 2H), 3.01 – 2.97 (m, 2H); ¹³C NMR (101 MHz, CDCl₃) δ 198.78, 134.22, 133.51, 133.37, 131.76, 129.93, 126.88, 126.41, 125.83, 125.68, 125.20, 38.65, 28.69.

2,3-Dihydro-1H-phenalen-1-ol; D

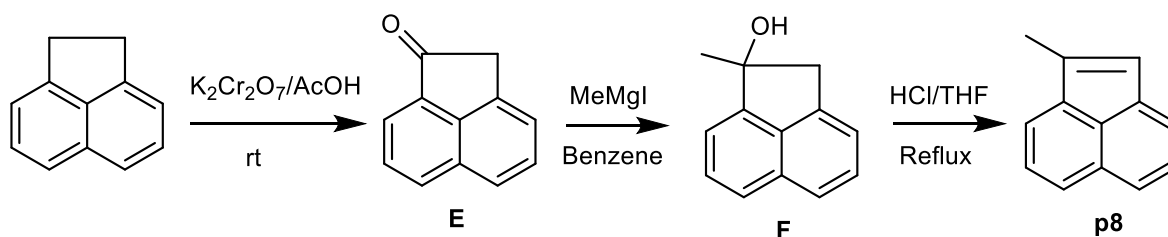
NaBH₄ (748 mg, 19.8 mmol) was added portion wise to a stirred solution of **C** (1.8 g, 9.88 mmol) in dry MeOH/THF (40 mL, 2;1) at 0 °C (ice-bath). After 5 min, the reaction mixture was allowed to warm to rt and stirring was continued for 30 min. Water (10 mL) was then added to quench the reaction. The mixture was concentrated under reduced pressure and extracted with EtOAc. The organic phase was separated, dried over anhydrous Na₂SO₄, filtered, and evaporated. The residue was column chromatographed (EtOAc in hexane 20 → 40%) to give **D**⁶ (1.64 g, 90%) as a white solid: ¹H NMR (600 MHz, Chloroform-*d*) δ 7.80 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.72 (d, *J* = 8.2 Hz, 1H), 7.56 (d, *J* = 7.0 Hz, 1H), 7.50 – 7.46 (m, 1H), 7.43 (dd, *J* = 8.2, 6.9 Hz, 1H), 7.31 (dd, *J* = 7.0, 1.5 Hz, 1H), 5.09 (dd, *J* = 6.8, 3.7 Hz, 1H), 3.33 (ddd, *J* = 16.1, 8.9, 4.6 Hz, 1H), 3.09 (ddd, *J* = 16.2, 7.3, 4.6 Hz, 1H), 2.24 – 2.14 (m, 2H), 1.96 (s, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 137.53, 135.21, 133.73, 128.79, 128.15, 126.01, 125.79, 125.72, 124.50, 123.59, 69.48, 31.41, 26.37.

1H-Phenylene; p1

The secondary alcohol **D** (1.0 g, 5.4 mmol) was dissolved in the mixture of THF/H₂O (20 mL, 1:1). Aqueous 4 N HCl (10.0 mL, 40 mmol) was then added and the reaction mixture was refluxed at 105 °C for 6 h. The reaction mixture was concentrated under vacuum to approximately 20 mL and was transferred to a separatory funnel and extracted with EtOAc. The organic phase was separated, dried over anhydrous Na₂SO₄, filtered, and evaporated. The residue was column chromatographed (*n*-hexane) to give **p1**⁶ (673 mg, 75%) as a light yellow solid: ¹H NMR (600 MHz, Chloroform-*d*) δ 7.56 (d, *J* = 8.2 Hz, 1H), 7.52 (d, *J* = 8.3 Hz, 1H), 7.36 (t, *J* = 7.6 Hz, 1H), 7.30 – 7.23 (m, 2H), 6.98 (d, *J* = 6.9 Hz, 1H), 6.60 (dt, *J* = 9.8, 2.3 Hz, 1H), 6.05 (dt, *J* = 9.8, 4.1 Hz, 1H), 4.09 – 4.06 (m, 2H); ¹³C NMR (101 MHz, CDCl₃) δ 134.36, 133.70, 132.13, 129.59, 127.91, 127.76, 126.82, 126.40, 126.17, 125.19, 125.04, 122.22, 32.19.

Synthesis of 1-methylacenaphthalene **p8**

The 1-methylacenaphthalene **p8** was prepared from commercially available acenaphthalene by modifying reported protocols.^{7,9} Shortly, oxidation of acenaphthalene with K₂Cr₂O₇ in acetic acid afforded acenaphthylenone **E** (Scheme 2). Reaction of ketone **E** with MeMgI in dry THF as reported¹⁰ led to the mixture of unidentified products. However, treatment of **E** with MeMgI in dry benzene¹¹ gave tertiary alcohol **F** in 81% yield. Dehydration of **F** with aqueous HCl in THF under reflux provided 1-methylacenaphthalene **p8** in high overall yield (80%).



Scheme S2. Synthesis of 1-methylacenaphthalene **p8**

Acenaphthylen-1(2H)-one; **E**.

Suspension of K₂Cr₂O₇ (9.53 g, 32.4 mmol) in acetic acid (40 mL) was added to an acetic acid (40 mL) solution of acenaphthalene (5.0 g, 32.4 mmol) at rt for overnight. The resulting mixture was poured into 200 mL of H₂O and extracted with 5 x 50 mL EtOAc. The combined organic portions were washed with saturated NaHCO₃ solution followed by brine. The organic layer was separated, dried over anhydrous Na₂SO₄, filtered, and evaporated. The residue was column chromatographed (0 → 10 % EtOAc/hexane) to give **E**⁷ (3.27 g, 60%) as off-white solid: ¹H NMR (400 MHz, Chloroform-*d*) δ 8.09 (dd, *J* = 8.1, 0.7 Hz, 1H), 7.96 (dd, *J* = 7.1, 0.8 Hz, 1H), 7.82 (dd, *J* = 8.4, 0.8 Hz, 1H), 7.71 (dd, *J* = 8.1, 7.0 Hz, 1H), 7.60 (dd, *J* = 8.4, 6.8 Hz, 1H), 7.46 (dq, *J* = 6.9, 1.0 Hz, 1H), 3.82 (t, *J* = 0.9 Hz, 2H); ¹³C NMR (101 MHz, CDCl₃) δ 203.11, 143.06, 135.13, 134.81, 131.61, 131.07, 128.50, 128.12, 124.08, 121.57, 121.16, 42.13.

1-Methyl-1,2-dihydroacenaphthylen-1-ol; **F**.

A solution of **E** (505 mg, 3.0 mmol) in benzene (10 mL) was added dropwise for 10 min to a cooled (ice-bath) solution of MeMgI (3 M, 1.5 mL, 4.5 mmol), and stirring was continued for an additional 10 min at rt. The reaction mixture was then refluxed at 85 °C for 2 h [progress of the reaction was monitored by TLC]. The reaction mixture was poured in ice-water and saturated NH₄Cl was added to quench the reaction. The mixture was extracted with EtOAc and organic layer was separated, dried over anhydrous Na₂SO₄, filtered, and evaporated. The residue was column chromatographed (0 → 20% EtOAc/hexane) to give **F**¹¹ (450 mg, 81.4%) as off-white solid: ¹H NMR (600 MHz, Chloroform-*d*) δ 7.76 (d, *J* = 8.1 Hz, 1H), 7.70 – 7.67 (m, 1H), 7.57 (dd, *J* = 8.1, 6.9 Hz, 1H), 7.52 (dd, *J* = 8.2, 6.8 Hz, 1H), 7.48 (d, *J* = 6.9 Hz, 1H), 7.31 (dq, *J* = 6.8, 1.1 Hz, 1H), 3.62 – 3.47 (m, 2H), 1.87 (brs, 1H), 1.77 (s, 3H).

1-Methylacenaphthalene; **p8**.

The tertiary alcohol **F** (400 mg, 2.17 mmol) was dissolved in THF/H₂O (10 mL, 1:1). Aqueous 6 N HCl (3.0 mL, 18 mmol) was then added and the reaction mixture was refluxed at 105 °C for 12 h. The reaction mixture was concentrated to ~6 mL and was transferred to a separatory funnel and extracted with EtOAc. The organic phase was separated, dried over anhydrous Na₂SO₄, filtered, and evaporated at reduced pressure. The residue was column chromatographed (*n*-hexane) to give **p8**¹¹ (356 mg, 98.6%) as a light orange liquid: ¹H NMR (600 MHz, Chloroform-*d*) δ 7.79 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.65 (d, *J* = 6.7 Hz, 1H), 7.58 – 7.47 (m, 3H), 6.72 (t, *J* = 1.8 Hz, 1H), 2.45 (t, *J* = 1.8 Hz, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 141.17, 140.46, 139.95, 129.10, 127.99, 127.90, 127.50, 127.27, 125.98, 125.41, 122.48, 121.83, 13.31.

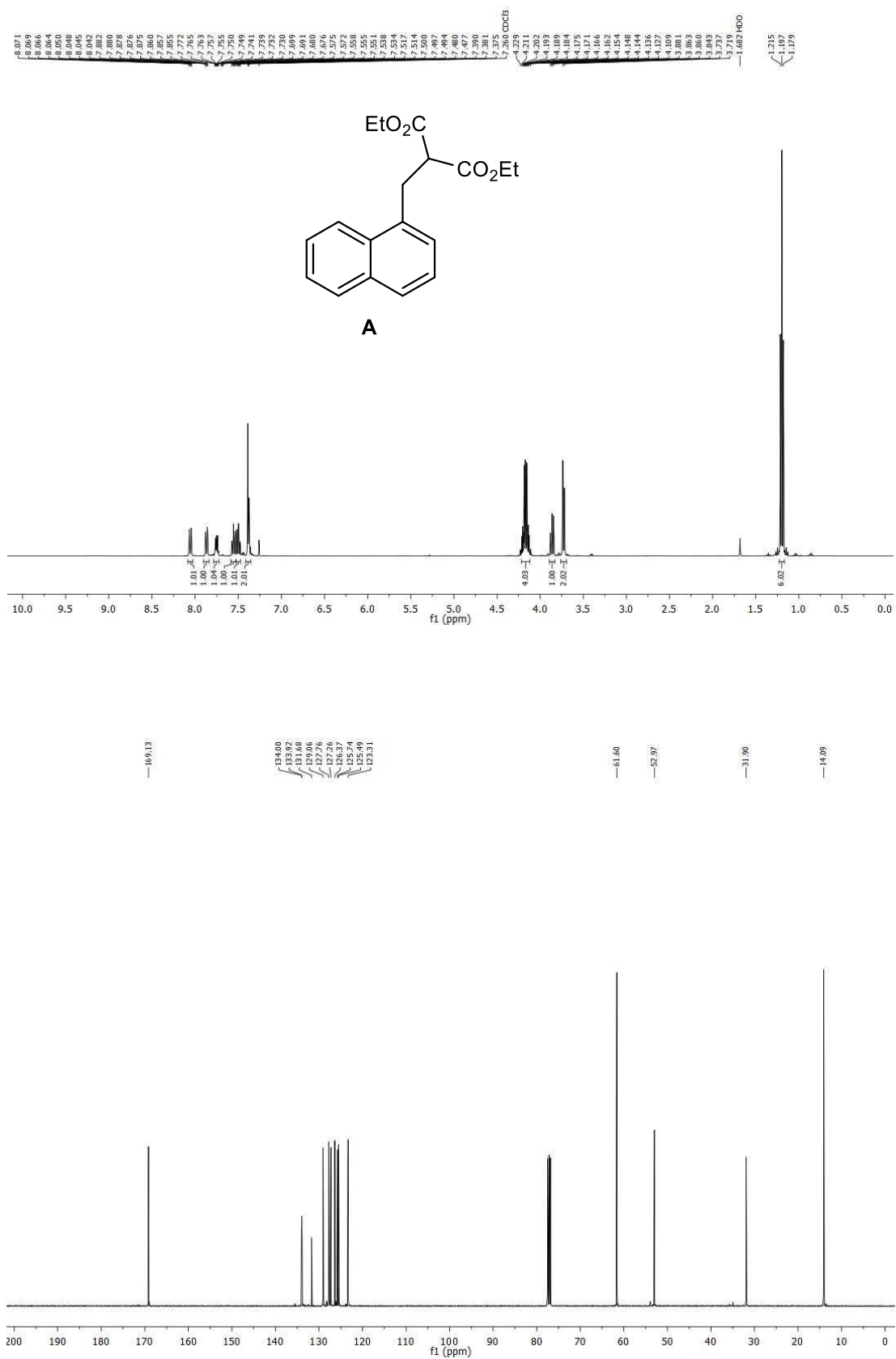


Figure S6. ¹H NMR and ¹³C NMR spectra of compound A in CDCl₃.

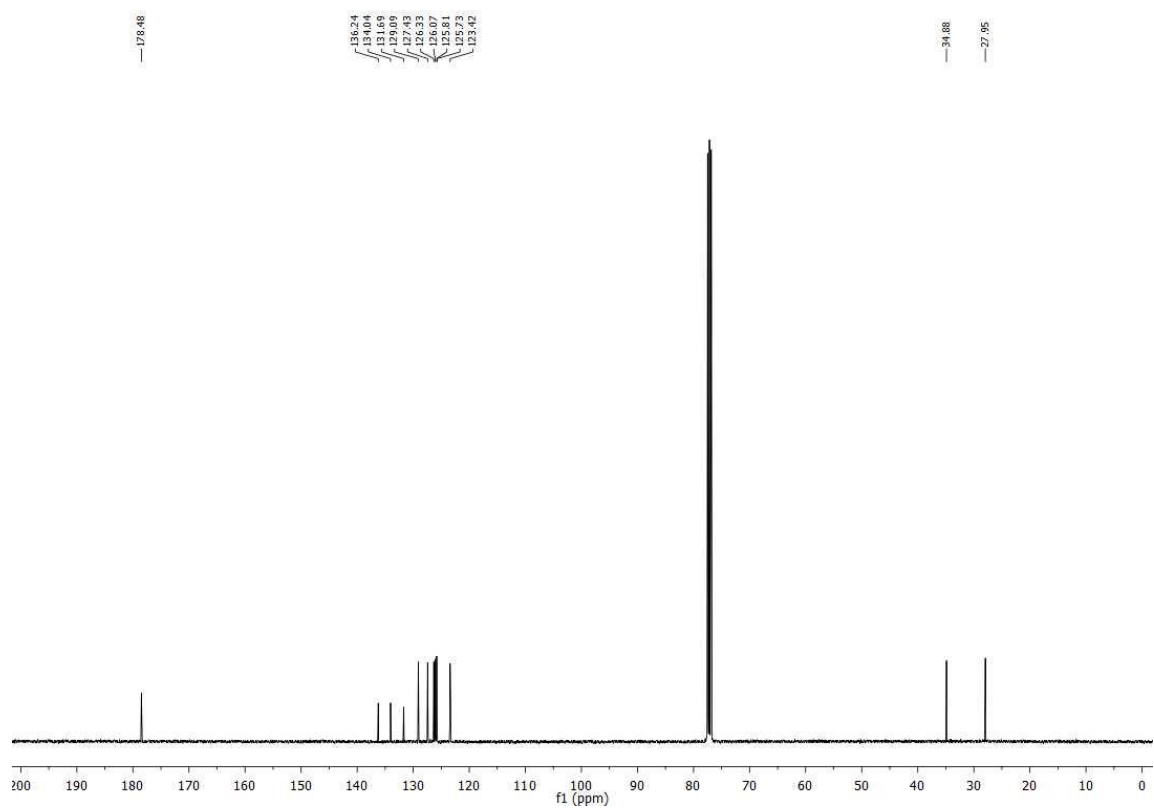
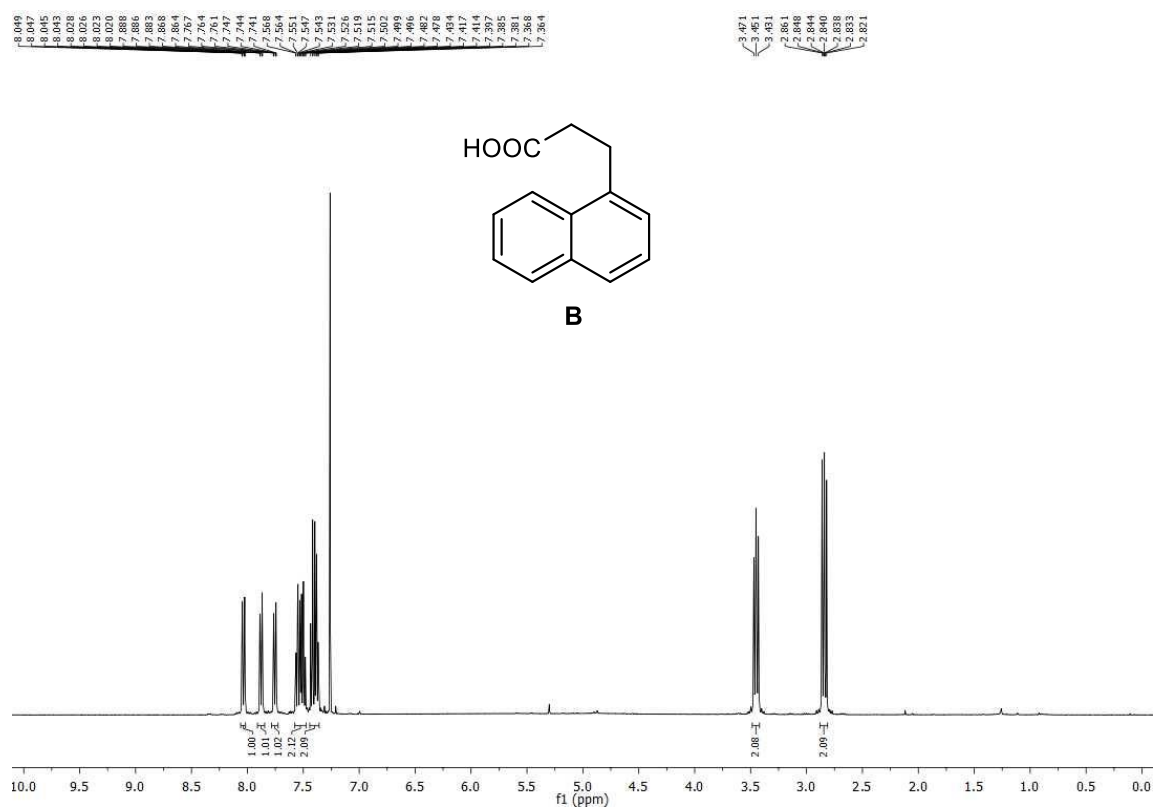


Figure S7. ¹H NMR and ¹³C NMR spectra of compound **B** in CDCl₃.

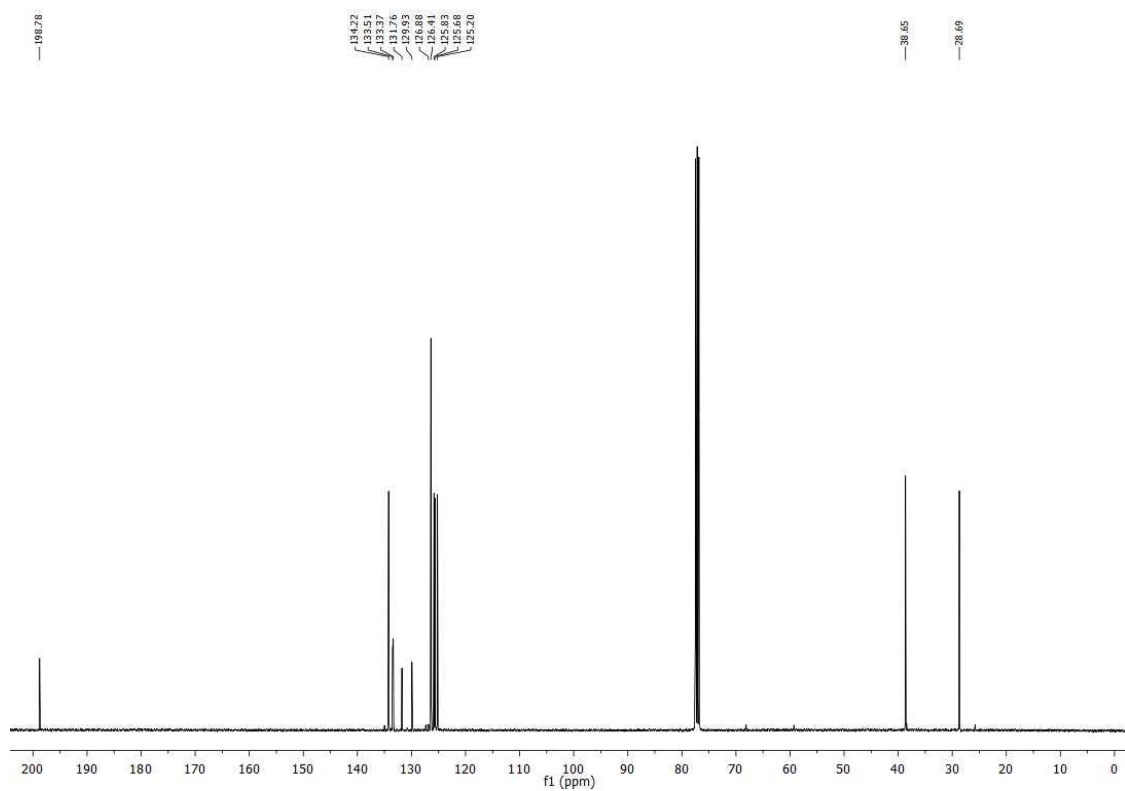
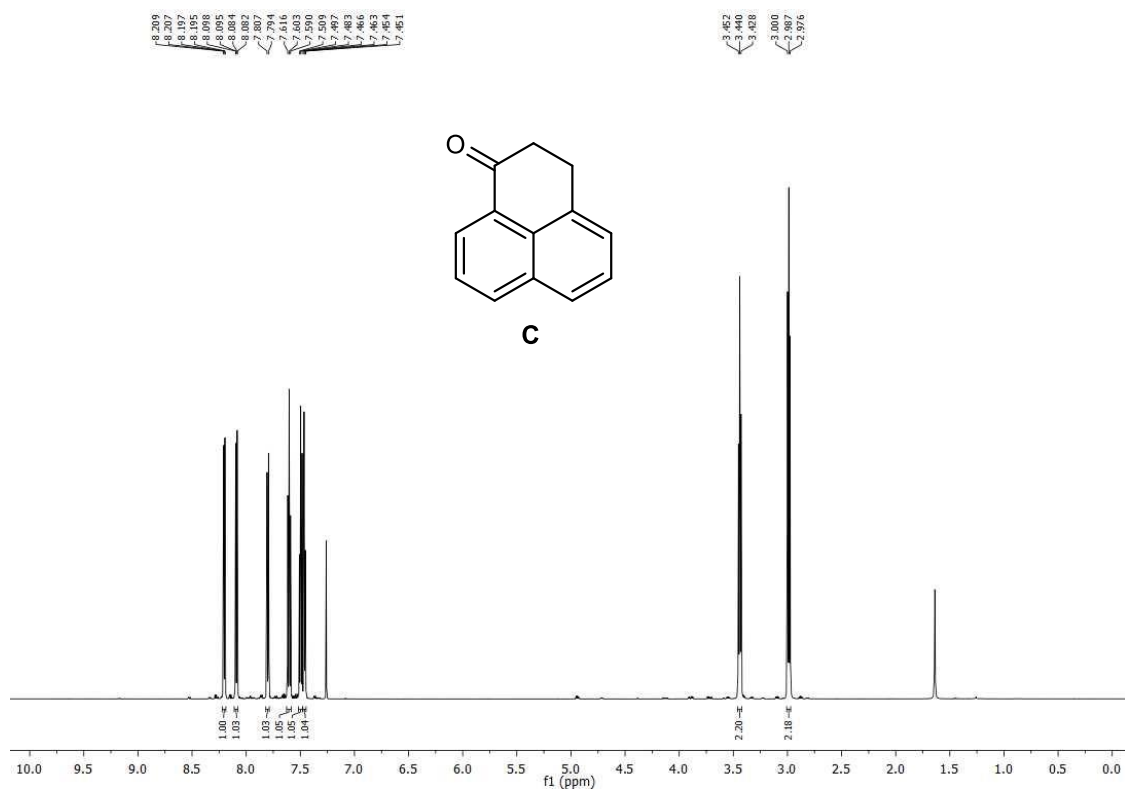


Figure S8. ¹H NMR and ¹³C NMR spectra of compound **C** in CDCl₃.

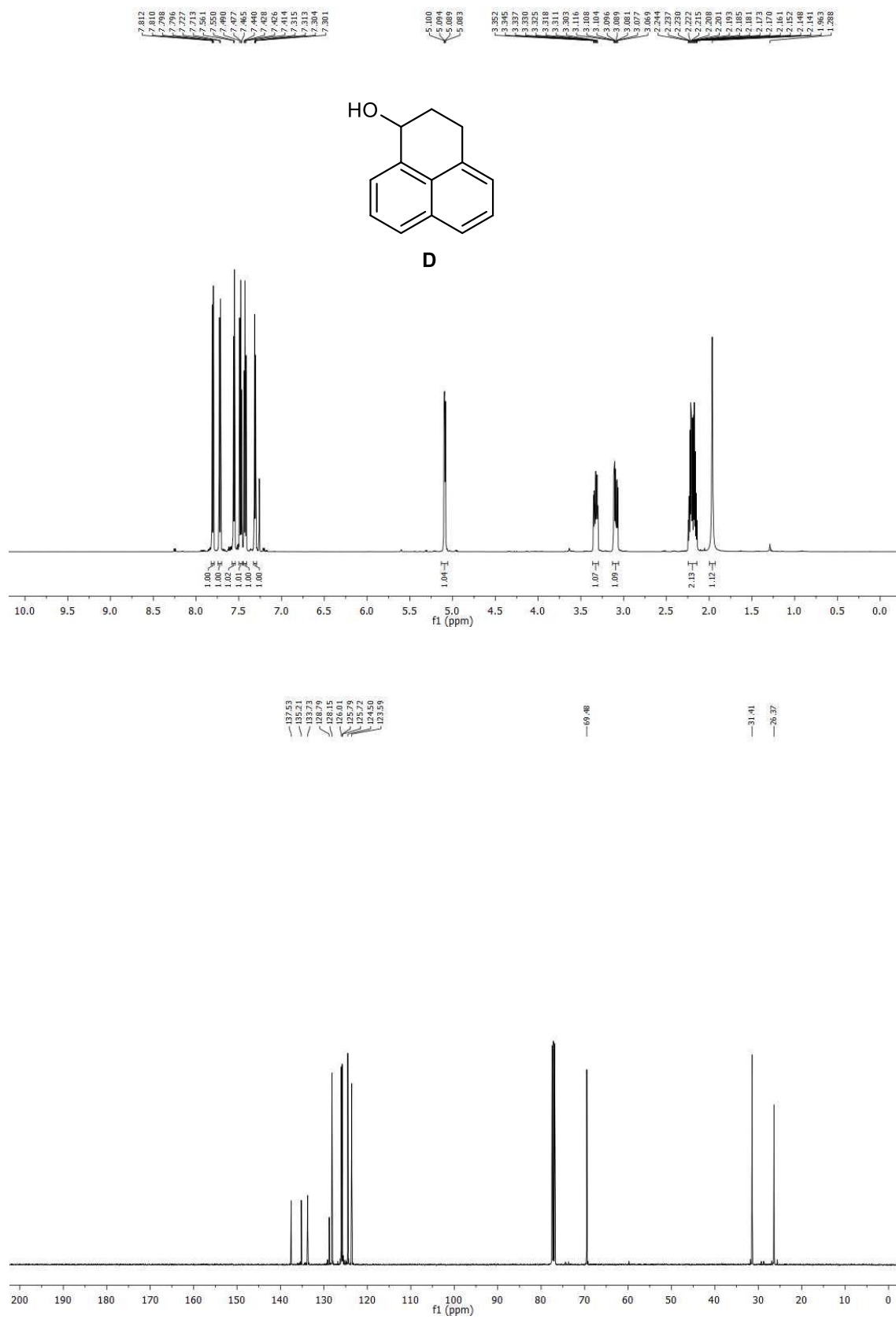


Figure S9. ¹H NMR and ¹³C NMR spectra of compound **D** in CDCl₃.

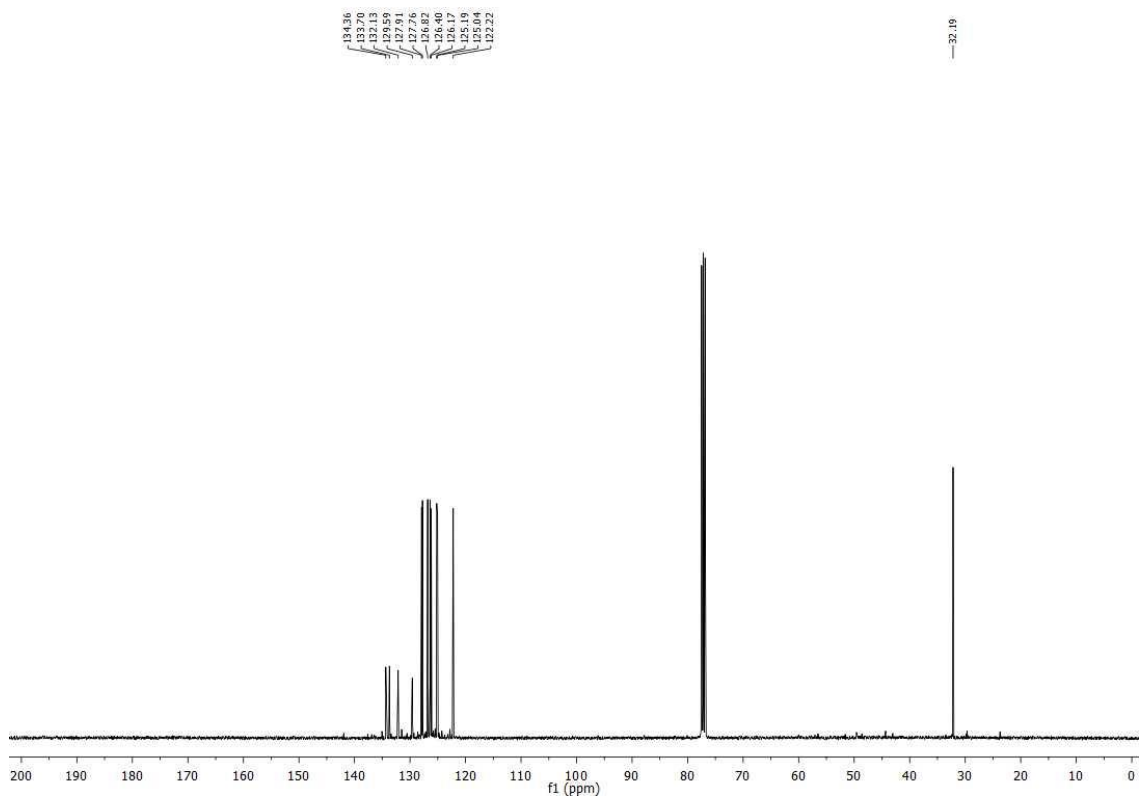
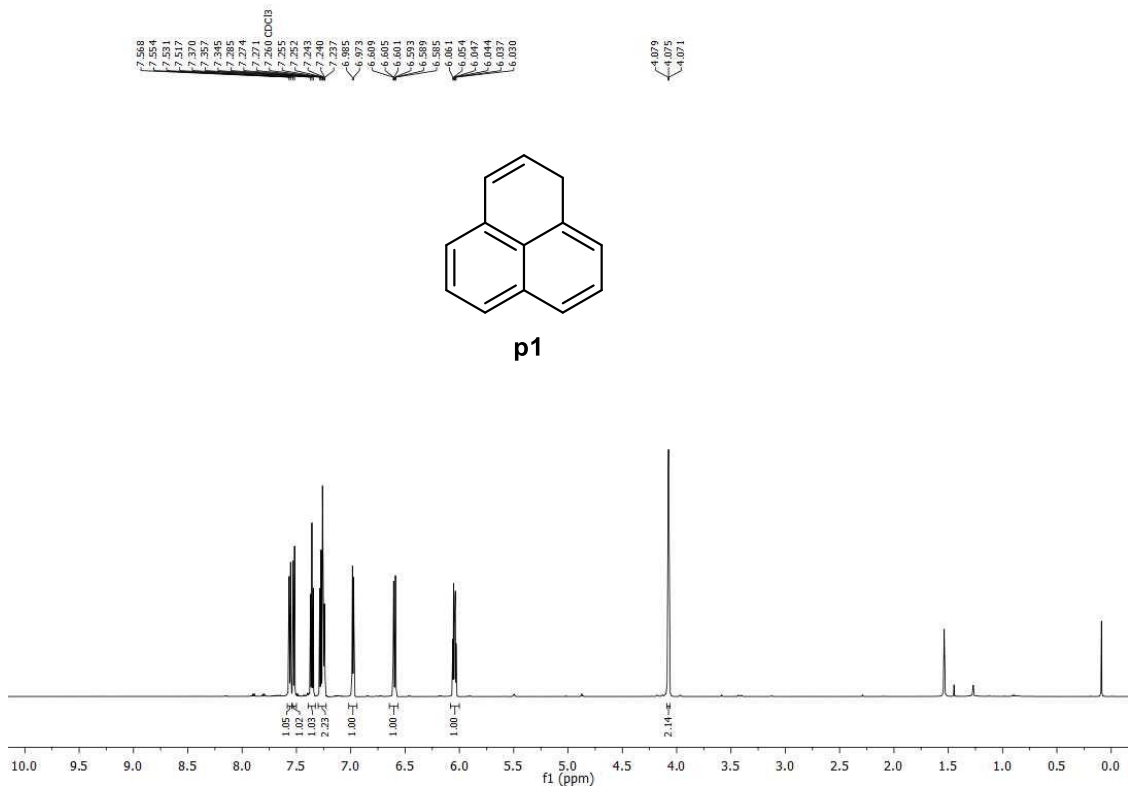


Figure S10. ^1H NMR and ^{13}C NMR spectra of compound **p1** in CDCl_3 .

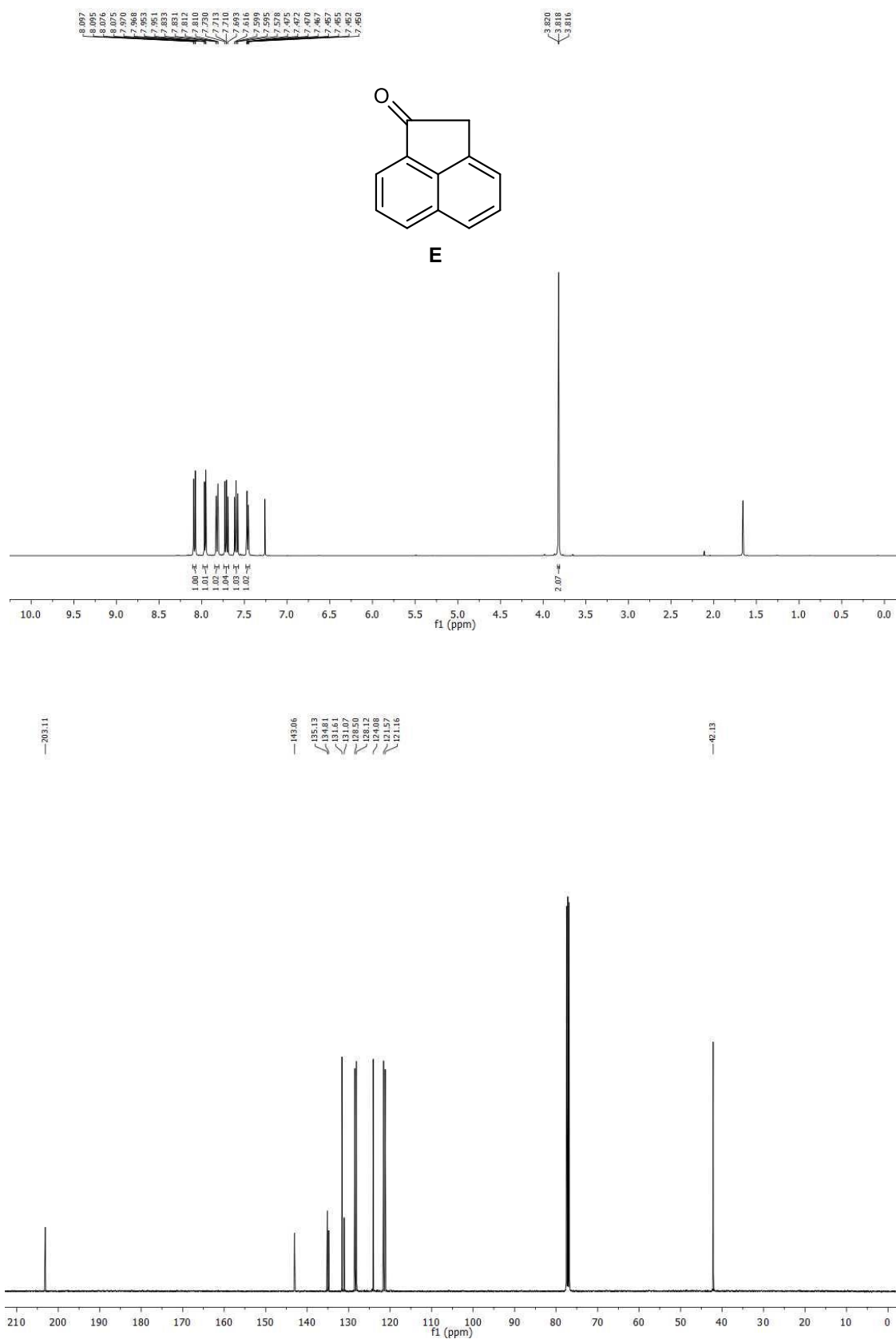


Figure S11. ¹H NMR and ¹³C NMR spectra of compound **E** in CDCl₃.

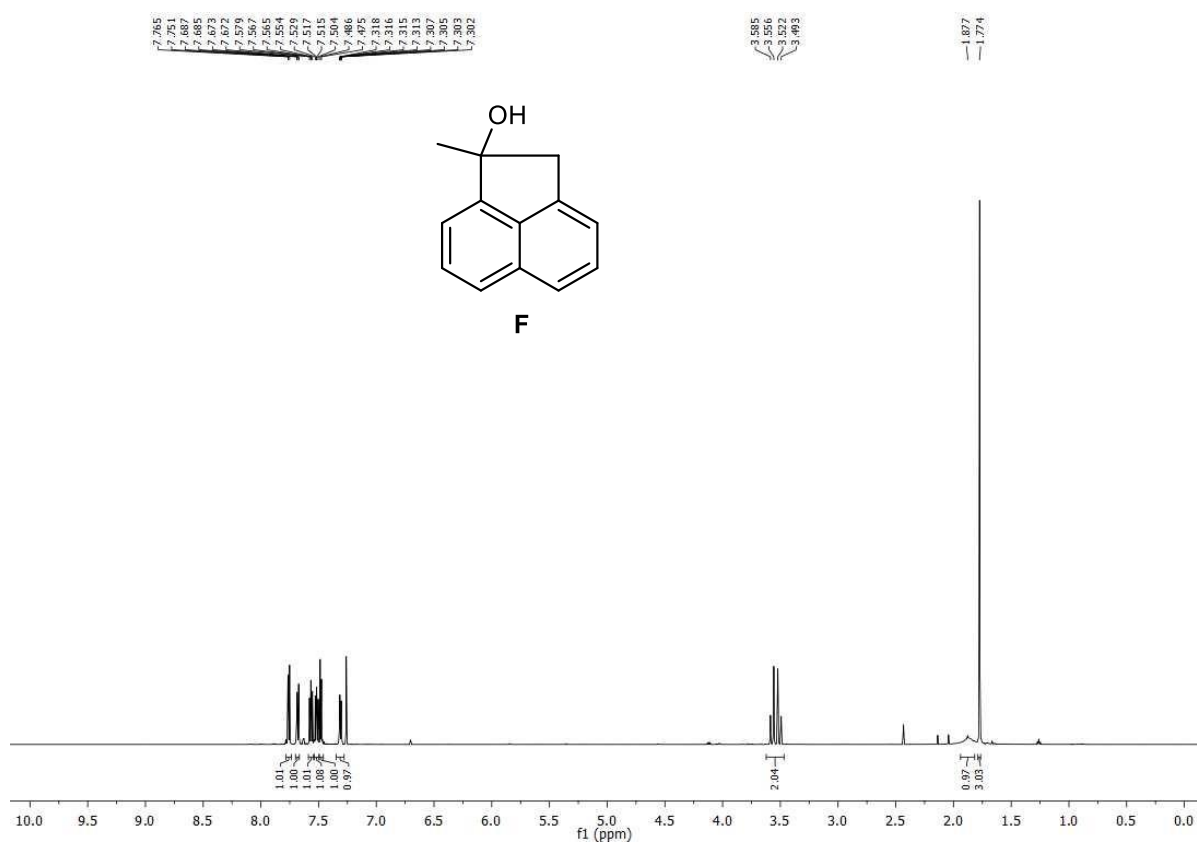


Figure S12. ¹H NMR spectrum of compound **E** in CDCl₃.

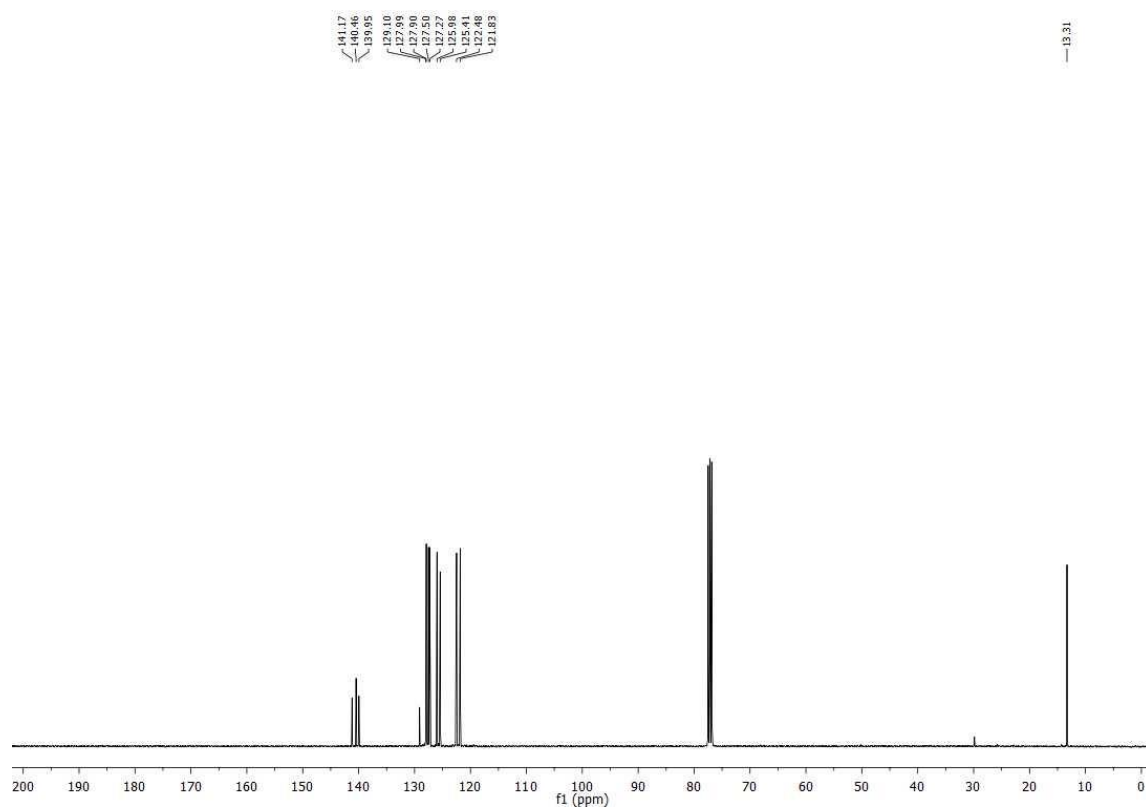
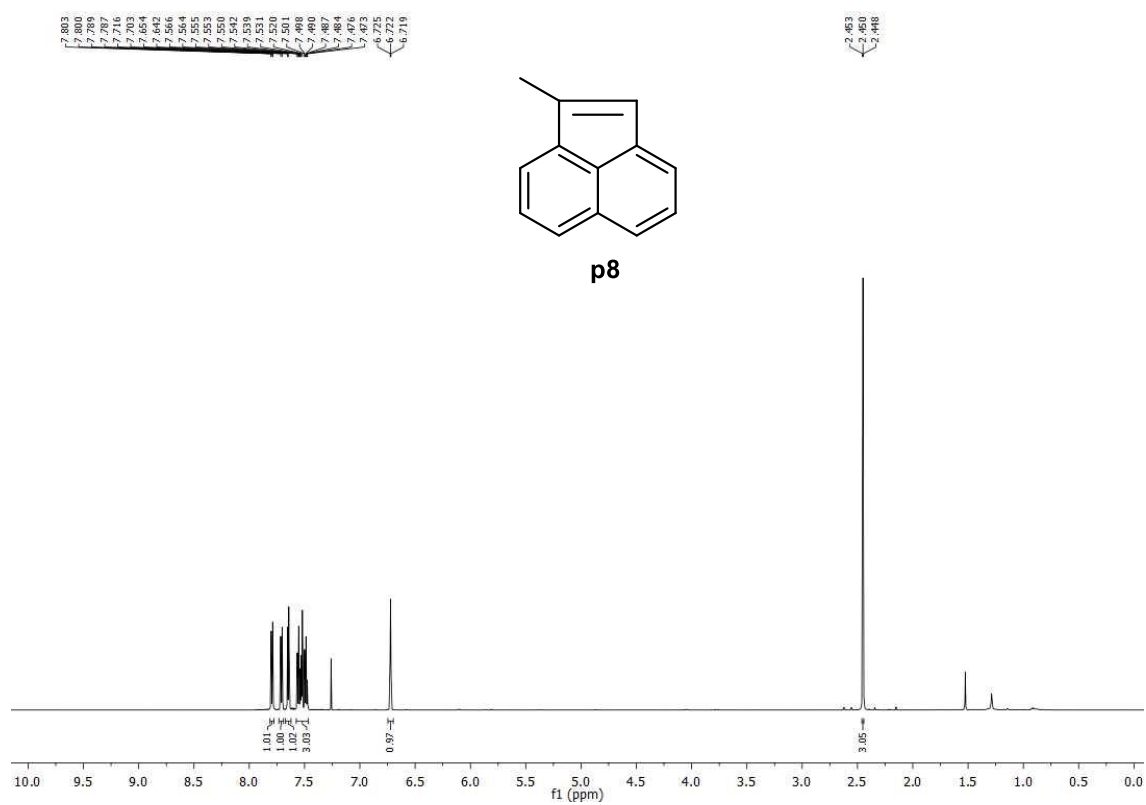


Figure S13. ^1H NMR and ^{13}C NMR spectra of compound **p8** in CDCl_3 .

Note S1. Input file for RRKM-ME calculations using the MESS package for the 1-naphthyl + C₃H₄ reactions, including coordinates and vibrational frequencies for all species involved.

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SymmetryFactor 0.5

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End

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C	2.8365136164	0.9166893997	0.0273963853
C	-0.4614502859	-0.1192789926	1.2334822232
C	-0.474522641	-0.0515979624	-1.2863589902
C	-1.2553936102	-1.2407997011	1.2007697544
C	-1.2934736503	-1.218233297	-1.2614362514
C	-1.6704689283	-1.805645239	-0.0108150478
H	-0.0420368999	3.0170688841	0.0973784691
H	3.0981357082	0.2868719968	0.882997621
H	3.093144529	0.3559128152	-0.8764135176
H	3.4426312283	1.8255309306	0.0609933415
H	-0.1493386697	0.3108227482	2.1791534286


```

H -1.5704622622 -1.6975432275 2.1336401879
H -2.2948174453 -2.6916144847 -0.0172907418
C -0.1398372221 0.5082864068 -2.5221280989
C -1.7291902061 -1.7695743852 -2.4864738721
C -0.581721293 -0.0507149843 -3.7178652956
C -1.3796672464 -1.1982417444 -3.6976016822
H 0.4759916944 1.4002090523 -2.5485093645
H -2.3527317204 -2.6575579777 -2.4637423898
H -0.3068066454 0.4058810671 -4.6620787963
H -1.7259402287 -1.6379528672 -4.6263981812

```

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

53.5715	92.8506	144.1585
165.5476	182.0764	254.8803
269.9684	379.9767	404.2973
435.5959	446.5756	503.1854
512.6592	526.9539	550.6847
560.6722	659.6081	688.6327
702.3243	721.9467	764.4998
792.3602	796.2180	798.4983
856.8429	881.6505	920.8665
954.6087	958.8596	974.5610
982.8894	1025.9717	1052.6059
1058.5059	1086.6716	1097.9137
1125.4074	1146.9156	1173.0285
1180.7995	1229.4966	1270.9152
1303.5742	1324.9566	1381.5283
1403.8539	1443.4151	1463.3272
1475.5945	1480.5247	1512.9358
1544.9943	1591.7334	1628.1291
1869.2451	3023.3935	3080.5813
3095.8738	3151.9525	3155.4159
3164.3951	3170.1335	3175.1946
3181.6512	3186.8380	3242.6981

ZeroEnergy[kcal/mol] -22.71

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i4-----

Well i4

Species

RRHO

Geometry[angstrom] 24

C	0.5528364458	-0.9816075716	-0.167231412
C	1.5444904696	0.0464849993	-0.064743573
C	-0.1895529122	1.6518732446	0.5175805335
C	1.1619691315	1.3315865044	0.2603157596
C	-1.15579445	0.6807241075	0.4466242644
C	-0.8154474554	-0.6528854002	0.1014186164
C	3.5640284305	0.0413027414	-1.4284214114
C	3.003535339	-0.2615264143	-0.2800092619
C	3.7576879915	-0.8803107315	0.8785498321
C	-1.4596433708	-2.9535872911	-0.3474117649
C	-0.1127065882	-3.2760124846	-0.6281102909
C	-1.7999284786	-1.6709577245	0.0047719552
C	0.8661586621	-2.3152730059	-0.5422263378
H	-0.4555941423	2.6709523902	0.7749927739
H	1.9181465022	2.1056769694	0.327035287
H	-2.1947885504	0.9198411107	0.6478626289
H	3.2519574484	0.4784967344	-2.3662489015
H	3.2842024293	-1.8130145651	1.1992638182
H	3.7450771766	-0.2035153003	1.7391613498
H	4.7941982812	-1.0846162968	0.6070593392
H	-2.2226006418	-3.7206318402	-0.418042514
H	0.1470228456	-4.2878312876	-0.9186072553
H	-2.8337735473	-1.4142785386	0.2116577373
H	1.8928929837	-2.5648763496	-0.780744173

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

44.6482	93.9982	149.4955
169.1939	183.6421	189.2130
294.5026	320.4277	381.1259
441.6107	479.0297	495.2312
499.4038	555.5961	579.3260
582.5278	660.4298	693.4082
710.7981	747.6614	792.8048
805.5905	813.5983	821.2044
859.0973	880.3005	924.1077
968.0383	985.5753	991.7336
998.4561	1026.5658	1045.3620

1051.0775	1082.5619	1138.9889
1168.5633	1182.6218	1197.7697
1234.2889	1258.1662	1290.1846
1361.4162	1388.9302	1401.3911
1418.9963	1464.8923	1480.8618
1483.3529	1490.9307	1542.7242
1611.0092	1632.3226	1660.7343
1671.7064	3022.3806	3074.1478
3115.3705	3158.0869	3160.7630
3169.0355	3172.6777	3182.9802
3186.3281	3193.0038	3229.2159

ZeroEnergy[kcal/mol] -36.71

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i5-----

Well i5

Species

RRHO

Geometry[angstrom] 24

C	0.4846848777	-0.9966854697	-0.1814615569
C	1.4741637901	0.0340287874	-0.0933277848
C	-0.2656014072	1.6456748715	0.4528031727
C	1.0875464527	1.3232959295	0.206272157
C	-1.2294140574	0.6713484672	0.3991216471
C	-0.8849386436	-0.6671415068	0.0782217226
C	3.5548603104	0.0725184102	-1.3851013583
C	2.9326939994	-0.2745450526	-0.2831617765
C	3.6442917319	-0.9470444744	0.8843443754
C	-1.524725999	-2.9747001089	-0.3420196052
C	-0.1770621797	-3.2975846353	-0.6190625375
C	-1.8674607064	-1.6883245462	-0.0065555303
C	0.7997370532	-2.3341211128	-0.5427643018
H	-0.5348447131	2.6691475453	0.6886527093
H	1.8419950014	2.0998957244	0.2587209633
H	-2.2693266689	0.9116373589	0.5941467532
H	4.5542948864	0.008945254	-1.7919996335
H	3.1465433423	-1.8823468543	1.1557818433
H	3.610613857	-0.295495888	1.7634437987
H	4.6881202214	-1.1606677146	0.6479163468
H	-2.2861019409	-3.7440496469	-0.4044822797

H 0.0841314243 -4.3116022568 -0.9005892972
H -2.9021639298 -1.4302843125 0.1942870904
H 1.8260722981 -2.5845427685 -0.782047918

Core RigidRotor

SymmetryFactor 0.5

End

Rotor Hindered ! 46 cm⁻¹
Group 7 9 17 18 19 20
Axis 2 8
Symmetry 1
Potential[kcal/mol] 8

0.07509219 3.240905055 5.159036836 0.738948391 0.335457214 0.033901833 0 0.246417368

End

Frequencies[1/cm] 65

94.7074 148.1626

168.8853	183.5304	191.8989
294.6737	327.6680	379.3976
444.1525	477.5062	479.5041
499.6196	551.6103	582.6395
594.7534	662.1872	690.3142
692.3489	747.7323	793.4618
806.6249	815.6198	844.7734
850.2385	880.3740	923.7703
963.6085	970.4569	985.5837
997.4492	1019.6540	1037.3963
1045.8682	1081.3057	1132.4680
1168.4150	1182.9180	1196.9811
1234.6087	1261.2342	1292.6974
1363.7595	1390.1869	1395.0350
1420.7674	1465.8169	1478.8524
1484.0882	1492.1226	1543.7902
1615.1090	1634.0198	1661.3250
1675.9832	3021.5751	3078.1617
3109.0398	3157.8422	3160.4870
3168.4700	3173.6365	3182.7158
3186.9137	3192.9829	3223.7123

ZeroEnergy[kcal/mol] -35.94

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i7-----

Well i7

Species

RRHO

Geometry[angstrom] 24

C	0.4746250402	-1.0011427781	0.0253216667
C	1.5123902508	-0.0172627637	-0.1008123113
C	-0.2145046441	1.7047650271	-0.2667740339
C	1.1388729345	1.3098501059	-0.2230532224
C	-1.2182131838	0.7743331225	-0.170514716
C	-0.9090007861	-0.6004661214	-0.0155869338
C	3.3883258026	-1.5320175907	-0.6575665122
C	2.9495949493	-0.4008443951	-0.0917574892
C	3.9182141938	0.5501649249	0.5750043125
C	-1.6190260866	-2.9139159926	0.3028045333
C	-0.2603550272	-3.3317629645	0.359248219
C	-1.9233517572	-1.5868927283	0.1217166535
C	0.6859362442	-2.3702133879	0.2273339273
H	-0.4555196816	2.7558878182	-0.3792406759
H	1.9013753487	2.0737844444	-0.309696931
H	-2.2595563309	1.0774900073	-0.2000570218
H	4.4387342222	-1.8000802056	-0.6245413358
H	3.5988948151	0.7884025993	1.5941108382
H	3.9944893663	1.4986535546	0.0335249315
H	4.917961416	0.1151191646	0.6158984273
H	-2.4090249297	-3.6499941267	0.407612811
H	-0.009186739	-4.3766524018	0.5065944467
H	-2.9592596504	-1.2670836982	0.0854847035
H	2.7273032328	-2.2111336143	-1.1803812871

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

38.4831	101.7593	165.7196
174.7445	192.8646	206.3873
320.8047	364.2097	393.9182
457.1323	469.6650	495.0524
503.8776	548.0520	580.5764
582.9704	630.6609	690.2538
723.9580	754.6836	773.1280
798.9498	825.0375	845.1010
884.0702	918.2311	923.6079
930.1562	971.3100	985.8592
1000.3975	1033.9537	1048.9428

1066.7061	1098.2296	1160.0378
1175.2875	1190.0696	1227.1139
1238.5642	1309.4770	1347.6211
1356.3372	1394.9983	1413.1858
1441.2282	1455.4707	1468.1459
1484.2703	1498.4660	1509.9611
1587.7431	1629.7145	1650.0065
1683.6888	3023.0025	3070.7998
3108.5719	3138.3431	3156.4779
3160.4185	3166.9340	3177.2493
3180.6535	3194.1921	3223.2819

ZeroEnergy[kcal/mol] -35.93

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i8-----

Well i8

Species

RRHO

Geometry[angstrom] 24

C	-0.277909	-0.187287	-0.010967
C	1.047942	0.352971	0.027509
C	0.119457	2.603484	0.102121
C	1.221419	1.720806	0.074174
C	-1.160198	2.110573	0.081037
C	-1.39349	0.71272	0.020471
C	2.537494	-1.307222	1.143267
C	2.257395	-0.536536	0.02057
C	3.079758	-0.537156	-1.096936
C	-2.926481	-1.170703	-0.094558
C	-1.828943	-2.059438	-0.142617
C	-2.709888	0.182557	-0.017719
C	-0.541372	-1.581195	-0.103064
H	0.294034	3.672659	0.146447
H	2.22776	2.123236	0.104521
H	-2.011914	2.782257	0.107309
H	3.414618	-1.943739	1.172864
H	1.899871	-1.284503	2.017295
H	2.842717	0.054761	-1.971231
H	3.98056	-1.140175	-1.122321
H	-3.937585	-1.561048	-0.124068

H -2.006169 -3.126728 -0.215011
H -3.547281 0.872132 0.011112
H 0.292281 -2.270299 -0.146648

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

33.6177	94.8354	159.2962
171.9887	192.1049	317.5311
338.2136	389.3128	448.4033
480.1284	501.8609	502.8165
546.6121	557.8267	562.3976
588.1096	630.8944	673.0416
699.5150	747.9578	776.6459
794.9349	806.6093	810.4702
818.0749	856.2024	880.3002
925.7461	967.4068	982.8495
985.4702	997.5163	1012.3426
1041.7356	1049.0168	1086.4933
1166.7802	1173.6917	1184.9083
1229.2340	1237.5760	1281.4046
1297.7522	1365.3819	1380.1033
1390.0870	1432.4655	1467.4117
1479.6263	1493.7251	1523.1051
1545.7795	1617.6504	1635.4140
1661.5950	3135.3818	3142.1803
3157.3096	3159.9953	3168.8382
3171.8436	3183.7228	3185.9316
3198.2308	3237.6701	3239.5885

ZeroEnergy[kcal/mol] -60.59

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i9-----

Well i9

Species

RRHO

Geometry[angstrom] 24

C -0.273246 -0.224245 0.079015
C 1.16693 0.174606 0.196786
C 0.470093 2.536276 -0.132324

C	1.468149	1.605528	0.012693
C	-0.87989	2.164812	-0.145265
C	-1.263915	0.789015	-0.055022
C	2.893323	-1.411412	-1.098857
C	2.241238	-0.805563	-0.126397
C	2.055124	-0.572138	1.292528
C	-2.996388	-0.925524	-0.07002
C	-2.016835	-1.917614	0.039774
C	-2.622422	0.404918	-0.121276
C	-0.673258	-1.562505	0.108468
H	0.733949	3.583119	-0.240948
H	2.510542	1.903211	0.016857
H	-1.653338	2.916467	-0.251363
H	3.698662	-2.108262	-0.887926
H	2.641308	-1.236578	-2.139268
H	1.53074	-1.311742	1.890217
H	2.76779	0.041856	1.835397
H	-4.0444	-1.19846	-0.123158
H	-2.300091	-2.963653	0.065886
H	-3.375985	1.179595	-0.219058
H	0.077416	-2.342476	0.172741

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

57.3542	101.1206	168.5949
183.5309	238.7150	279.0664
384.3867	390.1099	428.7733
443.7507	494.8447	501.2559
519.1099	546.3505	560.5739
657.3592	684.4954	691.1796
707.6675	760.7256	787.5948
790.2782	798.0569	842.7229
878.4845	895.2252	928.2150
928.7551	954.2541	957.5318
983.4671	1020.8540	1023.6909
1037.4408	1059.3590	1097.1440
1121.7669	1140.0962	1156.0303
1178.4405	1184.3611	1232.2546
1284.3905	1318.1903	1331.8320
1386.1391	1433.7369	1444.0179
1462.9019	1467.2126	1516.6051
1550.0404	1591.8662	1629.0183

1819.3689	3094.0011	3121.9060
3156.7840	3158.0718	3165.3998
3174.6633	3176.0725	3181.2748
3185.1380	3188.1312	3205.4716

ZeroEnergy[kcal/mol] -30.41

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i10-----

Well i10

Species

RRHO

Geometry[angstrom] 24

C	0.2484209625	-0.1339621248	-0.2932173862
C	-0.995487167	0.5468098689	-0.4897350552
C	0.047651617	2.6347205469	0.2082062096
C	-1.0738707213	1.8985816806	-0.2328125859
C	1.2540824407	2.0085990924	0.3897987061
C	1.388086057	0.6176765246	0.1442541467
C	-2.8311389194	-1.2275141965	1.3831655816
C	-2.9175886367	-0.9646125108	0.1046536011
C	-2.2387387593	-0.1967546558	-0.9641242678
C	2.7502002571	-1.3952769012	0.0908152667
C	1.6275677527	-2.1410630909	-0.3322256684
C	2.6287442882	-0.048114912	0.3244637232
C	0.4117427523	-1.5278280713	-0.5178107191
H	-0.0522991596	3.6978391074	0.3959893496
H	-2.0183293445	2.4126035512	-0.3789002094
H	2.1223737015	2.5669622225	0.7234567105
H	-2.0295934609	-0.8185565339	2.0042346337
H	-3.5506743668	-1.867166376	1.8880226164
H	-1.9893304619	-0.8706790366	-1.7918110936
H	-2.9465880246	0.5290164041	-1.3781960127
H	3.7040322225	-1.8907623051	0.2326825866
H	1.7265858827	-3.2063676401	-0.5079388822
H	3.484961749	0.5316889515	0.6534645637
H	-0.4402756613	-2.1219605952	-0.8223768149

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

46.1485	76.7145	141.5103
146.0508	175.8974	248.6691
284.2559	386.3108	431.6205
435.6599	462.0407	478.2063
508.4539	522.0077	558.9246
609.6911	664.0629	717.8786
745.1595	792.6506	804.1325
811.7218	864.1262	880.5941
888.1627	903.1385	921.5407
938.8723	964.6127	983.1086
995.5197	1008.2681	1037.8693
1057.2600	1095.4975	1168.3213
1183.5577	1187.3444	1208.8805
1237.9658	1259.1847	1288.0880
1313.0651	1381.3721	1393.5776
1409.3482	1422.5298	1467.5698
1478.7902	1493.8057	1547.3255
1615.0581	1638.7659	1664.0346
1737.9349	3019.4294	3043.5557
3047.8617	3143.8697	3156.8383
3158.4207	3164.8856	3169.7516
3183.4894	3184.3574	3199.7752

ZeroEnergy[kcal/mol] -37.16

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i11-----

Well i11

Species

RRHO

Geometry[angstrom] 24

C	-0.4491447986	-0.7659684195	-0.4039808257
C	-1.3308312859	0.3689659101	-0.5123534765
C	0.6149886039	1.8676551331	-0.2313798404
C	-0.736281958	1.5857561865	-0.4159532033
C	1.4615926672	0.7848026225	-0.13433052
C	0.9568266864	-0.5409197819	-0.2194692856
C	-2.8320686704	0.2331318572	-0.709562219
C	-4.4677930224	-1.1131499821	0.6595469129
C	-3.5752131524	-0.1340134385	0.552782031
C	1.3435747628	-2.9423852549	-0.2111676585

C	-0.0392373221	-3.164501707	-0.3901599783
C	1.8256701713	-1.6595680538	-0.1270618157
C	-0.9119156855	-2.105878004	-0.4827132857
H	0.9861051905	2.8842859264	-0.1690087219
H	2.5275648692	0.9334062419	0.0078580405
H	-3.2021322275	1.2008065987	-1.0641662628
H	-3.0520522855	-0.4949910204	-1.4964218293
H	-4.721006048	-1.7503782261	-0.1830978396
H	-4.983621491	-1.3116426733	1.5921431603
H	-3.3484701817	0.4813606809	1.4209209845
H	2.0204073289	-3.7861363634	-0.1389868466
H	-0.4157672401	-4.1795720187	-0.451391528
H	2.8869586127	-1.4810110082	0.011353096
H	-1.9700065239	-2.2953302054	-0.6037850883

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

51.0600	69.0946	106.8147
172.7584	191.5220	255.1185
296.2623	372.4337	426.4375
436.1319	480.7850	492.9414
520.3717	556.8542	565.7473
623.5784	668.5424	738.1547
742.6379	783.9648	792.2928
802.2545	867.5814	877.4951
916.1841	932.8291	946.0922
951.9860	966.9255	994.8589
1027.0481	1036.2738	1052.7509
1110.0520	1139.1452	1160.0872
1180.6957	1185.9380	1219.1773
1244.8690	1284.8684	1313.9559
1327.3463	1332.2966	1381.3055
1409.0112	1447.9889	1451.0468
1470.4462	1482.7514	1533.5251
1592.1335	1624.0681	1655.4261
1703.3560	3026.0843	3063.9801
3122.2237	3134.2495	3155.2857
3159.9322	3169.6693	3178.1615
3185.3787	3207.5535	3208.2649

ZeroEnergy[kcal/mol] -31.98

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i12-----

Well i12

Species

RRHO

Geometry[angstrom] 24

C	0.1943913493	-1.3242603157	-0.025109683
C	1.4355537785	-0.6506294206	-0.0082297025
C	0.3105604907	1.5104254756	-0.0150867385
C	1.4942519245	0.727056357	-0.0033290084
C	-0.949208093	0.8256464075	-0.0321223328
C	-0.9702526928	-0.595862192	-0.0367408612
C	2.8200223873	-1.2636394145	0.0063945785
C	2.9284101337	1.2164925146	0.0153957947
C	3.7144470772	-0.0608513927	0.0207512141
C	-0.8613572321	3.6397595351	-0.0217474603
C	-2.1032875652	2.9655098649	-0.0386060118
C	0.315791187	2.9295838267	-0.010635104
C	-2.143024338	1.591883006	-0.0440331459
H	0.1623678041	-2.4088454738	-0.0289384892
H	-1.9310277686	-1.1002178099	-0.049870609
H	2.9694074197	-1.9159998975	0.8818320135
H	2.9903536756	-1.9107211368	-0.8691349318
H	3.1375252911	1.8459151084	0.8955507336
H	3.1585557436	1.8514890195	-0.8554405529
H	4.795073097	-0.1067502587	0.0326211302
H	-0.8406745798	4.723925685	-0.0178300282
H	-3.0244076131	3.5373253286	-0.0472952666
H	1.2642167378	3.4546368863	0.0024514452
H	-3.0954672145	1.071829297	-0.0568969836

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

107.0347	128.5822	178.5528
226.0360	235.7459	276.7961
353.2598	420.6255	428.3238
460.9840	507.1061	519.1965
533.6438	603.7883	642.7840
671.0801	744.3952	751.4360
781.2758	788.6921	819.9104

868.7519	873.0958	911.2996
928.9603	930.0905	958.7096
960.1686	970.3396	993.5062
1025.4738	1045.4108	1072.8487
1129.5129	1137.3270	1167.6668
1177.4834	1184.1677	1211.9936
1234.2417	1271.5962	1283.4728
1324.5227	1345.9942	1377.9925
1400.1998	1412.7276	1457.6092
1463.8398	1470.8638	1497.5903
1552.6952	1612.0053	1636.2092
1665.8059	2947.8933	2949.9134
2952.4191	2952.4886	3155.0524
3157.4553	3165.2023	3173.7437
3178.2148	3188.1034	3204.6060

ZeroEnergy[kcal/mol] -66.29

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i13-----

Well i13

Species

RRHO

Geometry[angstrom] 24

C	0.261049	-0.089069	-0.216966
C	-0.79516	0.861023	-0.361462
C	0.788239	2.640725	0.15189
C	-0.51286	2.196729	-0.178266
C	1.815878	1.743195	0.29655
C	1.590333	0.354183	0.115933
C	-2.199608	0.389941	-0.68833
C	-3.416207	-1.424164	0.567835
C	-2.916686	-0.194094	0.504951
C	2.39137	-1.950033	0.068606
C	1.08528	-2.41084	-0.260585
C	2.627062	-0.608499	0.249284
C	0.117122	-1.471271	-0.38508
H	0.969263	3.701194	0.287115
H	-1.306717	2.927735	-0.293238
H	2.81536	2.083052	0.547222
H	-2.771047	1.246393	-1.064012

```

H -2.165734 -0.354058 -1.490121
H -3.329557 -2.115735 -0.264468
H -3.926126 -1.785086 1.453983
H -3.013656 0.468116 1.3633
H 3.197352 -2.668232 0.175565
H 0.892153 -3.468698 -0.401518
H 3.623833 -0.261639 0.500021

```

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

40.2572	67.2218	114.2085
168.6763	189.2897	239.6669
300.7709	377.9173	438.3903
447.0916	469.7792	492.6279
518.9589	564.6048	571.2018
617.4952	669.1613	734.7892
753.0874	774.5818	797.1910
817.9802	870.1966	884.1742
914.7536	920.3708	939.5138
947.1807	970.2855	985.1761
1025.1230	1030.7407	1053.7051
1086.5542	1124.1950	1163.2422
1186.1828	1193.4516	1226.0620
1250.5993	1261.7657	1316.6304
1329.4682	1352.7153	1373.5732
1395.2005	1449.2717	1454.4843
1471.8398	1478.6350	1511.5740
1591.5573	1636.9210	1655.3637
1703.3275	3018.4222	3063.1276
3123.2666	3132.4421	3156.0526
3157.2713	3163.4401	3168.2463
3180.6274	3183.3422	3211.2476

ZeroEnergy[kcal/mol] -32.71

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i14-----

Well i14

Species

RRHO

Geometry[angstrom] 24

C	1.030888025	-0.4131209403	0.3405528696
C	0.8779823504	0.8141811129	-0.3731879815
C	1.1265063657	2.0492277611	1.7078811452
C	0.9233765303	2.008536835	0.3121456091
C	1.2785487799	0.8844534124	2.4173893752
C	1.2329358268	-0.371275804	1.7603135824
C	0.6783770194	0.8046386159	-1.8782901368
C	0.7843530895	-1.758999396	-1.8178811619
C	0.2230112014	-0.5113397576	-2.4052423777
C	1.3277772364	-2.7920516625	1.8219671279
C	1.1245878035	-2.8340176431	0.4262282327
C	1.3812509128	-1.5866546142	2.475623363
C	0.9815635246	-1.6811252354	-0.3143862087
H	1.1570343188	3.0068469936	2.2157913136
H	0.7986758005	2.9391313789	-0.2330489695
H	1.4328659221	0.9071315945	3.4910278108
H	-0.0205538876	1.5980924879	-2.1621321471
H	1.6396888032	1.0855227674	-2.3521205861
H	1.7663247947	-1.9817604902	-2.2800413308
H	0.1535656039	-2.6197928449	-2.0623701061
H	-0.2817882916	-0.5548061034	-3.3633340369
H	1.436662743	-3.7189242004	2.3742265476
H	1.078517859	-3.7963752005	-0.0743094078
H	1.5347696682	-1.5458980674	3.5488424741

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

78.9096	133.8973	164.1190
235.4993	239.1190	388.1462
395.0495	437.3452	452.1558
470.1947	476.0541	477.5626
571.1033	574.5909	598.8709
635.5373	726.9066	759.0918
787.1068	806.5144	808.6198
832.0184	851.0386	911.7637
913.6174	918.1345	967.2240
976.6489	986.1117	1045.8801
1050.1993	1083.7823	1103.6479
1141.4497	1168.4922	1184.4790
1192.6991	1219.2144	1226.0687
1250.3849	1264.7307	1293.0811

1361.4426	1381.9365	1388.3936
1389.9532	1418.2059	1449.8624
1458.4621	1467.3333	1497.5369
1546.6549	1623.9166	1639.3150
1658.3129	2876.6264	2879.8878
3040.1730	3040.3073	3152.1672
3152.2942	3161.2850	3163.9993
3173.7231	3181.0291	3182.5125

ZeroEnergy[kcal/mol] -67.59

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i15-----

Well i15

Species

RRHO

Geometry[angstrom] 24

C	-0.267883467	-1.1131542874	0.0075401891
C	-1.3590207195	-0.1463893274	-2.25164E-4
C	0.3080853584	1.6586525622	-0.0233998281
C	-1.0184768093	1.2177889608	-0.0154426175
C	1.3473928714	0.7542721909	-0.0163936363
C	1.084399494	-0.6407760245	-8.625729E-4
C	-2.7203669229	-0.5710651066	0.007019508
C	-5.1459457263	-0.2274635296	0.008614099
C	-3.8712360018	0.2505901481	0.001152609
H	0.5135755966	2.7232912719	-0.0352719917
H	-1.8053272371	1.9606300103	-0.0214535437
H	-2.9191070731	-1.6359327538	0.0180694494
H	-5.9996252126	0.438299187	0.0037366832
H	-5.3496973425	-1.2931284422	0.0197363051
H	-3.7430035464	1.3289735621	-0.0099183379
C	1.9132980082	-2.9280015968	0.0218093937
C	0.5859685555	-3.3992844495	0.0302543985
C	2.1514419629	-1.5754431774	0.0066011962
C	-0.4704723032	-2.5147834159	0.0232842589
H	2.7388434743	-3.6306482838	0.0274011924
H	0.3927904731	-4.4660716365	0.0422629456
H	3.168312565	-1.1969382809	2.247798E-4
H	-1.474494032	-2.9168353855	0.0303298622
H	2.3774300343	1.0936208044	-0.0226621779

Core RigidRotor
SymmetryFactor 0.5
End

Frequencies[1/cm] 66

55.7169	66.7403	140.9919
152.4080	173.2745	260.6782
317.9342	360.2731	423.0701
448.7745	478.8529	510.1570
535.2604	543.7539	607.0310
641.2200	643.6401	735.2366
760.8168	775.5787	785.5649
799.9843	825.3613	863.8814
869.4634	875.6316	890.3688
956.5479	973.1059	983.1783
992.7291	998.7572	1044.5701
1059.5033	1118.9906	1161.3729
1185.7507	1188.9434	1209.5502
1221.9230	1252.3429	1274.9857
1313.4882	1334.0721	1373.2637
1391.6244	1422.9515	1464.4765
1484.9173	1494.5595	1533.2962
1558.3801	1592.2324	1606.6464
1652.9966	3135.4157	3148.1814
3159.1674	3163.2331	3169.8635
3177.7327	3179.6291	3186.5014
3199.1524	3207.6014	3229.2060

ZeroEnergy[kcal/mol] -64.08

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i16-----

Well i16

Species

RRHO

Geometry[angstrom] 24

C	-0.1774061305	-1.2620667521	-0.0893067904
C	-1.3549546384	-0.4235356263	-0.2236631984
C	0.1067759529	1.5454915899	-0.2358048395
C	-1.167842671	0.9614737738	-0.2906364731
C	1.2307700172	0.7617466408	-0.1194201315
C	1.1168514158	-0.6513732969	-0.0473111956

```

C -2.6608560836 -1.012345914 -0.3609766131
C -4.2348311562 0.6733538077 0.6366340117
C -3.9269574866 -0.4478673597 -0.0813836664
H 0.1993694212 2.6235251706 -0.3075787114
H -2.0271915497 1.5976708068 -0.4528430573
H -2.6903098569 -2.024355554 -0.7481332606
H -5.2682155511 0.9655223085 0.7769390031
H -3.4838828471 1.2745393269 1.1321507236
H -4.7696575849 -1.0274457677 -0.4536726813
C 2.1649567316 -2.8353853565 0.1695312955
C 0.8915833848 -3.4401556799 0.153891825
C 2.2695872621 -1.4691085941 0.0768042599
C -0.2452266471 -2.6724048868 0.0342654418
H 3.0543635993 -3.4479211372 0.2646766552
H 0.8061960928 -4.5171204281 0.2457515682
H 3.2428127482 -0.9899092938 0.1019793772
H -1.2098838565 -3.1621372652 0.0561401003
H 2.2179354336 1.2101294874 -0.086640643

```

Core RigidRotor

SymmetryFactor 0.5

End

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Rotor      Hindered      ! 58 cm^-1  CH3
Group              8 9 12 13 14 15
Axis              2 7
Symmetry          1
Potential[kcal/mol] 8

```

```
0 4.01606E-05 2.903614885 3.689028478 3.671993475 9.703104234 3.695189367 2.892052393
```

End

Frequencies[1/cm] 65

```

          95.8452          156.4647
178.3147          202.8461          268.8782
321.4872          411.1400          427.8340
445.8091          481.3369          508.7393
545.1694          547.4310          568.2200
637.7875          669.2575          741.3992
764.2918          769.7920          794.6788
804.0690          817.7148          856.7810
868.2623          882.7967          920.2123
964.0025          982.4033          988.6037
995.4822          1002.6832          1051.1844
1067.1235          1101.3716          1141.6305
1166.3798          1187.2048          1198.6973
1224.6438          1260.9722          1278.5363

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1292.7332	1343.6366	1378.1856
1413.3854	1446.4141	1456.5856
1473.5980	1485.5932	1536.5114
1561.4416	1592.8425	1614.7152
1654.9460	3121.0357	3149.9866
3158.7703	3162.3587	3166.9444
3171.4037	3179.2642	3185.2642
3199.9266	3204.8535	3239.2783

ZeroEnergy[kcal/mol] -61.17

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i17-----

Well i17

Species

RRHO

Geometry[angstrom] 24

C	0.2500308018	1.5403092821	-0.0233822633
C	1.4718288692	0.8123331749	-0.0976070745
C	0.2125923459	-1.3594684083	-0.1383547785
C	1.4883868688	-0.6512771951	-0.4848813804
C	-0.9215502726	-0.6664064138	0.0480178094
C	-0.9712352534	0.7926274165	0.0210657126
C	2.7968318161	1.1947235164	0.2286317343
C	2.8344632655	-1.1721746663	0.0904215694
C	3.6150823059	0.1017127491	0.3034241728
H	0.2080759883	-2.4450952958	-0.1160358937
H	1.591017133	-0.6897546637	-1.5870377083
H	3.1103545484	2.2084681003	0.4459269913
H	3.3320253927	-1.8865939309	-0.5715302115
H	2.6752794018	-1.684564201	1.0508592321
H	4.6641907469	0.1229404434	0.5693738706
C	-2.2308392333	2.8667670268	0.1687657163
C	-1.038532339	3.6008669495	0.1445096819
C	-2.1865846158	1.4771205204	0.1161672502
C	0.1804741575	2.9497614135	0.0595802265
H	-3.1842037107	3.377993258	0.2360938328
H	-1.0687660315	4.683902612	0.1896435578
H	-3.108689889	0.9059600047	0.1581720979
H	1.0972192341	3.5279785343	0.0326231139
H	-1.8543115308	-1.1894392269	0.2366527406

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

90.6488	106.4262	189.6997
238.6207	255.0841	361.1524
413.3124	425.0734	445.7761
496.5394	518.0739	541.0825
579.2870	649.8980	683.5008
698.1687	723.7031	747.7860
768.8834	790.7789	824.0169
854.9281	873.9721	921.4270
937.5715	945.3123	950.1509
977.2845	985.1344	989.3134
1047.1039	1061.9216	1075.8915
1104.3607	1137.1859	1152.6790
1170.0712	1181.3741	1204.1635
1228.5702	1261.0226	1279.9605
1292.8037	1331.3527	1339.8356
1351.2277	1416.1883	1424.1420
1458.1698	1477.4136	1488.5870
1513.6667	1573.0875	1618.3977
1666.4525	2873.9468	2978.5334
3058.2917	3144.5500	3155.5668
3163.1079	3165.9099	3176.4631
3185.0641	3188.5998	3205.7889

ZeroEnergy[kcal/mol] -60.54

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i19-----

Well i19

Species

RRHO

Geometry[angstrom] 24

C	0.6206530597	-0.4605060987	-0.245038274
C	1.3686992392	0.7237224546	-0.1458507559
C	-0.6881829697	1.9907176885	0.0892955037
C	0.7048727928	1.9476301958	0.0096507083
C	-1.4271280982	0.8205314502	0.0290606753
C	-0.787649979	-0.4285957074	-0.1367958281

C	2.8334253611	0.6390742112	-0.1671827856
C	2.7059469953	-1.8116639366	0.1958080674
C	3.4707576879	-0.5253835198	0.0083501027
C	-0.8555370926	-2.8950383505	-0.2167595441
C	0.5048385677	-2.9749061462	-0.3600424105
C	-1.5228941749	-1.6604792704	-0.1544287867
C	1.3547726331	-1.7536774404	-0.5463198513
H	-1.1919547373	2.9433731903	0.2098170031
H	1.2831234812	2.8629541757	0.0793230412
H	-2.5084370612	0.851605256	0.1122309577
H	3.3927524239	1.5641037162	-0.2688551086
H	3.2867571993	-2.6633330546	-0.1712458257
H	2.5376177286	-1.9900775296	1.2683166621
H	4.5544295129	-0.5547153449	0.0614397711
H	-1.4371543339	-3.8086856286	-0.1439405429
H	0.995665784	-3.9416570241	-0.4092602009
H	-2.6022235247	-1.6279343463	-0.0607007792
H	1.6228335048	-1.7055299406	-1.6219277991

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

117.6881	138.3197	197.6327
230.3082	361.4098	383.5760
420.6596	448.8591	459.1684
479.5070	489.3342	549.7250
568.3033	599.5874	634.4620
685.3026	713.3897	752.7517
761.4686	775.7725	798.6934
827.5272	836.1899	898.7177
944.5908	964.0838	972.0881
981.4039	990.4356	1015.4540
1044.9562	1077.2726	1101.6610
1104.5623	1174.4498	1177.5722
1187.7393	1197.5879	1212.0714
1236.2883	1254.9207	1274.2591
1322.3698	1324.6317	1362.5004
1379.2632	1414.5105	1433.1006
1475.0850	1477.2481	1493.1682
1548.3550	1600.8551	1609.8554
1684.3810	2857.4538	2982.5854
3053.9036	3148.0724	3149.7639
3157.3805	3165.4177	3166.5317

3169.9098 3181.2858 3183.4637

ZeroEnergy[kcal/mol] -66.13

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i20-----

Well i20

Species

RRHO

Geometry[angstrom] 24

C -0.3568356392 -0.9503959611 -0.1696642696

C -1.324671389 0.1532618425 -0.2040444128

C 0.5368707297 1.7413513423 0.0200909905

C -0.8244008288 1.4875908002 -0.1060652958

C 1.4581690012 0.7066506856 0.0555999294

C 1.0308027366 -0.6494881643 -0.0385998686

C -2.6583555933 -0.0681370037 -0.322674603

C -3.937415269 -0.2565434166 -0.4600107163

C -4.9328005369 -0.437706308 0.66632406

H 0.8782050994 2.7683813331 0.0911168443

H -1.5342229471 2.3050357638 -0.132555994

H -4.3578187 -0.2903154257 -1.4699997012

H -4.4437345405 -0.3952997853 1.6400540844

H -5.4453729175 -1.4009129349 0.574966908

H -5.7006176081 0.3418961457 0.6274865817

H 2.5173357694 0.9159940126 0.154867535

C 1.5430071383 -3.0279360638 -0.0987068076

C 0.1732635217 -3.3200404463 -0.2286636318

C 1.9599855722 -1.7185446201 -0.0059151812

C -0.7544943781 -2.2969136253 -0.2630492692

H 2.2680943829 -3.8336334408 -0.0717386643

H -0.1552797619 -4.3506097212 -0.3018382768

H 3.0150251829 -1.4856361204 0.0943324407

H -1.8093920249 -2.5246168884 -0.3644086817

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

52.4134 74.5911 124.7622

143.4908 174.8683 214.1369

233.6810 345.2472 380.6539

417.4539	481.3706	485.3626
500.0020	541.5363	556.7608
590.3862	634.3970	696.7137
726.4502	767.2286	782.0196
796.8542	799.3888	850.0816
852.8685	884.5450	933.1043
963.6443	968.7438	992.8568
1042.1795	1053.9296	1061.6849
1075.4953	1101.4720	1153.6398
1166.3883	1183.2988	1186.0348
1233.0620	1281.7745	1316.7667
1343.2225	1362.0033	1400.5062
1407.5653	1462.2382	1468.0289
1484.6354	1492.4315	1519.3916
1554.4512	1589.0504	1643.9989
1915.4934	3018.7667	3038.2257
3068.3592	3117.3523	3157.9489
3162.4189	3168.0479	3177.9747
3179.5281	3189.2598	3192.6879

ZeroEnergy[kcal/mol] -48.05

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i21-----

Well i21

Species

RRHO

Geometry[angstrom] 24

C	-9.2859674738	-0.4309097014	0.2025466707
C	-9.3093779291	-1.8112750965	0.0096190143
C	-8.0525873993	-2.4395706951	-0.1606143026
C	-6.8892815952	-1.6743525483	-0.2061378757
C	-6.9162140681	-0.2713784642	-0.1418346979
C	-8.150585479	0.3593461473	0.0401510575
C	-10.4927937247	0.4203937495	0.4145081482
C	-11.7136493242	-0.2095171246	-0.192457384
C	-11.7349188311	-1.5773758012	-0.3632552993
C	-10.6050098845	-2.4062316166	-0.1801888339
C	-8.608543469	1.7560140073	0.0016687261
C	-9.9535561607	1.8215780677	0.1252845267
C	-10.8153879227	3.0417051764	0.1286618887

H	-7.9989427615	-3.5140191836	-0.3009201536
H	-5.9369287436	-2.1750072515	-0.3437808756
H	-6.0003426838	0.2968711291	-0.260566556
H	-10.6849177263	0.4430447638	1.5107361755
H	-12.6071945604	0.3815265938	-0.3592606281
H	-12.66321824	-2.0456989547	-0.6759915699
H	-10.6937766701	-3.4768887498	-0.3247120383
H	-7.9563445217	2.6116602375	-0.1282390741
H	-11.366916219	3.140177008	1.0710839571
H	-10.2232647326	3.9482576331	-0.0122112285
H	-11.5640448797	2.9997806738	-0.67111136473

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

118.7913	157.0522	160.5839
196.8446	225.4279	292.2623
352.8514	405.1368	469.2695
481.5610	504.5838	530.9203
540.7660	577.8873	598.1561
631.4909	664.7759	711.9780
750.9904	776.6173	797.8826
806.0638	818.6475	875.9718
894.2700	932.5644	956.0805
968.4436	1010.7453	1034.0550
1053.3730	1068.1192	1070.4166
1083.3051	1142.4467	1164.4746
1168.3169	1190.1147	1202.3254
1232.4356	1276.7291	1292.9118
1318.7069	1338.8860	1385.3753
1415.8920	1422.0973	1469.3511
1478.6834	1481.0981	1490.6256
1524.7270	1605.1903	1622.0306
1643.0127	2834.0754	3007.4331
3047.1352	3098.4643	3151.3504
3157.7559	3170.1699	3173.7003
3181.7504	3183.1780	3186.2363

ZeroEnergy[kcal/mol] -59.27

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i22-----

Well i22

Species

RRHO

Geometry[angstrom] 24

C	-0.201397855	-0.0107686372	0.0818276784
C	-1.3411878734	0.780334085	-0.1322769652
C	-2.5672534631	0.0768100584	-0.3305487394
C	-2.589432867	-1.3156666903	-0.3057527692
C	-1.4429859868	-2.0985715069	-0.0916358821
C	-0.2074675918	-1.4488852274	0.1097296708
C	1.0839804802	0.4997692354	0.297365751
C	1.2611648506	1.8700035767	0.2996477147
C	0.1331890844	2.6988631755	0.0851540171
C	-1.1352184829	2.1831922521	-0.1251664169
C	1.1022674094	-1.8720152118	0.3477251779
C	2.032701582	-0.6784872484	0.4898271296
C	3.2212142901	-0.6994988794	-0.4911668386
H	-3.4852722685	0.6285778425	-0.5007395448
H	-3.5376676479	-1.8202769006	-0.4593067671
H	-1.5167130126	-3.1799919026	-0.082316788
H	2.2341790644	2.3212438794	0.4626613361
H	0.2701731024	3.7748851907	0.0872488474
H	-1.9733855292	2.8535026167	-0.2842713202
H	1.4397505948	-2.8973872752	0.4274028469
H	3.8518270616	0.1835335466	-0.3575789565
H	3.8426802993	-1.5841982226	-0.3284117647
H	2.8673262177	-0.7139935601	-1.5246979185
H	2.4411875412	-0.6554541965	1.5116155013

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

93.0384	167.6773	173.7045
235.0537	238.7650	283.1505
387.1133	420.9094	480.7843
495.9576	505.0357	526.6202
546.5100	597.6685	625.3395
654.6819	671.0319	702.1868
755.3628	779.5146	807.3659
818.8732	831.5125	862.0047
904.6750	908.8404	970.0565
975.7381	978.6399	1033.4482

1049.4102	1067.4763	1075.8978
1094.7036	1131.4514	1175.7350
1176.9393	1211.8116	1221.2722
1243.2087	1280.1966	1304.5661
1335.1422	1366.0235	1398.1368
1411.8916	1422.0644	1458.7169
1466.9905	1496.8708	1497.4516
1514.0950	1574.3678	1622.9528
1637.2044	2972.8779	3026.8250
3091.0097	3101.4387	3156.7370
3158.1104	3166.8993	3174.1911
3180.7678	3183.9661	3200.9834

ZeroEnergy[kcal/mol] -76.39

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----c10h7_c3h4_p0p-----

Bimolecular p0p

Fragment c3h4

RRHO

Geometry[angstrom] 7

C -0.823420841 0.0519880348 -0.0208571707

C 1.824711204 -0.1816552298 1.678957E-4

H -1.8820502847 0.1362504236 -0.0342313517

H 2.1265806386 -1.2327357481 0.0038417281

H 2.2515118512 0.2935470245 0.887798287

H 2.2667123243 0.2920674571 -0.8807572055

C 0.3727611076 -0.0556769621 -0.0121801829

Core RigidRotor

SymmetryFactor 3.0

End

Frequencies[1/cm] 15

339.4278 339.9763 666.0166

666.0469 943.1202 1056.2902

1056.6567 1416.3162 1479.4028

1479.6937 2229.8067 3026.9185

3085.7411 3086.1443 3478.9987

ZeroEnergy[kcal/mol] 0.0

ElectronicLevels[1/cm] 1

0 1

End

```

Fragment      c10h7
RRHO
Geometry[angstrom]  17
C  0.014468  -0.761638  0.0
C  1.273145  -1.416493  0.0
C  -1.226649  -1.409071  0.0
C  2.435985  -0.68536  0.0
C  2.394138  0.728582  0.0
C  1.190743  1.391526  0.0
C  -0.035299  0.677452  0.0
C  -2.446252  -0.820405  0.0
C  -1.301795  1.322885  0.0
C  -2.472747  0.604434  0.0
H  1.296576  -2.499829  0.0
H  3.394416  -1.191867  0.0
H  3.321619  1.290112  0.0
H  1.161733  2.476345  0.0
H  -3.369305  -1.389453  0.0
H  -1.330033  2.407247  0.0
H  -3.42943  1.115969  0.0
Core  RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]  45
169.5513          186.3331          361.7572
400.6956          462.4518          507.3376
508.4714          521.5661          610.9897
631.4357          731.1317          772.9822
773.8392          790.0839          800.0831
865.8314          893.2849          932.4053
964.6946          976.4209          998.9404
1033.6684         1046.5606         1138.8725
1169.0256         1175.9683         1197.8985
1236.3006         1270.8697         1359.7546
1378.0259         1389.4947         1451.5684
1484.0991         1520.9853         1582.9071
1637.0922         1662.7184         3157.5448
3159.0870         3169.4881         3170.4343
3181.2007         3182.1190         3192.4871
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  2
End

```

GroundEnergy[kcal/mol] 0.0
End
!-----c10h7_c3h4_p0a-----
Bimolecular p0a
Fragment c3h4
RRHO
Geometry[angstrom] 7
C -0.7953643067 0.0340930197 3.929351E-4
C 1.7999079767 -0.188313622 -0.0384040502
H -1.2789000818 0.9884787247 0.182918491
H -1.4365104427 -0.8255826572 -0.1664284561
H 2.3603730273 -0.4130354538 0.8635083944
H 2.3636835038 -0.0613232862 -0.9572540549
C 0.5024913234 -0.0757887252 -0.0189202593
Core RigidRotor
SymmetryFactor 4.0
End
Frequencies[1/cm] 15
371.2233 371.5183 865.8663
866.2617 884.0403 1016.3687
1016.5866 1109.0953 1422.1712
1479.1925 2051.9260 3118.9601
3123.0938 3193.6015 3194.4729
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
Fragment c10h7
RRHO
Geometry[angstrom] 17
C 0.014468 -0.761638 0.0
C 1.273145 -1.416493 0.0
C -1.226649 -1.409071 0.0
C 2.435985 -0.68536 0.0
C 2.394138 0.728582 0.0
C 1.190743 1.391526 0.0
C -0.035299 0.677452 0.0
C -2.446252 -0.820405 0.0
C -1.301795 1.322885 0.0
C -2.472747 0.604434 0.0
H 1.296576 -2.499829 0.0
H 3.394416 -1.191867 0.0
H 3.321619 1.290112 0.0

```

H  1.161733  2.476345  0.0
H -3.369305 -1.389453  0.0
H -1.330033  2.407247  0.0
H -3.42943  1.115969  0.0
Core  RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]  45
169.5513           186.3331           361.7572
400.6956           462.4518           507.3376
508.4714           521.5661           610.9897
631.4357           731.1317           772.9822
773.8392           790.0839           800.0831
865.8314           893.2849           932.4053
964.6946           976.4209           998.9404
1033.6684          1046.5606          1138.8725
1169.0256          1175.9683          1197.8985
1236.3006          1270.8697          1359.7546
1378.0259          1389.4947          1451.5684
1484.0991          1520.9853          1582.9071
1637.0922          1662.7184          3157.5448
3159.0870          3169.4881          3170.4343
3181.2007          3182.1190          3192.4871
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  2
End
GroundEnergy[kcal/mol] 1.14
End
!-----h_c13h10_p1-----
Bimolecular  p1
Fragment      c13h10
RRHO
Geometry[angstrom]  23
C -0.0437500061  0.0123095206  0.0252617316
C  0.6512048508  1.2535293387  0.0674946639
C -1.4811697898  2.4219864887  0.0295580341
C -0.0733849906  2.4297205801  0.0689110895
C -2.1697345502  1.2326288178  -0.0114837262
C -1.4723860618  4.463414E-4   -0.0147419459
C  2.1674259738  1.2854522682  0.1103769977
C  2.1271302562  -1.2065166299  0.0632193462
C  2.8216565622  -0.0652372226  0.1036075121

```

C	-1.4482975741	-2.4277915557	-0.0589128135
C	-0.0367694945	-2.4192400451	-0.0194545592
C	-2.1507497801	-1.2494370704	-0.0567039312
C	0.6679100113	-1.2321074712	0.0220911204
H	-2.0199183363	3.3631269993	0.0318430024
H	0.4509615944	3.3800208572	0.1009604327
H	-3.2541168815	1.2229121865	-0.0418266034
H	2.5455514135	1.8722361414	-0.7386036755
H	2.4970134376	1.8399994694	1.0003049323
H	2.6437836564	-2.1614699211	0.0598841027
H	3.9065563461	-0.0871677721	0.1334188125
H	-1.974612129	-3.3752899639	-0.0910812134
H	0.5049714574	-3.3593907628	-0.0217646563
H	-3.2351439657	-1.2535515946	-0.0869256535

Core RigidRotor

SymmetryFactor 1.0

End

Frequencies[1/cm] 63

89.1288	159.1117	202.1785
237.0345	378.2836	414.2774
432.7842	473.7832	478.3040
478.8314	504.4393	579.8259
580.2949	608.2522	646.5788
735.8134	763.3361	777.3378
793.2144	815.7311	824.6976
843.4769	897.7987	914.0571
954.4027	964.0034	979.9784
985.7081	1000.7368	1046.2329
1066.7674	1101.4892	1122.1096
1176.2572	1194.7653	1203.5052
1223.3532	1235.1670	1254.7218
1269.2080	1335.9060	1383.4596
1398.0764	1420.1847	1425.2403
1459.3047	1468.0401	1497.3962
1543.1068	1624.3055	1633.1183
1648.5874	1706.5838	2985.7361
2994.5071	3146.5544	3151.2918
3157.2425	3162.3213	3165.6717
3168.3035	3181.0060	3183.5965

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] -40.86
End
!-----h_c13h10_p2-----
Bimolecular  p2
Fragment      c13h10
RRHO
Geometry[angstrom]  23
C  -1.00819315  2.0029815592  -9.632184E-4
C  -1.628409413  0.7423855931  0.0011819134
C  0.5428905122  -0.3896342963  0.0020266231
C  -0.8788425691  -0.4297755539  0.0026152024
C  1.1693880937  0.9011689526  -1.452962E-4
C  0.3673101323  2.0745686408  -0.0016047233
C  -3.0944999782  0.3873861137  0.0023270246
C  -1.8036733799  -1.5679183356  0.0046518783
C  -3.0722254003  -1.1200886322  0.0045556658
C  2.7327038279  -1.4427688499  0.0027903843
C  3.3522129163  -0.1720040495  6.463853E-4
C  1.3622984979  -1.5473954491  0.0034644518
C  2.5875474865  0.9689121875  -7.786774E-4
H  -1.6038118374  2.9100381879  -0.0020854409
H  0.863146506  3.0395146806  -0.0032513242
H  -3.6160970822  0.7898381071  0.8802721015
H  -3.6169442175  0.7873346278  -0.8762454251
H  -1.5058101688  -2.6080462538  0.0064287965
H  -3.9648801754  -1.7311472901  0.0056825131
H  3.3450004555  -2.3376490281  0.0039081922
H  4.4342227121  -0.1023134772  1.303487E-4
H  0.896351355  -2.5261288065  0.0051186234
H  3.0613748766  1.9452413719  -0.002425999
Core  RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]  63
113.6369          131.8043          229.2486
241.8624          268.1795          387.6199
432.8761          438.9501          463.5555

```

506.1622	519.7898	564.9987	
613.2146	666.3128	682.0154	
723.1259	748.4914	753.1746	
798.3392	817.3539	841.0882	
879.1071	882.4464	933.1764	
950.2629	955.0476	958.7634	
966.8115	969.3634	992.8641	
1043.8602	1074.0915	1126.0872	
1143.1529	1166.9896	1178.4408	
1191.9357	1216.8143	1236.5436	
1283.2443	1293.4780	1351.7496	
1378.3128	1389.2441	1429.9837	
1431.5175	1469.3301	1486.4362	
1555.0881	1584.8304	1618.7769	
1634.2324	1664.4116	3014.4320	
3037.0896	3155.8948	3157.6475	
3165.4279	3174.7870	3178.0413	
3188.0239	3195.8059	3217.7140	
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]	-36.48		
End			
!-----h_c13h10_p3-----			
Bimolecular	p3		
Fragment	c13h10		
RRHO			
Geometry[angstrom]	23		
C	0.2079539949	-1.3236037336	-0.0293198595
C	1.4449134189	-0.6402904261	-0.0118366402
C	0.3131038156	1.5259732599	-0.0154327576
C	1.4940034378	0.7494297974	-0.0050686174
C	-0.9423550658	0.8281988632	-0.0331950759
C	-0.9561627666	-0.5939419797	-0.0396786718
C	2.8170545022	-1.1568678191	0.0017974887
C	2.9396634748	1.1836529957	0.013893014

C	3.6841614526	-0.1299061388	0.016655728
C	-0.8786352872	3.6449545064	-0.0196538428
C	-2.1155777833	2.9588961608	-0.0372446822
C	0.3041744388	2.946775239	-0.0091436667
C	-2.1423509347	1.585418576	-0.0439367221
H	0.1795566913	-2.4078678834	-0.0345179255
H	-1.9161098602	-1.0996153168	-0.053153079
H	3.0735818544	-2.2088713166	1.193785E-4
H	3.1813661716	1.7876833877	0.8977900664
H	3.2019767323	1.7956598273	-0.8585622442
H	4.7634660877	-0.2019802964	0.029108642
H	-0.8681963824	4.7293030031	-0.0145329232
H	-3.0418440058	3.5222031879	-0.0454370489
H	1.248232734	3.4801673323	0.0043765793
H	-3.090263721	1.0570647739	-0.05740314

Core RigidRotor
SymmetryFactor 1.0
End

Frequencies[1/cm] 63

111.6568	140.7102	235.6844
237.2977	257.3903	398.3061
432.9100	435.8335	465.2576
517.6351	520.4029	551.8127
616.8141	670.8690	681.8542
717.6867	751.4681	760.6125
787.6021	828.8345	839.7059
870.5954	872.9517	937.1086
954.6082	955.6063	959.7776
969.6397	982.1818	991.7866
1043.5437	1060.8248	1117.8038
1144.3104	1166.9374	1179.2839
1185.5663	1233.5486	1244.6810
1263.9404	1288.2738	1363.8797
1378.3823	1398.5186	1416.6139
1434.3843	1470.0655	1487.4275
1552.8417	1587.7447	1621.5463
1637.2740	1664.2119	3014.3619
3037.2215	3156.0943	3158.8407
3163.7816	3176.2621	3177.0994
3187.4040	3191.0726	3215.7707

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] -36.62
End
!-----h_c13h10_p4-----
Bimolecular  p4
Fragment      c13h10
RRHO
Geometry[angstrom]  23
C  -4.528101345071  -0.932478089845  0.03903978798
C  -3.187158947241  -0.363750657592  0.030039174806
C  -2.079371027764  0.115290359409  0.022527791082
C  -0.774578035774  0.693060520968  0.015885463092
C  -0.630125010456  2.0722604561  0.016198591032
C  0.644027596887  2.672338809846  0.010901996584
C  1.77811576128  1.897491116809  0.005267569479
C  0.397365620117  -0.13906510272  0.009418406193
C  1.686170994385  0.482073929924  0.004299595108
C  2.844080944149  -0.339537765781  -0.001658141
C  2.739457552364  -1.708368281295  -0.002860372657
C  0.324599776749  -1.554847127866  0.007827661382
C  1.465748911976  -2.320726459291  0.00177062926
H  -5.138168961711  -0.490168865641  0.832446511633
H  -5.038913318856  -0.754628808811  -0.912398498724
H  -4.4972196563  -2.013304229311  0.204373445384
H  -1.518324364398  2.692309059022  0.020835451
H  0.721151063548  3.753696311406  0.011450574214
H  2.760519662039  2.357695883854  0.001417712739
H  3.818783133071  0.137188944856  -0.005318459891
H  3.632271326669  -2.32354338991  -0.007451649299
H  -0.651919836009  -2.023481000559  0.011146352726
H  1.391125160311  -3.402434613576  4.88407428E-4
Core  RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]  63
6.2293          72.0222          74.4190
163.8638        176.6064          259.7311

```

265.9221	365.2929	387.5813
396.4508	453.9989	479.1291
499.2776	540.6374	583.2657
589.8083	653.5972	683.9733
747.3335	790.9499	804.9864
815.2779	833.1334	881.3513
922.9556	957.1114	967.7726
985.0968	998.8840	1042.0246
1049.3393	1054.5261	1075.7846
1120.3994	1168.7343	1180.8739
1201.9878	1237.0497	1267.9492
1308.1541	1357.2424	1391.6614
1414.6731	1427.6216	1467.7618
1477.6395	1478.9786	1492.4778
1543.6290	1613.6708	1627.8875
1661.0870	2331.6720	3019.6748
3073.9098	3079.7100	3158.9578
3162.5687	3169.8168	3178.2820
3183.0913	3192.5443	3194.4850

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] -10.28

End

!-----h_c13h10_p5-----

Bimolecular p5

Fragment c13h10

RRHO

Geometry[angstrom] 23

C	-4.480700820267	-0.629961654177	0.276907240784
H	-4.883330543335	-0.845664825687	1.263046932174
H	-5.182378932456	-0.281991534865	-0.476753053402
C	-3.216106576495	-0.782429591461	0.009512577434
C	-1.943993481034	-0.949328611635	-0.259307028182
C	-0.89480219054	0.08353548318	-0.135350503304
C	-1.235687965293	1.42488744264	-0.109824060823

C	-0.261110116228	2.435055562076	-0.013075947999
C	1.071529710913	2.109124129693	0.045614297446
C	0.491803531292	-0.28464263164	-0.05740954204
C	1.479838130069	0.752454756035	0.024441097473
C	2.853697580304	0.399742852961	0.091141295705
C	3.250807967076	-0.913431174679	0.088752389682
C	0.943782982531	-1.632151665434	-0.041828401882
C	2.281684853197	-1.938829071739	0.026260166657
H	-1.646738298276	-1.930062964247	-0.619001087913
H	-2.281780747416	1.700704923559	-0.179086995227
H	-0.571475388922	3.473836795685	0.001568624797
H	1.829009345928	2.883096848426	0.108308482195
H	3.588846875035	1.195822800966	0.147843018459
H	4.303400944928	-1.167670222384	0.141055046593
H	0.225112265248	-2.440709377754	-0.068875156227
H	2.596312873737	-2.976371269508	0.037280607587

Core RigidRotor

SymmetryFactor 1.0

End

Frequencies[1/cm] 63

34.9256	94.5729	134.8635
176.5932	239.6672	258.7652
321.8270	408.7192	413.7803
431.5133	476.8336	509.2602
516.6136	542.7298	607.4089
655.0582	678.4938	744.1389
766.6646	793.9369	805.8972
813.9631	869.5746	877.3258
878.9295	901.5681	925.3020
962.5839	984.9457	995.8558
1011.6259	1016.7775	1052.7399
1100.3751	1128.3501	1169.4513
1190.5669	1197.2151	1233.1650
1264.1030	1280.9695	1339.1628
1383.9795	1393.8708	1424.5484
1463.5509	1484.0357	1496.2001
1550.0010	1613.5941	1634.1732
1662.6119	2033.8783	3104.0534
3144.5264	3158.7888	3161.3806
3169.4659	3173.3218	3173.5683
3184.2770	3186.1441	3198.6078

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] -5.04
End
!-----h_c13h10_p6-----
Bimolecular  p6
Fragment      c13h10
RRHO
Geometry[angstrom]  23
C  0.2417293017  -0.1231029792  -0.2663292228
C  -0.9998538449  0.5615351061  -0.4565573225
C  0.0708264558  2.6610063627  0.154617934
C  -1.0638962028  1.9203122781  -0.2460227709
C  1.2738839602  2.030357528  0.3377267714
C  1.393403319  0.6312828386  0.1315794027
C  -2.2501629942  -0.185015172  -0.9038100881
C  2.7390925835  -1.3927402926  0.108905572
C  1.6049695864  -2.1402234371  -0.2781734669
C  2.6314490257  -0.0388708254  0.3098826501
C  0.3902309487  -1.5229669912  -0.4593099951
H  -0.018242751  3.7299138517  0.3120805565
H  -2.0068760763  2.4371793268  -0.3906819199
H  2.151755128  2.5909440572  0.6412577803
H  -2.0253973669  -0.8015835174  -1.7819178023
H  -2.9949295799  0.546250848  -1.2317265779
H  3.6912805545  -1.8918978632  0.2489313828
H  1.6937681179  -3.210254916  -0.4289239071
H  3.4972539485  0.5424020194  0.6098342153
H  -0.4705422556  -2.1182979108  -0.7355054762
C  -3.3369946642  -1.7267744707  0.9797615886
C  -2.8467194933  -1.0312891624  0.1316469445
H  -3.7647307007  -2.3388746787  1.7352007517
Core  RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]  63
53.0973          76.9056          149.9481

```

175.6043	256.3389	262.6339
344.3904	392.1855	427.5207
434.2643	478.9520	512.5606
522.8119	557.3915	616.0057
664.2892	670.7530	675.1393
724.1538	745.4770	793.0457
804.2224	812.7617	866.3796
886.7231	917.7622	935.9585
957.0324	966.2268	983.7392
996.3317	1040.3698	1061.1259
1097.2954	1168.7413	1184.8333
1188.5373	1216.9966	1240.8398
1261.9381	1289.0032	1334.8405
1383.4957	1397.2626	1424.7856
1469.8395	1481.4292	1495.3975
1548.5129	1618.6270	1641.8188
1665.8494	2221.0616	3020.8864
3059.0888	3158.0483	3159.4820
3165.9205	3170.1972	3184.2919
3185.3131	3198.5910	3477.3261
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] -2.0		
End		
!-----ch3_c12h8_p7-----		
Bimolecular p7		
Fragment c12h8		
RRHO		
Geometry[angstrom] 20		
C 0.5443045687 0.2005444428 0.8505882989		
C -0.7487312176 0.8012408473 1.0254685357		
C 0.1899684447 2.9782201099 0.4807434526		
C -0.9031654786 2.1660967544 0.8395463005		
C 1.4365711371 2.4278504078 0.3075436019		
C 1.6464170241 1.036488149 0.4860751955		

C	-2.8274825718	-0.6655359612	1.6986686947
C	-1.8760325877	0.0054170134	1.3890740191
C	3.1132088224	-0.9005879857	0.4886319094
C	2.0232635745	-1.7249183022	0.8487972933
C	2.9266177105	0.4479222943	0.3120605133
C	0.7705583185	-1.1879268817	1.0253007116
H	0.0378789474	4.0424551849	0.3424740129
H	-1.8831391325	2.6072680104	0.9743656549
H	2.2798709967	3.0518173445	0.0310687068
H	-3.6671176836	-1.2572572886	1.9693598738
H	4.0961079551	-1.3373744707	0.3526289688
H	2.1789602544	-2.7890059356	0.9863991687
H	3.7587351911	1.0869079361	0.0355849516
H	-0.0639252734	-1.8208156691	1.301348136

Core RigidRotor
SymmetryFactor 1.0
End

Frequencies[1/cm] 54

102.4513	138.5306	175.2683
202.9107	353.7725	364.1458
445.2477	451.3350	478.8168
495.6215	551.3867	582.9265
593.9030	628.1577	655.4881
690.7284	705.6784	749.1842
791.0004	806.2552	817.0283
872.6489	882.9997	928.0044
970.7953	988.0719	1001.9896
1036.9341	1053.1978	1096.1872
1169.1937	1182.5636	1192.3821
1237.0354	1251.8741	1292.9297
1360.3674	1392.3362	1422.9748
1468.9275	1491.9413	1544.4621
1614.1481	1628.4663	1661.8362
2200.7963	3160.2690	3164.1854
3171.2083	3180.3108	3184.6645
3194.7060	3196.0618	3476.9162

ZeroEnergy[kcal/mol] 0.0

ElectronicLevels[1/cm] 1

0 1

End

Fragment ch3

RRHO

Geometry[angstrom] 4

```

C 3.465073663 -1.8287770054 7.55108E-5
H 2.9494866157 -1.9893536196 -0.9357821139
H 2.9493016592 -1.9893430857 0.9358330347
H 4.4960410621 -1.5052722892 1.755672E-4
Core RigidRotor
SymmetryFactor 6.0
End
Frequencies[1/cm] 6
505.5776 1403.1131 1403.3797
3103.7859 3282.6714 3283.0465
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 2
End
GroundEnergy[kcal/mol] -15.82
End
!-----h_c13h10_p8-----
Bimolecular p8
Fragment c13h10
RRHO
Geometry[angstrom] 23
C -0.3922641251 -3.7210691382 -0.7554262317
H 0.2746093546 -4.0794398649 -1.547498267
H -0.1056249533 -4.2452469846 0.1630690935
H -1.4103649088 -4.0208934777 -1.0107602649
C -0.2888064764 -2.2383332731 -0.5887224039
C -1.2858886378 -1.3174067893 -0.7209568027
C -0.7520806394 0.0301584592 -0.4716092601
C -1.2534664645 1.3134238365 -0.4583786661
C -0.3707375699 2.3912574429 -0.1575458971
C 0.9681699968 2.2010281547 0.1215218544
C 0.6221112346 -0.1452112921 -0.1832868457
C 1.5142132215 0.8835472895 0.1149195091
C 2.8573393181 0.4862980786 0.3749499554
C 3.2051079076 -0.8501991807 0.3225521757
C 0.9582196352 -1.5168399569 -0.2416799826
C 2.2646067242 -1.8739000349 0.0141224001
H -2.3146302076 -1.5419044156 -0.9713539439
H -2.2966790271 1.5238680338 -0.6697448321
H -0.772317769 3.3986876206 -0.1489316319
H 1.6029981452 3.051847095 0.3452455161
H 3.6079263432 1.2323642518 0.6142521081
H 4.2319736923 -1.1355302456 0.5231621048

```



```

H 2.5945912054 -2.907291609 -0.0127926876
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 63
123.6554 145.0837 165.2801
219.8869 230.4511 299.8964
406.4497 409.7388 461.9884
498.2425 533.6410 547.7805
588.7086 592.9362 630.4302
677.6053 678.8317 764.1281
781.7886 800.5684 816.5086
819.6503 855.7291 919.6885
926.7661 971.3683 973.6004
984.0718 1017.1347 1035.4674
1056.9106 1059.6228 1086.5646
1158.4683 1179.7372 1204.9284
1220.3426 1247.6447 1280.5653
1322.0509 1386.5098 1406.3004
1414.8708 1450.0206 1461.5859
1480.8588 1488.1775 1492.6846
1515.2612 1595.3952 1635.7790
1654.5020 1659.5208 3013.6915
3055.3217 3102.0961 3158.4831
3159.0177 3167.6841 3168.9914
3182.1158 3183.1647 3202.5868
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] -37.58
End
!-----ch3_c12h8_p9-----
Bimolecular p9
Fragment c12h8
RRHO
Geometry[angstrom] 20

```

C	0.2474731132	-0.0017353973	-0.0873576261
C	1.3842839801	0.7912130642	0.0631843178
C	2.6211177064	0.0927337572	0.1769335129
C	2.6397734955	-1.2884002657	0.1345710569
C	1.4571493826	-2.0659726552	-0.0206678822
C	0.2467795828	-1.4157010294	-0.1328995413
C	-1.0721757537	0.4912806987	-0.2171557552
C	-1.2563572511	1.8573028204	-0.1938781882
C	-0.1179086697	2.6987294075	-0.0414534636
C	1.1643548377	2.1989735178	0.0839332276
C	-1.1609899217	-1.8133931398	-0.3009625416
C	-1.9347504468	-0.694645335	-0.3504080449
H	3.547655231	0.644337076	0.2966603007
H	3.5891074108	-1.805169376	0.2224427509
H	1.5313070623	-3.1481130452	-0.0474108747
H	-2.2402605978	2.3048545329	-0.2881547269
H	-0.2686285616	3.7725003934	-0.0237709184
H	2.0025413527	2.8783100067	0.1980333929
H	-1.5146548296	-2.8329483454	-0.3726936943
H	-3.0095781232	-0.6714536857	-0.4682813022

Core RigidRotor
SymmetryFactor 1.0
End

Frequencies[1/cm] 54

160.5077	212.2102	229.3073
375.5763	423.1391	461.5454
470.8274	518.8992	561.3635
583.0543	615.6679	668.6491
675.1331	695.7926	741.1577
766.9659	788.4054	818.0424
848.4967	879.4882	917.5353
929.4159	935.3924	975.8155
985.5792	1027.4923	1034.8022
1056.5181	1102.5586	1113.1093
1176.0904	1203.3361	1224.4432
1246.4128	1273.1232	1331.5419
1385.4527	1419.4808	1447.3262
1457.4011	1489.6834	1515.4936
1540.3868	1636.3596	1652.3436
1660.5778	3159.6761	3160.0774
3168.9918	3169.7302	3183.0860
3184.0689	3201.8299	3221.8770
ZeroEnergy[kcal/mol]	0.0	

```

ElectronicLevels[1/cm]      1
0 1
End
Fragment      ch3
RRHO
Geometry[angstrom]  4
C  3.465073663  -1.8287770054  7.55108E-5
H  2.9494866157  -1.9893536196  -0.9357821139
H  2.9493016592  -1.9893430857  0.9358330347
H  4.4960410621  -1.5052722892  1.755672E-4
Core  RigidRotor
SymmetryFactor 6.0
End
Frequencies[1/cm]  6
505.5776          1403.1131          1403.3797
3103.7859         3282.6714          3283.0465
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]      1
0 2
End
GroundEnergy[kcal/mol] -43.96
End
!-----bar_ts0-1-----
Barrier      ts0-1  i1  p0p
RRHO
Geometry[angstrom]  24
C  0.470333  -0.151755  -0.227133
C  0.449763  -1.563667  -0.377451
C  -0.644568  0.682915  -0.423588
C  1.586643  -2.306482  -0.170219
C  2.798294  -1.675591  0.197213
C  2.852382  -0.311765  0.353075
C  1.701052  0.492696  0.149145
C  -0.634277  2.03374  -0.269051
C  1.719711  1.904931  0.304404
C  0.588517  2.658055  0.103
H  -0.483637  -2.038988  -0.653952
H  1.55915  -3.384126  -0.287332
H  3.687271  -2.275671  0.356724
H  3.782358  0.171412  0.635841
H  -1.526587  2.631415  -0.424013
H  2.651089  2.383703  0.588309
H  0.620519  3.735669  0.22709

```

C -2.706114 -0.229668 -1.107978
 C -4.016101 -0.780731 1.143374
 C -3.385692 -0.514233 -0.139583
 H -2.417312 -0.099501 -2.124349
 H -4.280436 -1.837516 1.24136
 H -4.931025 -0.193191 1.261822
 H -3.34106 -0.52387 1.967251

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 299.7862

WellDepth[kcal/mol] 41.68

WellDepth[kcal/mol] 1.74

End

Rotor	Hindered	! 57 cm ⁻¹	CH3
Group		22 23 24	
Axis		19 20	
Symmetry		3	
Potential[kcal/mol]		4	

0 0.071106877 0.179382401 0.070254091

End

Rotor	Hindered	! 17 cm ⁻¹
Group		19 20 21 22 23 24
Axis		3 18
Symmetry		1
Potential[kcal/mol]		8

0 0.534680841 1.8736721 0.477881183 0.001157755 0.456316189 1.721036667 0.406609899

End

Frequencies[1/cm] 63

35.6533

89.6241

101.7003

171.2419	193.3488	316.2767
350.8434	372.2125	405.7979
469.0672	499.7525	511.3195
519.9559	595.3877	621.3856
658.8588	704.9756	737.3383
777.2651	784.1230	797.3976
802.6777	869.5187	898.8601
926.2114	939.4749	965.1524
976.3497	997.7390	1035.0451
1039.8818	1050.7858	1057.8464
1135.8799	1167.7238	1176.2465

1201.3652	1234.8784	1269.8281
1362.2137	1381.3859	1385.4874
1411.6407	1452.7598	1473.9049
1474.4423	1482.6103	1522.9826
1582.3819	1634.4438	1659.9137
2111.4609	3015.3060	3070.5633
3083.8860	3151.3024	3154.9701
3162.0807	3166.9013	3175.9532
3181.0882	3192.6782	3431.3587

ZeroEnergy[kcal/mol] 1.74

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts0-5-----

Barrier ts0-5 i5 p0p

RRHO

Geometry[angstrom] 24

C	-0.6298601875	0.0377674688	-0.0719979277
C	0.6524726573	0.6163319424	-0.0342907811
C	-0.2240210352	2.8312377667	0.1473707096
C	0.890209868	1.9527618813	0.0529792832
C	-1.5040290197	2.3326274155	0.1361907611
C	-1.7487313472	0.937545357	0.0256020902
C	2.8147164319	-0.8320574423	-1.2552498255
C	2.5290544979	-0.731770059	-0.0723467724
C	2.6596728171	-0.9381032217	1.3779468423
C	-3.2624602123	-0.9589616646	-0.1159436465
C	-2.1612039688	-1.8405598022	-0.2199636389
C	-3.0598275207	0.3945533937	0.0021578808
C	-0.8761645236	-1.3550883225	-0.1987224665
H	-0.0546922104	3.90014717	0.226893282
H	1.8992866473	2.3523564785	0.0535294324
H	-2.3527837499	3.0047361659	0.2074443514
H	2.8682482804	-0.7806970661	-2.3162997093
H	1.7653771684	-1.4104024513	1.7903527459
H	2.7965500558	0.0124034107	1.8979172139
H	3.5214934568	-1.5783249885	1.5848130852
H	-4.2707351611	-1.3574885825	-0.1330246105
H	-2.3366332497	-2.9058945244	-0.3199529839
H	-3.9052547508	1.071117136	0.0779359683
H	-0.028704944	-2.0236464614	-0.291911284

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 373.6138

WellDepth[kcal/mol] 38.61

WellDepth[kcal/mol] 2.67

End

Rotor Hindered ! 153 cm⁻¹ CH3

Group 18 19 20

Axis 8 9

Symmetry 3

Potential[kcal/mol] 4

0 0.445792225 1.291397166 0.480834243

End

Rotor Hindered ! 33 cm⁻¹

Group 7 9 17 18 19 20

Axis 2 8

Symmetry 1

Potential[kcal/mol] 8

0 1.670964539 5.143005849 1.476119674 0.004166664 1.095134757 3.594033566 0.980218298

End

Frequencies[1/cm] 63

50.8858

76.0292

156.6214

174.3989

221.9524

237.7945

361.1689

385.4939

409.6355

469.4145

506.9269

515.8877

520.8724

562.1984

620.7239

623.2516

681.9563

738.4206

766.2118

777.7233

797.7613

802.9552

869.9148

899.1608

911.4459

933.0302

966.2199

977.4450

997.8735

1035.1833

1041.0399

1052.5316

1066.9174

1136.4488

1168.2513

1177.0022

1202.0869

1235.0661

1270.1387

1362.8351

1382.0931

1384.8985

1414.8405

1453.1780

1477.1258

1482.0330

1482.7686

1523.6535

1582.4641

1634.2063

1659.6334

2062.3549

3034.1763

3098.9727

3101.3672

3150.7134

3155.2397

3161.0345

3167.3229

3176.1997

```

3181.3630          3192.6561          3452.9220
ZeroEnergy[kcal/mol] 2.67
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts1-2-----
Barrier      ts1-2  i1  i2
RRHO
Geometry[angstrom] 24
C -4.5171805107 -0.8423526916 -0.5353990485
H -4.7670491551 -0.2983009596 0.3868636789
H -4.98681165 -0.3047960468 -1.3670284715
H -5.0063700026 -1.8261491921 -0.4683528024
C -3.0857439214 -0.9442775989 -0.7319065319
C -1.7885548436 -1.0293076712 -0.8633874057
H -1.3580366323 -1.9556462355 -1.2601938247
C -0.8038046579 0.0409341123 -0.5446700341
C -1.1853856996 1.3697769287 -0.5936793284
C -0.2800739202 2.4131064203 -0.3210380258
C 1.0269044138 2.1316968983 -0.0084163719
C 0.5532743867 -0.2795648919 -0.2016918141
C 1.4750417529 0.7885842149 0.0585459799
C 2.8209905469 0.4790737042 0.3882136212
C 3.2502910025 -0.8215238615 0.4727040284
C 1.0327020368 -1.6128410652 -0.0858371102
C 2.3419601151 -1.8773535544 0.2380185155
H -2.2061134412 1.6083580449 -0.871373871
H -0.6198587695 3.4415174478 -0.3757164831
H 1.7337638369 2.9304312955 0.1897890674
H 3.5080850959 1.2975093691 0.5771341176
H 4.2810361923 -1.0424791596 0.726228087
H 0.3523199436 -2.4401252826 -0.2398861439
H 2.6798968807 -2.9044012251 0.3202711713
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 245.6869
WellDepth[kcal/mol] 5.45
WellDepth[kcal/mol] 4.94
End
Frequencies[1/cm] 65

```

38.6772	75.7988	
96.6580	174.3311	178.3561
250.0129	287.6780	317.1825
419.7192	428.7456	479.1015
498.5213	530.6029	544.4188
612.8207	643.3423	727.8498
742.9960	776.4607	798.2513
806.2131	823.0574	846.3765
880.8846	917.5401	924.2758
963.5913	981.4319	986.7625
994.9548	1036.6889	1039.1692
1053.4624	1102.7993	1168.6065
1187.0623	1189.5157	1231.4727
1246.3664	1274.0143	1302.5161
1378.0923	1389.3009	1405.5653
1420.2367	1451.3958	1468.1461
1470.2281	1491.8040	1546.7016
1611.1012	1632.8419	1661.5621
1810.6603	2951.9893	2985.5872
3003.3333	3046.2402	3156.8249
3158.5773	3167.6715	3169.3056
3182.3441	3183.4266	3198.3909

ZeroEnergy[kcal/mol] -34.49

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts2-3-----

Barrier ts2-3 i2 i3

RRHO

Geometry[angstrom] 24

C	-1.1218021334	0.2086494433	0.348449078
C	-2.3969774405	-0.8527578207	-0.4601107843
C	-2.1715580343	-0.7543548436	0.8016824568
C	-3.0048554205	-1.2987292436	-1.7136671143
C	-1.4047429382	1.6082236847	0.2692723695
C	0.2759941379	-0.2139281695	0.1911423142
C	-0.4223067318	2.5280794904	-0.0776604043
C	1.2597999954	0.7588849606	-0.1662042588
C	0.8851510671	2.1269922451	-0.3133599734
C	0.6819574389	-1.5472251264	0.3796318549
C	2.6001289996	0.3382004529	-0.3422338252
C	2.0022444399	-1.9288389089	0.2124711343

C	2.9676020175	-0.9782344756	-0.1573595718
H	-2.4991489278	-1.1332283808	1.7661324197
H	-3.403347227	-0.4497805407	-2.2773251936
H	-2.2620148796	-1.7931983731	-2.3471603454
H	-3.82585664	-2.0062392082	-1.5335172961
H	-2.4202034118	1.9369532958	0.4587786241
H	-0.6838363306	3.5782589975	-0.1553601415
H	1.6439610109	2.8517388037	-0.5861235171
H	-0.0596685679	-2.2893116052	0.651287869
H	3.3430705863	1.0781277252	-0.6221505121
H	2.2902759012	-2.9628990473	0.3653735247
H	4.0002660887	-1.2795093553	-0.2945717073

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 527.591

WellDepth[kcal/mol] 22.28

WellDepth[kcal/mol] 5.56

End

Frequencies[1/cm] 65

72.0040	79.0329	
125.0441	152.5167	187.4163
248.3727	267.8324	305.6232
397.2511	439.9563	463.0052
490.4843	513.0152	522.3483
561.1917	614.2876	699.6667
716.2729	751.6211	770.8325
783.0948	800.7536	827.2984
871.8468	874.3250	880.6119
955.6688	959.9654	985.6399
1019.4823	1033.9774	1052.2172
1058.5672	1095.3235	1122.8887
1154.8165	1175.6522	1181.2612
1216.2226	1232.7161	1286.2288
1323.2070	1345.9205	1393.6696
1399.4417	1461.0555	1465.4299
1466.5200	1468.9988	1522.0634
1552.1682	1587.0143	1637.6655
1869.0831	2983.4018	3054.6990
3077.9842	3121.6978	3155.0061
3156.7397	3165.5034	3172.8406
3177.4463	3182.9760	3187.9248

```

ZeroEnergy[kcal/mol] -17.15
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts2-15-----
Barrier      ts2-15  i2  i15
RRHO
Geometry[angstrom]  24
C  -4.1959291577  -0.2252471692  0.3388039885
C  -3.1674028602  -0.9852853422  -0.2641068791
C  -1.8233969966  -1.1131474823  -0.2029014073
C  -0.8457646924  -0.0302498501  -0.1020489159
C  -1.250455554   1.3017658   -0.0706587521
C  -0.3325347172  2.360992005  0.0151523527
C  1.0173508613   2.1109812341  0.0687683367
C  0.571941155   -0.3133985888 -0.0555737193
C  1.4986585742   0.7783905143  0.034297865
C  2.8917320101   0.5085145902  0.0883372481
C  3.3696287355  -0.7770910628  0.0581258909
C  1.1090255179  -1.6280803978 -0.0820791165
C  2.4640890361  -1.855887274  -0.0274049809
H  -4.0308108141  0.4105063042  1.2132877013
H  -5.149803819  -0.1232342486 -0.170052949
H  -1.4322367777  -2.1149305809 -0.3355645429
H  -2.3055431687  1.5359215044  -0.1323935865
H  -0.6999231389  3.3811400636  0.0349561244
H  1.7309804049   2.925100376  0.1353852062
H  3.5765786947   1.3476338658  0.1551913079
H  4.4362171779  -0.967109334  0.0997064467
H  0.4468564638  -2.4808794549 -0.144580033
H  2.8394554983  -2.8728533149 -0.0504803147
H  -4.1270184335  -1.5436691571  0.4146927288
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  1821.0623
WellDepth[kcal/mol]  42.85
WellDepth[kcal/mol]  67.5
End
Frequencies[1/cm]  65
24.5570              88.5183

```

138.6199	173.0926	222.7249
231.6450	337.0042	371.4037
429.4101	439.4516	448.1297
480.5899	513.9683	546.3480
570.6956	652.4600	658.0382
738.6691	764.2337	784.7169
796.8756	802.5624	832.7083
868.5124	872.1961	889.7324
911.6693	956.5716	978.6669
992.2053	1004.3906	1034.7307
1055.0035	1074.8652	1114.5311
1137.9787	1167.7300	1191.2353
1199.3517	1228.9580	1257.7121
1280.9828	1335.9036	1381.0205
1402.3980	1423.8258	1459.6559
1471.1287	1490.5226	1544.6356
1561.1442	1615.6520	1627.0746
1658.7431	2176.4022	3027.1524
3157.2697	3160.9658	3163.2910
3168.4863	3169.9198	3177.4308
3184.7206	3195.1024	3206.7257

ZeroEnergy[kcal/mol] 3.42

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts2-20-----

Barrier ts2-20 i2 i20

RRHO

Geometry[angstrom] 24

C	-4.1318147367	-1.5680126573	0.7498767696
C	-3.1326913707	-1.1543414517	-0.2768956784
C	-2.0580317228	-0.4751988407	-0.4945959933
C	-0.9615467859	0.4226627712	-0.3191741303
C	-1.1586963869	1.7978519204	-0.4614783251
C	-0.0850531897	2.6976436895	-0.3679699554
C	1.1956381057	2.2457576193	-0.1414994539
C	0.3728687356	-0.076443014	-0.0845850832
C	1.4532868976	0.8565370038	0.0047458183
C	2.7628145368	0.3642570799	0.2425752307
C	3.0018036934	-0.9816274712	0.384906089
C	0.6526082452	-1.4552554607	0.0676465297
C	1.9348847672	-1.9007108938	0.2962405437

H	-3.9163587493	-1.0814048295	1.7107363875
H	-5.14377441	-1.2988139289	0.437906544
H	-4.1088076866	-2.6508240116	0.8956506201
H	-2.1601118129	2.1689181918	-0.6441557131
H	-0.2758583468	3.7599938128	-0.473382864
H	2.0234939523	2.9428626097	-0.0717751229
H	3.5790992956	1.0761070302	0.3096646539
H	4.0089699748	-1.3403183869	0.5655420717
H	-0.164298935	-2.1647026469	0.0021793698
H	2.1274432248	-2.9616973274	0.409332644
H	-2.4943872957	-1.1899008079	-1.4424499525

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 2065.9969

WellDepth[kcal/mol] 44.24

WellDepth[kcal/mol] 52.86

End

Frequencies[1/cm] 65

44.3047	67.4441	
108.5518	149.7766	173.2941
211.3223	244.1321	248.3056
366.5553	390.2747	418.7057
451.3949	480.8590	496.5940
542.3458	568.8739	589.9472
643.1330	685.5769	741.3225
784.6179	802.2427	806.3972
822.9596	874.1045	895.3511
923.2403	963.6458	974.3860
993.7160	1021.6229	1029.8288
1043.1492	1065.2080	1101.3867
1165.6561	1179.6643	1191.5957
1224.9092	1237.8435	1289.2888
1344.6786	1378.6522	1384.7855
1414.0733	1464.7212	1465.9989
1475.7461	1481.7120	1537.7997
1588.5422	1609.9906	1653.3699
1969.4389	2293.0449	2986.4971
3073.9564	3095.7218	3157.2810
3161.0997	3166.9927	3175.6156
3178.7686	3187.9517	3189.0465

ZeroEnergy[kcal/mol] 4.81

```

ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts2-21-----
Barrier      ts2-21  i2  i21
RRHO
Geometry[angstrom]  24
C  -0.7958293728  -3.749870677  -1.0778023626
H  -0.1953539919  -4.0418612044  -1.945333378
H  -0.4871733416  -4.3920960093  -0.2447667368
H  -1.8488738152  -3.9759224459  -1.2977062858
C  -0.6081061341  -2.3269432153  -0.7466296921
C  -1.3862366938  -1.2610213579  -0.5919350204
C  -0.7415491146  -0.0115188233  -0.1801947424
C  -1.2501231472  1.272406747  -0.3031100582
C  -0.3876304372  2.3777622044  -0.1582727206
C  0.9698452795  2.1999077611  0.0212539457
C  0.6129531957  -0.1942617615  0.1900568567
C  1.5137361415  0.8957411505  0.1582447007
C  2.9114769076  0.6099575926  0.1742997295
C  3.3581780226  -0.6996636655  0.2012431878
C  1.0785556184  -1.5418152603  0.4092438832
C  2.4668573228  -1.7740991606  0.3569096359
H  -2.4513519299  -1.2777894469  -0.8303256476
H  -2.2864785755  1.4278055981  -0.5832017975
H  -0.7882086069  3.3800836137  -0.2631388018
H  1.6377934124  3.0547113617  0.0256765956
H  3.6200124925  1.4297992866  0.1282638023
H  4.4243717623  -0.8990252399  0.1784405729
H  0.4954368111  -2.1902436873  1.0580643017
H  2.8564541942  -2.7690233606  0.5408360319
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 526.0228
WellDepth[kcal/mol] 15.2
WellDepth[kcal/mol] 35.04
End
Frequencies[1/cm] 65
104.4394          141.2395
163.9178          184.7534          208.0470

```

275.7736	333.9873	379.3355
417.5868	469.2378	480.3732
515.3011	538.7697	582.1135
613.2457	640.1586	693.9858
743.2674	766.3065	778.1941
800.6839	814.1341	837.2865
865.7739	896.1273	908.6810
960.5699	967.1173	975.0022
1030.5138	1043.7442	1053.4717
1081.2541	1095.5883	1144.2360
1171.8212	1184.3216	1202.7859
1221.0353	1245.8291	1294.3537
1356.7593	1380.7674	1398.0694
1401.0162	1448.4761	1458.4621
1475.4991	1476.7469	1518.2838
1563.2066	1598.1268	1630.6378
1688.8901	2978.8909	3041.7983
3060.2654	3081.6924	3107.1283
3157.2454	3158.1524	3168.0082
3171.8584	3181.6637	3182.9745

ZeroEnergy[kcal/mol] -24.23

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts3-4-----

Barrier ts3-4 i3 i4

RRHO

Geometry[angstrom] 24

C	0.3187108343	-0.1767089183	-0.0272686108
C	-1.0459028795	0.3622690251	-0.0800842402
C	-0.1012498593	2.6324108134	-0.137362571
C	-1.1973528981	1.7780956308	-0.1862135001
C	1.188377714	2.1357442002	-0.0259585365
C	1.4216864212	0.7298818768	0.017361579
C	-2.3029059511	-0.4462703255	1.0109368992
C	-2.2294484174	-0.539296435	-0.2706857418
C	-2.8653082689	-1.1429383809	-1.4764817969
C	2.9601101483	-1.156209376	0.1005815252
C	1.873999943	-2.0461843509	0.046053004
C	2.7345050154	0.2034418585	0.0883205608
C	0.5807035826	-1.5592944546	-0.0134272501
H	-0.2616124613	3.7038333992	-0.1951805235

H	-2.199863189	2.1801385629	-0.2779274848
H	2.0373618104	2.8089627412	0.0123823453
H	-2.7159616178	-0.6344747042	1.9860153803
H	-2.1462959345	-1.761790188	-2.0214974597
H	-3.1975824312	-0.3571447505	-2.1620649818
H	-3.724580196	-1.7571752654	-1.2004776792
H	3.9729517275	-1.539827518	0.1535069638
H	2.049229227	-3.1160977252	0.0556543457
H	3.5688269559	0.8961072105	0.1311155504
H	-0.2513222752	-2.2532889261	-0.0297297774

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 604.1172

WellDepth[kcal/mol] 6.46

WellDepth[kcal/mol] 20.46

End

Frequencies[1/cm] 65

81.0246	91.5021	
134.3827	168.4294	183.3953
226.3361	276.1962	369.7836
397.4020	470.9722	472.7723
493.7575	522.7610	536.9735
561.3816	605.7633	639.3156
647.7566	691.3615	722.1578
771.6290	784.6987	799.1007
826.5922	841.7650	880.8534
908.7783	958.3105	962.4797
987.6116	1014.4673	1040.3793
1051.8062	1085.9397	1115.3429
1156.7620	1176.3407	1182.6957
1231.7724	1238.6704	1288.6103
1324.6277	1349.2580	1393.4134
1399.3780	1461.0697	1467.3328
1475.8596	1483.2000	1521.8367
1554.4534	1587.6479	1640.3774
1814.0237	3024.5870	3078.5508
3109.5238	3156.2613	3158.2804
3166.9640	3173.7544	3179.4834
3183.9743	3189.8070	3286.0267

ZeroEnergy[kcal/mol] -16.25

ElectronicLevels[1/cm] 1

```

0 2
End
!-----
!-----bar_ts4-5-----
Barrier      ts4-5  i4  i5
RRHO
Geometry[angstrom]  24
C -0.2728869063 -0.1794948736 -0.0715451777
C  1.0403223592  0.3891326112 -0.088185117
C  0.0709062394  2.6154031337  0.0661597993
C  1.1898275879  1.7584599978 -0.029558364
C -1.1978759071  2.095084759  0.1023544476
C -1.4046300406  0.6932157549  0.0312940929
C  2.9121784187 -0.6597035052 -1.2574169759
C  2.2673293278 -0.491788879 -0.1387064153
C  2.696547237 -1.1051290867  1.1898744885
C -2.8956842907 -1.2259944637 -0.0374825004
C -1.7814699602 -2.0874687052 -0.1545198561
C -2.7082116846  0.1312570396  0.0491130246
C -0.5056976478 -1.5772907055 -0.1732491708
H  0.2240717663  3.6878003104  0.1136932551
H  2.1878621357  2.1815582819 -0.0532207015
H -2.0609278038  2.7479779391  0.1802607539
H  3.4537218091 -0.815344814 -2.1606594751
H  1.8793221816 -1.6838072835  1.6306368504
H  2.9480782208 -0.3111934886  1.900724377
H  3.5641940931 -1.7538506253  1.0638893366
H -3.897458693 -1.6404639889 -0.0235202584
H -1.937219154 -3.1574291562 -0.2360814719
H -3.5598628534  0.7990815508  0.128678734
H  0.3416045648 -2.2427618029 -0.285805676
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  710.1939
WellDepth[kcal/mol]  4.66
WellDepth[kcal/mol]  3.89
End
Frequencies[1/cm]  65
42.5911          94.2169
147.8980         168.6124         174.3170
189.3461         299.8491         327.9163

```


380.7559	443.7658	478.6877
497.9453	500.7314	557.0123
584.3111	587.1113	641.3337
663.5846	694.9807	747.3138
793.5222	805.6236	815.1449
842.6506	879.5232	921.2243
952.1095	968.3694	984.3516
997.3084	1015.3916	1035.2289
1044.9419	1078.9626	1115.1994
1167.9818	1181.9849	1190.1677
1233.7553	1252.2229	1287.6074
1362.1785	1389.0889	1391.5558
1418.5800	1465.0498	1479.5251
1481.6929	1491.1070	1542.9816
1612.3824	1633.1191	1660.9463
1673.4829	3020.7469	3075.7576
3115.9315	3157.2995	3159.8189
3168.1880	3171.4658	3182.4042
3185.1551	3192.6877	3435.1637

ZeroEnergy[kcal/mol] -32.05

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts5-7-----

Barrier ts5-7 i5 i7

RRHO

Geometry[angstrom] 24

C	-0.3214924007	-0.1477460768	0.0393666974
C	1.0385202238	0.3076420197	-0.0172515398
C	0.1969231152	2.5924467213	-0.1684579409
C	1.2654894469	1.667206225	-0.119833952
C	-1.1071705302	2.1678107953	-0.1150519121
C	-1.4035138685	0.7830727992	-0.0094309101
C	-2.977922561	-1.0692811879	0.1522855961
C	-1.9054735973	-1.9969381459	0.2010275078
C	-2.7300522733	0.2803123025	0.050044089
C	-0.6288334843	-1.5134332735	0.1438112454
H	0.4202205908	3.6504033254	-0.2490945978
H	2.278506514	2.0473242869	-0.1649604582
H	-1.9231774719	2.8818804015	-0.1527313984
H	-3.9992413512	-1.4324387735	0.1963405081
H	-2.1094129074	-3.0592600795	0.2816644641

H	-3.5551964316	0.9839180882	0.0132809065
C	1.8544389772	-1.9851094198	0.135019243
C	2.1392611086	-0.687183183	0.035866783
C	3.5716178816	-0.1969530522	-0.0245430492
H	2.534220374	-2.8278912751	0.1843938732
H	3.7935887902	0.4781034206	0.8080062462
H	3.7630087534	0.3504841787	-0.952868809
H	4.2671431955	-1.0352332373	0.0241304002
H	0.5341429061	-2.1578318598	0.1704540074

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 1618.6465

WellDepth[kcal/mol] 8.92

WellDepth[kcal/mol] 8.91

End

Frequencies[1/cm] 65

91.5438	155.0625	
178.3413	214.3170	220.2743
266.7426	354.0256	394.8654
458.3114	466.8088	467.4779
506.2533	519.8291	561.9771
591.8543	612.8501	643.1957
696.5611	722.1389	754.9205
782.0968	806.3781	825.5849
865.3707	898.4603	921.9498
960.6959	975.4195	986.9299
990.2819	1023.4004	1030.0156
1049.4184	1056.1112	1091.3990
1167.4744	1170.5969	1217.5366
1224.0975	1242.2008	1291.1239
1357.8408	1380.7492	1404.3939
1408.0878	1452.9985	1474.5921
1485.4757	1488.8274	1517.0213
1577.7994	1592.9711	1633.7815
1642.8269	1688.5869	3021.8643
3073.2333	3114.3371	3155.5331
3160.5483	3166.5555	3177.0521
3179.4874	3181.6004	3193.5496

ZeroEnergy[kcal/mol] -27.02

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts7-8-----

Barrier ts7-8 i7 i8

RRHO

Geometry[angstrom] 24

C -0.3254724974 -0.1742138486 -0.0223713799

C 1.0351062139 0.28083458 -0.0193136404

C 0.2169462753 2.5700855852 0.1049894304

C 1.2766401695 1.6386975316 0.0611453868

C -1.0920800148 2.1521907797 0.0719925657

C -1.4023736546 0.770150578 0.0091769164

C -2.9992150512 -1.0705608232 -0.0428218947

C -1.9366462725 -2.0140944873 -0.0640394194

C -2.7354289685 0.2779666425 -0.0061559612

C -0.6585905285 -1.5404349534 -0.0625594066

H 0.4460384116 3.6278869921 0.1708380276

H 2.2987087605 1.996593219 0.1043600954

H -1.9021513739 2.8731550508 0.108154516

H -4.0249270525 -1.4240753041 -0.0522749022

H -2.1537142959 -3.0767363779 -0.0852087562

H -3.552300534 0.9916412913 0.0168722651

C 3.2450206285 -0.4793382251 -0.8393629914

C 2.1182037148 -0.7296078538 -0.1535671386

H 4.0157885844 -1.2343519745 -0.9435295585

H 3.4233137306 0.4761059253 -1.3182387583

C 1.8178638886 -2.0689436584 0.41636178

H 1.7401920961 -2.0924820645 1.5051281256

H 2.4178326838 -2.8890396348 0.0253129941

H 0.5944940864 -2.2244329698 0.0863437045

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 1546.5932

WellDepth[kcal/mol] 7.57

WellDepth[kcal/mol] 32.23

End

Frequencies[1/cm] 65

91.9233 127.1667

176.5707 208.3510 283.8831

351.9265 397.5545 405.7644

463.4072 475.3999 496.6039

508.5375	549.6622	565.4009
588.6311	626.6960	637.9787
718.3839	726.3157	760.4659
786.6744	805.4182	832.4306
870.5335	896.2646	908.3704
925.9550	946.6200	976.1335
987.9089	1015.7012	1047.5989
1058.0831	1073.1203	1088.4866
1165.3315	1174.5001	1212.5955
1217.5962	1238.7022	1302.6665
1317.0487	1358.7184	1373.0926
1400.9795	1429.5776	1455.4412
1459.8232	1467.5657	1513.8395
1564.9151	1593.5657	1629.4450
1650.8943	1660.3468	3062.9622
3138.2760	3145.6685	3154.7455
3159.4783	3165.6074	3173.8271
3178.7223	3187.2570	3222.7124

ZeroEnergy[kcal/mol] -28.36

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts8-9-----

Barrier ts8-9 i8 i9

RRHO

Geometry[angstrom] 24

C	-0.2343235937	-0.2474583139	0.0448693616
C	1.1826828393	0.1442193298	0.1163855599
C	0.5076585572	2.4957394436	-0.1213783103
C	1.5043645592	1.53400043	-0.0539681774
C	-0.8359252466	2.1452363342	-0.0739768852
C	-1.2276261399	0.7751243809	-0.0110990405
C	3.0168015688	-1.512279841	-0.7432689316
C	2.2555475344	-0.8631549003	0.1215448833
C	2.0829951683	-0.6342795311	1.5399233957
C	-2.9642782811	-0.9326540462	-0.0284734355
C	-1.9820984945	-1.9354866262	3.20617E-4
C	-2.5912135544	0.3952694591	-0.038945613
C	-0.640461488	-1.5923326039	0.0319517043
H	0.7865111118	3.5393140255	-0.2210846892
H	2.5490250396	1.8190730792	-0.0998651538
H	-1.6051084845	2.9077042024	-0.1195443838

```

H  3.8002072258  -2.1823375242  -0.4055106436
H  2.8753862851  -1.3950813802  -1.8117766945
H  1.3918510569  -1.2339089866  2.1181506096
H  2.7478572996  0.0327166295  2.0758984732
H  -4.01408714  -1.2030111816  -0.0514556145
H  -2.2725352783  -2.9799110948  -0.0079757336
H  -3.3455727778  1.1744326208  -0.075805202
H  0.1131952326  -2.3717519052  0.0410029039

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Core RigidRotor
SymmetryFactor 0.5
End

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Tunneling      Eckart
ImaginaryFrequency[1/cm] 527.5157
WellDepth[kcal/mol] 32.6
WellDepth[kcal/mol] 2.42

```

```

End
Frequencies[1/cm] 65
83.8037          87.9406
156.8416        191.3936      212.4967
293.5545        364.3537      387.2803
436.5984        473.1645      495.7832
499.1882        519.4853      562.0430
605.4042        647.8815      694.4712
715.1016        725.8550      761.7327
773.7603        802.8424      807.0948
831.6882        865.2739      882.0326
931.8923        958.0647      960.3596
962.1068        989.0570     1017.6192
1025.2346       1052.4578     1094.3964
1129.1472       1154.9949     1176.4612
1183.6363       1212.8615     1234.1721
1287.9674       1325.2809     1344.8315
1390.5692       1423.7171     1458.5931
1462.8509       1464.9851     1522.1713
1548.4294       1587.2459     1636.6569
1800.3540       3128.6502     3131.6025
3157.4601       3160.3729     3166.7806
3175.7366       3177.3689     3185.9360
3188.3226       3218.4461     3233.0557

```

```

ZeroEnergy[kcal/mol] -27.99
ElectronicLevels[1/cm] 1
0 2
End

```

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!-----
!-----bar_ts9-10-----
Barrier      ts9-10  i9  i10
RRHO
Geometry[angstrom]  24
C  0.3813595401  -0.1625442929  -0.3045860264
C  -0.9221762555  0.4871285395  -0.4069860656
C  0.1122199133  2.6189152021  0.2172810774
C  -0.9995152681  1.8878751263  -0.1936465416
C  1.3434618027  2.0090272435  0.384505822
C  1.5040359823  0.6203932166  0.1113554841
C  -2.7757566494  -0.8437846506  1.6445792787
C  -2.2979143751  -0.4602055329  0.493437405
C  -2.147995194  -0.2527617192  -0.9189616271
C  2.9363201705  -1.3421608339  -0.0692675833
C  1.8328854149  -2.1102345575  -0.4793093691
C  2.7701757732  -0.0060955914  0.2206721815
C  0.584465069  -1.5277750678  -0.5907527818
H  0.0096783338  3.6848024994  0.3903461858
H  -1.9532814052  2.3846563074  -0.3337123763
H  2.2065861406  2.5837996556  0.7003773303
H  -2.2896402491  -0.59440594  2.5857203259
H  -3.6896574509  -1.4404616725  1.7200574481
H  -1.9562761285  -1.1294204578  -1.5390383108
H  -2.887510595  0.396543187  -1.392472632
H  3.9140082266  -1.8024322999  0.0198669964
H  1.9587987763  -3.163303272  -0.7038647478
H  3.6172056816  0.5937271794  0.5373685364
H  -0.2536402542  -2.1474222684  -0.8851210096
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  554.0274
WellDepth[kcal/mol]  13.42
WellDepth[kcal/mol]  20.17
End
Frequencies[1/cm]  65
66.7900          72.2580
143.5806         177.5793         235.6246
265.1868         326.2018         393.8315
419.0436         460.5338         480.2076
487.5819         509.3165         522.3780

```

561.2409	614.7866	698.2004
719.8195	768.9232	781.7030
800.2420	829.2506	855.5641
873.4457	905.3043	919.8081
931.9982	948.7144	959.4926
984.8778	1003.0798	1034.2985
1061.3482	1092.8397	1117.8189
1161.0717	1176.7441	1186.4041
1195.5724	1217.6068	1237.8866
1290.7419	1350.9133	1357.9356
1405.3306	1432.9317	1460.4835
1468.2415	1475.5719	1530.8640
1566.5219	1589.0399	1642.7188
1816.9615	3029.7562	3042.9735
3102.4365	3124.1631	3156.9564
3158.4818	3168.3768	3170.6086
3180.5063	3183.4255	3191.9733

ZeroEnergy[kcal/mol] -16.99

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts10-11-----

Barrier ts10-11 i10 i11

RRHO

Geometry[angstrom] 24

C	0.2347665409	-0.2262891961	-0.2946780018
C	-1.027216237	0.3962883076	-0.5059845728
C	-0.0980972527	2.5815101413	0.0924330575
C	-1.1486279502	1.7459608134	-0.3102537539
C	1.1332673466	2.0002808114	0.3030074374
C	1.3310638548	0.6032051174	0.118437322
C	2.7785118216	-1.3512714457	0.1530065705
C	1.6981511913	-2.1660483424	-0.2536579851
C	2.5966675096	-0.001270828	0.3336787604
C	0.4569465119	-1.6166131268	-0.472018971
H	-0.2419066253	3.6467372668	0.2349176546
H	1.9775056443	2.6070201353	0.6157749188
H	3.7525254567	-1.7963966331	0.3220203986
H	1.8523594402	-3.230209866	-0.3933580509
H	3.4260443358	0.6249845301	0.6459959151
H	-0.3673025869	-2.2480805409	-0.7839239776
C	-4.5879613441	0.9869901539	-1.2971710123

```

C  -3.3117528571   0.8693460469  -0.9979463219
C  -2.322861548   -0.2652045645  -0.9407810705
H  -5.098406967   1.9445704586  -1.2643719135
H  -5.1921356609   0.1277845541  -1.5920552563
H  -2.6438119367  -1.0376801246  -0.2307712943
H  -2.2220832077  -0.7550566839  -1.9173738907
H  -2.4860734803   1.8615850151  -0.6253309625
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  1833.0551
WellDepth[kcal/mol]  24.03
WellDepth[kcal/mol]  18.85
End
Frequencies[1/cm]  65
50.9686          132.0657
165.0610         165.8899         230.6505
270.2842         299.7142         402.2211
413.4286         477.7128         486.0750
507.4578         525.3486         562.0049
569.3533         636.6257         641.0730
746.2028         748.0058         783.6219
810.0418         812.3970         867.3448
876.4532         902.4877         910.7373
955.5949         957.1595         971.2516
995.6617         1029.5780        1045.8982
1052.8331        1093.5681        1137.8956
1163.1177        1168.3030        1178.4497
1196.5920        1228.9233        1260.0945
1289.7426        1365.2701        1390.4807
1399.5570        1424.2806        1459.1406
1462.8010        1473.0831        1541.0193
1600.7317        1613.8429        1658.7002
1727.2821        1745.4615        3003.7837
3028.6754        3075.0453        3153.5676
3158.5476        3166.1206        3169.2225
3176.1923        3178.3035        3188.8393
ZeroEnergy[kcal/mol]  -13.13
ElectronicLevels[1/cm]  1
0  2
End
!-----

```


!-----bar_ts11-12-----

Barrier ts11-12 i11 i12

RRHO

Geometry[angstrom] 24

C	1.5731967121	0.7393682913	0.0343768815
C	3.0873832812	0.5254960066	0.0672469418
C	3.2858994963	-0.918112022	-0.3129234979
C	2.5070072885	-1.8500763997	0.3053898789
C	0.7892339261	-0.3777623067	-0.0120221203
C	-0.608268829	-0.38016287	-0.0390181819
C	-1.2484692568	0.8409717418	-0.0320360623
C	-0.5086500528	2.0535465467	0.0180636171
C	0.926235513	2.0134803235	0.0578236672
H	3.6046091396	1.1966251731	-0.6231574781
H	3.4751767169	0.7473486036	1.0712315667
H	3.7580311199	-1.1464207115	-1.2627364524
H	2.1876014597	-1.725886996	1.334160279
H	2.4185089874	-2.8560121247	-0.0917512877
C	-0.4392407239	4.4842041537	0.0952623118
C	0.972213183	4.4449337179	0.1403512983
C	-1.1582383314	3.3152771713	0.0357695203
C	1.6367291839	3.2414121094	0.1219691808
H	-0.9515358577	5.4395809183	0.1089276036
H	1.532973978	5.3718173714	0.1896416775
H	-2.2426651082	3.3412914691	0.0032065456
H	2.7195731928	3.2258180831	0.1590201058
H	-1.1745220088	-1.3048386035	-0.0705441186
H	-2.33275101	0.8916563534	-0.0631638767

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 430.6211

WellDepth[kcal/mol] 10.51

WellDepth[kcal/mol] 44.82

End

Frequencies[1/cm] 65

76.2656	126.0891	
191.8347	214.9594	220.0327
282.7316	414.2004	437.2419
444.2483	478.5834	491.9855
519.0362	536.4077	594.0266
627.0391	671.2436	742.4772

747.4524	779.1685	781.5584
807.8639	860.7825	872.4651
898.2019	919.6443	938.7477
952.2561	958.5119	967.0725
993.8520	1015.5241	1046.7745
1085.3975	1121.8683	1161.7864
1178.5042	1184.3502	1200.7156
1229.1145	1268.7050	1283.5513
1298.7740	1354.7271	1383.9578
1397.8017	1424.9884	1452.2609
1465.2323	1483.9789	1534.1954
1568.4587	1593.9945	1615.4399
1656.6957	2991.5055	3066.7773
3126.5677	3149.7292	3157.8216
3161.5619	3166.3667	3169.7498
3180.5622	3189.8157	3206.7585

ZeroEnergy[kcal/mol] -21.47

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts10-13-----

Barrier ts10-13 i10 i13

RRHO

Geometry[angstrom] 24

C	0.2276865416	-0.1368191378	-0.1011589787
C	-0.8583758916	0.7819681878	-0.2274376871
C	0.7293658056	2.6174575637	-0.0657581646
C	-0.5900047632	2.1324199041	-0.21678688
C	1.784806276	1.7501530865	0.0764757615
C	1.5667290022	0.3492729756	0.0598896058
C	-2.2899461786	0.2653610479	-0.3077824605
C	-3.2980605992	-1.7584695429	-1.5365353711
C	-2.396202337	-1.1417723175	-0.7976044712
C	2.3709903771	-1.9500383216	0.1478715783
C	1.0494038582	-2.438461719	-0.0308763438
C	2.6177381968	-0.5979860418	0.1871673195
C	0.036001791	-1.531888074	-0.1425074456
H	0.9021492384	3.687943093	-0.0611467723
H	-1.4051772424	2.8418993133	-0.3189985382
H	2.795553502	2.125645375	0.1972790358
H	-2.7169829561	0.3090913729	0.7048239037
H	-2.8941121155	0.9387202402	-0.9273401736

```

H -4.1834157373 -1.2419240906 -1.9095687424
H -3.2033731062 -2.8060640377 -1.8037869775
H 3.1901214702 -2.6546974448 0.2459192581
H 0.8669973098 -3.5066651246 -0.0786049586
H 3.6320636048 -0.2338393267 0.3129826091
H -1.2867890467 -1.7281069809 -0.4345301068
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1612.9218
WellDepth[kcal/mol] 17.14
WellDepth[kcal/mol] 12.69
End
Frequencies[1/cm] 65
64.0491 121.4037
167.2366 214.2931 237.1582
263.3501 361.5032 405.2792
431.7413 450.6593 468.7786
501.7915 549.4655 567.6019
571.3980 627.6223 634.2803
739.9182 754.3754 778.8162
806.8934 816.8009 879.5719
887.5257 908.8948 913.2310
931.5828 945.6762 975.8842
985.3594 1028.9105 1061.5163
1084.7478 1106.1838 1126.3204
1166.9548 1188.0727 1210.8467
1219.7882 1238.8482 1253.1837
1292.2772 1365.3427 1375.0004
1401.7320 1431.9973 1451.0381
1456.4723 1477.8489 1517.3203
1588.3498 1603.1943 1635.1404
1655.8295 1720.0860 2981.3017
3028.0518 3077.1092 3154.0513
3154.3779 3162.4304 3165.6962
3173.4882 3177.9762 3181.9837
ZeroEnergy[kcal/mol] -20.02
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts13-14-----

```

Barrier ts13-14 i13 i14

RRHO

Geometry[angstrom] 24

C	-0.0085582509	-0.0313097756	0.0936804925
C	0.7122419613	1.2067109396	0.1341886638
C	-1.3870138455	2.4152899397	-0.1253502284
C	0.018841552	2.3906223259	0.0129703445
C	-2.1021917764	1.2449815294	-0.1476289278
C	-1.4418250703	-0.0062930049	-0.0438608633
C	2.2238591442	1.217940462	0.3476724272
C	2.9572791977	-1.1280854198	0.0641812957
C	2.8793797084	0.1220698329	-0.4392269466
C	-1.5076563667	-2.4415306314	0.0177158884
C	-0.0924629071	-2.483534609	0.1410502425
C	-2.1558615408	-1.2344431304	-0.0751524597
C	0.5867731252	-1.3056462162	0.1762009779
H	-1.896712834	3.3684772914	-0.2117944867
H	0.5636526829	3.329091558	0.0338437339
H	-3.182561488	1.2596185125	-0.2485134282
H	2.6119455021	2.203160822	0.0757059999
H	2.4289349892	1.0718224708	1.4155084075
H	2.8932608705	-1.3065974772	1.1315322983
H	3.2815336755	-1.965056277	-0.544211557
H	3.043285813	0.2925319525	-1.4995169849
H	-2.0707456688	-3.3688572849	-0.0090602278
H	0.4176956809	-3.4399455996	0.2013172511
H	-3.2354561544	-1.2012842108	-0.177495913

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 307.9882

WellDepth[kcal/mol] 5.43

WellDepth[kcal/mol] 40.31

End

Frequencies[1/cm] 65

86.2408	127.1758	
171.8267	237.8031	257.8402
330.1055	407.6493	440.0152
454.4478	469.3721	483.6747
515.7923	558.8908	578.4343
623.4799	644.7406	741.6489
755.3921	776.1504	801.3225

816.6011	854.9871	882.9753
902.1229	923.6859	936.4560
956.1878	971.4011	973.7813
983.6439	1022.0629	1055.3707
1090.3419	1109.3951	1161.5448
1184.8730	1199.0582	1231.1661
1244.1374	1256.9500	1292.1740
1301.5092	1358.4898	1374.5380
1387.5333	1435.3263	1455.0553
1467.6640	1482.3781	1513.0873
1588.8843	1608.9243	1634.9399
1650.2733	3008.7264	3067.8606
3132.3336	3146.7346	3150.1920
3154.0850	3158.1474	3161.5179
3175.0032	3181.4977	3217.1804

ZeroEnergy[kcal/mol] -27.28

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts15-16-----

Barrier ts15-16 i15 i16

RRHO

Geometry[angstrom] 24

C	0.5554711997	-0.3337005282	-0.0664577434
C	-0.8875260392	-0.0846260171	-0.1254075513
C	-0.4251604613	2.3306542306	-0.0223778563
C	-1.3211570578	1.2649731139	-0.0946789254
C	0.9368101785	2.1055030195	0.0268519162
C	1.4506861036	0.7784420515	0.0081203838
C	-1.8211690958	-1.1244910167	-0.2136520239
C	3.3570707277	-0.733149371	0.0494181295
C	2.4793686903	-1.8301244223	-0.0211008194
C	2.8474083058	0.5442233742	0.0637767881
C	1.1148894193	-1.6297234311	-0.0775159027
H	-0.8068873087	3.3456577371	-0.0044307882
H	-2.3852023106	1.4631583644	-0.1244400887
H	1.6330714372	2.9350016354	0.0830074726
H	-1.4730172186	-2.1501982971	-0.2649217473
H	4.4279763584	-0.8962789065	0.0930173814
H	2.8755932625	-2.8392701543	-0.0308971088
H	3.5130209686	1.3993830645	0.1192067277
H	0.4681509175	-2.4959165061	-0.1287575579

```

C -4.1403613334 -0.9253340279 0.6875192537
C -3.2825449743 -0.9397766717 -0.3307945015
H -5.2068555759 -0.8142361403 0.5240567266
H -3.8052514531 -1.0243434202 1.7148241701
H -3.6782997405 -0.8391416807 -1.3441943347
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 178.3067
WellDepth[kcal/mol] 8.8
WellDepth[kcal/mol] 5.89
End
Frequencies[1/cm] 65
70.0450 86.4537
161.7942 182.6467 231.8001
277.5198 399.5872 417.7644
448.7769 473.8670 489.4586
520.9606 529.4487 563.7424
623.5875 675.1314 695.5232
733.9795 779.2380 788.1655
801.3506 807.3677 869.2729
878.1920 888.0023 954.8812
957.5465 967.4235 976.5757
990.6159 1013.3486 1049.2723
1062.9121 1106.8866 1122.8839
1160.1980 1180.3261 1192.2259
1222.9197 1258.4767 1274.9988
1315.3575 1327.2311 1366.1326
1396.3965 1434.4340 1461.4595
1475.8556 1477.5601 1528.9563
1572.4719 1594.6614 1648.8104
1686.6048 3070.8139 3128.6306
3158.6536 3162.0999 3162.2558
3170.2973 3178.2366 3184.8418
3193.6998 3199.7146 3212.9798
ZeroEnergy[kcal/mol] -55.28
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts16-17-----
Barrier ts16-17 i16 i17

```

RRHO

Geometry[angstrom] 24
C -0.2504511843 -0.326586861 0.5146476007
C 1.1294051074 -0.3705697921 0.1873108387
C 1.0988825107 2.0469859584 -0.2957189866
C 1.824424441 0.8126869892 -0.2047701493
C -0.2315972034 2.0904867783 0.0017991766
C -0.9429635911 0.9300248124 0.4381806123
C 1.8935961184 -1.5826154192 -0.109330575
C 2.6169709281 -0.19383494 -1.9476385141
C 2.6796539034 -1.464704157 -1.1977473599
C -2.9978626142 -0.1452728785 1.1656265232
C -2.3275197996 -1.3855766839 1.2232892629
C -2.3124680287 0.9855084176 0.7736751341
C -0.9936862465 -1.4772770258 0.8986438908
H 1.6285374209 2.9532019281 -0.5678737873
H 2.8806142659 0.8787221043 0.0335268384
H -0.7713845545 3.0307601115 -0.0547509197
H 1.8027397495 -2.5027625925 0.455660528
H 3.544023444 0.2513386716 -2.3006092182
H 1.7754838237 -0.0580379538 -2.6234309039
H 3.3332093172 -2.2722073863 -1.5204133512
H -4.0491977628 -0.0860687971 1.4224094465
H -2.8709678378 -2.2748891377 1.5231680301
H -2.8245206807 1.9406363888 0.7127143391
H -0.4967975265 -2.4391665354 0.940753544

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 638.9894

WellDepth[kcal/mol] 29.89

WellDepth[kcal/mol] 29.26

End

Frequencies[1/cm] 65

87.1305	118.1877	
188.7124	221.0112	247.1189
361.7480	430.8089	453.6761
465.4662	477.0079	487.3062
550.2862	555.5941	565.9527
652.6072	680.3497	723.9664
741.1664	755.5491	788.0304
790.3671	814.6247	844.1904

868.7334	878.4520	919.1932
950.4209	961.4855	976.4356
985.1273	1009.3608	1040.3130
1054.5038	1062.6004	1097.1515
1152.3983	1158.5208	1178.9352
1187.0448	1219.4395	1234.8126
1287.0703	1356.7609	1368.5685
1384.4543	1424.1980	1449.3518
1452.2211	1477.2910	1527.7850
1557.8524	1605.0039	1617.3051
1636.6673	3091.6994	3127.9531
3136.7910	3154.1144	3157.4472
3165.1164	3173.4710	3178.1989
3180.0678	3186.3668	3191.6573

ZeroEnergy[kcal/mol] -31.28

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts16-19-----

Barrier ts16-19 i16 i19

RRHO

Geometry[angstrom] 24

C	-0.2507039602	0.0180002894	-0.4623630246
C	0.8383192003	0.9386011455	-0.5360926765
C	-0.6512737157	2.7155770917	0.1961437115
C	0.6091291609	2.2765390893	-0.2504427427
C	-1.6699496166	1.8122717421	0.3974227895
C	-1.4905526144	0.4400366687	0.0856975756
C	2.1896150675	0.4308079296	-0.8045558689
C	1.6720977994	-1.7343400823	0.2590729872
C	2.567094073	-0.8146339919	-0.4301185239
C	-2.3151966563	-1.8552111762	-0.0041796641
C	-1.1440739052	-2.2677156129	-0.654319929
C	-2.5103589853	-0.5283830204	0.3271188658
C	-0.079963309	-1.3733388201	-0.8732913003
H	-0.8019582306	3.7651237302	0.4230710985
H	1.4285263235	2.9840229478	-0.3233005888
H	-2.6216664875	2.1373532672	0.8043133898
H	2.9032756571	1.0956322964	-1.2806125389
H	1.9013477372	-2.7949011859	0.2136052112
H	1.226813302	-1.4174105823	1.1960871212
H	3.5553436128	-1.1711691699	-0.7121286303


```

H -3.104488502 -2.5762304224 0.1803155674
H -1.0660485626 -3.2838055346 -1.0250380378
H -3.446234987 -0.2032340171 0.7681248294
H 0.5611565987 -1.5613975821 -1.7264466213
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 688.5853
WellDepth[kcal/mol] 22.63
WellDepth[kcal/mol] 27.59
End
Frequencies[1/cm] 65
135.8869 141.3535
185.9715 243.0352 310.8670
361.0165 412.7008 457.6790
469.1912 490.3113 504.6763
558.2994 567.7446 630.6723
639.0723 687.9795 705.0774
729.2566 766.4812 771.3669
800.5419 811.6540 843.7867
866.4548 895.8233 911.3173
944.5004 970.1342 980.1015
988.8157 1007.8306 1036.3488
1065.9161 1089.8702 1106.2390
1148.3335 1177.0570 1187.3347
1208.3370 1220.2956 1239.6934
1262.6145 1353.7025 1372.2863
1396.9944 1413.7495 1443.6882
1469.0565 1479.5661 1515.5788
1577.4307 1586.5189 1600.9472
1638.4690 3112.6181 3125.6165
3147.4975 3157.3305 3158.6564
3163.1880 3166.5872 3171.4042
3182.1083 3183.7341 3196.5064
ZeroEnergy[kcal/mol] -38.54
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts21-22-----
Barrier ts21-22 i21 i22
RRHO

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```

Geometry[angstrom] 24
C -0.4669755963 -3.701610993 -0.7560042591
C -0.364658677 -2.2380042685 -0.4431040042
C -1.3640496721 -1.2537253662 -0.5628174146
C -0.7973304566 0.0406128192 -0.3653411155
C -1.3009585392 1.3643330878 -0.3403581275
C -0.406241838 2.4127602614 -0.1124781808
C 0.9648263413 2.2136192807 0.09387206
C 0.5781252599 -0.1335175259 -0.1138547409
C 1.5019984483 0.9014135934 0.0965529322
C 2.8641641787 0.5110653771 0.2370575235
C 3.2280388973 -0.8394577274 0.1267637061
C 0.9207842022 -1.5223831006 -0.1299950314
C 2.3127304635 -1.8690650968 -0.0792158496
H 0.198005059 -4.3009096379 -0.1285987292
H -1.4855089415 -4.067114074 -0.6094754263
H -0.1863958334 -3.8883830579 -1.7983647747
H -2.4088271522 -1.4741510029 -0.7347272831
H -2.3519040625 1.5708474573 -0.5082078687
H -0.787265167 3.4286581874 -0.1052444201
H 1.6171206965 3.0672972954 0.242300734
H 3.6295614802 1.261909983 0.3975647804
H 4.2802344038 -1.0959708939 0.193772702
H 0.2199655632 -2.0546391529 0.8068349307
H 2.6464559421 -2.8960414448 -0.1663301432

```

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 1321.6917

WellDepth[kcal/mol] 19.62

WellDepth[kcal/mol] 36.74

End

Frequencies[1/cm] 65

```

129.3272          152.6303
186.2525          207.1028          228.3477
294.3726          384.5954          412.2917
487.4940          492.2843          521.1271
543.3617          563.8827          588.3376
620.0803          664.1652          683.2639
724.3769          742.1932          783.9967
788.9082          813.0639          826.0473
830.9283          867.1503          954.1646

```

957.1588	967.8940	1013.5285
1053.7376	1057.0375	1073.3256
1097.4201	1134.5796	1153.4463
1170.3095	1186.1486	1202.6743
1237.2615	1285.0202	1320.0586
1358.2714	1375.4241	1396.4872
1422.2314	1446.8197	1460.6445
1483.1567	1490.1960	1509.1882
1515.3927	1541.8323	1577.5859
1618.5504	1910.4369	3020.3598
3074.3564	3101.6903	3157.2610
3158.7205	3172.4807	3177.4032
3182.9537	3187.4991	3207.9837

ZeroEnergy[kcal/mol] -39.65

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts14-p1-----

Barrier ts14-p1 i14 p1

RRHO

Geometry[angstrom] 24

C	-0.0633239864	0.0011982866	0.0475940345
C	0.6354222909	1.2415683388	0.0320952331
C	-1.4910121067	2.4143721182	-0.0938669567
C	-0.083454048	2.4184258167	-0.0353308166
C	-2.1838336617	1.227416816	-0.0780496278
C	-1.4921025928	-0.0061103217	-0.0042810531
C	2.1508318985	1.2713800704	0.0871729332
C	2.1040697552	-1.226165482	0.1974829814
C	2.7961111871	-0.0660522168	0.2726262744
C	-1.4810653956	-2.4322994519	0.0995798982
C	-0.0704999792	-2.4276580534	0.1524851239
C	-2.1765794633	-1.252130742	0.0215199557
C	0.6380732665	-1.2441267028	0.1258599353
H	-2.025193034	3.3564597626	-0.1481553979
H	0.4444698481	3.3672043936	-0.0429499113
H	-3.2677929119	1.2200903054	-0.1200801506
H	2.539872688	1.72343872	-0.8384739367
H	2.4794481366	1.949054969	0.8862416868
H	2.6032854961	-2.1668361833	0.4027675117
H	3.8728443929	-0.086140795	0.4046431939
H	-2.0120784395	-3.3773574274	0.1200799783

```

H 0.4666997481 -3.3685923269 0.2085011021
H -3.2605685526 -1.2526300658 -0.0208715052
H 2.4957754636 -1.7021548282 -1.6753144868
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 654.3176
WellDepth[kcal/mol] 31.32
WellDepth[kcal/mol] 4.59
End
Frequencies[1/cm] 65
77.7429 155.9644
198.1064 233.7055 257.4250
360.2480 402.2492 432.1628
439.3368 474.0601 476.7943
478.4899 519.8273 577.5389
594.6595 607.5869 655.2759
735.6529 764.1114 778.1287
792.9817 815.1477 823.4318
842.9291 899.3350 915.9988
951.4987 962.5704 979.9930
987.3014 1005.3515 1047.2960
1064.5692 1102.4606 1118.2720
1173.2163 1193.5163 1199.9750
1219.1200 1234.1637 1252.8575
1267.6933 1333.7497 1384.2505
1397.0186 1418.5977 1421.6223
1452.5798 1467.2531 1497.4050
1541.1712 1609.8521 1625.3637
1637.3509 1666.0553 2966.7481
3003.8122 3152.0865 3156.9158
3159.1933 3163.5131 3167.4729
3174.7765 3181.8740 3184.8758
ZeroEnergy[kcal/mol] -36.27
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts19-p1-----
Barrier ts19-p1 i19 p1
RRHO
Geometry[angstrom] 24

```

C	-0.0600934276	-0.0174735345	0.0518734566
C	-0.3769357849	1.374639625	0.0311127042
C	-2.743538218	0.8144064086	0.0243139557
C	-1.7045859051	1.7669342216	0.0197339062
C	-2.4569720293	-0.5293962913	0.0263373068
C	-1.1097725428	-0.9810922141	0.033550237
C	0.7143267301	2.3437945619	-0.0200189424
C	2.4104737639	0.5549284235	0.3125314137
C	1.9973223002	1.9804433174	0.0834334294
C	0.539697061	-2.7663281199	0.0550856968
C	1.576756005	-1.8228697483	0.0792932656
C	-0.7772440932	-2.3601445397	0.0301536221
C	1.3084298328	-0.453094308	0.0332110393
H	-3.7745798994	1.1499179892	0.0171181651
H	-1.9465417219	2.8243674824	-2.592871E-4
H	-3.2552227202	-1.263826085	0.0188919633
H	0.4491304755	3.3884551963	-0.1498992824
H	3.3015553587	0.3138268448	-0.2743769678
H	2.7155578341	0.4487798055	1.3658468218
H	2.7826942036	2.7284083657	0.0474992951
H	0.7807730633	-3.8234677302	0.0643254589
H	2.6080013049	-2.1586547869	0.1125955078
H	-1.5775064875	-3.0923162562	0.0180927538
H	1.4968378966	-0.2568276279	-1.8785255192

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 721.9896

WellDepth[kcal/mol] 30.54

WellDepth[kcal/mol] 5.27

End

Frequencies[1/cm] 65

113.9477	156.4338	
202.2847	239.7456	372.9049
387.4188	415.7992	425.8074
450.6250	476.5690	483.0602
503.7095	509.2932	573.3572
596.0444	613.1110	645.7605
729.0293	761.3059	779.4538
788.8410	815.9835	822.4566
846.2760	895.6429	913.7229
955.9012	959.5731	979.7623

985.8237	997.0472	1048.4061
1066.3522	1104.3991	1122.1488
1175.7537	1193.0175	1204.0232
1217.5079	1229.0593	1251.9467
1267.3358	1331.2121	1381.5721
1390.8294	1410.1336	1424.3944
1461.3140	1465.1456	1487.8280
1535.2097	1605.6250	1616.8584
1636.7616	1699.3217	2961.6450
3050.8807	3150.7025	3158.1255
3159.2497	3166.1013	3168.1987
3172.3959	3183.2037	3184.7577

ZeroEnergy[kcal/mol] -35.59

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts12-p2-----

Barrier ts12-p2 i12 p2

RRHO

Geometry[angstrom] 24

C	-1.010282092	2.0058058373	-0.0457078139
C	-1.631988179	0.7469614412	0.0278370486
C	0.5370052173	-0.3862457896	0.0672678421
C	-0.8833740316	-0.4213140832	0.0855424869
C	1.1655400551	0.9012081522	-0.0010847807
C	0.3646477745	2.0744814579	-0.0565369427
C	-3.100341405	0.4005773588	0.0604700451
C	-1.8094401942	-1.5638077869	0.1491350655
C	-3.0869152013	-1.0983933583	0.1833029486
C	2.7232350207	-1.4438801175	0.0900224226
C	3.3454007186	-0.1760612918	0.0293783262
C	1.3526103652	-1.5454766794	0.1083049247
C	2.5834554701	0.9659543857	-0.0158623113
H	-1.6049386933	2.9122416263	-0.0901424898
H	0.8618007313	3.0373264661	-0.1089773222
H	-3.6240750117	0.8754577253	0.9001385685
H	-3.6203950271	0.7292562801	-0.850031292
H	-1.516940653	-2.5876792857	0.3349157806
H	-1.6848304688	-2.2060767569	-1.7564388697
H	-3.9795911463	-1.7039685769	0.2592689758
H	3.3336633179	-2.3394579301	0.1203413484
H	4.4274800622	-0.1094053724	0.0162535667

```

H 0.8840637682 -2.5219185658 0.1493675803
H 3.0593896019 1.9399188638 -0.0660121082
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 586.3837
WellDepth[kcal/mol] 33.77
WellDepth[kcal/mol] 3.96
End
Frequencies[1/cm] 65
112.3577 129.5063
220.1278 236.9661 257.1050
277.2873 325.6929 411.5057
432.8427 459.7626 465.0112
506.8749 520.0614 573.5601
612.4584 680.1111 681.7438
715.7034 749.0580 752.7241
795.8303 818.3469 838.5436
878.6747 881.4479 931.3597
955.4761 958.4054 964.1298
968.9099 971.0319 994.0632
1044.3349 1071.3736 1118.2310
1141.5153 1167.5446 1178.7616
1190.5546 1216.4718 1236.7107
1283.2014 1295.0506 1351.1799
1378.1811 1391.3769 1426.5539
1430.1135 1469.1562 1486.5530
1534.1178 1559.4663 1606.6464
1630.8977 1665.1776 3005.2631
3029.5507 3156.8165 3158.7557
3166.8129 3175.6793 3179.5578
3189.4202 3204.2843 3222.7327
ZeroEnergy[kcal/mol] -32.52
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts17-p2-----
Barrier ts17-p2 i17 p2
RRHO
Geometry[angstrom] 24
C -0.5561474778 -0.4019702496 0.0025529198

```

C	0.8616160091	-0.4996742827	0.0030965122
C	1.0807770774	1.9419054508	-0.0590289665
C	1.6649861946	0.6530355615	0.0561873677
C	-0.2838614868	2.0577425177	-0.0830675805
C	-1.1319258617	0.9113793989	-0.0325388803
C	1.7367799817	-1.6648227637	-0.0658740081
C	3.1104251811	0.2377641315	-0.1349828799
C	3.0218781382	-1.2660410179	-0.1320312758
C	-3.3533813084	-0.0769684086	-0.0161561656
C	-2.7851599281	-1.3692876533	0.0119276572
C	-2.5430781562	1.0345273777	-0.0395183665
C	-1.4188658633	-1.5269266759	0.0185972128
H	1.7112020163	2.8237367234	-0.0932258704
H	-0.7466058838	3.0371288215	-0.1424322493
H	1.3995320219	-2.6927083253	-0.0691049124
H	3.7874954055	0.6279818047	0.6300731319
H	3.4825740189	0.602265051	-1.1026942759
H	3.8864417149	-1.9137899466	-0.1889421224
H	-4.4316515397	0.0358812165	-0.0204457732
H	-3.4315844058	-2.2395147415	0.0304107135
H	-2.9789429034	2.0279557598	-0.0639863919
H	-0.9910599616	-2.5224518711	0.0440398481
H	1.8032910169	0.6888871213	1.9727033556

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 702.9684

WellDepth[kcal/mol] 29.37

WellDepth[kcal/mol] 5.31

End

Frequencies[1/cm] 65

111.0437	128.7695	
224.3494	241.8118	274.3638
370.0890	401.9669	422.8161
441.9605	458.8567	504.7338
515.1000	521.2554	567.5127
611.3282	674.3077	684.2630
726.0641	748.9940	752.3363
801.3682	815.6097	840.6904
879.1104	881.2481	932.1632
952.0595	954.6435	959.7125
966.9878	971.0966	993.3931

1045.5647	1076.6118	1126.2267
1144.7269	1168.1011	1177.8986
1192.3943	1211.6341	1234.0192
1284.4908	1286.4325	1353.0052
1372.6451	1385.3220	1430.7513
1435.4219	1467.9125	1475.0613
1544.8633	1567.5875	1611.2070
1625.8175	1654.9415	3007.8916
3067.7580	3158.1861	3160.9656
3167.2543	3178.5258	3179.7087
3189.4376	3197.2353	3218.5505

ZeroEnergy[kcal/mol] -31.17

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts12-p3-----

Barrier ts12-p3 i12 p3

RRHO

Geometry[angstrom] 24

C	0.2003578984	-1.3234899668	0.136586655
C	1.4365421729	-0.6405377373	0.1382952226
C	0.3117157251	1.5227823086	0.0091383506
C	1.4910471609	0.744908703	0.0769664475
C	-0.9444560277	0.8272974254	0.0108376283
C	-0.9616660409	-0.5936215939	0.0762809094
C	2.8114396447	-1.164291235	0.1882705451
C	2.9359723366	1.1835303956	0.0972011125
C	3.6808114085	-0.1202680357	0.2140317415
C	-0.8736010771	3.6406916603	-0.1205880972
C	-2.1115934464	2.9569993091	-0.1185404464
C	0.307290221	2.9414983542	-0.0579673274
C	-2.142258741	1.5849618059	-0.0541637426
H	0.1712759852	-2.4066401231	0.179347513
H	-1.9223616559	-1.0978963345	0.0752810747
H	3.0635780645	-2.200727516	0.3682863244
H	3.0015989967	-1.7655012927	-1.7225285686
H	3.1609382573	1.8548369618	0.9358912383
H	3.2169517918	1.7281032542	-0.8148535544
H	4.7579041462	-0.1909570867	0.2793120534
H	-0.8603989731	4.7237261563	-0.1721997829
H	-3.0361847524	3.5208865179	-0.1682701045
H	1.2523864646	3.4731765806	-0.060545173

```

H -3.0912735597  1.0585864888  -0.0528560193
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 589.7493
WellDepth[kcal/mol] 33.74
WellDepth[kcal/mol] 4.07
End
Frequencies[1/cm] 65
109.5949          136.2490
229.1342          235.9127          245.0849
272.8001          327.5149          415.3074
433.4025          456.8020          466.0928
520.4309          520.7384          559.3707
616.6653          680.9680          682.6272
714.6219          751.3348          759.5826
787.1020          827.9301          837.1024
870.3640          873.6152          934.1113
956.0219          958.5093          969.0526
972.1631          981.2720          993.1048
1044.0550         1059.1820         1110.1578
1143.6833         1167.3814         1179.3699
1185.0116         1232.9099         1241.4073
1266.3998         1288.5925         1361.1544
1377.9750         1397.9458         1415.9543
1432.6410         1467.9526         1488.4605
1535.2006         1561.8214         1611.9018
1630.6206         1663.3786         3004.8701
3029.4209         3157.2641         3160.7871
3164.7169         3177.0352         3179.4718
3188.0144         3199.0250         3219.6406
ZeroEnergy[kcal/mol] -32.55
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts2-p4-----
Barrier      ts2-p4  i2  p4
RRHO
Geometry[angstrom] 24
C -4.5390052317 -0.8030966877 1.2088351288
C -3.3033248329 -0.0830534569 0.9520765945

```

C	-2.2577195624	0.407898198	0.5613023452
C	-1.0846751629	1.2333794144	0.443326404
C	-1.2303169031	2.5863996177	0.1896150277
C	-0.1070998138	3.4301188299	0.0785020157
C	1.1604165731	2.9206485732	0.2174975872
C	0.2279592833	0.674670959	0.5908751939
C	1.3612134041	1.5403908702	0.4759177954
C	2.6621144938	0.9922907649	0.6258909583
C	2.8402757991	-0.345702983	0.8764262444
C	0.4466459083	-0.7017540546	0.8511194816
C	1.7200873632	-1.1997389549	0.9896282625
H	-4.4870531479	-1.3604217575	2.1486745126
H	-5.3901411027	-0.119039386	1.2692286679
H	-4.7396101864	-1.5194781777	0.4031419616
H	-2.0667112493	-0.5860483885	-1.0532299332
H	-2.2264647278	2.995735038	0.0744647706
H	-0.2538554153	4.4857713178	-0.1193814423
H	2.0268493094	3.5678281748	0.1312236487
H	3.5175524821	1.6539898329	0.5385550641
H	3.8395227877	-0.7512298899	0.9884234791
H	-0.4103729283	-1.3580447518	0.9375724877
H	1.8688868603	-2.2553881023	1.1871447441

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 706.1139

WellDepth[kcal/mol] 34.95

WellDepth[kcal/mol] 5.8

End

Frequencies[1/cm] 65

47.2621	71.2991	
77.9395	158.2765	160.5429
175.8722	243.7666	262.4663
354.5689	385.1569	404.1424
446.5882	478.7933	500.2188
531.7432	542.8026	587.8280
604.3266	655.6980	690.1442
747.0397	791.1077	805.6297
815.3470	833.1670	881.1620
924.9642	957.6110	967.6782
985.7296	999.3818	1037.0870
1042.5812	1055.2557	1076.3271

1119.6429	1168.7724	1182.3772
1200.9802	1237.4349	1266.4944
1301.8607	1360.7203	1392.6782
1410.0495	1425.6910	1468.1055
1470.7639	1475.1882	1492.8365
1544.3146	1613.0113	1629.5928
1661.8480	2233.5965	3009.1703
3065.0897	3083.3039	3159.0145
3162.7282	3170.3651	3178.9945
3183.9017	3193.7088	3196.3476

ZeroEnergy[kcal/mol] -4.48

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts20-p4-----

Barrier ts20-p4 i20 p4

RRHO

Geometry[angstrom] 24

C	0.4520731587	-0.1396946256	0.0489447314
C	-0.7313529035	0.6771046821	0.0908504394
C	0.653443589	2.6771367973	-0.0178134153
C	-0.6089948422	2.0599245685	0.0561191636
C	1.7978500366	1.9173188091	-0.0567929246
C	1.7288753378	0.5008599407	-0.0250094438
C	-2.0211037092	0.0856361416	0.17097991
C	-3.1293631686	-0.4097830462	0.1715293908
C	-4.4439857854	-0.9851948334	0.4465317425
C	2.8159267234	-1.6724564073	-0.0376823875
C	1.5537734265	-2.3036610244	0.0339431731
C	2.898694939	-0.3023610221	-0.0666668323
C	0.4013505912	-1.5554862665	0.0761377859
H	0.7148016262	3.7590586819	-0.0442296543
H	-1.5060427274	2.6661828817	0.0861893784
H	2.7718877237	2.3915679103	-0.113396253
H	-3.3160901902	-0.5398815694	-1.94390215
H	-4.6175625497	-1.039450619	1.5256539983
H	-4.5267045554	-1.9945444975	0.0355879922
H	-5.2384843092	-0.3801260853	0.0025126681
H	3.7172684155	-2.2740681777	-0.0705485431
H	1.4962931318	-3.3861454189	0.0546658651
H	3.8643561515	0.1890884778	-0.1228030275
H	-0.5659721101	-2.0398162975	0.1290973928

```

Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 415.8985
WellDepth[kcal/mol] 40.99
WellDepth[kcal/mol] 3.22
End
Frequencies[1/cm] 65
52.1117          71.5811
74.2595          136.6391          163.9678
177.7013         274.4205          275.0017
343.8571         378.8381          407.6289
413.8758         471.5166          480.4276
499.2670         541.0993          584.0272
590.4129         653.0752          684.6341
747.6880         790.3669          804.7850
816.1606         833.0399          882.1945
924.2946         954.6183          968.9802
986.6926         1000.4394         1042.4203
1044.2063        1060.3610         1076.4707
1119.7825        1168.8892         1181.6404
1202.2683        1237.6208         1266.9255
1308.3161        1356.5778         1390.7028
1412.8599        1426.8259         1467.7051
1475.9276        1480.3572         1491.4179
1543.0525        1609.3770         1625.2395
1660.4924        2273.6239         3025.6362
3084.5928        3091.8607         3160.1195
3163.8492        3171.0304         3179.7801
3184.0883        3194.1663         3195.4235
ZeroEnergy[kcal/mol] -7.06
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts2-p5-----
Barrier      ts2-p5  i2  p5
RRHO
Geometry[angstrom] 24
C -4.3533905647 -0.510217511 0.7115720434
C -3.0960738432 -0.6412416486 0.366557573
C -1.8514758722 -0.8399528623 0.0139571871

```

C	-0.7892730529	0.1865534873	-0.0290127347
C	-1.120637176	1.5278962867	-0.1101516262
C	-0.1357979158	2.5307868687	-0.1736809098
C	1.1955262252	2.1947722284	-0.1706891053
C	0.5963815082	-0.1907539421	-0.0062650429
C	1.5936761139	0.8371814216	-0.0888164127
C	2.9665426659	0.4751931314	-0.0791434077
C	3.3539202529	-0.8373994481	0.0177328775
C	1.0389113462	-1.5364319616	0.1089756506
C	2.3764572011	-1.8519150801	0.1176788559
H	-4.6677026442	-0.6057173723	1.7468641072
H	-5.1026304174	-0.1778603507	-0.0013047094
H	-5.1935841979	-2.47824175	0.4417353164
H	-1.5895589785	-1.8511865692	-0.2880318055
H	-2.1674352452	1.8082729112	-0.1397561491
H	-0.437895536	3.5699850032	-0.2389020697
H	1.9602030139	2.9617318777	-0.231908376
H	3.7089582875	1.2635426847	-0.1472649925
H	4.4059487231	-1.0990187375	0.0246578049
H	0.3142141633	-2.3341449402	0.2075924748
H	2.6847589428	-2.887488727	0.2074594508

Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 357.7577
WellDepth[kcal/mol] 37.23
WellDepth[kcal/mol] 2.84
End
Frequencies[1/cm] 65

36.5788	87.5914	
120.6938	166.0537	176.6909
226.0967	259.4551	262.9401
357.1700	419.0076	426.2693
432.6091	478.2649	513.7969
526.7005	543.5507	618.0513
655.6935	689.0048	744.7060
764.2745	794.1602	805.9207
814.8087	868.3656	878.9819
893.2214	902.7002	925.7164
963.5513	985.2184	996.8898
1014.0947	1017.3089	1052.4984
1096.0389	1121.7256	1169.6668

1190.1902	1195.5037	1232.9137
1264.0128	1279.5211	1336.4346
1383.1544	1392.8609	1424.7388
1461.7609	1481.0422	1495.7246
1549.7271	1613.5587	1634.3695
1662.6503	2001.0535	3109.0217
3130.5323	3159.3992	3161.9891
3169.8897	3173.6210	3181.6871
3184.6032	3186.5446	3197.9931

ZeroEnergy[kcal/mol] -2.2

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts10-p5-----

Barrier ts10-p5 i10 p5

RRHO

Geometry[angstrom] 24

C	0.5309185348	-0.2657386867	-0.0753144147
C	-0.7985186755	0.1257935313	0.2986957771
C	0.0093839876	2.3745358718	0.7769453768
C	-1.0280535418	1.4257778577	0.7093561671
C	1.2925574219	2.0214237515	0.4407146444
C	1.5850810199	0.7034241452	0.0101309446
C	-4.4453552875	-0.2995739385	0.6635403999
C	-3.1820621867	-0.5677681401	0.5261797128
C	-1.9132453141	-0.8542730711	0.2650589486
C	3.1903564296	-0.9442542477	-0.7782528275
C	2.1536223629	-1.8975340483	-0.8799019952
C	2.9068337133	0.3265089503	-0.3458211343
C	0.8635281169	-1.5666834169	-0.5403281807
H	-0.2130688051	3.3832882179	1.1060230554
H	-2.0320336983	1.7173912821	0.9958943211
H	2.099382528	2.7441471822	0.4992907601
H	-4.9138197105	-0.2197927623	1.641534438
H	-5.0861436337	-0.1464494866	-0.2034027446
H	-1.652129541	-1.9076481666	0.2729519072
H	4.2040811671	-1.2179476179	-1.0479059028
H	2.3768062772	-2.897604279	-1.2342164057
H	3.6934849713	1.0701464437	-0.2717187024
H	0.0895992284	-2.3145036132	-0.649341079
H	-2.0233763648	-1.1249307587	-1.6749450662

Core RigidRotor

```

SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 670.7499
WellDepth[kcal/mol] 36.95
WellDepth[kcal/mol] 4.83
End
Frequencies[1/cm] 65
45.2001          106.0587
123.5117         176.4943      213.9752
248.5106         260.4308      364.9655
403.3492         422.1199      434.4510
452.1806         478.4215      514.5551
523.8723         542.1603      602.0572
652.1209         673.5545      743.1356
765.8695         792.9350      806.3842
812.9614         868.3921      876.3565
881.1238         926.5930      943.6714
962.2858         986.5699      994.4425
996.3063         1011.2629     1053.0150
1096.6676        1119.7558     1169.6641
1191.7536        1196.6841     1233.8341
1262.4955        1280.6567     1335.6908
1384.0842        1394.4412     1424.1116
1454.0661        1480.0666     1496.0628
1550.6472        1613.7095     1636.1978
1663.4989        1981.2230     3088.7629
3151.7328        3157.7635     3159.5346
3162.3227        3170.6475     3173.8011
3185.1720        3186.7880     3203.1758
ZeroEnergy[kcal/mol] -0.21
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts15-p5-----
Barrier      ts15-p5  i15  p5
RRHO
Geometry[angstrom] 24
C -0.4992521186 -0.3173368125 0.0360054166
C 0.8677635987 0.1275956826 -0.035949809
C 0.0904951842 2.4141345947 -0.3820826249
C 1.1255676839 1.4747015725 -0.2408756352

```


C	-1.2221700869	2.0144520038	-0.3125362156
C	-1.5482950685	0.6518321978	-0.1033278873
C	1.9776101285	-0.8236662059	0.1074769089
C	4.4866602882	-0.3426509916	-0.4539766453
C	3.2609972461	-0.5485819913	-0.0599675768
C	-3.2246409713	-1.0897721972	0.1643276716
C	-2.1971307686	-2.0494721032	0.2939119512
C	-2.9019892078	0.2289010242	-0.0314020072
C	-0.8767051281	-1.6735135784	0.2295621983
H	0.3370955262	3.45819914	-0.5385481812
H	2.1555891322	1.8094930067	-0.2827983495
H	-2.026425725	2.7351317055	-0.414651778
H	1.7456373412	-1.8328637116	0.4318019424
H	5.2618616203	0.0119338117	0.2159030981
H	4.7675314841	-0.5298896375	-1.4878564823
H	-4.262440105	-1.3985559019	0.2171763826
H	-2.4523140371	-3.0925604624	0.4433656711
H	-3.6819328896	0.975810855	-0.1366120588
H	-0.1174878926	-2.4385749536	0.3229799643
H	3.5674247656	-0.1685980477	2.031474046

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 487.7839

WellDepth[kcal/mol] 62.28

WellDepth[kcal/mol] 3.24

End

Frequencies[1/cm] 65

22.2570	84.0729	
120.3893	126.6883	175.9574
241.5962	259.5355	365.3472
396.1572	415.3698	420.1932
440.5641	477.0014	511.7776
520.0771	543.4342	609.2635
655.1899	681.3478	742.9924
767.5304	792.4481	805.3679
812.5573	871.7810	876.7425
885.5229	892.1358	926.4910
961.1696	987.1901	996.5448
1005.9913	1016.2488	1053.6649
1101.4745	1123.9559	1169.6763
1192.1512	1201.5932	1233.1387

1263.7761	1280.1672	1337.9869
1384.4245	1396.4665	1424.7521
1460.3564	1481.9424	1494.6993
1550.2335	1609.9485	1631.7369
1662.2742	1983.6281	3109.5037
3156.6846	3160.0260	3162.9532
3170.8221	3175.3703	3185.4935
3187.6683	3190.5477	3201.8766

ZeroEnergy[kcal/mol] -1.8

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts16-p5-----

Barrier ts16-p5 i16 p5

RRHO

Geometry[angstrom] 24

C	-0.2575223884	-0.0327404005	0.0125427607
C	0.825947297	0.9138760084	0.0952173987
C	-0.78633698	2.7484089674	-0.1005644519
C	0.5295583296	2.2698387762	0.0254309557
C	-1.8324840221	1.8636545875	-0.1666536197
C	-1.5969970731	0.4657942569	-0.1164377692
C	2.2445628669	0.5833878307	0.2575752938
C	3.5733677237	-1.5961900978	0.8222620816
C	2.8792282491	-0.5679667891	0.416476637
C	-2.4623929723	-1.805907651	-0.1613751048
C	-1.1468993181	-2.3005912968	-0.0455516856
C	-2.6770725885	-0.4506933897	-0.1975708934
C	-0.0770877227	-1.4391236626	0.039300432
H	-0.964521794	3.8166911951	-0.1447923025
H	1.343998641	2.9844159702	0.0778356983
H	-2.8531871289	2.2182053496	-0.2622973587
H	2.9009534179	1.4516880208	0.2017195583
H	4.0329177506	-2.2969737576	0.1344059223
H	3.6959040607	-1.7876787752	1.8857162048
H	-3.296938441	-2.4949590168	-0.2255926194
H	-0.975468948	-3.371077151	-0.025511718
H	-3.6831609659	-0.0557207424	-0.2926183541
H	0.9193520826	-1.8446443842	0.124170638
H	3.061903924	-0.9186618483	-1.6895657037

Core RigidRotor

SymmetryFactor 0.5

```

End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  487.0267
WellDepth[kcal/mol]  60.08
WellDepth[kcal/mol]  3.95
End
Frequencies[1/cm]  65
36.7032          101.8680
136.5124         142.3226          176.9138
247.5559         277.4011          366.0295
386.1574         415.3938          424.7488
442.2608         480.0651          512.0620
520.7546         551.3736          612.7407
646.0492         680.4563          722.6458
744.9662         791.3461          808.3120
815.6813         877.3851          888.6322
892.9783         895.4110          926.3566
967.8929         984.5027          999.8032
1009.8839        1041.9383         1052.8918
1088.8628        1143.9365         1169.9407
1189.4866        1206.3704         1236.0389
1245.0021        1293.9863         1349.6380
1385.3061        1398.4769         1427.7581
1465.1950        1482.4649         1494.3745
1550.0954        1606.3177         1630.5263
1661.6893        1978.0754         3102.3256
3109.4832        3159.5480         3161.2205
3168.2370        3171.2228         3186.0919
3187.3094        3190.1109         3233.6803
ZeroEnergy[kcal/mol]  -1.09
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----bar_ts10-p6-----
Barrier      ts10-p6  i10  p6
RRHO
Geometry[angstrom]  24
C  0.2733794815  -0.0339281707  -0.199476254
C  -0.9506643831  0.6971958561  -0.3134957167
C  0.2720271911  2.7826300708  -0.0289962974
C  -0.9322942859  2.0709471388  -0.2277297554
C  1.4596925313  2.1068924915  0.0785217716

```

C	1.4945361831	0.6905871246	-0.0053748263
C	-3.2090669399	-1.4059689712	1.5340873346
C	-2.7835779738	-0.7311735397	0.6264061795
C	-2.2765390436	-0.0173118198	-0.5434382197
C	2.7403171669	-1.3961595399	0.0155630268
C	1.5382402053	-2.1135299977	-0.1713741208
C	2.7149728765	-0.0258916295	0.0975931583
C	0.3381022059	-1.4513477543	-0.2747717997
H	0.2480718535	3.8645551592	0.0344912088
H	-1.8626813376	2.6224493258	-0.3151670295
H	2.3899994267	2.6447063612	0.2278160997
H	-3.5728158374	-1.8279747949	2.4392796715
H	-2.1854301432	-0.7279651155	-1.3747617084
H	-3.0229577603	0.7188258875	-0.8563185424
H	3.679894875	-1.9309926513	0.0962038589
H	1.5628025864	-3.1958604896	-0.2293866286
H	3.6336226721	0.5328958534	0.2431988528
H	-0.5721104661	-2.0239098974	-0.3987446594
H	-3.3786230843	-3.2987528974	0.6880063957

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 449.3232

WellDepth[kcal/mol] 38.5

WellDepth[kcal/mol] 3.34

End

Frequencies[1/cm] 65

45.3091	54.0144	
78.8575	150.9509	176.8174
217.7525	262.1258	275.6250
378.5677	416.1950	433.2491
436.0754	478.8597	513.7825
523.8740	557.5711	616.5222
663.2079	664.9663	724.1107
746.8152	755.0295	793.0110
804.7137	813.3714	867.0211
886.4878	918.0674	933.3033
956.2360	967.6476	984.6778
998.0466	1040.2011	1061.4485
1097.8132	1169.2296	1185.2944
1188.8542	1214.6533	1240.7487
1262.0586	1289.3159	1332.5679

1383.7810	1397.5236	1425.2570
1467.6405	1479.7013	1495.8324
1549.3139	1618.7591	1641.9892
1665.9763	2169.9616	3010.5530
3058.5398	3158.3558	3159.9913
3166.1673	3171.1324	3184.9135
3185.7463	3200.5033	3463.2959

ZeroEnergy[kcal/mol] 1.34

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts4-p7-----

Barrier ts4-p7 i4 p7

RRHO

Geometry[angstrom] 24

C	0.4733024465	0.0997196019	0.7155802006
C	-0.8425080651	0.6611477346	0.8072935849
C	0.0685944495	2.8673674122	0.3452159867
C	-1.0234603465	2.0193967281	0.6219845344
C	1.33874363	2.3555758824	0.2484351748
C	1.5743306778	0.9686286297	0.4310940699
C	-2.8088162408	-0.6732143015	1.8665730106
C	-1.9875548715	-0.1810973492	1.0934394503
C	-2.4578444954	-0.85177211	-1.0056752447
C	3.0922564	-0.927580627	0.5261057751
C	2.0047905412	-1.7842883588	0.8100776686
C	2.8791722197	0.4163017939	0.3430870955
C	0.7285648092	-1.2828861688	0.903866978
H	-0.1052154634	3.9287948236	0.2096805175
H	-2.0222771683	2.4325409415	0.6949653922
H	2.1803573932	3.0053274159	0.0330980248
H	-3.6332702381	-1.2254076828	2.2532151272
H	-1.4844315021	-1.2159221724	-1.3101648229
H	-2.7703179148	0.1031966194	-1.4093093048
H	-3.2318577128	-1.5941749772	-0.8585820985
H	4.0944228581	-1.3352446808	0.4560924311
H	2.1813981395	-2.8437920745	0.9578040698
H	3.7101856495	1.0801722176	0.1286305403
H	-0.1026691954	-1.9392532977	1.1306058386

Core RigidRotor

SymmetryFactor 0.5

End

```

Tunneling      Eckart
ImaginaryFrequency[1/cm]  541.7243
WellDepth[kcal/mol]  31.85
WellDepth[kcal/mol]  10.96
End
Frequencies[1/cm]  65
41.8345          83.7354
89.4065          136.3084          155.5747
173.8321         229.1338          316.2761
355.7762         433.5588          447.1053
474.8120         479.0291          508.3359
518.1158         546.0993          562.8477
575.5390         606.9517          650.0449
697.0455         705.4575          747.3657
791.4012         806.0677          815.4793
864.7867         881.3995          893.8615
924.0189         969.6221          985.5888
999.6514         1032.5655         1049.1644
1091.7810        1167.9840         1179.8628
1188.0629        1234.2161         1245.8766
1288.1620        1359.9581         1391.5726
1417.2908        1419.7836         1422.6493
1467.3793        1490.7375         1543.3199
1611.9100        1629.8501         1661.1185
1989.8059        3087.1778         3159.2705
3163.0248        3170.1622         3178.1029
3183.8262        3191.6227         3194.8727
3247.3856        3248.2445         3431.7594
ZeroEnergy[kcal/mol]  -4.86
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----bar_ts21-p8-----
Barrier      ts21-p8  i21  p8
RRHO
Geometry[angstrom]  24
C  -0.2685444226  -0.0159566706  0.0445457761
C  -1.4119320204  0.7803454707  0.068592984
C  -2.6550056245  0.0895963888  -0.0139253368
C  -2.6696860752  -1.2866014028  -0.1444101104
C  -1.4793929387  -2.0610081463  -0.2176768969
C  -0.261492027  -1.4158266789  -0.1273919233

```

C	1.0668275347	0.4763195031	0.1031904946
C	1.2424306945	1.8579244066	0.0301351653
C	0.0988020339	2.6908521192	0.071559232
C	-1.1921172522	2.188224707	0.1123251468
C	1.1511912282	-1.810906949	-0.2110220878
C	1.9483414701	-0.7145130771	-0.0918308336
C	3.4407584963	-0.6570256505	-0.129097286
H	-3.5874474379	0.6433283639	0.0115224748
H	-3.623445682	-1.7984147826	-0.2119619237
H	-1.5491744827	-3.1345527465	-0.3571504401
H	1.3306216829	0.2881211789	1.9650792311
H	2.2297705331	2.304886656	-0.0090031388
H	0.2430279045	3.7656775626	0.0652536079
H	-2.0365200117	2.8685693053	0.1422798743
H	1.504461339	-2.8249403368	-0.3461779679
H	3.7929931404	-0.0175882981	-0.9463818334
H	3.8423546062	-0.2400960439	0.8007009304
H	3.870847311	-1.6503588789	-0.2694431384

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 813.9111

WellDepth[kcal/mol] 27.56

WellDepth[kcal/mol] 5.87

End

Frequencies[1/cm] 65

125.6299	150.6479	
170.2657	215.9667	229.9769
294.6746	322.1176	409.8960
414.5657	432.5569	474.3070
496.4841	533.5039	548.3305
584.8000	592.3271	623.4650
664.0912	684.7728	761.3242
774.8164	799.2438	816.4866
818.3943	858.1695	909.1416
920.0877	968.4812	974.2899
982.7933	1018.9768	1040.5504
1058.4725	1062.6814	1088.5472
1155.7303	1178.6472	1202.6261
1211.2809	1245.6208	1282.6925
1315.2457	1381.5807	1396.3056
1412.5757	1443.2018	1452.3463

1476.8563	1480.6916	1489.6370
1514.0051	1597.0222	1611.6854
1643.6810	1649.9083	3014.3549
3057.7275	3103.8709	3160.1606
3161.0276	3170.4641	3172.2479
3183.4047	3184.5564	3202.5384

ZeroEnergy[kcal/mol] -31.71

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts22-p8-----

Barrier ts22-p8 i22 p8

RRHO

Geometry[angstrom] 24

C	0.4596999626	-0.0183589649	0.4175197111
C	1.5993581458	0.7843306008	0.363755708
C	2.8451419883	0.0952015744	0.2926452893
C	2.8689078063	-1.2867114876	0.2777272108
C	1.6856429174	-2.074909556	0.3333464389
C	0.4648694479	-1.434378789	0.4070908001
C	-0.8640105199	0.465199561	0.4893984071
C	-1.0573375567	1.8288063507	0.5203184295
C	0.0823648942	2.6800417444	0.4745191026
C	1.3722606356	2.1897051035	0.3959509845
C	-0.9353498537	-1.8450330095	0.4884158675
C	-1.7462440351	-0.7311861993	0.5085135282
C	-3.2202220064	-0.6929038928	0.7824287613
H	3.773901483	0.6543241624	0.2523022516
H	3.8250480935	-1.7954922552	0.2228478507
H	1.7645193097	-3.1567685853	0.3193062201
H	-2.0477802163	2.2684466571	0.5718091455
H	-0.0728280021	3.752984529	0.4990198247
H	2.2114929567	2.876375058	0.3596947228
H	-1.2867343278	-2.8679142242	0.5169706193
H	-2.0243974714	-0.7487585974	-1.5712597031
H	-3.7298748221	0.0433020683	0.1562789334
H	-3.6806703925	-1.666146407	0.6035300275
H	-3.4040824369	-0.4182334413	1.8276578686

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 529.6788

WellDepth[kcal/mol] 42.21

WellDepth[kcal/mol] 3.4

End

Frequencies[1/cm] 65

129.1800	160.1892	
170.2600	211.3810	233.4819
280.1370	299.9895	383.4010
413.6668	425.2039	463.2951
502.1416	534.0570	548.7563
584.0311	594.2354	628.9343
670.8247	678.7660	763.9168
782.0881	800.1689	815.6987
819.2675	852.8184	918.9508
927.2557	969.3909	975.7484
985.8815	1014.9023	1037.4315
1052.0649	1058.3718	1090.1006
1157.5797	1179.6633	1205.6641
1219.0924	1248.2245	1283.6499
1316.8059	1381.8489	1404.4596
1414.6630	1449.7032	1457.7280
1481.4118	1489.0792	1490.2839
1516.4341	1544.0966	1631.8043
1649.1711	1658.0720	3017.7763
3074.5312	3109.0404	3160.2465
3160.7976	3169.8678	3171.0169
3183.6104	3184.5386	3207.6626

ZeroEnergy[kcal/mol] -34.18

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts22-p9-----

Barrier ts22-p9 i22 p9

RRHO

Geometry[angstrom] 24

C	0.5159982963	-7.20132E-5	-0.492847879
C	1.6246888237	0.77993161	-0.1585828951
C	2.8330455757	0.0696490158	0.1026460013
C	2.8557721935	-1.3102872775	0.0119825928
C	1.7110987601	-2.0756943787	-0.3391567481
C	0.5225899311	-1.4158977375	-0.5980261158
C	-0.7653836025	0.5098428114	-0.795533479

C	-0.9418346742	1.8768506647	-0.7753471284
C	0.1673403279	2.7032519682	-0.4445058696
C	1.4131703033	2.1873295104	-0.1390182748
C	-0.8231926698	-1.8018016645	-0.9986836261
C	-1.6191574688	-0.6703723803	-1.0668858292
C	-2.8753224937	-0.652257174	1.0217696321
H	3.7352329762	0.6113258669	0.3662141733
H	3.7843172074	-1.8340171593	0.2118533658
H	1.7900625038	-3.1557995275	-0.4021506108
H	-1.8995433072	2.3347677917	-0.9995109479
H	0.0246866342	3.7782548051	-0.4308534677
H	2.230716367	2.8557241048	0.1099092874
H	-1.151796581	-2.8128175142	-1.1961222996
H	-2.5989953108	-0.6265727707	-1.5189363886
H	-3.4309188724	0.2660073111	0.8808617741
H	-3.4109582641	-1.5872949824	0.9235686246
H	-2.0177906557	-0.6265468803	1.679491108

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 366.3596

WellDepth[kcal/mol] 37.84

WellDepth[kcal/mol] 5.42

End

Frequencies[1/cm] 65

74.4637	91.3835	
94.0092	165.6382	222.6769
240.2713	371.7494	421.0985
437.7108	462.5129	465.7981
482.5491	517.7196	558.1013
566.9208	621.3854	657.1732
670.6948	698.7810	735.4363
765.4992	772.1013	787.8468
815.5952	841.9975	870.8753
891.3854	910.3856	922.5380
973.7400	983.4085	1027.5981
1037.4318	1058.2189	1082.8727
1113.8368	1175.2964	1203.3418
1218.0263	1245.2760	1270.4810
1326.8448	1356.2402	1411.8834
1412.8360	1414.7422	1426.4946
1450.6166	1469.3841	1484.6337

1515.5058	1623.2050	1643.6288
1654.7724	3093.3538	3158.6149
3159.0151	3168.2901	3169.7184
3182.0155	3183.1360	3208.1301
3226.9033	3256.3208	3267.0270

ZeroEnergy[kcal/mol] -38.54

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_tsa-8-----

Barrier tsa-8 i8 p0a

RRHO

Geometry[angstrom] 24

C	-0.0181814664	0.7086009756	-0.0048916025
C	-1.2903001756	1.33872805	-0.0330515354
C	1.2100558863	1.394494446	0.0041781266
C	-2.4426251461	0.5908698687	-0.0395232797
C	-2.3806262132	-0.8221104634	-0.0221893513
C	-1.1663094148	-1.4637452734	8.107336E-4
C	0.0480672705	-0.7292696573	0.0109171847
C	2.4299195646	0.7953695331	0.0440965981
C	1.319970436	-1.3615207251	0.0363254043
C	2.4799340579	-0.6258240453	0.0500725768
H	-1.3316059004	2.4209673019	-0.0565685152
H	-3.408271412	1.0835346955	-0.0607792734
H	-3.2990535726	-1.3984184129	-0.0291818624
H	-1.1189085843	-2.548100694	0.0112946722
H	3.3487683685	1.3719312671	0.0665537011
H	1.360755325	-2.4456417762	0.0477109089
H	3.443504797	-1.1243818272	0.0701490883
C	1.3359900477	3.9895442144	1.2973392299
C	1.1737136609	3.9922747978	-1.296714175
C	1.2455681988	3.7621918736	-0.0088784955
H	0.4550293852	3.9818281243	1.9309740742
H	2.3012587	4.0399706367	1.7908060048
H	1.1418117511	3.204729807	-2.036806635
H	1.1419924357	5.0198932828	-1.6500885779

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 379.4546

```

WellDepth[kcal/mol] 63.89
WellDepth[kcal/mol] 2.16
End
  Rotor      Hindered      ! 25 cm^-1
  Group              18 19 21 22 23 24
  Axis              3 20
  Symmetry          2
  Potential[kcal/mol] 4
0 0.67478177 3.46828441 0.453420232
End

```

```

Frequencies[1/cm] 64
                    50.9563
72.8522             110.7348             157.2665
174.6022           223.1429             243.3183
366.9442           393.2684             410.0668
469.0025           508.9215             516.9695
521.3382           617.7680             620.6303
737.0222           762.4501             776.3415
796.1755           802.4918             808.4932
811.1414           868.1593             895.2839
897.1112           919.6938             964.9512
976.3016           997.3881            1006.6860
1021.4819          1036.4483            1051.1197
1062.5129          1137.4093            1168.4723
1177.4855          1202.2841            1235.3393
1270.8517          1362.3854            1381.9267
1384.6280          1427.9280            1452.7938
1471.3812          1483.2696            1523.5377
1582.4280          1634.6617            1659.8925
1927.3981          3118.5100            3122.0573
3152.6952          3155.4395            3163.2401
3167.7575          3177.0998            3181.7773
3193.2148          3198.4771            3222.0054

```

```

ZeroEnergy[kcal/mol] 3.3
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_tsa-10-----
Barrier      tsa-10  i10  p0a
RRHO
Geometry[angstrom] 24
C 0.161836292 0.7384373026 0.0516065949

```

C -1.0500266585 1.4604970248 0.2171078634
 C 1.4355393165 1.3291468619 -0.0413813256
 C -2.253959728 0.8030650913 0.2932224941
 C -2.3076971853 -0.6075188134 0.208540251
 C -1.1546917662 -1.337377914 0.0515097563
 C 0.1094437509 -0.6979066546 -0.0312063754
 C 2.59606856 0.6361650901 -0.1883498522
 C 1.3194700393 -1.4250942737 -0.1908353975
 C 2.5304902076 -0.7823093466 -0.266993503
 H -1.0079937871 2.5400976998 0.2915559036
 H -3.1713755613 1.3667306415 0.4207612139
 H -3.2656355822 -1.1117342138 0.2700093302
 H -1.1952839182 -2.420176956 -0.0118545971
 H 3.5588848491 1.1343136475 -0.2480282659
 H 1.2707214292 -2.5072680694 -0.2510267029
 H 3.4459783692 -1.3521598504 -0.3875283968
 C 1.6872242817 3.6776823202 0.0084696252
 C 0.8296465628 4.4970124473 2.3454445861
 C 1.2712855741 4.1578672728 1.1702269984
 H 2.7454227244 3.5158029027 -0.1649932936
 H 1.0586753231 3.7491266132 -0.8725951159
 H 0.4387812513 3.75231135 3.0362316198
 H 0.8355206558 5.5291928264 2.6857295889

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 259.2179

WellDepth[kcal/mol] 39.65

WellDepth[kcal/mol] 1.35

End

Rotor	Hindered	! 23 cm ⁻¹
Group		19 20 21 22 23 24
Axis		3 18
Symmetry		1
Potential[kcal/mol]		8

0 0.431762366 0.46246641 0.447822219 0.495196683 0.024928446 0.404301919 0.633293973

End

Frequencies[1/cm] 64

35.3008

88.0958	118.9646	170.9919
192.4061	330.1983	340.4464
367.6939	381.2228	406.4605

468.1632	501.3107	512.2570
521.7083	603.8213	619.8811
735.1939	749.6154	777.2654
794.3458	801.9431	855.0737
865.4989	874.6043	875.1544
895.2766	936.6288	963.9005
975.5462	996.0347	998.1067
1033.8730	1037.3348	1054.6759
1064.7385	1138.5142	1168.1506
1178.3226	1204.6261	1234.7166
1270.6161	1362.1951	1383.4993
1386.3815	1420.1487	1453.5688
1466.0069	1483.5514	1524.0002
1582.7839	1635.4745	1659.9757
1969.6019	3092.9368	3124.8194
3146.7906	3155.5575	3159.5184
3162.9212	3168.1407	3176.4823
3182.1328	3194.9055	3200.5618

ZeroEnergy[kcal/mol] 2.49

ElectronicLevels[1/cm] 1

0 2

End

!-----

End

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