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

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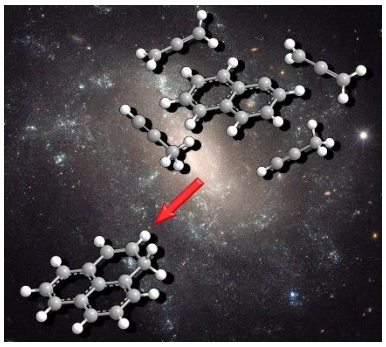
Abstract: For the last decades, the Hydrogen-Abstraction/aCetylene-Addition (HACA) mechanism has been fundamental in aiding our understanding of the source of polycyclic aromatic hydrocarbons (PAHs) in combustion processes and in circumstellar envelopes of carbon rich stars. However, the reaction mechanisms 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 ($[C_{10}H_7]^{\bullet}$) 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 ($C_{13}H_9^{\bullet}$) (**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 ($C_6H_5^{\bullet}$) and tertiary butyl ($C(CH_3)_3^{\bullet}$) 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 ($C_{26}H_{14}$).[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 C_2–C_4 alkenes and recombination of phenalenyl **(2)** with arylmethyl radicals such as naphthylmethyl ($C_{11}H_9^{\bullet}$) or phenanthrenylmethyl ($C_{14}H_{11}^{\bullet}$). 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**) ($C_{13}H_{10}$; 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 ($C_{10}H_7^{\bullet}$; 127 amu) with allene and methylacetylene (C_3H_4; 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-napthyl 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 ($C_{10}H_7^{\bullet}$) with allene (H_2CCCH_2) and methylacetylene (CH_3CCH) 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).

(1a) $[C_{10}H_7]^{\bullet}$ (127 amu) + C_3H_4 (40 amu) → $C_{13}H_{10}$ (166 amu) + H (1 amu)

(1b) $[C_{10}H_7]^{\bullet}$ (127 amu) + C_3H_4 (40 amu) → $C_{12}H_8$ (152 amu) + CH_3 (15 amu).

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 $C_{13}H_{11}$ 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[G3(MP2,CC)] = E[CCSD(T)/6-311G(d,p)] + E[MP2/G3Large)] – E[MP2/6-311G(d,p)] + ZPE[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, 1–2º 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 09[45] and MOLPRO 2010[46] program packages were used for the ab initio calculations. Pressure- and temperature-dependent rate constants for the 1-naphthyl + C_3H_4 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 C_6H_5 + C_3H_4[49] and 1-naphthyl + C_3H_4 reactions;[38] the Lennard-Jones parameters were taken as (ε/cm^{-1}, σ/Å) = (390, 4.46) and the temperature dependence of the range parameter α for the deactivating wing of the energy transfer function was expressed as $\alpha(T) = \alpha_{300}(T/300\ K)^n$, with n = 0.62 and α_{300} = 424 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 publications[49] 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-naphtyl 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-napthyl – 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-isotoplogue 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 ($C_{13}H_{10}$) (**p1**) along with two of its isomers (1-methylacenaphthylene (**p8**), 3H-cyclopenta(a)naphthalene (**p2**)) and acenaphthylene ($C_{12}H_8$) (**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 ($C_{13}H_{10}$) (**p1**, via **i8**, **i9**, **i10**, **i13**, and **i14**) and 3H-cyclopenta(a)naphthalene ($C_{13}H_{10}$) (**p2**, via **i8**, **i9**, **i10**, **i11**, and **i12**) are open, whereas 1-methylacenaphthylene ($C_{13}H_{10}$) (**p8**), and acenaphthylene ($C_{12}H_8$) (**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 10π 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** → **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-ethynylnaphtahlene ($C_{12}H_8$) (**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 biphenylyl ($C_{12}H_9^{\bullet}$)[50] and 4-phenanthryl ($C_{14}H_9^{\bullet}$)[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.

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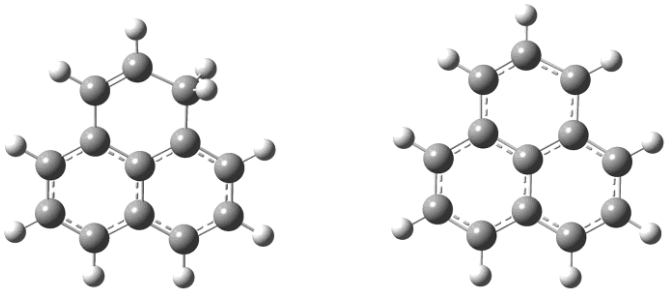
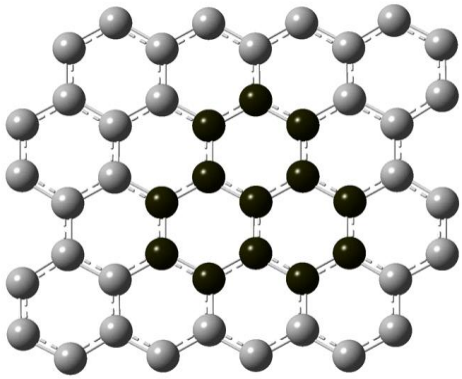
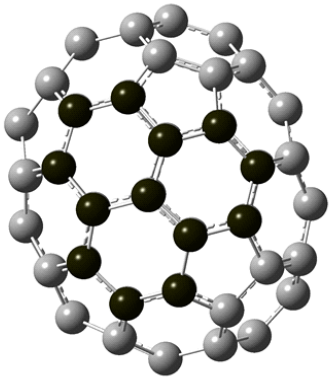


Scheme 1. Molecular structures of the 1H-phenalene molecule (**1**) and the phenalenyl radical (**2**).



(3)



(4)

Scheme 2. Molecular building blocks of the 1H-phenalene carbon skeleton (black) in graphene (**3**) [51] and C_{70}-fullerene (**4**).[52-54]

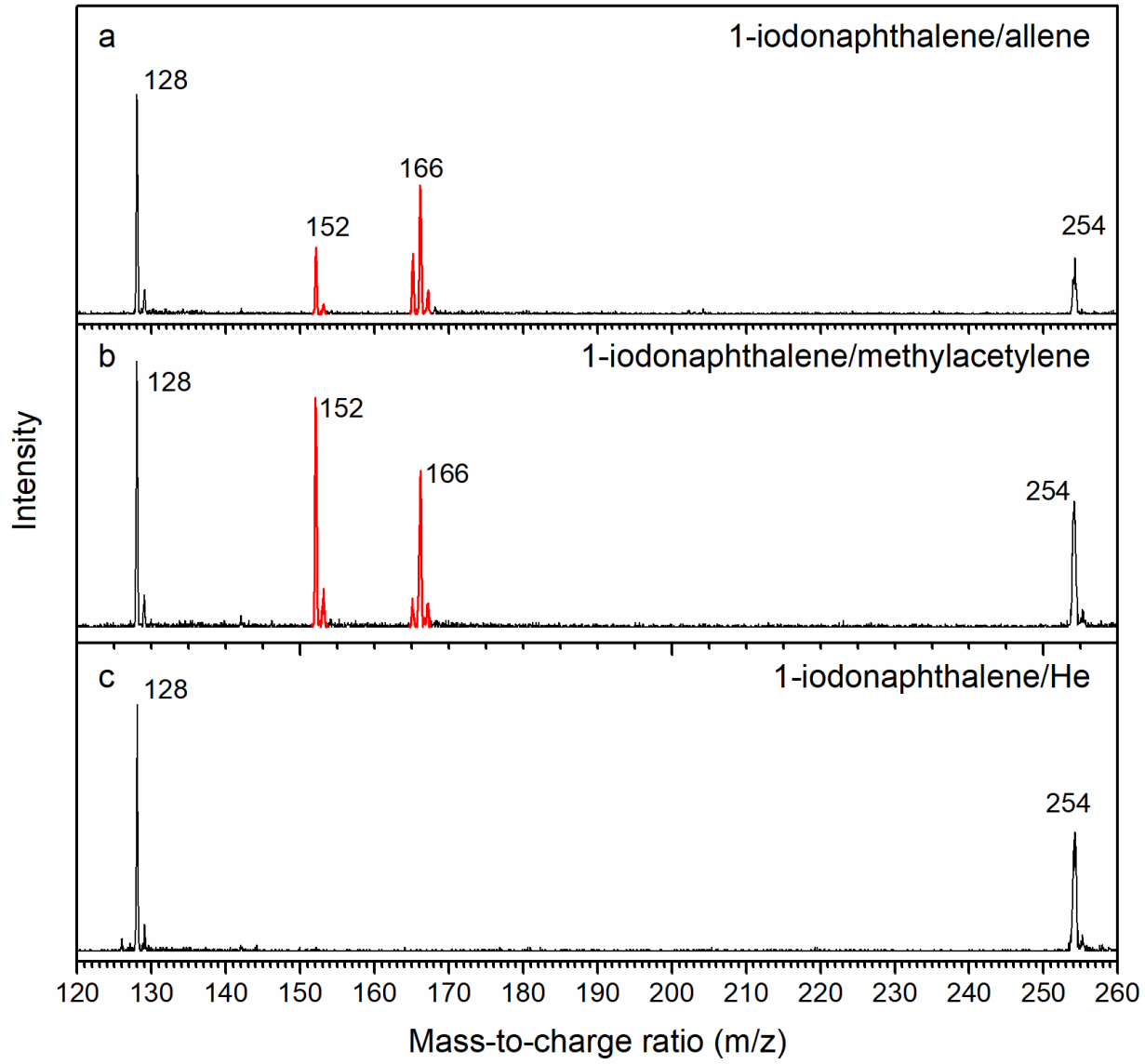


Figure 1. Comparison of photoionization mass spectra recorded at a photon energy of 9.50 eV. (a) 1-iodonaphthalene ($C_{10}H_7I$) - allene (C_3H_4) system; (b) 1-iodonaphthalene ($C_{10}H_7I$) - methylacetylene (C_3H_4) system; and (c) 1-iodonaphthalene ($C_{10}H_7I$) - helium (He) system. The mass peaks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

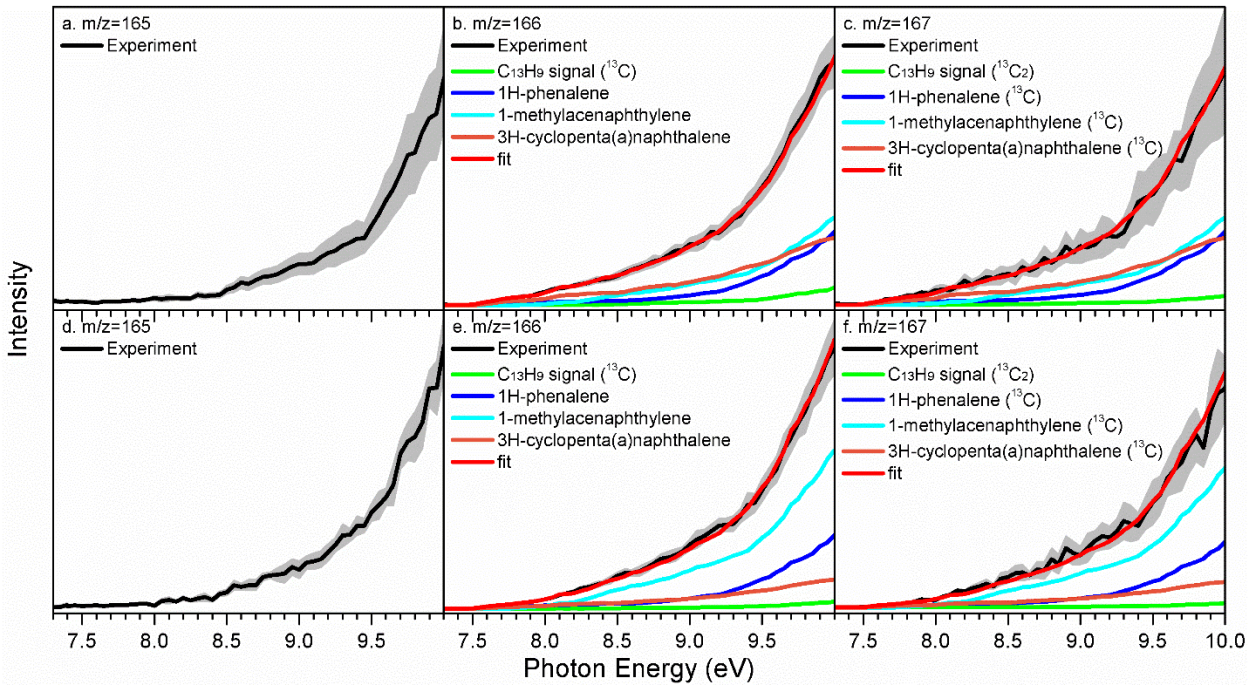


Figure 2. Photoionization efficiency (PIE) curves for signal at *m/z* = 165 to 167 in the systems of (a), (b) and (c): 1-iodonaphthalene ($C_{10}H_7I$) + allene (C_3H_4); (d), (e) and (f): 1-iodonaphthalene ($C_{10}H_7I$) + methylacetylene (C_3H_4). Black: experimentally derived PIE curves; colored lines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

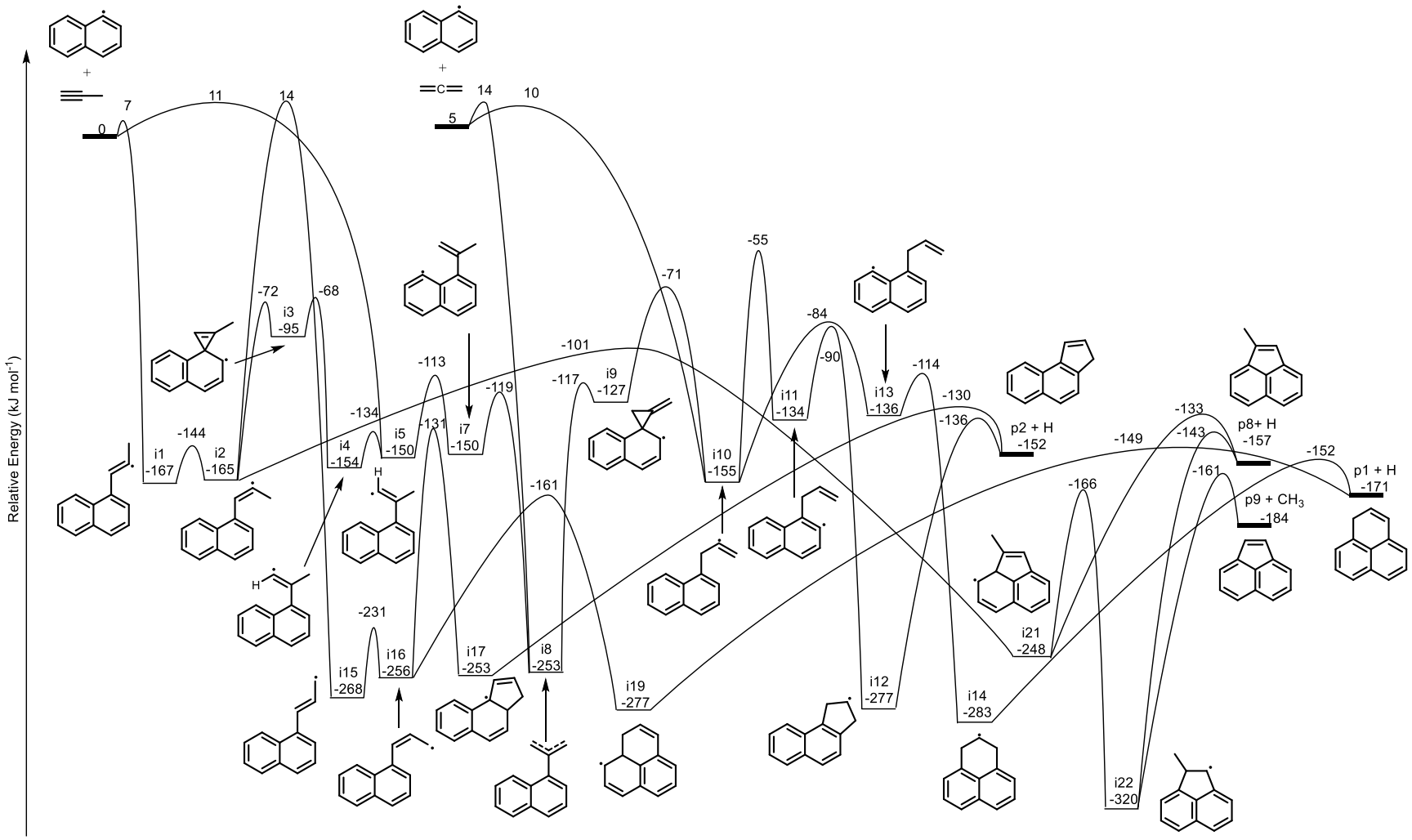
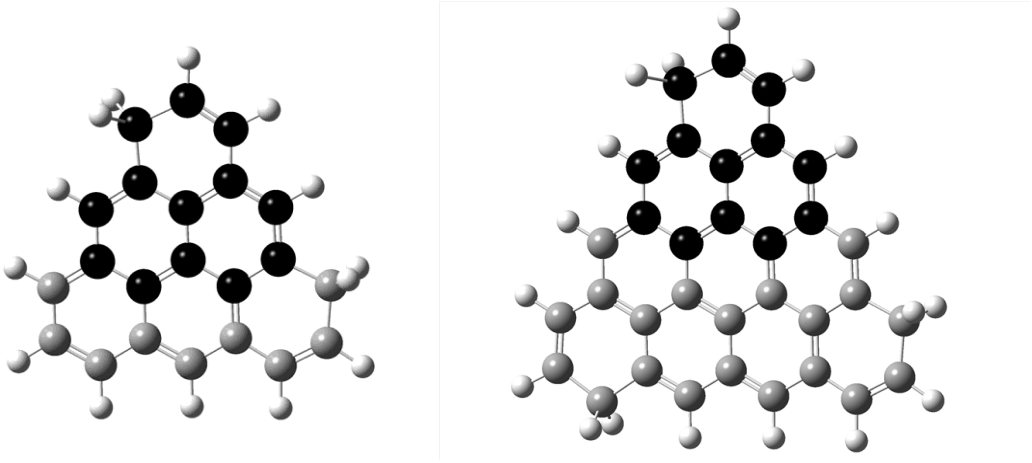


Figure 3. Potential energy surface (PES) for the 1-naphthyl ($C_{10}H_7^{\bullet}$) reaction with allene/methylacetylene (C_3H_4). This PES was calculated at the G3(MP2,CC)//B3LYP/6-311G(d,p) level of theory for the channels leading to 1H-phenalene (**p1**), 3H-cyclopenta(a)naphthalene (**p2**), 1-methylacenaphthylene (**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 10π-Aromatic, Resonantly Stabilized Free Radical Intermediates

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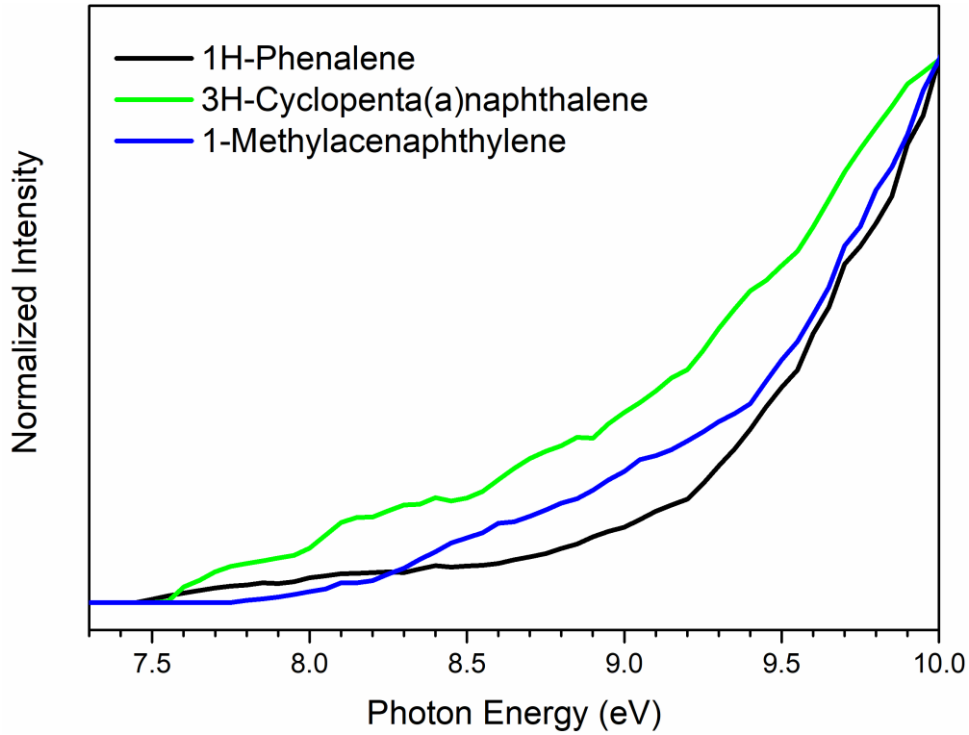


Figure S1. PIE calibration curves for distinct $C_{13}H_{10}$ isomers along with their adiabatic ionization energies: 1H-phenalene (**p1**; 7.45 ± 0.05 eV), 3H-cyclopenta(a)naphthalene (**p2**; 7.55 ± 0.05 eV), 1-methylacenaphthylene (**p8**; 7.75 ± 0.05 eV). The measured ionization energy of 1H-phenalene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

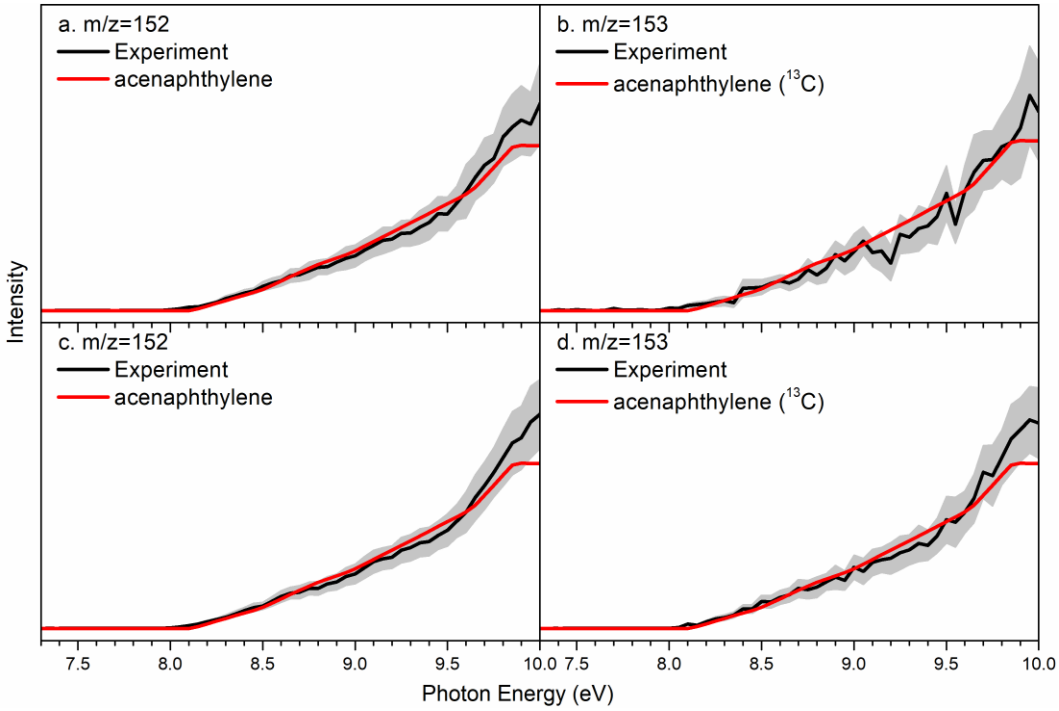


Figure S2. Photoionization efficiency (PIE) curves for signal at *m/z* = 152 and 153 in the reaction systems of (a) and (b): 1-iodonaphthalene ($C_{10}H_7I$) + allene (C_3H_4); (c) and (d): 1-iodonaphthalene ($C_{10}H_7I$) + methylacetylene (C_3H_4). Black: experimentally derived PIE curves; red: reference PIE curves. The overall error bars consist of two parts: ±10% based on the accuracy of the photodiode and a 1 σ 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.

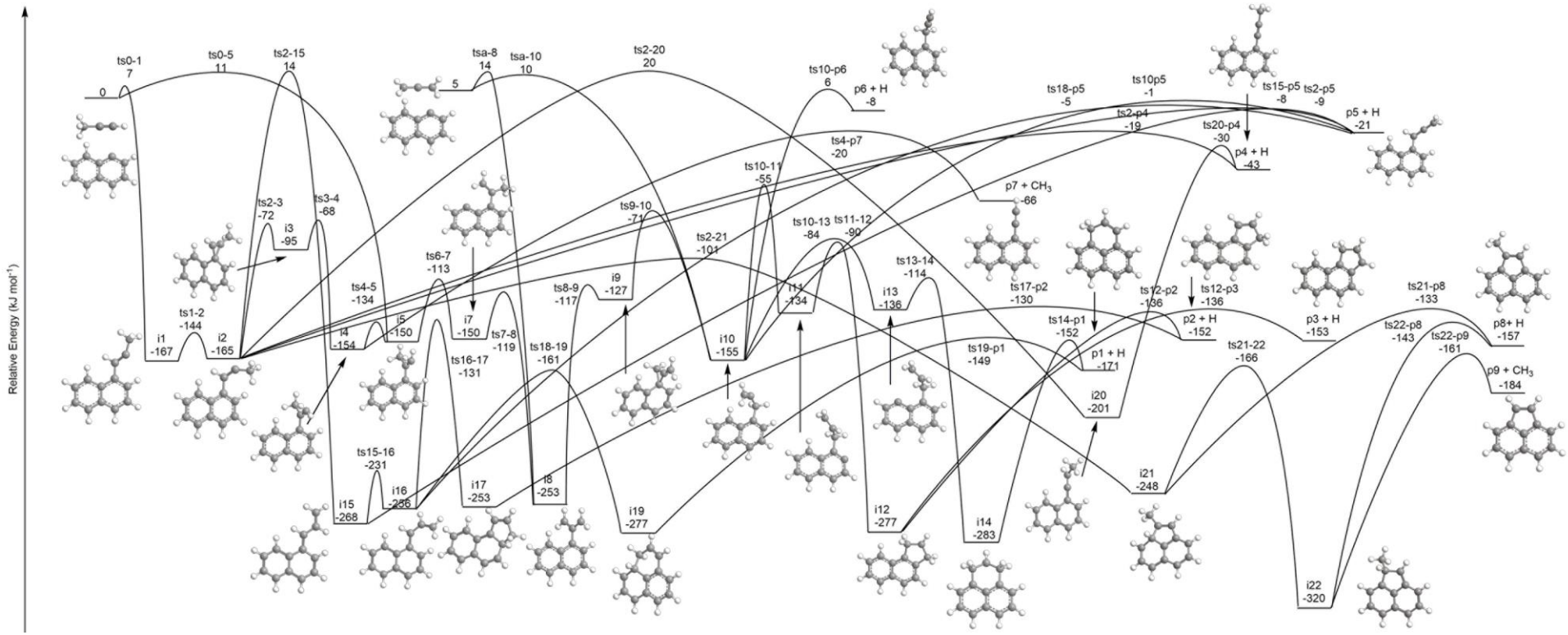
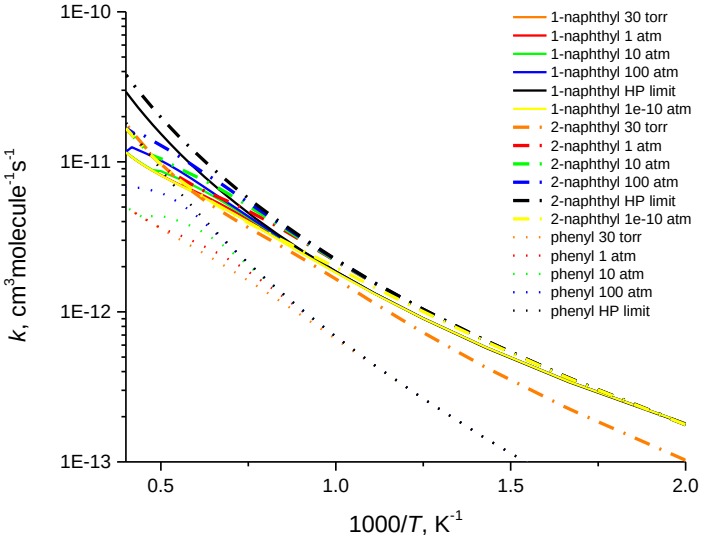
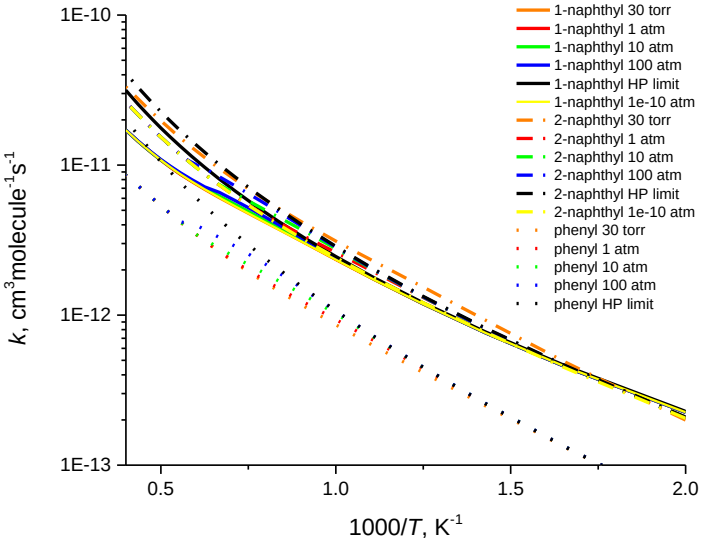


Figure S3. Complete potential energy surface (PES) for the 1-naphthyl ($C_{10}H_7^{\bullet}$) reaction with allene/methylacetylene (C_3H_4) calculated at the G3(MP2,CC)//B3LYP/6-311G(d,p) level. The relative energies are given in kJ mol^{-1}.



(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/methylacetylene[1] and phenyl + allene/methylacetylene.[3]

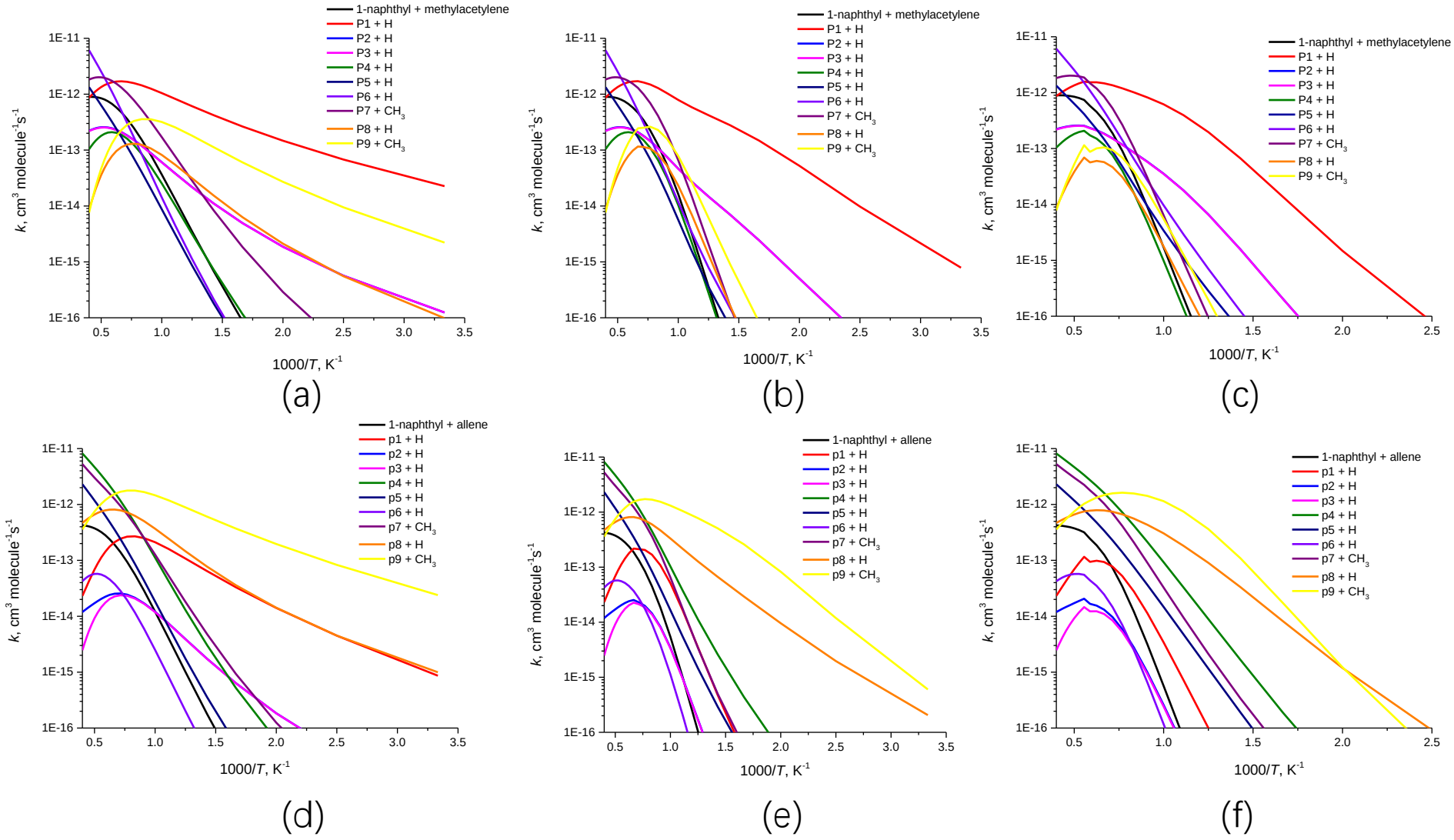


Figure S5. Calculated rate constants for individual reaction channels leading to various bimolecular products: (a) 1-naphthyl + allene at zero-pressure limit; (b) 1-naphthyl + allene at 30 Torr; (c) 1-naphthyl + allene at 1 atm; (d) 1-naphthyl + methylacetylene at zero-pressure limit; (e) 1-naphthyl + 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 (cm^3 $molecule^{-1}$ 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 (cm^3 $molecule^{-1}$ 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 (cm^3 $molecule^{-1}$ 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 (cm^3 $molecule^{-1}$ 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 (cm^3 $molecule^{-1}$ 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%

[a]R-ma indicates formation of 1-naphthyl + methylacetylene as the product of the 1-naphthyl + allene reaction.

[b]Total 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 (cm^3 $molecule^{-1}$ 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 (cm^3 $molecule^{-1}$ 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 (cm^3 $molecule^{-1}$ 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 (cm^3 $molecule^{-1}$ 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 (cm^3 $molecule^{-1}$ 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%

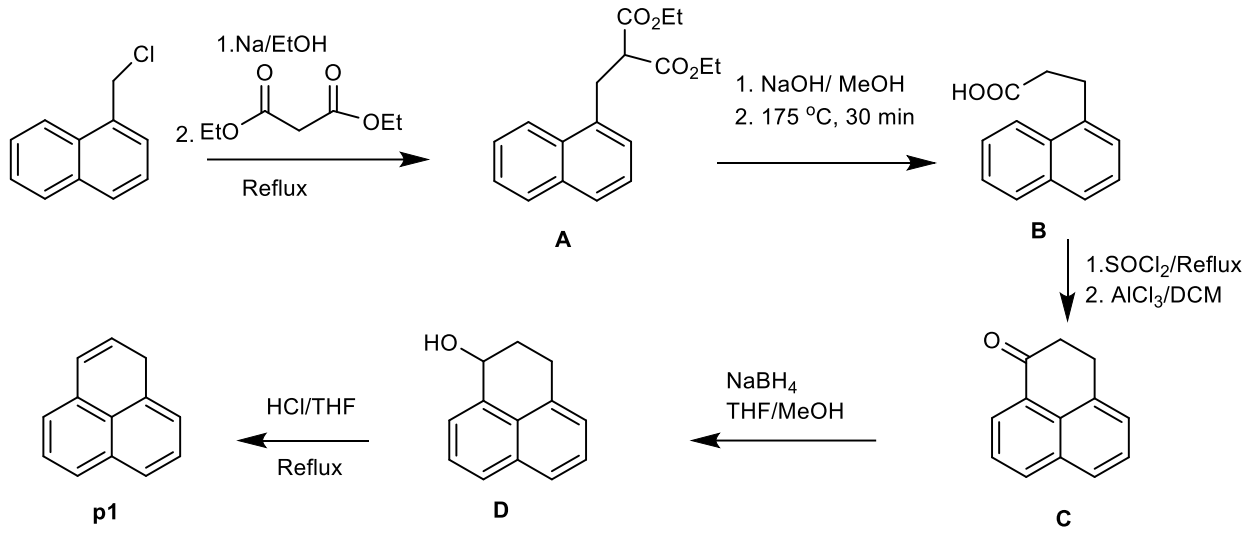
[a]R-a indicates formation of 1-naphthyl + allene as the product of the 1-naphthyl + methylacetylene reaction.

[b]Total reaction rate constant at the high-pressure limit.

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

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

The 1H-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 $SOCl_2$ and cyclization with $AlCl_3$ provided perinaphthanone-7 **C** in 75% yield. Reduction of ketone **C** with $NaBH_4$ and dehydration of the resulting **D** with HCl gave 1H-Phenalene **p1** in high overall yields (67%). Described here method uses $SOCl_2/AlCl_3$ instead of HF for the cyclization of B to C.



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

Diethyl 2-(naphthalen-1-ylmetyl)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 $NaHCO_3$ and brine. The EtOAc layer was separated, dried over anhydrous Na_2SO_4, filtered, and evaporated. The residue was column chromatographed (0 → 5 % EtOAc/hexane) to give **A**[8] (6.8 g, 80%) as a clear liquid: ^{1}H 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); ^{13}C NMR (101 MHz, $CDCl_3$) 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: ^{1}H 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); ^{13}C NMR (101 MHz, $CDCl_3$) 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-1*H*-phenalen-1-one; C.

Compound **B** (2.8 g, 13.98 mmol) was dissolved in $SOCl_2$ (40 mL) and the solution was refluxed at 85 °C for 1 h. The $SOCl_2$ 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 Na_2SO_4, filtered, and evaporated. The residue was column chromatographed (5 → 10 % EtOAc/hexane) to give **C**[5] (1.91 g, 75%) as off-white solid: ^{1}H 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); ^{13}C NMR (101 MHz, $CDCl_3$) 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-1*H*-phenalen-1-ol; D

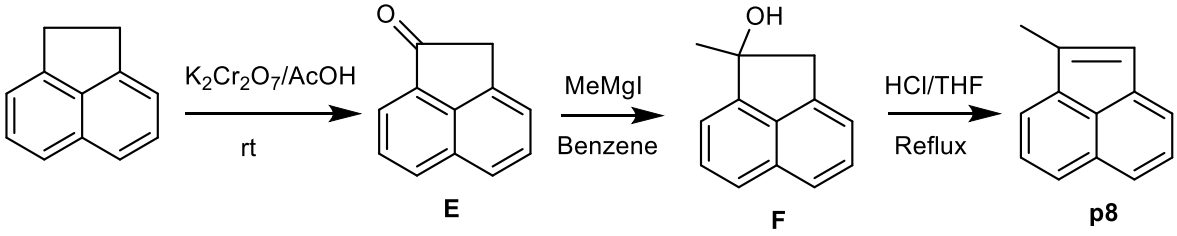
$NaBH_4$ (748 mg, 19.8 mmol) was added portion wise to a stirred solution of **C** (1.8 g, 9.88 mmol) in dry MeOH/THF (40 mL, 2;1) at 0 °C (ice-bath). After 5 min, the reaction mixture was allowed to warm to rt and stirring was continued for 30 min. Water (10 mL) was then added to quench the reaction. The mixture was concentrated under reduced pressure and extracted with EtOAc. The organic phase was separated, dried over anhydrous Na_2SO_4, 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: ^{1}H 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); ^{13}C NMR (101 MHz, $CDCl_3$) 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.

1*H*-Phenalene; p1

The secondary alcohol **D (**1.0 g, 5.4 mmol) was dissolved in the mixture of THF/H_2O (20 mL, 1:1). Aqueous 4 N HCl (10.0 mL, 40 mmol) was then added and the reaction mixture was refluxed at 105 ^oC 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 Na_2SO_4, filtered, and evaporated. The residue was column chromatographed (*n*-hexane) to give **p1**[6] (673 mg, 75%) as a light yellow solid: ^{1}H 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); ^{13}C NMR (101 MHz, $CDCl_3$) 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 $K_2Cr_2O_7$ in acetic acid afforded acenaphthylenone **E** (Scheme 2). Reaction of ketone **E** with MeMgI in dry THF as reported[10] led to the mixture of unidentified products. However, treatment of **E** with MeMgI in dry benzene[11] 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 $K_2Cr_2O_7$ (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 H_2O and extracted with 5 x 50 mL EtOAc. The combined organic portions were washed with saturated $NaHCO_3$ solution followed by brine. The organic layer was separated, dried over anhydrous Na_2SO_4, filtered, and evaporated. The residue was column chromatographed (0 → 10 % EtOAc/hexane) to give **E**[7] (3.27 g, 60%) as off-white solid: ^{1}H 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); ^{13}C NMR (101 MHz, $CDCl_3$) 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-1,2dihydroacenaphthylen-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 continues for an additional 10 min at rt. The reaction mixture was then refluxed at 85 ^{o}C for 2 h [progress of the reaction was monitored by TLC]. The reaction mixture was poured in ice-water and saturated NH_4Cl was added to quench the reaction. The mixture was extracted with EtOAc and organic layer was separated, dried over anhydrous Na_2SO_4, filtered, and evaporated. The residue was column chromatographed (0 → 20% EtOAc/hexane) to give **F**[11] (450 mg, 81.4%) as off-white solid: ^{1}H 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/H_2O (10 mL, 1:1). Aqueous 6 N HCl (3.0 mL, 18 mmol) was then added and the reaction mixture was refluxed at 105 ^{o}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 Na_2SO_4, 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: ^{1}H 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); ^{13}C NMR (101 MHz, $CDCl_3$) 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.

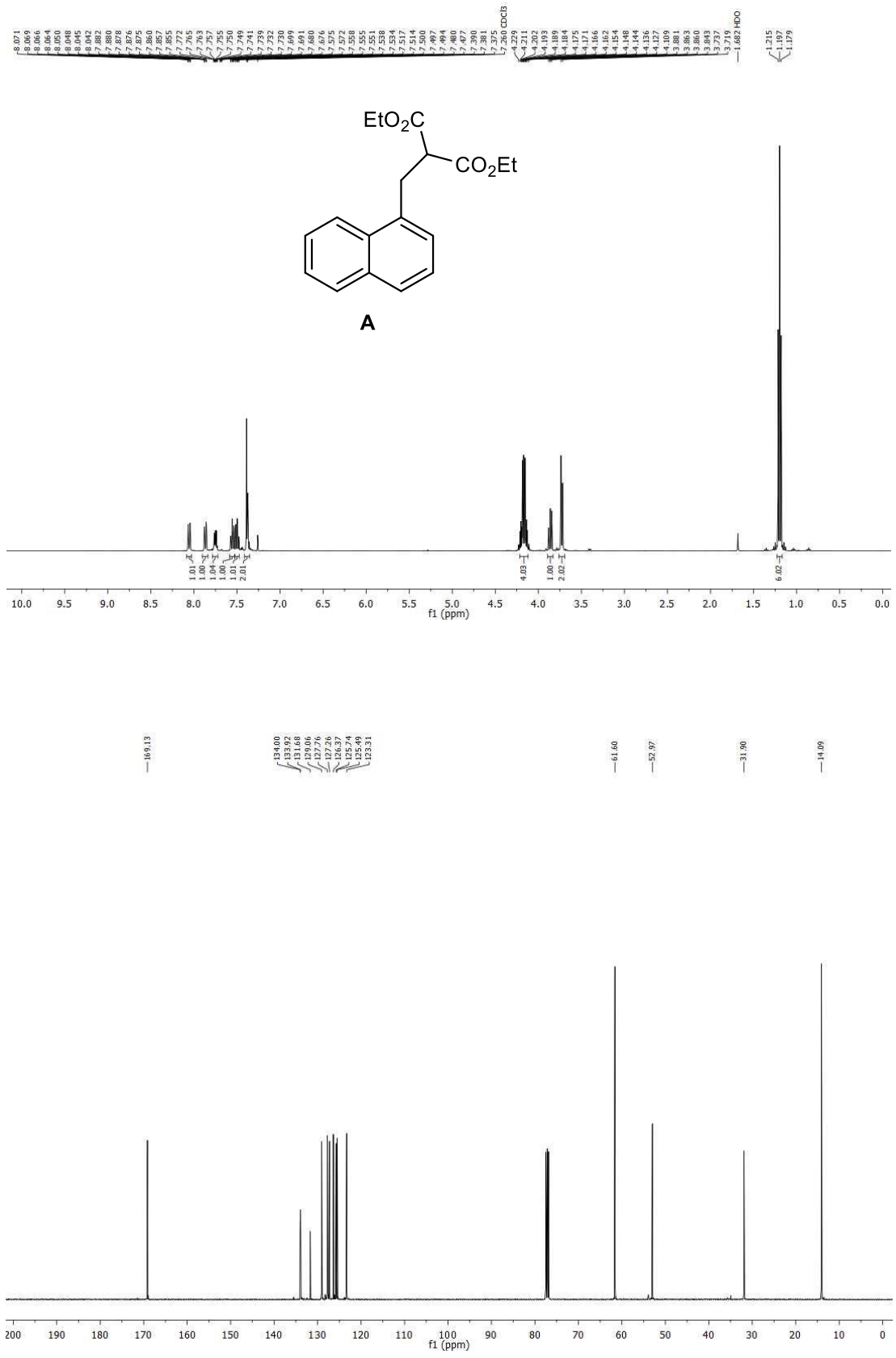


Figure S6. ^{1}H NMR and ^{13}C NMR spectra of compound **A** in $CDCl_3$.

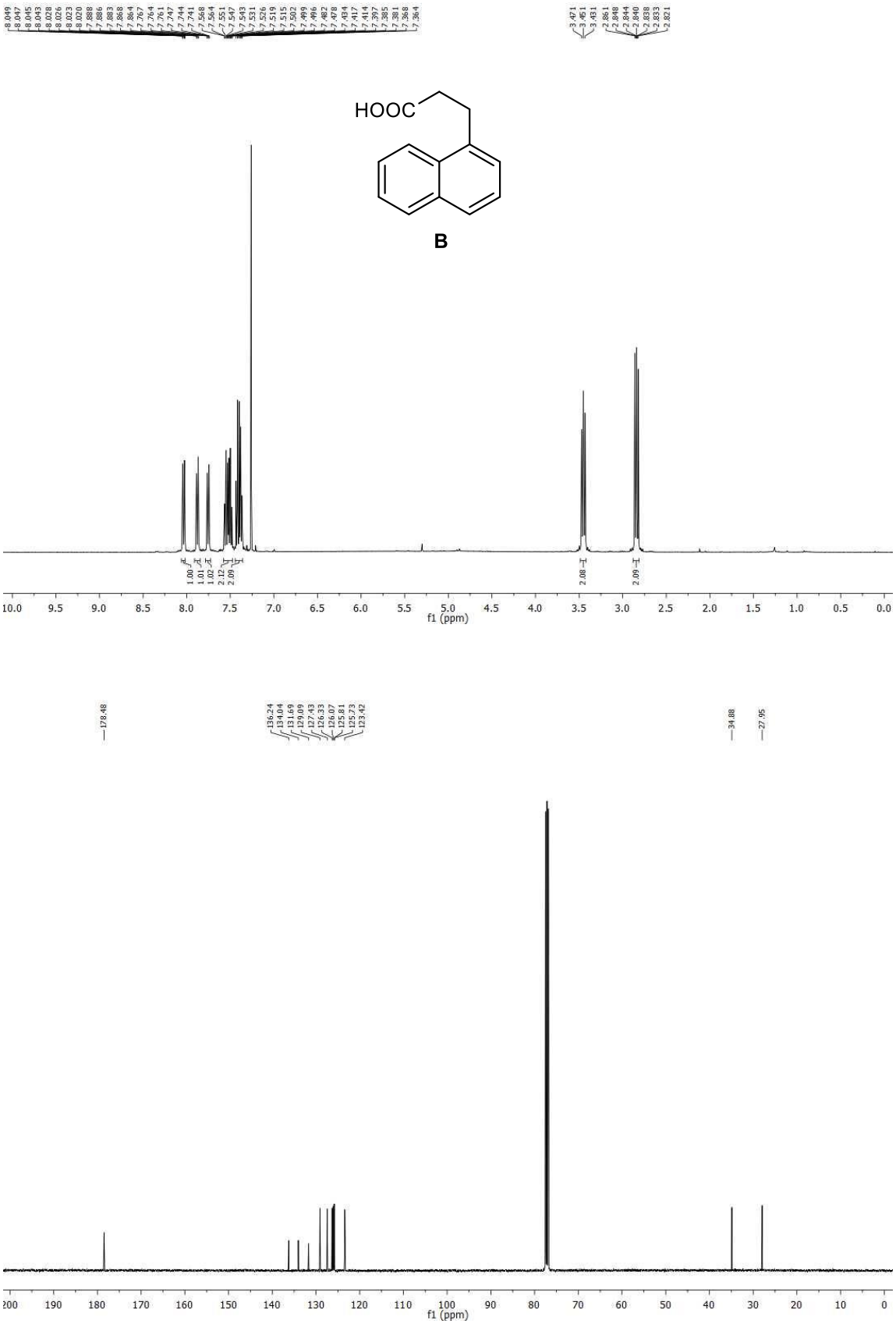


Figure S7. ^{1}H NMR and ^{13}C NMR spectra of compound **B** in $CDCl_3$.

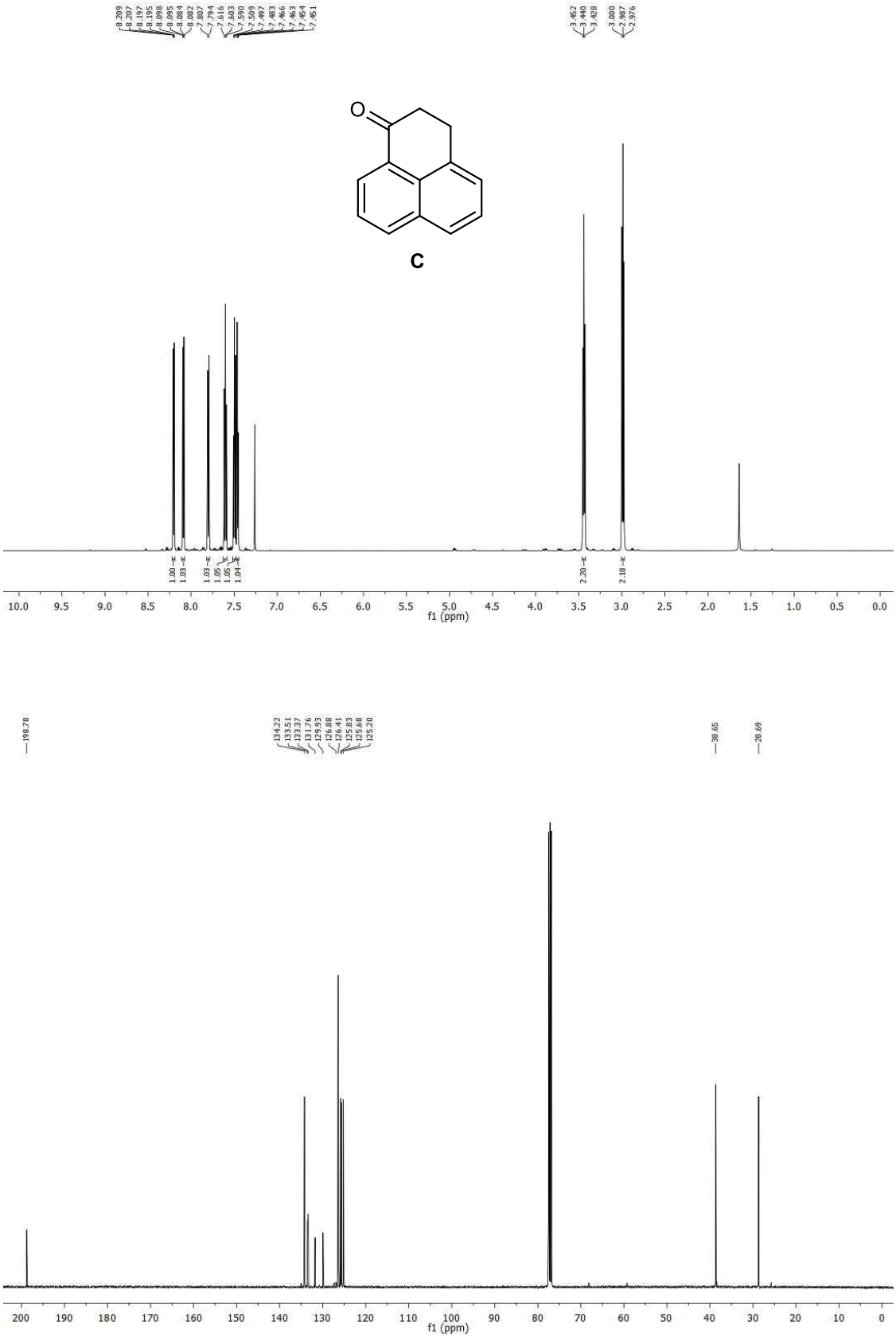


Figure S8. ^{1}H NMR and ^{13}C NMR spectra of compound **C** in $CDCl_3$.

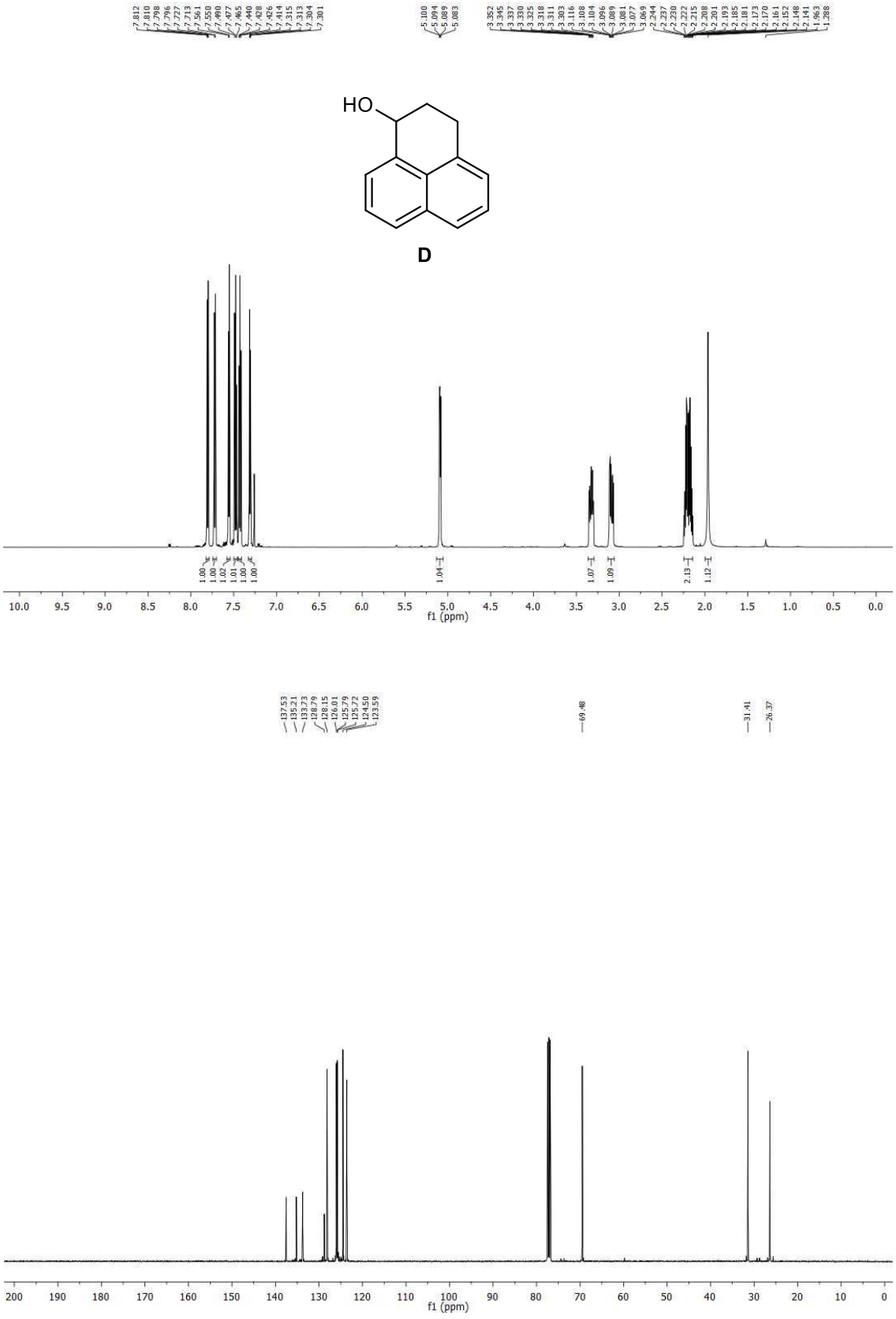


Figure S9. ^{1}H NMR and ^{13}C NMR spectra of compound **D** in $CDCl_3$.

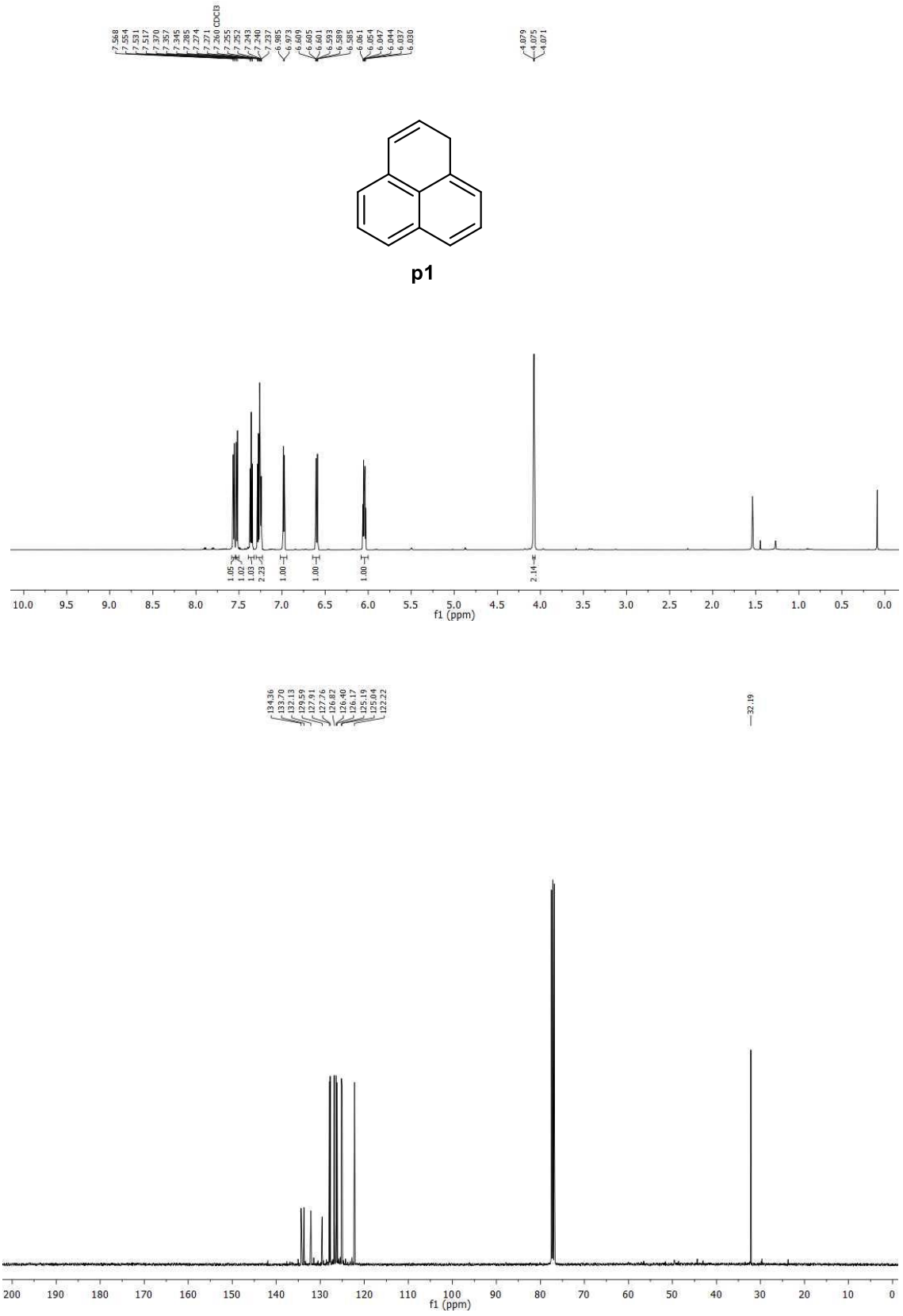


Figure S10. ^{1}H NMR and ^{13}C NMR spectra of compound **p1** in $CDCl_3$.

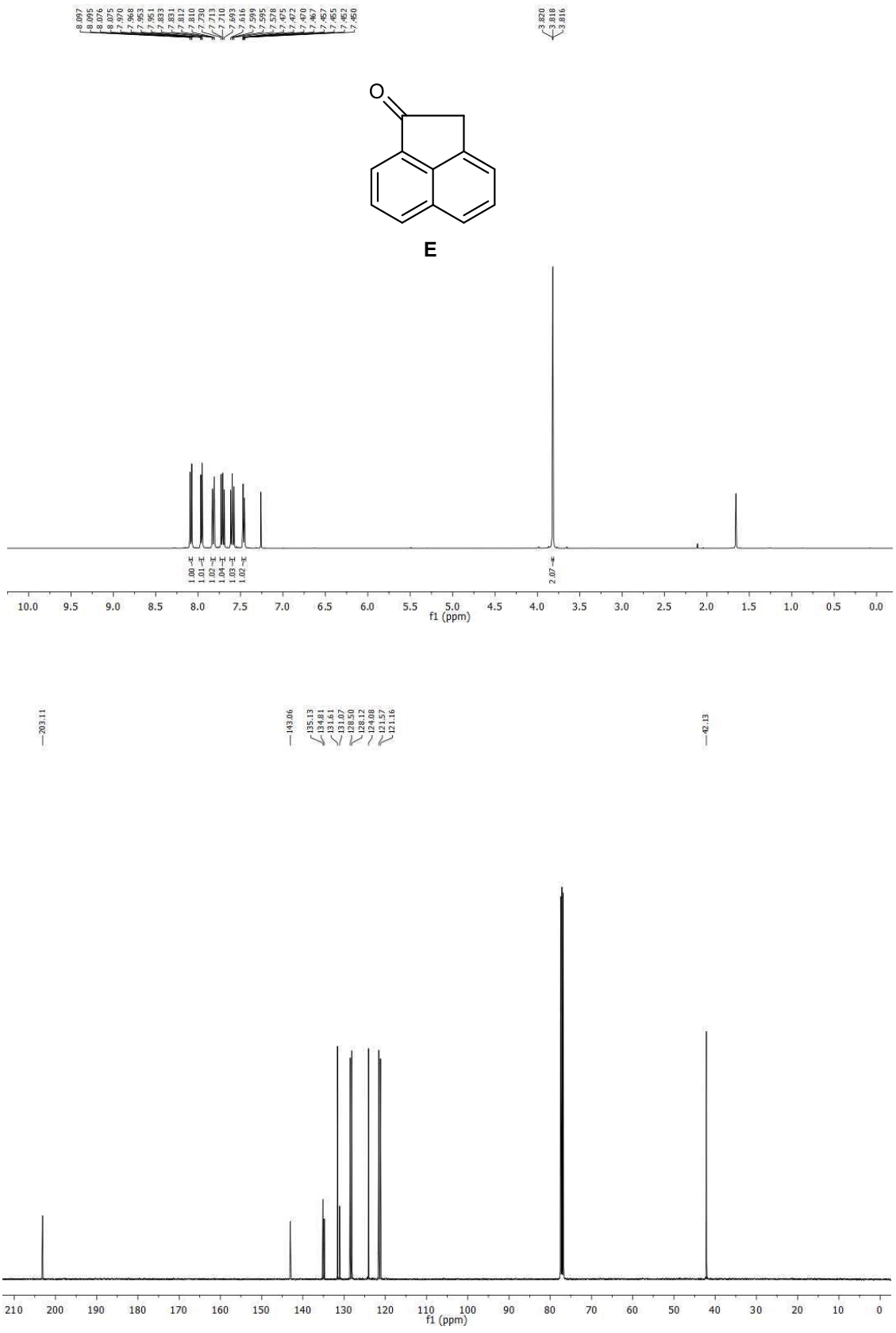


Figure S11. ^{1}H NMR and ^{13}C NMR spectra of compound **E** in $CDCl_3$.

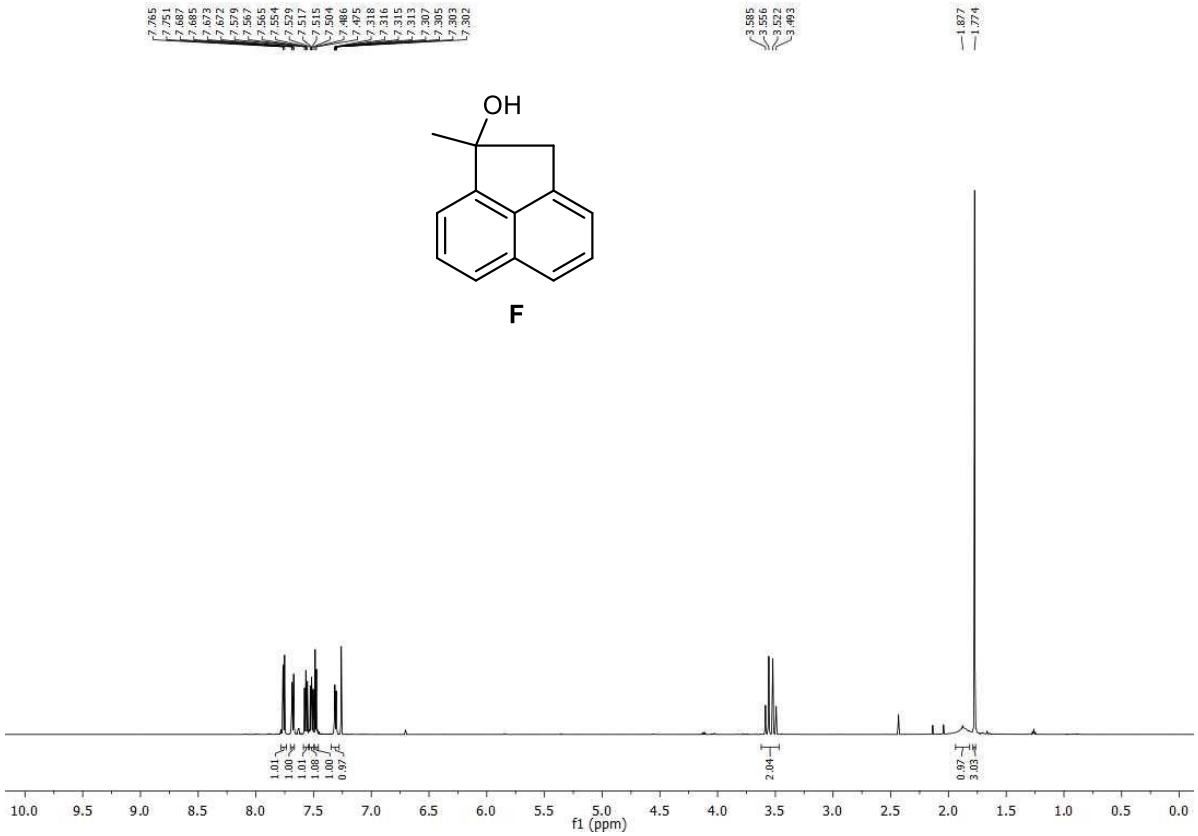


Figure S12. ^{1}H NMR spectrum of compound **E** in $CDCl_3$.

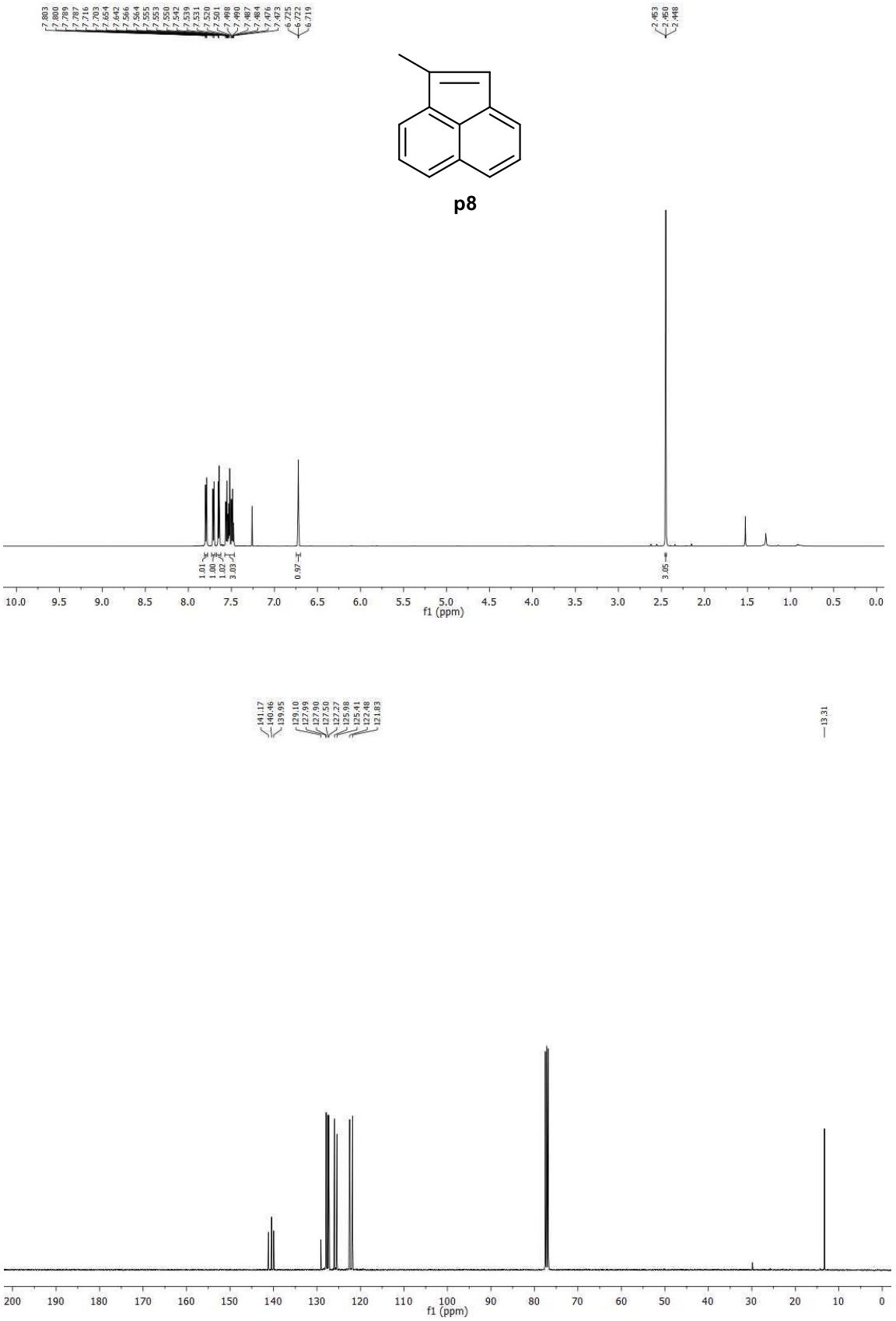


Figure S13. ^{1}H NMR and ^{13}C NMR spectra of compound **p8** in $CDCl_3$.

Note S1. Input file for RRKM-ME calculations using the MESS package for the 1-naphthyl + C_3H_4 reactions, including coordinates and vibrational frequencies for all species involved.

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H -0.0053442043 3.6756196076 -0.0766070885
H 2.2531764477 2.7063004221 0.1910688485
H 3.7147024425 0.7429028288 0.3266782013
H 4.0237158253 -1.7060739629 0.3348780273
H -0.1951506358 -2.2736481653 -0.1525038556
H 2.0532742547 -3.206917166 0.098483872
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 66
42.2735 87.8768 136.4419
160.1998 180.5972 223.3749
244.2594 374.3249 392.8798
432.6205 445.9414 480.8198

510.9639 536.2310 554.7665
626.2304 663.3195 737.4691
748.7638 789.4189 799.2751
809.2722 824.8445 859.9272
885.3938 922.4455 926.3534
965.7695 982.8095 996.6789
1035.2265 1038.5090 1044.6602
1054.2184 1099.2856 1168.2936
1183.2084 1189.1448 1231.6391
1253.2343 1276.2703 1301.0625
1372.3072 1389.4254 1394.2218
1420.6350 1458.4557 1467.3218
1470.9361 1491.6067 1544.9071
1611.4148 1632.7519 1661.0809
1734.5659 2972.0473 3044.0034
3063.9135 3088.0838 3157.7277
3160.4495 3168.9337 3174.3289
3183.5970 3187.4022 3196.4680
ZeroEnergy[kcal/mol] -39.43
ElectronicLevels[1/cm] 1
0 2
End
End
!----------
!-------well_i3----------
Well i3
Species
RRHO
Geometry[angstrom] 24
C 0.0108561018 0.5425057255 0.0053570418
C 1.3949064632 1.2309915061 0.0418821584
C 0.3853246135 2.0275843306 0.0676996182
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
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

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 -0.6711136473
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
Core RigidRotor
SymmetryFactor 0.5
End
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

!---------------------------------
!-------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

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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