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A Free Radical Pathway to Hydrogenated Phenanthrene in Molecular Clouds – Low Temperature Growth of Polycyclic Aromatic Hydrocarbons

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Abstract: The Hydrogen-Abstraction/Acetylene-Addition mechanism has been fundamental to unravelling the synthesis of polycyclic aromatic hydrocarbons (PAHs) detected in combustion flames and carbonaceous meteorites like Orgueil and Murchison. However, the fundamental reaction pathways accounting for the synthesis of complex PAHs such as the tricyclic anthracene and phenanthrene along with their dihydrogenated counterparts remain elusive to date. By investigating the hitherto unknown chemistry of the 1-naphthyl radical with 1,3-butadiene, we reveal a facile *barrierless* synthesis of dihydrophenanthrene adaptable to low temperatures. These aryl-type radical additions to conjugated hydrocarbons via resonantly stabilized free radical intermediates defy conventional wisdom that PAH growth is predominantly a high temperature phenomenon and thus may represent an overlooked path to PAHs as complex as coronene and corannulene in cold regions of the interstellar medium like in the Taurus Molecular Cloud.

The Hydrogen-Abstraction/Acetylene-Addition (HACA) mechanism[1] has been instrumental for rationalizing the synthesis of polycyclic aromatic hydrocarbons (PAHs) – organic molecules carrying fused benzene rings – in high temperature combustion systems[2-3] and in circumstellar envelopes of carbon-rich asymptotic giant branch (AGB) stars.[3-4] The ubiquity of PAHs along with their (de)hydrogenated, ionized, and side-chain-substituted counterparts in the interstellar medium (ISM)[5-6] is surmised from the unidentified infrared (UIR) emission bands (3 to 20 μm)[7-8] and the UV-bump[9-11] – an absorption feature superimposed on the interstellar extinction curve near 217.5 nm – that correlate with laboratory spectra of aromatic hydrocarbons. Although individual PAHs have not been detected in the ISM yet, the explicit identification of PAHs like phenanthrene and anthracene ($C_{14}H_{10}$) in carbonaceous chondrites like Murchison and Orgueil bearing anomalous $^{13}C/^{12}C$ and D/H isotopic ratios[12-15] strongly suggests an inter-stellar origin with fashionable astrochemical reaction networks mainly loaned from the combustion chemistry community.

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Here, under fuel rich conditions, acetylene (C_2H_2) has been proposed to react with aromatic hydrocarbons undergoing ring formation and expansion through a series of bimolecular reactions assembled in the HACA mechanism. Kinetic modeling[16-19] along with electronic structure calculations[20-24] suggest recurring progressions of hydrogen atom abstractions from the aromatic hydrocarbon followed by sequential addition of two acetylene molecules to the radical sites prior to cyclization and aromatization. Recent studies exploiting tunable vacuum ultraviolet (VUV) light exposed that the naphthalene molecule ($C_{10}H_8$) can be formed via the reaction of the phenyl radical (C_6H_5·) with two acetylene molecules (C_2H_2)[25] through key transients in the HACA framework – styrenyl (C_8H_7·) and *ortho*-vinylphenyl (C_8H_7·).[26] HACA-type reactions involving naphthyl ($C_{10}H_7$·) and of biphenylyl radicals ($C_6H_5C_6H_4$·) with acetylene have also lead to the three-membered ring PAHs acenaphthylene ($C_{12}H_8$)[27] and phenanthrene ($C_{14}H_{10}$),[28] respectively, under high temperature combustion-relevant conditions.

High temperatures along with acetylene enrichment near the photosphere of carbon-rich Asymptotic Giant Branch (AGB) stars underscore HACA's applicability to describing soot production in these outflows. Aromatic species [benzene (C_6H_6) or phenyl (C_6H_5)] likely form within the envelope and undergo processing into polycyclic compounds via HACA[4] before exiting to the ISM as 'free' PAHs, or condensed as carbonaceous grains or fullerenes.[4, 29-30] Carbonaceous grains comprising aromatic interiors[31] could contribute to the interstellar PAH budget through shattering facilitated by turbulence or supernova-induced shockwaves that release aromatic content to the ISM.[32-33] However, in recent years, astronomical models combined with observations revealed that the destruction of interstellar PAHs and carbonaceous grains by, for example, high velocity shockwaves, limit their lifetime to a few 10^8 years.[34-35] This time span is much shorter than the PAH injection time from stellar sources, including C-rich AGB stars such as CW Leo (IRC+10216), of some 10^9 years, and thus the ubiquitous distribution of PAH-like species in the interstellar medium coupled with the less-than-expected production of PAHs in circumstellar envelopes suggests that crucial routes for the fast chemical growth of PAHs are missing. These routes may involve low temperature interstellar environments such as cold molecular clouds that hold temperatures down to 10 K. Considering the barriers of acetylene addition to aromatic radicals of typically 10 to 20 kJ mol^{-1},[20] HACA cannot operate in cold molecular clouds, since these entrance barriers cannot be overcome. Therefore, key production routes to PAH-like species in the interstellar medium associated with molecular growth processes are clearly missing.

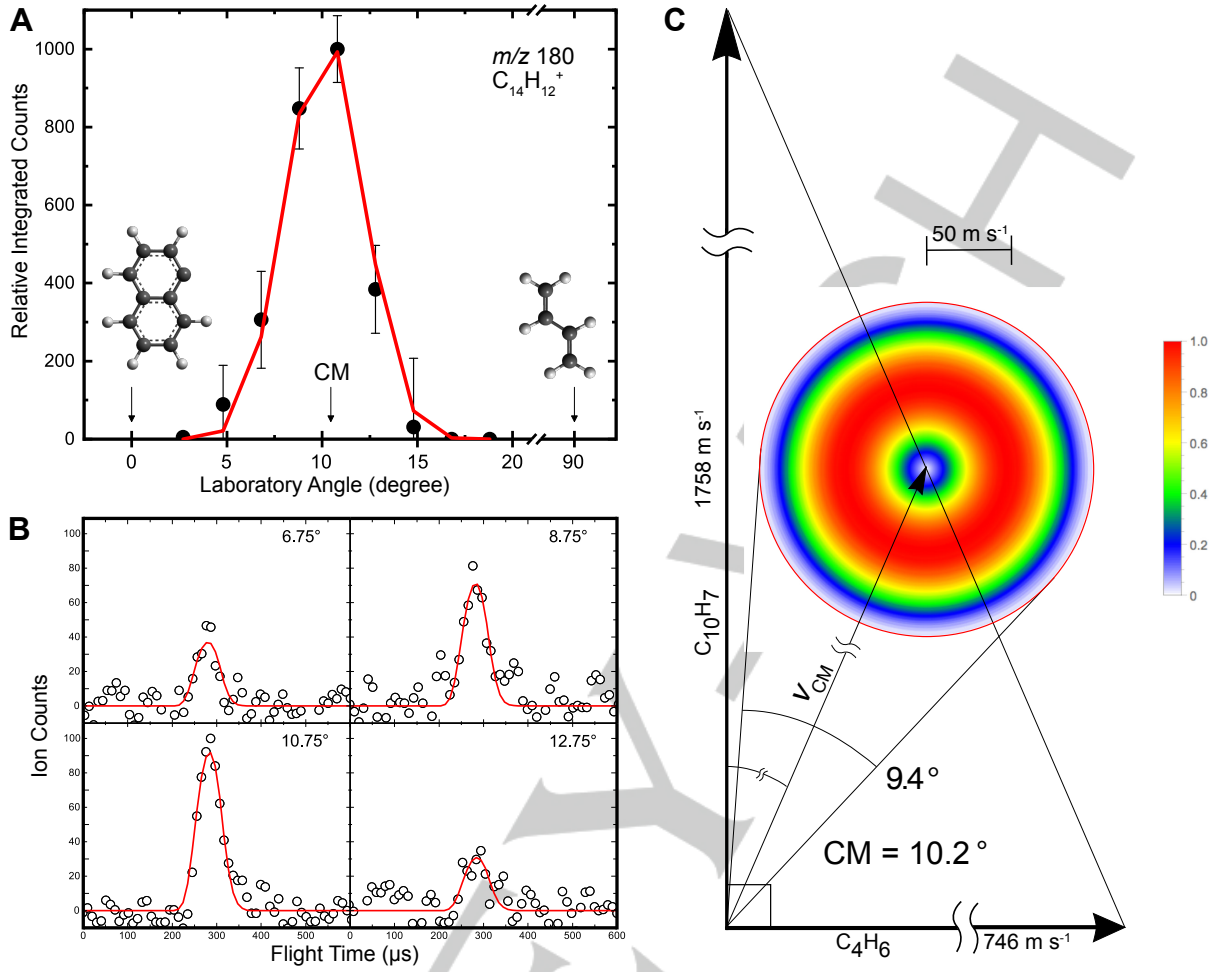


Figure 1. Laboratory angular distribution (A) and time-of-flight spectra (B) recorded at mass-to-charge 180 ($C_{14}H_{12}^+$) in the reaction of 1-naphthyl with 1,3-butadiene. The circles define the experimental data and the red lines represent the fitting based on the best-fit center-of-mass functions, as depicted in Figure 3. Error bars are standard error of the mean. The CM arrow indicates the center-of-mass angle. (C) Newton Diagram depicting the distribution of $C_{14}H_{12}$ produced in the crossed molecular beams reaction of 1-naphthyl + 1,3-butadiene. The differential cross section has a radius equal to the maximum center of mass velocity of $C_{14}H_{12}$.

Herein, we report the reaction dynamics of the aromatic 1-naphthyl radical [$C_{10}H_7$· (X^2A')] with 1,3-butadiene [C_4H_6 (X^1A_g)] under single collision conditions in a crossed molecular beam experiment (Experimental Methods; Supporting Information) as a prototype system of a barrier-less ring expansion in PAHs via aryl radical reactions with conjugated hydrocarbons.[36] A recent combined experimental, computational, and modeling study suggests that 1,3-butadiene can be synthesized in the gas phase via the reaction of the methylidyne radical (CH) with propylene (C_3H_6),[37] which are known constituents of the ISM. Combined with electronic structure calculations, our study exposes the first *barrierless* synthesis of a tricyclic PAH – 1,4-dihydrophenanthrene ($C_{14}H_{12}$) – via ring expansion involving resonantly stabilized free radical (RSFR) intermediates that underscore PAH mass growth processes in the cold interstellar medium beyond the classical HACA framework. This system is also interesting from the viewpoint of a physical–organic chemist as a benchmark to unravel the chemical reactivity, bond breaking processes, and the synthesis of truly combustion and astrochemically relevant cyclic and aromatic hydrocarbons via bimolecular gas-phase reactions in single collision events.

In the crossed molecular beam reaction of the 1-naphthyl radical with 1,3-butadiene, scattering signal was probed for the adduct at *m/z* 181 ($C_{14}H_{13}^+$) and for the atomic and molecular hydrogen loss channels at *m/z* 180 ($C_{14}H_{12}^+$) and *m/z* 179 ($C_{14}H_{11}^+$), respectively. Considering that no signal was detectable at *m/z* 181 and that the time-of-flight spectra (TOF) at *m/z* 180 and *m/z* 179 are superimposable after scaling, only the atomic hydrogen loss channel leading to a hydrocarbon with the molecular formula $C_{14}H_{12}$ is open under the current experimental conditions. Therefore, TOF spectra were collected at *m/z* 180. TOF spectra were integrated and scaled to yield the laboratory angular distribution of $C_{14}H_{12}$, which depicts a relatively narrow spread of 10° holding a maximum close to the center-of-mass angle of 10.2 ± 1.1° (Figure 1). This shape proposes a complex forming reaction mechanism (indirect scattering dynamics) involving $C_{14}H_{13}$ reaction intermediate(s). However, considering that the hydrogen atom can be emitted from the 1-naphthyl radical and/or from the 1,3-butadiene reactant, the latter was substituted

ceteris paribus by the isotopologue 1,3-butadiene-d_6 (C_4D_6). In this system, reactive scattering signal was probed at *m/z* 186 ($C_{14}H_6D_6^+$) and *m/z* 185 ($C_{14}H_7D_5^+$) at the center-of-mass angle 11.3 ± 1.1°. Signal was detected at *m/z* 186 and *m/z* 185. Within the signal-to-noise, the TOF of the *m* = 2 loss channel (*m/z* 185) overlays agreeably with that of the atomic hydrogen loss channel (*m/z* 186). Therefore, we can conclude that atomic hydrogen is

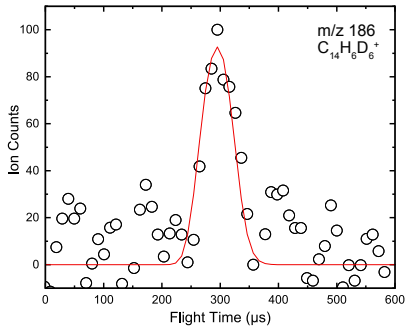


Figure 2. Time-of-flight spectrum taken at the center-of-mass angle for the reaction of 1-naphthyl with 1,3-butadiene-d_6 recorded at mass-to-charge ratio 186 ($C_{14}H_6D_6^+$). The circles define the experimental data and the red line represents the fitting based on the best-fit center-of-mass functions.

emitted from the 1-naphthyl radical leading to signal at *m/z* 186, and that the signal observed at *m/z* 185 likely results from dissociative ionization of $C_{14}H_6D_6$. The corresponding TOF spectrum taken at *m/z* 186 at the center-of-mass is depicted in Figure 2. In summary, our laboratory data alone suggest that in the reaction of the 1-naphthyl radical with 1,3-butadiene, a hydrocarbon molecule of the formula $C_{14}H_{12}$ is formed via indirect reaction dynamics with the hydrogen atom displaced from the naphthyl moiety (Reaction (1)).

(1) $$C_{10}H_7\cdot + C_4H_6 \rightarrow C_{14}H_{12} + H\cdot$$

The goal of our investigation is not only to obtain the molecular formula of the reaction product ($C_{14}H_{12}$), but also to explore the structure(s) of the product isomer(s) together with the underlying reaction mechanism(s) and chemical dynamics possibly leading to PAH(s). This is accomplished through a forward-convolution routine that transforms the laboratory data into the center-of-mass reference frame.[38-39] The outcome is two 'best-fit' center-of-mass functions: the translational energy $P(E_T)$ and angular $T(\theta)$ flux distributions (Figure 3). It is important to highlight that the laboratory data could be fit with a single reaction channel leading to $C_{14}H_{12}$ plus atomic hydrogen via the 1-naphthyl radical and 1,3-butadiene reactants. The best fit center-of-mass (CM) angular flux distribution, $T(\theta)$, is isotropic and depicts flux over the complete scattering range. This finding is indicative of an indirect reaction mechanism that proceeds through the formation of rovibrationally excited $C_{14}H_{13}$ intermediate(s). Within the error limits, a slightly forward $T(\theta)$ distribution could fit the experimental data as well. The (nearly) isotropic distribution results from the inability of the light hydrogen atom to carry away a significant fraction of the initial total angular momentum.[40] Most important, the translational energy flux distribution, $P(E_T)$, reveals a maximum product translational energy (E_{max}) of 173 ± 25 kJ mol^{-1}. For molecules born without rovibrational excitation, E_{max} represents the sum of the collision energy plus the reaction exoergicity. Therefore, a subtraction of the collision energy from E_{max} reveals that the reaction to form $C_{14}H_{12}$ along with atomic hydrogen is exoergic by 104 ± 25 kJ mol^{-1}. Also, the $P(E_T)$ shows a distribution maximum at 14 ± 4 kJ mol^{-1}, which suggests that the unimolecular decomposition of the $C_{14}H_{13}$ complex involves a tight exit transition state. Therefore, the reverse reaction is characterized by an entrance barrier of hydrogen atom addition to a closed shell (unsaturated) hydrocarbon. Taken together, the center-of-mass functions $P(E_T)$ and $T(\theta)$ reveal that 1-naphthyl plus 1,3-butadiene reactively scatters forming a hydrogen atom plus the heavy $C_{14}H_{12}$ product via a (long-lived) $C_{14}H_{13}$ intermediate in an overall exoergic reaction.

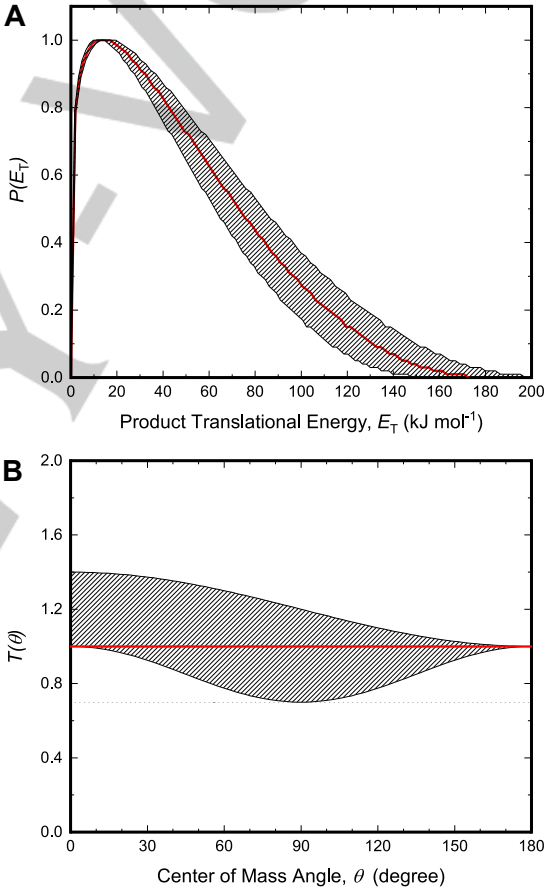


Figure 3. Center-of-mass translational energy flux distribution $P(E_T)$ (A) and angular flux distribution $T(\theta)$ (B) leading to the formation of the $C_{14}H_{12}$ molecule plus atomic hydrogen in the reaction of 1-naphthyl with 1,3-butadiene. Shaded areas indicate the acceptable upper and lower error limits of the fits. The red solid lines define the best-fit functions.

We now merge these experimental results with the computational data to untangle the underlying reaction mechanism(s) and to evaluate to what extent reaction (1) can lead to the formation of a tricyclic PAH (Figure 4). The computations at the G3(MP2,CC)//B3LYP/6-311 G** level of theory (Computational Methods; Supporting Information) reveal five

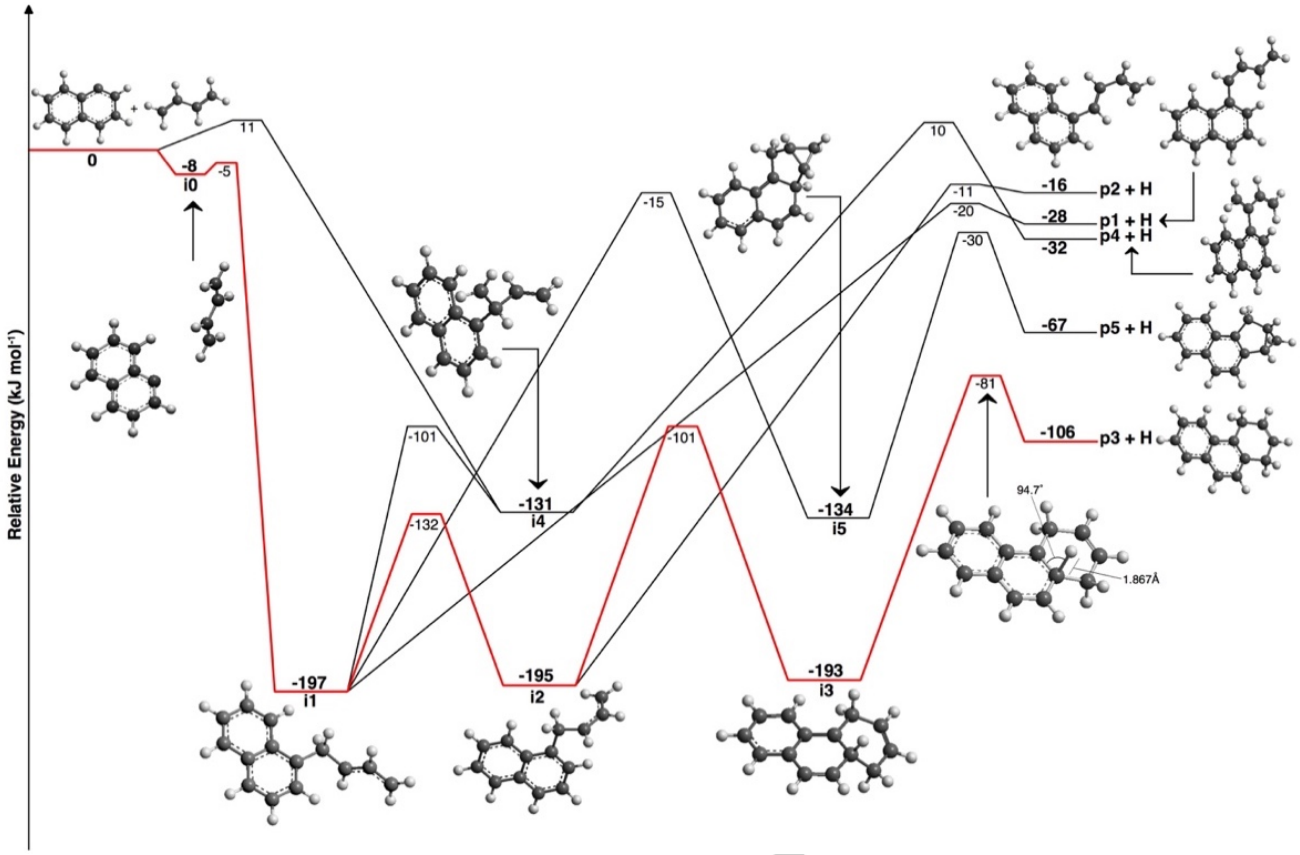
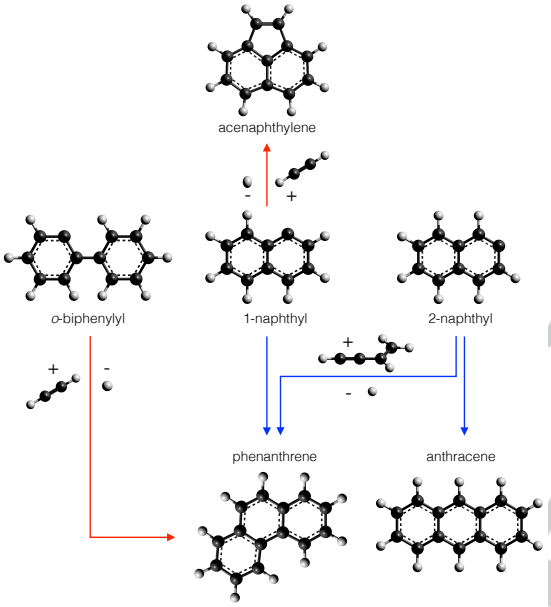


Figure 4. Potential energy surface for the reaction of 1-naphthyl [$C_{10}H_7$· (X^2A')] plus 1,3-butadiene [C_4H_6 (X^1A_g)] depicting hydrogen-loss channels. Energies are relative to the separated reactants; energies are given in kJ mol^{-1}. The minimum energy path leading to the 1,4-dihydrophenanthrene ($C_{14}H_{12}$) plus atomic hydrogen products is highlighted in red. Details on the structures and vibrational frequencies are compiled in the Supporting Information.

exit channels leading to distinct $C_{14}H_{12}$ isomers, **p1** to **p5**, with overall exoergicities ranging from 16 to 106 kJ mol^{-1}. A comparison of these data with the experimental reaction energy of 104 ± 25 kJ mol^{-1} reveals that the formation of the thermodynamically most favorable isomer **p3** (1,4-dihydrophenanthrene) can account for the experimentally derived reaction energy; based on the energetics alone, we cannot eliminate contributions of the thermodynamically less favorable isomers. The electronic structure calculations exposed a barrierless pathway to 1,4-dihydrophenanthrene initiated by the formation of a van-der-Waals complex **i0** from the separated reactants. This complex is weakly bound by 8 kJ mol^{-1} and isomerizes via a barrier of only 3 kJ mol^{-1} through addition of the radical center of the 1-naphthyl radical to the C1-carbon of 1,3-butadiene forming a resonantly stabilized intermediate **i1**. After a facile *cis-trans* isomerization from **i1** to **i2**, cyclization leads to intermediate **i3**, which is bound by 193 kJ mol^{-1} with respect to 1-naphthyl plus 1,3-butadiene. A hydrogen elimination from the bridging carbon atom leads to aromatization and formation of **p3** (1,4-dihydrophenanthrene) through a tight exit transition state that lies 25 kJ mol^{-1} above the separated products. This order of magnitude is in line with the experimental observation of an exit barrier close to 14 ± 4 kJ mol^{-1} with the hydrogen atom eliminated almost perpendicularly to the plane of the decomposing complex. It is important to recall that in the reaction of 1-naphthyl with 1,3-butadiene-d_6, a hydrogen atom loss was observed. Tracing the deuterium atoms in the 1,3-butadiene reactant supports this finding. Here, all deuterium atoms stay with the 1,3-butadiene moiety, and in the formation of 1,4-dihydrophenanthrene, the hydrogen atom is eliminated exclusively from the bridged carbon atom. Considering the energies of the barriers to isomerization, formation of **p1** (from **i1**), **p2** (from **i2**), **p4** (from **i1** via **i4**), and **p5** (from **i1** via **i5**) is unfavorable. At the low temperatures of the interstellar medium, alternative hydrogen abstraction pathways forming naphthalene plus C_4H_5 isomers along with the addition of the naphthyl radical to the C2 position of 1,3-butadiene are closed (Figure S1). However, these pathways may be open at elevated collision energies and equivalent higher temperatures.

Our experimental and computational investigation of the 1-naphthyl plus 1,3-butadiene reaction provides compelling evidence on the facile and barrierless formation of a three-ringed PAH – 1,4-dihydrophenanthrene – under single collision conditions. The reaction follows indirect scattering dynamics and is initiated by the formation of a weakly-bound van-der-Waals complex, followed by the addition of the naphthyl radical to the C1-carbon of C_4H_6 yielding a resonantly stabilized free radical intermediate. The latter isomerized in two steps ultimately leading to 1,4-dihydrophenenthrene accompanied by hydrogen atom loss and aromatization. In the cold interstellar medium, due to the absence of an entrance barrier and location of all inherent barriers

to isomerization residing below the energy of the separated reactants, this reaction leads *exclusively* to 1,4-dihydrophenanthrene. Indeed, statistical (Rice−Ramsperger−Kassel−Marcus; RRKM) calculations carried out for zero-pressure conditions corresponding to crossed molecular beam experiments as well as to cold molecular clouds showed that the relative yield of 1,4-dihydrophenanthrene changes only very slightly from 100% at zero collision energy to 99.5% at the collision energy of 100 kJ mol^{-1} if one considers the barrierless addition channels of 1-naphthyl to 1,3-butadiene. At the high collision energy, about 0.4% of the **p1** product is predicted to be formed. However, under combustion-relevant conditions at finite pressures, the reaction changes likely to a multichannel process that produces energetically less favorable $C_{14}H_{12}$ isomers along with potential hydrogen abstraction products. It is worth mentioning however that the difference in the barrier heights to form 1,4-dihydrophenanthrene and **p1** is 61 kJ mol^{-1}, that is 15 kJ mol^{-1} higher than the difference in the barrier heights to form 1,4-dihydronaphthalene and the one-ring analog of **p1** in the phenyl + 1,3-butadiene reaction.[41] This change originates from the additional aromatic stabilization due to the presence of the extra ring and results in a higher yield of 1,4-dihydrophenanthrene as compared to that of 1,4-dihydronaphthalene from C_6H_5 + C_4H_6.[41] Therefore, for larger PAHs, the analogous reactions of their radicals with 1,3-butadiene are anticipated to lead to a one-ring extension even more efficiently.



Scheme 1. C_2H_2 addition to *o*-biphenylyl, 1-napthyl, and 2-naphthyl is inhibited by an entrance barrier (red), while that of C_4H_4 proceeds barrierlessly and is thus viable at extremely low temperatures (blue). All paths shown are exoergic overall.

Considering that the related reactions of the phenyl radical with 1,3-butadiene[41] and vinylacetylene[42] synthesize 1,4-dihydronaphthalene and naphthalene, respectively, via submerged barriers, and that the 1-naphthyl-1,3-butadiene system leads solely to 1,4-dihydrophenanthrene at ultralow temperatures, our present works leads us to the prediction that the reaction of the 1-napthyl and 2-napthyl radicals with vinylacetylene is likely to result in the barrierless formation of phenanthrene and anthracene ($C_{14}H_{10}$) in the cold interstellar medium, such as in the Taurus Molecular Cloud TMC-1 (Scheme 1). Our recent RRKM – Master Equation calculations have shown that in the prototype phenyl plus vinylacetylene reaction naphthalene remains a major or significant low-temperature product up to the pressure of 10^{-7} bar.[43] This mechanism represents a hitherto overlooked low-energy (temperature) pathway to PAH growth – among them catacondensed $C_{14}H_{10}$ and $C_{14}H_{12}$ isomers - in the interstellar medium, and may resemble a key pathway for the addition of six-membered rings to existing PAHs that lack a bay-region. Once those pathways of 1- and 2-napthyl radicals with vinylacetylene have been unraveled, astrochemists and combustion scientists will be in the position to quantify the contribution of vinylacetylene and 1,3-butadiene mediated routes to PAHs in distinct extreme environments.

In conclusion, our study reveals the first low temperature pathway accounting for the barrierless formation of a tricyclic (polycyclic) aromatic hydrocarbon - 1,4-dihydrophenanthrene ($C_{14}H_{12}$) - via the elementary bimolecular gas phase reaction of the 1-naphthyl radical ($C_{10}H_7$·) with 1,3-butadiene (C_4H_6). The reaction proceeds by a de-facto barrierless addition of the naphthyl radical with its radical center to the H_2C moiety of the 1,3-butadiene reactant – facilitated by a weakly bound van der Waals complex – followed by isomerization and atomic hydrogen loss accompanied by aromatization to form 1,4-dihydrophenanthrene. Statistical (RRKM) calculations confirm that the pathway leading to 1,4-dihydrophenanthrene plus atomic hydrogen accounts for 100% of all products in the limit of zero collision energy as closely present in cold molecular clouds such as TMC-1. This combination of experimental, *ab initio*, and statistical methodologies presented in this work reveals a novel reaction mechanism of aryl-type radical additions to conjugated hydrocarbon systems like 1,3-butadiene and vinylacetylene (C_4H_4), and changes how we think about molecular growth processes to PAHs in the cold regions of space.

Experimental Section

See Supportingl Information.

Acknowledgements

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The authors declare no conflicts of interest.

Keywords: gas phase chemistry • polycyclic aromatic hydrocarbon • astrochemistry • aryl radicals • mass spectrometry

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COMMUNICATION

At low temperature extremes like those found in Taurus Molecular Cloud, polycyclic aromatic hydrocarbons increase their complexity via conjugated hydrocarbons. By probing the reaction of the aromatic naphthyl radical with 1,3-butadiene under single-collision conditions, we find that the tricyclic dihydrophenanthrene molecule constitutes 100% of product formation at conditions relevant to the cold interstellar medium. The underlying reaction type, namely aryl addition to conjugated hydrocarbons, defies conventional PAH growth schemes and may be key to understanding the reappropriation of interstellar carbon into macromolecules.

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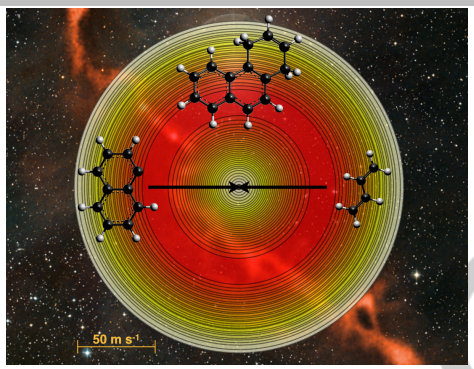

Gas-Phase Chemistry

A. M. Thomas, M. Lucas, T. Yang, R. I. Kaiser, L. Fuentes, D. Belisario-Lara, A. M. Mebel**

Page No. – Page No.

A Free Radical Pathway to Hydrogenated Phenanthrene in Molecular Clouds – Low Temperature Growth of Polycyclic Aromatic Hydrocarbons

Experimental Methods

The reaction of the 1-naphthyl ($C_{10}H_7$·) radical with 1,3-butadiene (C_4H_6) was performed in a universal crossed molecular beams machine at the University of Hawaii.[1] A pulsed supersonic beam of naphthyl radicals was generated via photodissociation (ArF, 193 nm, 30 mJ/pulse) of helium (99.9999%; AirGas; 1034 Torr) seeded 1-chloronaphthalene ($C_{10}H_7Cl$: >97.0%; Tokyo Chemical Industry). Here, the precursor was purified through two freeze-thaw cycles and heated to 448 K to reach a seeding fraction of 8%. After photodissociation of the pulsed precursor beam 1 mm downstream of the nozzle, the 1-naphthyl radical beam was skimmed then velocity-selected by a 4-slot chopper wheel before colliding perpendicularly with a supersonic beam of 1,3-butadiene released by a second pulsed valve at a backing pressure of 550 Torr. The peak velocities and speed ratios of the 1-naphthyl and 1,3-butadiene beams were determined to be v_p = 1758 ± 10 m s^{-1} and S = 13.5 ± 1.3 as well as v_p = 746 ± 10 m s^{-1} and S = 8.4 ± 0.4, respectively, where the secondary pulsed valve was triggered 100 μs prior to the primary valve. The 1-naphthyl plus 1,3-butadiene reaction was repeated using the 1,3-butadiene-d_6 (1,3-C_4D_6: 98% D; Icon Isotopes) isotopologue.

Product detection was accomplished by using a triply differentially pumped universal detector that is rotatable in the plane defined by the reactant beams. Neutral products entered the detector and were ionized with 40 eV electrons, mass-filtered by a quadrupole mass spectrometer (1.2 MHz), and detected by a Daly detector. The latter employs an aluminum-coated stainless steel target (-25 kV), an aluminum-coated scintillator, and a photomultiplier tube (1.35 kV). Data were interpreted in the center-of-mass frame via a forward convolution routine that accounts for the machine and beam parameters.[2-3] The best fits were achieved iteratively through the comparison of the experimentally recorded data and the computed outputs from the resulting differential cross section (DCS). The DCS $I(E_T, \theta)$ is assumed to be separable into the translational energy E_T and angularly θ dependent components, i.e. $I(E_T, \theta) = P(E_T)$ x $T(\theta)$. Upper and lower error bounds of the $P(E_T)$ and $T(\theta)$ fits were determined through the error limits of the laboratory angular distribution along with the uncertainties in the beam velocities.

Computational Methods

Geometries of the reactants, products and various intermediates and transition states on the $C_{14}H_{13}$ potential energy surface were optimized at the hybrid density functional B3LYP level of theory[4-5] with the 6-311G** basis set. The same B3LYP/6-311G** method was employed to calculate vibrational frequencies, which were then used to compute zero-point energy (ZPE) corrections, to characterize the stationary points as minima or first-order saddle points, and to evaluate rate constants for unimolecular reaction steps. Single-point energies were refined using the G3(MP2,CC)//B3LYP modification[6-7] of the original Gaussian 3 (G3) scheme,[8] which provides accuracy for relative energies within 10 kJ mol^{-1}. The ab initio and DFT calculations were carried out using the GAUSSIAN 09[9] and MOLPRO 2010[10] program packages. Relative reaction product yields under single-collision conditions were computed using Rice− Ramsperger−Kassel−Marcus (RRKM) theory.[11-13] The rate constants were calculated as functions of available internal energy, where the internal energy was taken as a sum of the energy of chemical activation in the reaction of 1-naphthyl with 1,3-butadiene and the collision energy, assuming that a dominant fraction of the latter is converted to internal vibrational energy. Only a single

total-energy level was considered throughout, as for single-collision conditions (zero-pressure limit).[14] The harmonic approximation was employed to compute numbers and densities of state required for evaluating the rate constants. Using the calculated rate constants, product branching ratios were computed by solving first-order kinetic equations within the steady-state approximation for unimolecular isomerization and fragmentation steps of initial reaction intermediates formed as a result of the addition of 1-naphthyl to 1,3-butadiene.

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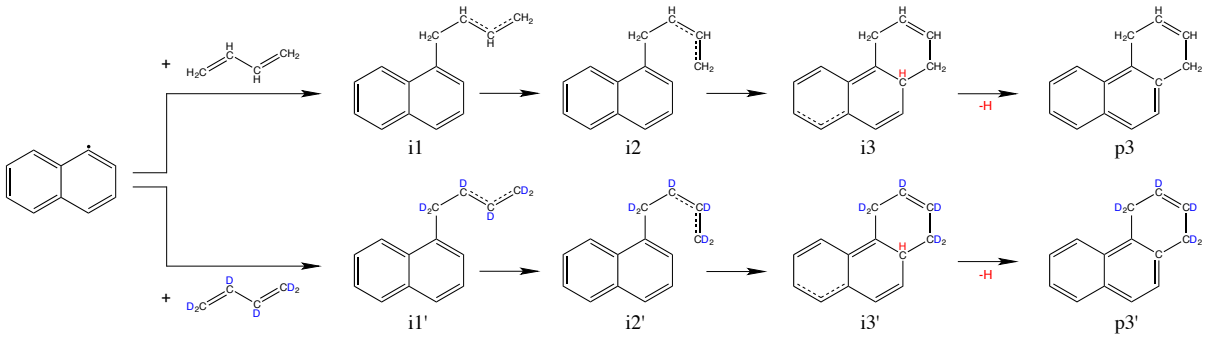


Figure S1. Structural schematic of the 1-napthyl + 1,3-butadiene(-d_6) reaction coordinate leading to the formation of 1,4-dihydrophenanthrene(-1,1,2,3,4,4-d_6) derived from the potential energy surface depicted in Figure 4.

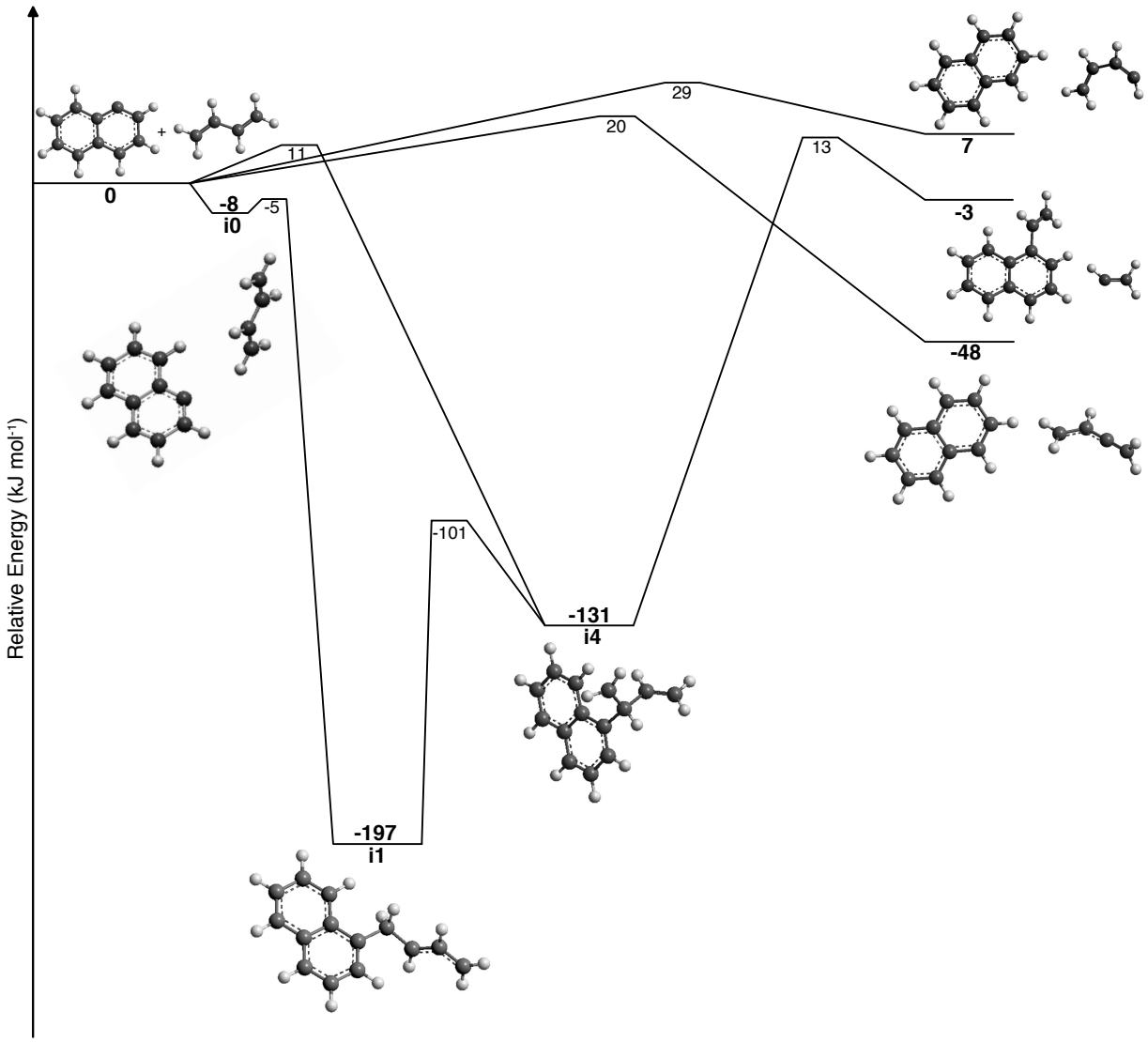
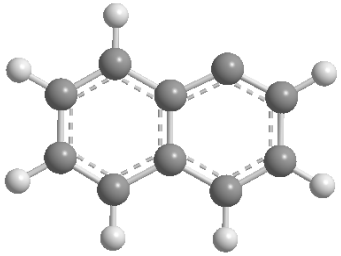
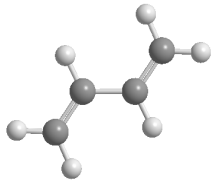
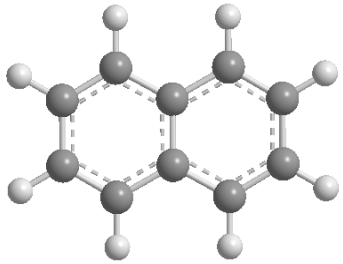
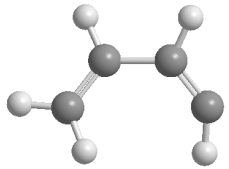
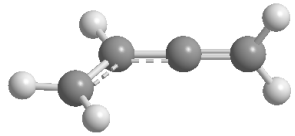
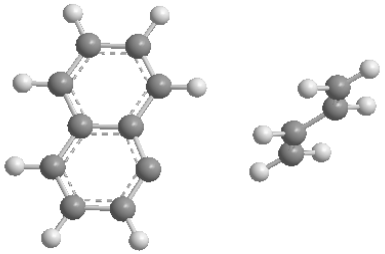


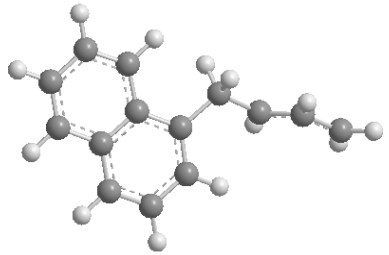
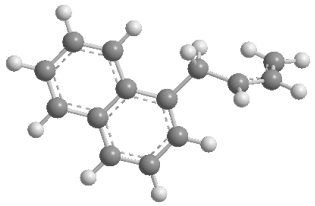
Figure S2. Potential energy surface for the reaction of 1-naphthyl [$C_{10}H_7$· (X^2A')] plus 1,3-butadiene [C_4H_6 (X^1A_g)] at the G3(MP2,CC)//B3LYP/6-311G** level of theory. Energies are relative to the separated reactants and given in kJ mol^{-1}.

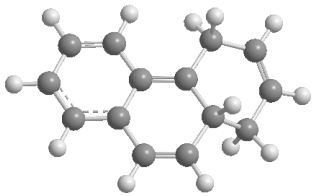
Table S1. Optimized cartesian coordinates and vibrational frequencies of various species involved in the 1-napthyl + 1,3-butadiene reaction.

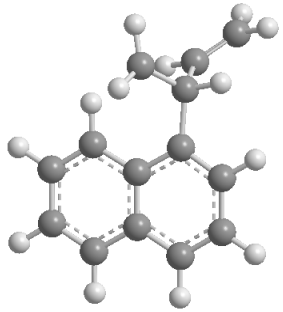
Structure	Coordinates	Frequencies		
1-naphthyl 	C 0 0.023 0.87 -0.005 C 0 -1.245 1.506 -0.011 C 0 1.254 1.536 -0.007 C 0 -2.397 0.757 -0.009 C 0 -2.333 -0.656 0 C 0 -1.12 -1.301 0.006 C 0 0.095 -0.568 0.003 C 0 2.483 0.967 -0.001 C 0 1.372 -1.194 0.009 C 0 2.531 -0.457 0.007 H 0 -1.285 2.588 -0.017 H 0 -3.363 1.249 -0.013 H 0 -3.252 -1.232 0.001 H 0 -1.074 -2.385 0.012 H 0 3.397 1.551 -0.003 H 0 1.417 -2.277 0.016 H 0 3.496 -0.954 0.012	169.0815 400.4761 508.4015 631.436 774.2017 865.775 964.7622 1033.4616 1169.2441 1236.259 1378.4397 1483.7947 1637.5411 3159.128 3181.3196	186.4021 462.3548 521.6622 731.0985 790.0047 893.207 976.4435 1046.5316 1175.9502 1270.7261 1389.6675 1520.9957 1663.0357 3169.2163 3182.2589	361.6147 507.2935 610.9118 772.9352 800.1065 932.4236 998.9149 1138.8633 1197.8391 1360.445 1451.6278 1583.074 3157.6021 3170.3996 3192.7115
1,3-butadiene 	C 0 -1.763 -0.556 0.000 C 0 -0.688 0.239 0.000 C 0 0.688 -0.239 0.000 C 0 1.763 0.556 0.000 H 0 -1.667 -1.637 0.000 H 0 -2.768 -0.154 0.000 H 0 -0.822 1.319 0.000 H 0 0.822 -1.319 0.000 H 0 2.768 0.154 0.000 H 0 1.667 1.637 0.000	174.7307 539.5033 935.2888 1004.0979 1314.7141 1473.4839 3122.6088 3136.0574	299.7384 781.1108 936.3672 1058.2456 1319.9258 1653.2799 3131.6187 3219.197	518.7089 899.2131 1001.4607 1226.8727 1415.4793 1706.0528 3135.2663 3219.64

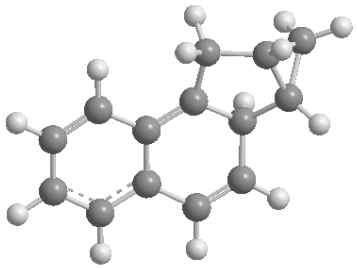
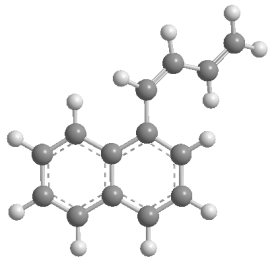
naphthalene 	C 0 -1.81 0.479 0.000 C 0 -2.415 -0.754 0.000 C 0 -1.633 -1.933 0.000 C 0 -0.262 -1.854 0.000 C 0 0.396 -0.596 0.000 C 0 0.262 1.854 0.000 C 0 1.81 -0.479 0.000 C 0 1.633 1.933 0.000 C 0 -0.396 0.596 0.000 C 0 2.415 0.754 0.000 H 0 -2.409 1.384 0.000 H 0 -3.497 -0.829 0.000 H 0 -2.122 -2.901 0.000 H 0 0.34 -2.758 0.000 H 0 -0.34 2.758 0.000 H 0 2.409 -1.384 0.000 H 0 2.122 2.901 0.000 H 0 3.497 0.829 0.000	173.4641 186.503 365.6943 395.8173 479.6536 488.2683 518.9789 519.9213 634.9425 636.11 729.1005 773.1528 786.8972 798.3575 808.8587 849.4725 896.8187 950.9586 956.9713 974.2974 992.4737 999.8054 1035.578 1046.283 1151.05 1169.144 1171.906 1185.142 1232.356 1270.067 1287.044 1391.18 1398.354 1418.015 1490.58 1491.658 1548.692 1613.751 1641.301 1671.224 3156.238 3158.023 3160.299 3163.757 3174.368 3175.703 3187.244 3188.402
$CH_2CHCHCH$ 	C 0 -1.343 -0.291 0.078 C 0 -0.323 0.461 0.495 C 0 1.108 0.212 0.214 C 0 1.597 -0.329 -0.879 H 0 -1.186 -1.195 -0.5 H 0 -2.367 -0.03 0.318 H 0 -0.527 1.333 1.114 H 0 1.804 0.543 0.987 H 0 1.237 -0.704 -1.826	139.3725 263.6516 485.2365 612.1843 725.0418 847.0438 886.2099 943.99 946.1638 1023.389 1078.421 1269.114 1324.422 1441.915 1631.761 1683.745 3081.93 3127.543 3138.763 3221.527 3234.545

CH_2CHCCH_2 	C 0 -1.626 -0.157 -0.631 C 0 -0.48 0.592 -0.371 C 0 0.64 0.135 0.227 C 0 1.717 -0.304 0.803 H 0 -1.687 -1.201 -0.355 H 0 -2.478 0.296 -1.119 H 0 -0.475 1.639 -0.672 H 0 2.539 -0.738 0.233 H 0 1.851 -0.262 1.884	206.2749 524.9901 883.6799 981.0715 1376.856 1909.844 3126.936	213.5512 573.2105 907.7026 1090.359 1449.111 3068.407 3151.733	496.0615 741.2263 937.2938 1193.552 1492.056 3111.5 3252.499
i0 	C 0 2.688481 -2.361042 -0.280065 C 0 3.322052 -1.142844 -0.323987 C 0 2.608842 0.072542 -0.138727 C 0 1.189494 0.020305 0.100344 C 0 0.630967 -1.263108 0.128245 C 0 1.284774 -2.436287 -0.045356 H 0 3.250778 -3.277416 -0.424136 H 0 0.782054 -3.396497 -0.011308 C 0 -3.150892 -0.716310 1.354029 C 0 -3.681496 -0.440222 0.157466 C 0 -4.985371 0.176705 -0.041551 C 0 -5.515800 0.449571 -1.238058 H 0 -2.175350 -1.178523 1.447725 H 0 -3.120096 -0.685966 -0.741778 H 0 -5.545538 0.421526 0.858862 H 0 -6.491736 0.909387 -1.336881 H 0 -4.986555 0.219308 -2.157451 H 0 4.390766 -1.093471 -0.503345 C 0 3.235803 1.344668 -0.179242 C 0 2.509255 2.496159 0.004316 C 0 1.115350 2.437083 0.238694 C 0 0.466654 1.227306 0.286443 H 0 4.305002 1.392969 -0.358734 H 0 3.004526 3.460003 -0.029960 H 0 0.557873 3.355791 0.381366 H 0 -0.600579 1.173401 0.466042 H 0 -3.679828 -0.487673 2.274278	3.7681 21.5988 169.0406 298.2164 462.3644 518.3938 609.5571 771.5036 790.6618 892.9695 936.4394 976.4178 1004.6748 1059.2199 1176.5984 1236.2603 1319.8658 1388.9349 1472.9939 1582.3835 1662.2981 3128.8816 3156.5692 3169.6702 3191.9234	7.3767 33.5656 175.7855 362.1299 507.1734 521.5714 631.3737 773.6884 799.7785 899.9194 942.2319 1000.7013 1033.7619 1138.7058 1198.122 1272.8432 1359.1251 1415.0531 1483.8804 1636.9168 1703.9057 3133.748 3158.1452 3180.5257 3217.1934	13.9408 48.7704 186.9135 400.4949 508.0127 543.6658 731.1536 783.3021 866.5518 931.9012 965.3773 1003.2153 1046.9684 1168.8455 1226.1727 1314.3884 1378.6301 1451.3555 1520.9965 1650.6586 3121.646 3135.2438 3168.251 3181.7412 3218.9727
i1	C 0 -2.215 -0.633 0.541	34.2819	44.2654	117.343

	C 0 -1.976 -2.015 0.322 C 0 -0.743 -2.446 -0.092 C 0 0.301 -1.518 -0.313 C 0 0.12 -0.165 -0.126 C 0 -1.158 0.309 0.319 C 0 1.259 0.821 -0.366 C 0 2.449 0.279 -1.093 C 0 3.729 0.214 -0.564 C 0 4.847 -0.25 -1.232 C 0 -3.481 -0.166 0.98 C 0 -1.43 1.683 0.564 C 0 -2.668 2.102 0.993 C 0 -3.707 1.17 1.202 H 0 -2.783 -2.72 0.491 H 0 -0.558 -3.502 -0.253 H 0 1.269 -1.884 -0.632 H 0 1.577 1.243 0.596 H 0 0.86 1.666 -0.943 H 0 2.291 -0.065 -2.112 H 0 3.861 0.557 0.461 H 0 5.819 -0.274 -0.756 H 0 4.784 -0.603 -2.255 H 0 -4.273 -0.89 1.14 H 0 -0.649 2.418 0.416 H 0 -2.847 3.156 1.173 H 0 -4.679 1.512 1.538	139.3304 238.9196 416.3863 499.7969 544.2789 639.0191 770.1833 806.8639 869.1447 961.375 996.554 1051.9268 1169.0318 1205.6798 1253.5272 1300.0951 1398.0087 1471.6405 1519.3753 1641.3182 3025.0996 3139.3214 3167.9568 3184.4755	178.7399 275.9113 416.9379 518.2524 561.5695 719.1145 789.2609 810.5521 906.0626 973.0111 996.8124 1096.8268 1184.2198 1215.4155 1279.441 1364.6162 1424.8369 1495.7597 1548.3997 1664.0877 3114.1931 3157.5602 3172.2826 3196.1963	207.3438 301.7059 479.6005 534.4393 613.3209 743.4374 803.2892 861.0085 930.945 987.718 1028.2642 1118.3405 1189.6965 1232.3677 1285.557 1383.3474 1468.9998 1499.2739 1618.9051 2986.0572 3132.1496 3159.654 3182.919 3234.2987
i2 	C 0 -2.057 -0.899 0.268 C 0 -1.664 -2.244 0.045 C 0 -0.341 -2.561 -0.111 C 0 0.648 -1.553 -0.043 C 0 0.323 -0.233 0.182 C 0 -1.057 0.126 0.335 C 0 1.403 0.844 0.246 C 0 2.808 0.343 0.391 C 0 3.806 0.411 -0.574 C 0 3.695 0.902 -1.861 C 0 -3.423 -0.547 0.422	25.2957 144.6196 248.1019 415.5216 500.1444 541.6261 640.0331 767.6658 805.7636 869.267 964.0261	31.0964 178.2394 287.1782 433.8808 530.3732 579.1827 704.6147 789.581 809.3498 904.3238 985.4379	118.3627 219.835 348.6634 479.579 534.0146 610.0754 743.6109 791.1158 857.6026 930.4393 995.3405

	C 0 -1.49 1.464 0.543 C 0 -2.822 1.772 0.685 C 0 -3.802 0.757 0.627 H 0 -2.429 -3.012 -0.004 H 0 -0.041 -3.588 -0.288 H 0 1.688 -1.826 -0.174 H 0 1.192 1.488 1.109 H 0 1.314 1.491 -0.633 H 0 3.06 -0.105 1.347 H 0 4.782 0.031 -0.278 H 0 4.548 0.907 -2.527 H 0 2.763 1.287 -2.256 H 0 -4.169 -1.333 0.373 H 0 -0.759 2.262 0.588 H 0 -3.124 2.802 0.842 H 0 -4.85 1.011 0.742	996.0539 1047.4294 1168.7518 1189.3169 1245.2458 1305.3649 1424.9347 1472.7131 1525.1589 1641.244 3043.6691 3156.4431 3167.7576 3185.3879	1005.0769 1053.6765 1177.0309 1231.8806 1258.6262 1381.0275 1432.3918 1487.7246 1548.3324 1663.9407 3125.0902 3156.9635 3173.2192 3197.26	1034.8784 1097.3212 1185.5569 1240.5169 1281.116 1395.9387 1470.686 1496.8422 1618.6527 3002.0947 3147.0932 3159.3982 3183.4872 3237.1894
i3 	C 0 -2.407 1.924 1.485 C 0 -3.382 0.927 1.35 C 0 -1.1 1.687 1.103 C 0 -3.022 -0.314 0.831 C 0 -0.696 0.431 0.56 C 0 -1.711 -0.586 0.439 C 0 -1.345 -1.886 -0.092 C 0 0.626 0.158 0.153 C 0 1.038 -1.2 -0.353 C 0 1.736 1.17 0.26 C 0 -0.089 -2.183 -0.452 C 0 2.858 0.956 -0.725 C 0 2.88 -0.027 -1.622 C 0 1.81 -1.081 -1.697 H 0 -2.677 2.891 1.896 H 0 -4.406 1.118 1.65 H 0 -0.368 2.474 1.229 H 0 -3.769 -1.094 0.726 H 0 -2.131 -2.63 -0.185 H 0 1.784 -1.605 0.36 H 0 2.151 1.173 1.283	54.0793 191.4149 378.5158 434.2611 511.4515 599.776 711.3542 793.8207 858.8217 938.8527 987.1776 1009.974 1066.0465 1172.7546 1205.7025 1284.5589 1326.2399 1409.246 1454.9197 1491.1763 1681.8412	103.0051 238.0062 392.6154 451.0257 527.6245 674.7642 745.3928 801.7636 915.6865 960.1189 993.5756 1046.1019 1131.8564 1182.982 1220.33 1293.11 1342.5665 1413.3991 1464.8184 1560.9573 1721.5624	141.1685 248.5803 407.9959 494.1989 70.218 685.6595 765.1222 835.6719 927.1854 973.678 994.6329 1056.2575 1165.2135 1186.5154 1238.4496 1316.2562 1376.1554 1429.6167 1481.1516 1606.3031 2876.5873

	H 0 1.347 2.184 0.116 H 0 0.152 -3.169 -0.838 H 0 3.666 1.682 -0.698 H 0 3.7 -0.091 -2.332 H 0 1.102 -0.855 -2.505 H 0 2.253 -2.053 -1.942	2932.7224 3036.6273 3155.2277 3165.213	3004.7946 3133.2614 3156.3114 3185.8594	3026.305 3140.6055 3162.3744 3196.5732
i4 	C 0 -1.669 0.153 -0.198 C 0 -2.838 -0.518 -0.465 C 0 -2.886 -1.928 -0.404 C 0 -1.758 -2.635 -0.071 C 0 0.769 0.115 0.426 C 0 -0.534 -1.974 0.212 C 0 0.629 -2.709 0.557 C 0 -0.476 -0.542 0.146 C 0 0.943 1.635 0.343 C 0 1.867 -0.651 0.757 C 0 1.805 -2.06 0.827 C 0 0.937 2.127 -1.095 C 0 -0.01 2.407 1.206 C 0 1.95 2.764 -1.672 H 0 -1.66 1.235 -0.232 H 0 -3.732 0.039 -0.723 H 0 -3.814 -2.447 -0.618 H 0 -1.785 -3.718 -0.017 H 0 0.569 -3.791 0.605 H 0 1.959 1.836 0.721 H 0 2.81 -0.158 0.966 H 0 2.694 -2.62 1.094 H 0 0.031 1.936 -1.664 H 0 -0.431 1.963 2.099 H 0 -0.141 3.47 1.04 H 0 1.895 3.103 -2.701 H 0 2.874 2.969 -1.139	61.9432 159.9421 203.6557 323.3209 449.1076 518.9166 637.1624 728.7634 806.7642 880.4038 946.9536 992.3405 1045.6065 1112.0927 1186.2762 1240.4757 1301.4405 1390.1952 1451.644 1546.7639 1662.9407 3123.6203 3156.2674 3168.5698 3192.8486	64.93181 169.1835 273.0227 400.098 481.7482 551.5951 653.25 749.6083 818.091 885.7505 969.973 998.7138 1051.4199 1154.5785 1189.6705 1261.8101 1328.0789 1422.0707 1473.5886 1616.0271 1696.5957 3134.3597 3158.2474 3182.7132 3208.4514	04.873 172.6631 314.0156 440.9628 496.3474 577.4917 695.3891 796.1499 868.0675 921.4273 985.3682 1026.9719 1083.9965 1168.4776 1230.1698 1281.2861 1382.1844 1443.945 1493.1533 1639.0826 2928.0497 3149.56 3164.6428 3183.8275 3245.1366
i5	C 0 -0.978 -2.143 0.305 C 0 -0.058 -1.078 0.099 C 0 -0.542 -3.404 0.665 C 0 -0.453 0.218 -0.271	55.0668 203.4926 365.3892 457.6983	111.2069 224.5361 383.6412 482.4101	170.0945 297.6984 414.5611 505.6131

	C 0 1.34 -1.338 0.333 C 0 2.282 -0.231 0.274 C 0 1.745 -2.621 0.703 C 0 0.824 -3.655 0.859 C 0 -1.836 0.812 -0.162 C 0 0.547 1.284 -0.647 C 0 1.927 1.001 -0.126 C 0 -1.589 2.314 0.041 C 0 -0.124 2.605 -0.221 C 0 -1.182 3.149 -1.146 H 0 -2.035 -1.964 0.147 H 0 -1.261 -4.205 0.797 H 0 3.303 -0.428 0.587 H 0 2.799 -2.806 0.887 H 0 1.161 -4.646 1.141 H 0 -2.383 0.387 0.685 H 0 -2.451 0.623 -1.055 H 0 0.64 1.307 -1.752 H 0 2.657 1.804 -0.155 H 0 -2.11 2.806 0.853 H 0 0.435 3.287 0.409 H 0 -1.396 4.211 -1.11 H 0 -1.263 2.712 -2.138	527.1633 677.3285 751.3961 804.2979 861.3619 939.7906 986.382 1048.1183 1076.2789 1139.8745 1180.1952 1223.4277 1284.2327 1345.5056 1421.3269 1488.0071 1605.4029 2971.2866 3143.8925 3161.5506 3178.2411	564.0382 700.9446 778.44 813.511 869.4681 973.0254 996.0605 1051.7343 1101.0163 1157.5767 1191.2329 1255.375 1297.9397 1378.7946 1456.534 1490.6448 1663.9242 3044.3244 3154.3045 3162.539 3186.8518	644.4648 717.8225 794.7237 843.4683 903.13 974.4498 1001.7454 1059.77 1110.2573 1173.5701 1210.6289 1279.6244 1332.9074 1410.7197 1478.1566 1560.2132 2843.911 3098.7293 3155.1098 3165.9797 3188.598
p1 	C 0 -2.152 0.092 -0.149 C 0 -3.26 -0.633 -0.516 C 0 -0.924 -0.548 0.165 C 0 -3.2 -2.041 -0.6 C 0 -2.024 -2.693 -0.321 C 0 0.251 0.18 0.558 C 0 -0.862 -1.975 0.063 C 0 0.36 -2.641 0.34 C 0 1.414 -0.524 0.823 C 0 0.195 1.641 0.746 C 0 1.473 -1.929 0.708 C 0 1.084 2.561 0.32 C 0 2.246 2.338 -0.525 C 0 3.126 3.296 -0.841	35.9009 162.9468 251.1516 418.8282 489.7887 567.4946 698.409 797.9308 827.7933 931.2322 966.8558 999.2255 1055.3365 1168.5464	75.6634 182.2447 320.3734 457.1064 522.1276 630.1574 744.5358 803.943 867.965 934.5583 986.0008 1035.0127 1095.965 1182.3772	127.0957 196.6156 373.7855 481.5319 547.8821 687.013 767.3197 813.1828 887.0651 941.3922 996.6793 1049.1259 1148.6139 1191.2111

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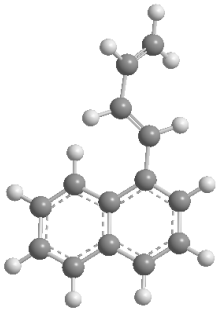
p2 	C 0 -1.837 0.792 -2.135 C 0 -3.135 0.451 -1.696 C 0 -0.736 0.489 -1.37 C 0 -3.296 -0.224 -0.512 C 0 -0.863 -0.173 -0.119 C 0 -2.179 -0.569 0.294 C 0 -2.349 -1.319 1.486 C 0 0.258 -0.513 0.72 C 0 0.032 -1.295 1.844 C 0 1.642 -0.08 0.482 C 0 -1.26 -1.693 2.234 C 0 2.074 1.097 -0.008 C 0 3.479 1.468 -0.18 C 0 4.49 0.636 -0.451 H 0 -1.707 1.288 -3.091 H 0 -3.996 0.705 -2.304 H 0 0.25 0.731 -1.74 H 0 -4.285 -0.518 -0.178 H 0 -3.351 -1.605 1.785 H 0 0.878 -1.579 2.46 H 0 2.398 -0.778 0.84 H 0 -1.389 -2.284 3.133 H 0 1.349 1.869 -0.249 H 0 3.694 2.532 -0.098 H 0 4.332 -0.426 -0.605	55.7633 156.0784 240.9506 434.322 483.0494 570.6014 671.5896 791.3174 877.6656 925.961 982.896 1009.8906 1062.9843 1168.6603 1233.7322 1316.1828 1378.5848 1452.1962 1546.3887 1653.7418 3124.1184 3155.03 3166.8155 3185.7874	69.8469 176.804 292.4842 444.0873 525.705 630.2366 746.5982 805.5662 890.2045 934.2756 987.4508 1029.0444 1087.5932 1185.4375 1246.3094 1328.368 1384.7851 1471.9555 1610.5194 1663.7592 3128.1088 3157.9877 3170.3 3215.4824	116.0843 205.5016 327.1769 479.0529 550.3524 646.7226 750.6219 814.0017 901.8403 970.639 997.1021 1045.009 1112.1508 1198.4986 1284.0654 1352.5505 1425.7298 1492.0727 1628.4077 1689.8234 3137.2852 3159.6582 3184.5544 3220.3363

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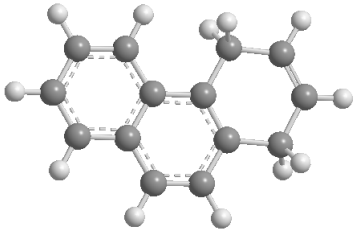
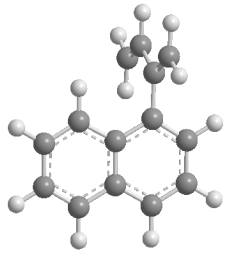
p3 	C 0 -2.197 0.381 0.044 C 0 -3.349 -0.368 0.124 C 0 -0.915 -0.232 0.042 C 0 -3.285 -1.774 0.207 C 0 -2.063 -2.402 0.208 C 0 0.303 0.524 -0.041 C 0 -0.859 -1.659 0.127 C 0 0.409 -2.296 0.126 C 0 0.228 2.035 -0.13 C 0 1.517 -0.135 -0.038 C 0 1.554 -1.553 0.047 C 0 2.841 0.595 -0.122 C 0 1.558 2.724 -0.212 C 0 2.724 2.086 -0.209 H 0 -2.275 1.459 -0.019 H 0 -4.314 0.127 0.124 H 0 -4.199 -2.354 0.27 H 0 -2.001 -3.484 0.272 H 0 0.455 -3.378 0.19 H 0 -0.325 2.428 0.735 H 0 -0.378 2.322 -1.001 H 0 2.521 -2.048 0.047 H 0 3.457 0.324 0.747 H 0 3.404 0.219 -0.989 H 0 1.537 3.809 -0.277 H 0 3.65 2.65 -0.272	66.9445 218.4781 392.265 444.6533 536.4157 647.4787 710.5671 821.4682 873.8948 961.0556 985.1892 1014.2907 1168.9084 1202.0015 1236.6804 1324.5955 1407.3673 1463.5234 1505.9139 1645.6301 2981.1844 2991.2458 3157.3248 3171.2459	99.185 230.5184 396.0913 484.8997 538.2855 680.0159 753.2769 830.084 935.1699 978.1444 993.6225 1052.4536 1172.5077 1209.0593 1242.188 1373.1057 1419.9457 1469.7251 1548.121 1663.9726 2982.1504 3135.4725 3158.4574 3183.6541	142.813 291.3286 420.2034 511.0493 598.511 692.7309 785.0991 863.4701 957.154 981.5039 996.6423 1096.5081 1199.7623 1227.7955 1288.3804 1384.6569 1424.4849 1474.9807 1614.2531 1742.6789 2990.5347 3150.0455 3167.3222 3198.627
p4 	C 0 -1.58 -0.037 -0.559 C 0 -2.453 -0.938 -1.119 C 0 -0.363 -0.469 0.034 C 0 -2.16 -2.32 -1.115 C 0 -0.996 -2.773 -0.545 C 0 0.568 0.438 0.635 C 0 -0.07 -1.871 0.043 C 0 1.131 -2.328 0.645 C 0 0.314 1.915 0.648 C 0 1.72 -0.056 1.211	33.5397 151.6084 252.3335 422.1028 487.2514 565.7511 690.7859 791.4521 816.899 912.5893	81.0927 161.4624 326.0819 460.2352 524.7125 602.7639 716.1328 795.492 843.5358 927.8522	139.0546 177.6271 376.4035 480.5576 537.8825 677.4568 747.7729 808.5938 879.6558 934.0712

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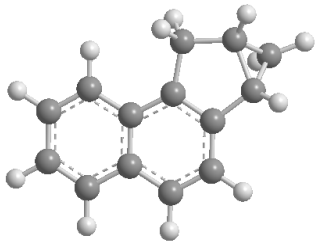
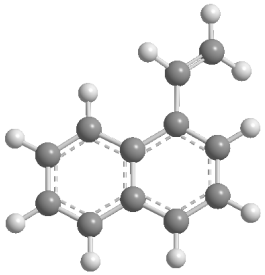
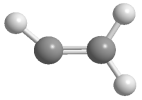
p5 	C 0 -2.218 0.364 -0.37 C 0 -3.318 -0.408 -0.659 C 0 -0.959 -0.233 -0.095 C 0 -3.216 -1.818 -0.686 C 0 -2.013 -2.428 -0.422 C 0 0.204 0.513 0.222 C 0 -0.856 -1.664 -0.12 C 0 0.394 -2.278 0.162 C 0 1.408 -0.119 0.475 C 0 0.332 2.019 0.361 C 0 1.509 -1.527 0.449 C 0 1.824 2.24 0.622 C 0 2.49 0.874 0.728 C 0 2.801 1.801 -0.434 H 0 -2.305 1.444 -0.352 H 0 -4.272 0.064 -0.868 H 0 -4.091 -2.415 -0.916 H 0 -1.933 -3.51 -0.442 H 0 0.456 -3.362 0.141 H 0 -0.013 2.554 -0.531 H 0 -0.269 2.385 1.202	90.32 213.3272 375.3046 459.2409 550.1834 683.2702 759.2717 818.4384 873.2934 957.3938 992.8884 1045.4154 1095.7205 1177.9383 1207.933 1282.5768 1373.1338 1412.4373 1488.6833 1608.1359 3011.496	124.5715 230.2183 421.0466 516.6884 594.4263 721.132 788.0454 830.6689 891.0246 967.5811 997.6609 1057.7609 1108.907 1185.2857 1223.0658 1296.8393 1381.8922 1469.3786 1497.8602 1632.8421 3038.8951	200.609 343.433 451.4276 530.7434 656.9103 753.2974 796.5092 869.8101 930.5561 984.3383 1036.583 1071.4445 1167.4421 1187.8654 1235.2307 1349.0689 1397.8576 1476.7508 1552.827 1663.8602 3110.2461

	H 0 2.459 -2.009 0.653 H 0 2.12 3.046 1.282 H 0 3.267 0.662 1.453 H 0 3.772 2.282 -0.44 H 0 2.427 1.523 -1.414	3155.3861 3164.7514 3177.8153	3157.6982 3169.0006 3187.7254	3158.701 3175.961 3197.5874
naprene 	C 0 -1.464 0.448 -0.86 C 0 -2.617 -0.296 -0.932 C 0 -0.359 0.023 -0.074 C 0 -2.729 -1.515 -0.228 C 0 0.861 0.776 0.028 C 0 -0.47 -1.224 0.623 C 0 -1.675 -1.967 0.527 C 0 0.628 -1.696 1.387 C 0 1.001 2.083 -0.642 C 0 1.897 0.269 0.793 C 0 1.788 -0.966 1.464 C 0 2.118 2.55 -1.203 H 0 -1.392 1.369 -1.425 H 0 -3.447 0.052 -1.538 H 0 -3.643 -2.094 -0.292 H 0 -1.748 -2.908 1.063 H 0 0.533 -2.64 1.912 H 0 0.114 2.71 -0.666 H 0 2.803 0.853 0.903 H 0 2.622 -1.326 2.056 H 0 2.152 3.537 -1.648 H 0 3.028 1.961 -1.249	85.8137 205.337 411.6963 496.571 607.0323 721.22 806.0462 881.4519 965.1727 1023.3987 1058.7177 1185.2716 1260.6432 1370.5385 1453.7803 1546.3834 1661.1751 3141.9642 3169.4341 3188.0997	118.6477 257.914 441.5407 513.882 635.1311 748.4969 817.4546 925.2972 985.1518 1032.3658 1113.8993 1191.9432 1287.9812 1389.3623 1470.7121 1615.3459 1684.6818 3157.9901 3174.7895 3197.6957	178.2874 342.701 479.1751 547.0604 708.1703 795.6451 868.7295 944.7125 996.8835 1049.6011 1168.6357 1232.6247 1331.555 1418.722 1494.0121 1632.8052 3133.2046 3161.1406 3184.0981 3219.3603
C_2H_3 	C 0 -0.852 -0.153 0.000 C 0 0.453 -0.141 0.000 H 0 -1.666 0.556 0.000 H 0 1.022 0.793 0.000 H 0 1.042 -1.056 0.000	710.263 1045.4745 3036.774	818.8584 1391.1849 3134.7552	921.5323 1650.6757 3235.4777
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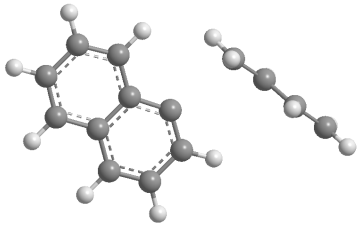
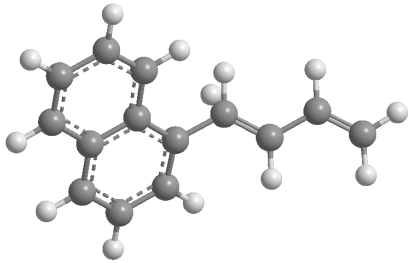
	C 0 -2.189708 0.919117 0.239764 C 0 -4.530903 0.273186 0.610443 C 0 -2.552594 2.260328 0.531425 C 0 -4.848012 1.581125 0.885522 C 0 -3.850305 2.582754 0.845935 H 0 -3.609019 -2.210406 0.025698 H 0 -1.286198 -2.813471 -0.541838 H 0 0.488852 -1.047870 -0.624326 H 0 -5.297040 -0.494967 0.642116 H 0 -1.787223 3.026593 0.503214 H 0 -5.867825 1.851286 1.135573 H 0 -4.115200 3.610731 1.066300 C 0 1.121619 2.136695 -0.176276 C 0 2.104602 1.477475 -0.825947 C 0 3.074718 0.619902 -0.178225 C 0 4.041693 -0.052792 -0.820172 H 0 1.054678 2.122971 0.905595 H 0 0.460610 2.813483 -0.701258 H 0 2.173538 1.562255 -1.908243 H 0 2.995744 0.531427 0.903627 H 0 4.747376 -0.679677 -0.288874 H 0 4.154148 0.009867 -1.897977	517.0973 614.5319 762.0449 796.7637 886.7395 925.2238 977.1443 1008.1320 1051.2776 1177.1351 1235.7227 1317.9063 1386.4706 1472.5182 1582.6891 1655.4927 3134.9450 3154.4834 3168.3382 3192.2226	521.8080 617.1710 774.0689 801.5533 901.9347 934.2584 980.1435 1036.0192 1136.5455 1200.9463 1269.8810 1360.6699 1405.8566 1484.0123 1607.2470 1661.1607 3138.0314 3156.9452 3178.0340 3222.2315	579.2284 737.2080 782.3221 867.7801 905.7383 962.8960 995.7319 1046.7762 1168.5744 1228.2380 1299.6614 1381.3128 1452.3206 1522.7614 1636.3835 3125.2332 3145.1108 3166.2396 3181.4003 3235.7725
ts **i1-p1** 	C 0 -3.111696 -0.285837 0.622774 C 0 -3.316925 -1.537567 -0.010039 C 0 -2.339269 -2.085409 -0.802801 C 0 -1.124290 -1.403382 -1.004121 C 0 -0.864367 -0.181253 -0.406494 C 0 -1.870839 0.407518 0.434589 C 0 0.416595 0.506073 -0.646539 C 0 1.620310 -0.115070 -0.761222 C 0 2.871527 0.581047 -0.949766 C 0 4.063696 -0.024021 -1.057596 C 0 -4.112146 0.291537 1.448086 C 0 -1.691413 1.642761 1.113228 C 0 -3.907481 1.495268 2.074284 C 0 -2.680578 2.173867 1.906310 H 0 -4.260773 -2.051016 0.139251	-509.4810 116.8525 181.1210 302.5242 409.3594 495.9978 566.9080 672.9375 793.3305 875.0603 922.8427 966.2443 997.1400 1056.2064 1183.5509	44.6155 147.1873 243.9086 314.2322 440.2766 526.2935 631.0468 745.0658 805.0172 884.4075 929.4169 974.0382 1037.1560 1109.2041 1190.3738	73.5043 176.1370 254.7309 362.5315 481.2260 549.3580 648.3601 758.4254 814.0706 894.3757 962.1835 985.9670 1040.1178 1169.1626 1197.0050

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	H 0 0.416909 1.589303 -0.584843	1372.5419	1388.6368	1421.2383
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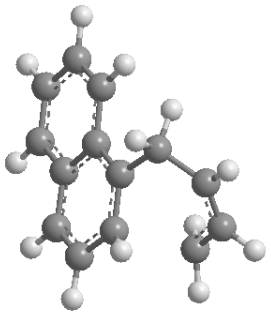
ts **i2-i3** 	C 0 -0.449352 -0.332686 0.853568	-586.7024	54.1658	106.5734
	C 0 -0.598012 -1.744329 0.877599	133.5324	188.4624	235.1787
	C 0 1.688943 -0.555707 2.222160	239.5917	348.6813	391.8412
	C 0 0.482842 0.288834 1.874440	415.0313	436.4636	471.9364
	C 0 -1.047858 0.417015 -0.196534	485.9977	515.0739	544.4334
	C 0 -1.846539 -0.262626 -1.183329	569.3760	613.2733	651.6899
	C 0 -2.036542 -1.674858 -1.079405	683.6325	699.2924	743.2081
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	C 0 -2.448853 0.476224 -2.223534	868.6143	919.3116	936.2529
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	H 0 -3.045340 -0.056218 -2.957534	3042.8860	3099.4407	3109.9579
	H 0 1.412752 -1.623796 -0.538236	3153.0678	3153.3445	3156.9084
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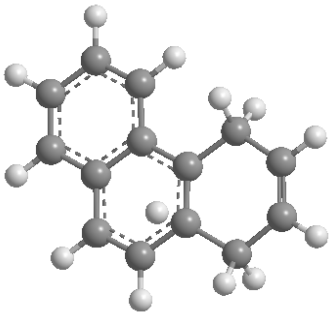
ts **i3-p3** 	C 0 0.172134 -0.032104 0.438253 C 0 0.287312 -1.411990 0.237458 C 0 1.533771 -2.175384 0.656911 C 0 2.389972 -1.444029 1.645343 C 0 2.198564 -0.168379 1.963585 C 0 1.116821 0.689399 1.373181 C 0 -0.903886 0.685224 -0.173445 C 0 -1.807294 0.000956 -1.048246 C 0 -1.612460 -1.388397 -1.292606 C 0 -0.599099 -2.062852 -0.684958 C 0 -1.114891 2.074214 0.041834 C 0 -2.863014 0.716403 -1.659098 C 0 -3.037603 2.061526 -1.426319 C 0 -2.152450 2.743332 -0.566958 H 0 -0.642061 -1.871199 1.790099 H 0 2.123287 -2.390799 -0.247179 H 0 1.247802 -3.154544 1.056518 H 0 3.203484 -2.000826 2.101038 H 0 2.852697 0.312790 2.685177 H 0 0.538788 1.147609 2.188934 H 0 1.579786 1.537420 0.848504 H 0 -2.284533 -1.898951 -1.974459 H 0 -0.455306 -3.121761 -0.873416 H 0 -0.450477 2.620401 0.698760 H 0 -3.538670 0.182361 -2.319351 H 0 -3.851989 2.597747 -1.900543 H 0 -2.291685 3.802833 -0.383017	-782.0153 143.7405 297.7133 393.1649 487.0533 544.2244 656.9013 708.1697 819.6282 874.8373 960.5837 988.7909 1013.4868 1164.9432 1201.7417 1235.1510 1323.6515 1408.3861 1459.7494 1493.0441 1639.2696 2975.3248 3031.3618 3158.6977 3174.5442	76.3073 210.9560 374.6603 427.2843 511.6798 558.4175 678.4331 753.9677 827.1285 933.8851 976.4519 993.8672 1053.2636 1171.7712 1203.6514 1237.9811 1367.6912 1415.4226 1465.9679 1541.6919 1652.1722 2979.2894 3138.7319 3161.5344 3183.7825	102.8023 229.6975 390.9332 438.8348 518.5147 600.3735 700.4331 786.4496 860.1251 956.7567 979.2139 997.5292 1095.7025 1197.5549 1228.4931 1288.4539 1378.4370 1422.6602 1473.6576 1589.0226 1739.9181 2989.9879 3155.3114 3168.7845 3199.3156
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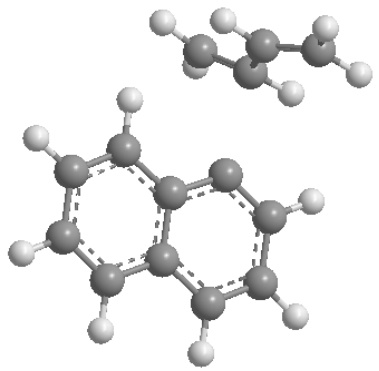
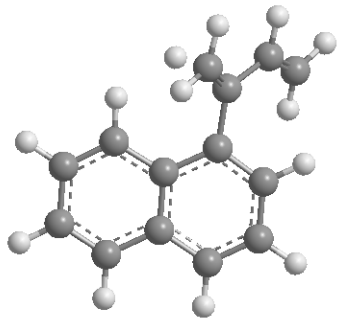
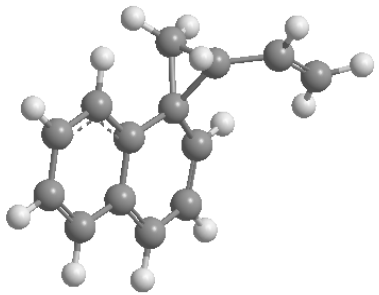
	C 0 -1.363031 -0.072802 2.661348 C 0 -1.392113 -1.484001 2.741113 H 0 -0.199112 -3.486906 -0.599386 H 0 0.547890 -2.392944 -2.681684 H 0 0.615307 0.089259 -2.839970 H 0 -0.929838 1.631473 1.450102 H 0 -1.027910 -3.328895 1.724037 H 0 -1.672157 0.517983 3.516407 H 0 -1.721843 -1.963034 3.656207 C 0 -1.205390 3.076479 -1.049704 C 0 0.074015 2.614843 -1.197653 C 0 1.147698 2.983131 -0.265257 C 0 2.450899 2.896523 -0.536976 H 0 -1.529023 3.557464 -0.133177 H 0 -1.953987 2.917536 -1.815289 H 0 0.394030 2.299919 -2.186051 H 0 0.829954 3.379017 0.696986 H 0 3.201182 3.209553 0.178957 H 0 2.809270 2.504750 -1.483579	794.3104 865.5036 917.4747 974.7591 1000.8343 1058.8707 1178.3068 1234.7277 1320.3163 1384.7315 1467.3289 1550.5639 1660.1145 3136.5261 3149.7806 3168.3905 3206.7323	802.5585 878.3645 935.7953 989.9669 1037.5297 1137.8560 1205.1356 1267.4706 1362.7797 1394.1936 1483.6049 1584.1264 1689.5321 3139.1724 3155.5020 3176.4351 3220.7125	839.4369 894.7371 962.7063 995.0455 1040.0143 1168.4440 1212.7284 1270.3993 1382.8462 1454.5591 1524.1853 1635.6986 3128.5823 3144.4324 3159.1902 3183.8611 3231.7790
ts **i4-p4** 	C 0 0.090978 -0.371956 0.518184 C 0 0.063826 -1.806784 0.473459 C 0 1.263073 -2.527228 0.246778 C 0 2.448968 -1.863169 0.071103 C 0 2.483160 -0.453995 0.105875 C 0 1.344877 0.301598 0.317951 C 0 1.196478 2.410418 1.602982 C 0 1.494067 1.795643 0.421597 C 0 2.304985 2.545324 -0.574169 C 0 2.777081 2.110098 -1.743339 C 0 -1.138964 0.302107 0.755862 C 0 -1.167362 -2.488228 0.663776 C 0 -2.313340 -0.389322 0.934682 C 0 -2.332128 -1.800373 0.891416 H 0 1.224971 -3.611143 0.220911 H 0 3.368940 -2.413292 -0.091427 H 0 3.433254 0.049346 -0.020933 H 0 1.394408 3.467010 1.744885	-901.7182 144.2312 188.5834 382.7417 459.6736 522.1971 581.4583 684.2309 762.4235 816.8830 890.3660 947.2409 996.1998 1049.3909 1167.2728 1226.5679 1310.2327 1384.5036	59.4148 164.0038 248.2144 406.3045 480.3995 535.2225 605.6914 695.6265 795.7520 829.1289 908.8731 967.4444 1016.0666 1064.2243 1172.3418 1239.3905 1331.6715 1401.9778	95.1438 181.6425 340.8275 421.2629 483.1111 556.2953 646.7236 746.4680 805.6570 878.8523 934.6649 987.3816 1025.5751 1095.4557 1187.1824 1278.8104 1360.8212 1428.7067

	H 0 0.720709 1.878143 2.415925 H 0 2.507699 3.573312 -0.283133 H 0 3.354939 2.768274 -2.381152 H 0 2.594556 1.106788 -2.107820 H 0 -1.151051 1.382454 0.788565 H 0 -1.167643 -3.572625 0.625234 H 0 -3.234903 0.154917 1.108520 H 0 -3.264735 -2.334027 1.035928 H 0 0.006156 2.325712 -0.600657	1453.3305 1545.2311 1635.9648 3133.2880 3158.6355 3179.0023 3206.2931	1469.9515 1562.4019 1660.5115 3142.1503 3162.0243 3185.2948 3230.6448	1493.3339 1613.5631 1684.0453 3148.9391 3170.1224 3195.7367 3238.2557
ts **i1**-**i4** 	C 0 -2.238267 -0.366115 1.062022 C 0 -1.984023 -1.412815 1.913612 C 0 -0.678721 -1.750999 2.283304 C 0 0.428044 -0.951922 1.857078 C 0 0.219373 0.158509 0.988362 C 0 -1.156736 0.417258 0.446952 C 0 -1.511644 1.795902 -0.091107 C 0 -1.202498 0.738680 -1.107222 C 0 -2.160107 0.240252 -2.126361 C 0 -3.318095 -0.407263 -2.003104 C 0 1.736221 -1.225219 2.316434 C 0 1.319012 0.952467 0.648567 C 0 2.598367 0.670598 1.119318 C 0 2.807998 -0.430537 1.953881 H 0 -3.259541 -0.079847 0.849194 H 0 -2.816143 -1.974874 2.324683 H 0 -0.494072 -2.590413 2.943414 H 0 -0.805004 2.603103 0.064892 H 0 -2.552263 2.083907 0.008844 H 0 -0.192137 0.796061 -1.498549 H 0 -1.825599 0.461203 -3.139718 H 0 -3.884496 -0.677147 -2.887062 H 0 -3.735200 -0.710208 -1.053096 H 0 1.886177 -2.075849 2.973272 H 0 1.188644 1.811712 0.000323 H 0 3.428360 1.307650 0.835952 H 0 3.803350 -0.657096 2.319113	-117.4564 160.8639 252.2407 407.3907 501.2698 561.2098 678.2406 763.0141 808.9067 876.7805 949.0084 982.1148 1059.2039 1102.8779 1153.2320 1233.0380 1319.6954 1391.4920 1456.8161 1519.0350 1627.9990 3112.0212 3157.1935 3175.4746 3195.3761	59.7709 213.8078 321.8073 434.8270 508.0753 638.5980 697.7143 785.9499 811.9220 929.5483 960.4221 1000.5413 1074.2026 1114.3175 1179.2955 1245.2728 1340.6240 1419.9327 1464.9230 1552.3344 1700.2398 3142.6409 3159.4147 3180.6276 3200.5396	99.8591 224.6157 381.2001 476.1864 532.5519 649.1745 706.2458 790.8602 856.3262 937.7965 977.9008 1025.6893 1077.1239 1146.0310 1186.5040 1284.4900 1348.7349 1451.2297 1485.0747 1592.0986 3103.6830 3152.6134 3164.2710 3188.9693 3239.4533
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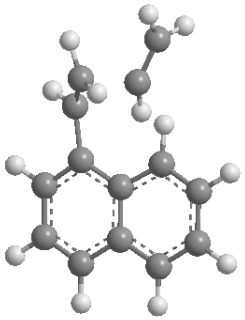
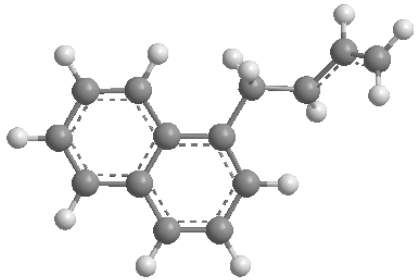
	C 0 -2.257204 -2.240704 0.139704 C 0 -1.112087 -2.836590 0.602225 C 0 0.016849 -2.050903 0.949033 C 0 -0.047674 -0.622237 0.834760 C 0 -1.276902 -0.017010 0.401274 C 0 -1.188731 2.343765 1.313894 C 0 -1.510799 1.448512 0.339018 C 0 1.221012 -2.658985 1.391432 C 0 1.130641 0.119861 1.119782 C 0 2.284588 -0.502806 1.533428 C 0 2.329549 -1.905626 1.686406 H 0 -3.252395 -0.382308 -0.310730 H 0 -3.115023 -2.841848 -0.140042 H 0 -1.048246 -3.915354 0.697968 H 0 -1.555029 3.362278 1.264420 H 0 -0.552493 2.088862 2.151207 H 0 -2.299156 1.737379 -0.349755 H 0 1.250791 -3.739852 1.482948 H 0 1.125138 1.190905 0.978614 H 0 3.171719 0.087583 1.734052 H 0 3.243429 -2.384103 2.020285 C 0 -0.160021 1.963023 -1.496578 C 0 0.322840 3.172061 -1.637931 H 0 -0.140173 1.074937 -2.115339 H 0 0.882681 3.470067 -2.526593 H 0 0.194345 3.935779 -0.873933	68.3190 171.5817 271.7627 434.2751 495.1523 589.0020 703.6256 793.6844 857.4116 881.9760 957.9178 998.7457 1082.3327 1168.2719 1236.6263 1300.3006 1389.4720 1473.4558 1566.5402 1646.4139 3138.8270 3156.8669 3169.5275 3204.1704	125.4839 211.5569 326.7593 450.0303 509.4453 603.5603 748.2794 806.2734 869.7759 919.6795 971.9720 1006.5481 1094.1988 1185.8104 1242.6582 1363.6541 1423.2278 1493.3061 1614.0045 1662.2641 3141.7432 3158.4240 3183.6079 3221.4263	170.2495 223.4836 370.1917 478.3564 563.5392 669.5426 789.0936 818.3191 878.1508 935.6389 983.9155 1048.8114 1104.8859 1193.0366 1283.1797 1386.4343 1443.2627 1545.8690 1635.6414 3060.8925 3147.2528 3165.4651 3184.7919 3237.0909
ts **i1-i2** 	C 0 1.399746 0.393332 -0.346477 C 0 2.830618 0.306985 -0.329974 C 0 3.452661 -0.912224 0.045099 C 0 2.692635 -2.000724 0.381933 C 0 1.281750 -1.917072 0.370091 C 0 0.624914 -0.755288 0.027788 C 0 -0.894748 -0.688008 0.010375 C 0 -1.615318 -1.792300 0.720214 C 0 -3.000034 -2.147682 0.369673 C 0 -3.364035 -3.183151 -0.385279 C 0 0.814022 1.624676 -0.748110	-207.8576 124.6709 229.3630 360.1677 479.4387 534.1886 638.8764 742.9896 807.8361 901.4530 963.0402	31.9199 150.0522 272.3540 414.1976 499.8462 543.2162 670.8903 788.9791 856.6155 928.9245 983.0855	39.0071 178.9037 284.8917 437.0298 519.2678 611.2783 738.2409 804.6904 870.0363 955.4971 990.5459

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	C 0 1.588116 2.705021 -1.101140	1120.1662	1168.2656	1185.4950
	H 0 4.536200 -0.966713 0.054429	1189.3444	1213.6172	1230.1323
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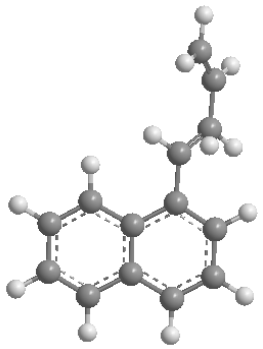
ts **i2-p2** 	C 0 1.522644 0.097762 -0.250406	-432.5288	60.6116	67.0535
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	C 0 3.629331 -1.033683 0.343322	187.1907	221.0352	260.0166
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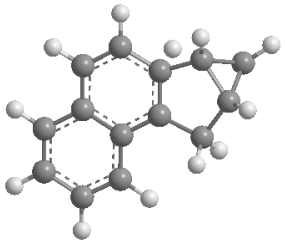
ts **i5-p5** 	C 0 -1.713952 1.530563 0.109446 C 0 -1.726096 0.190382 -0.380031 C 0 -0.524495 -0.593990 -0.321895 C 0 0.639617 0.008840 0.208226 C 0 0.660319 1.371506 0.536124 C 0 -0.565742 2.109831 0.570751 C 0 1.952469 -0.660012 0.558096 C 0 2.769996 0.437243 1.247288 C 0 1.944155 1.720174 1.234901 C 0 3.223117 1.615689 0.433789 C 0 -2.905252 -0.405713 -0.886570 C 0 -0.571299 -1.945153 -0.757275 C 0 -1.735988 -2.490169 -1.245062 C 0 -2.913816 -1.714411 -1.313790 H 0 -2.643873 2.089426 0.106754 H 0 -0.563432 3.134447 0.925195 H 0 2.467535 -1.063754 -0.322352 H 0 1.783079 -1.504445 1.235858 H 0 3.350824 0.167967 2.121150 H 0 1.907466 2.391864 2.084536 H 0 3.130716 1.578857 -0.646411 H 0 4.082567 2.167078 0.798395 H 0 -3.811686 0.189232 -0.932169 H 0 0.330436 -2.545355 -0.713094 H 0 -1.752261 -3.520495 -1.582628 H 0 -3.825550 -2.154358 -1.701682 H 0 1.045147 2.044755 -1.113550	-875.4008 191.4219 329.8066 425.9967 513.2521 587.8563 691.2878 758.7215 816.4111 874.9674 957.3396 992.4482 1047.0466 1097.7602 1175.6681 1205.3992 1282.4534 1368.8358 1412.1377 1485.5145 1580.2813 3009.8404 3157.1265 3164.1811 3181.7667	86.7455 223.9004 361.4605 456.5201 534.6412 626.6983 718.4738 784.4892 828.8256 887.5618 972.0629 1004.5720 1055.9241 1112.2434 1186.0622 1214.0389 1296.7070 1376.4316 1465.1874 1487.3898 1625.0260 3036.1124 3157.6282 3166.2594 3188.9669	123.9152 236.0709 367.4444 474.4769 552.1933 662.6673 750.3867 792.9829 865.0002 926.6962 978.4459 1037.5813 1067.7114 1167.6157 1187.8408 1232.1763 1339.6816 1396.1248 1470.2982 1539.3448 1651.1685 3108.0585 3161.4285 3178.8495 3196.5529
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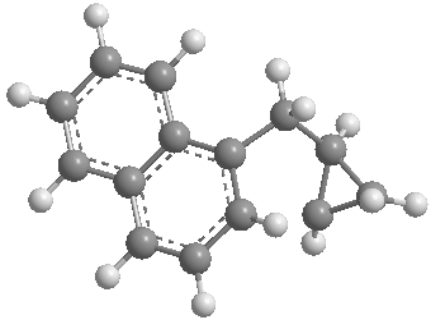
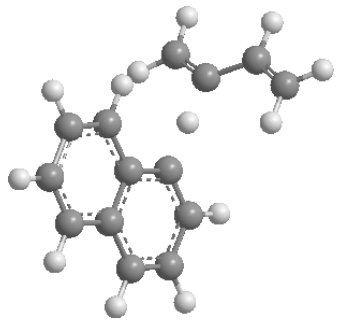
	C 0 0.590620 -1.171660 0.835925 C 0 -0.432618 -2.152222 0.640761 C 0 1.593593 1.034893 0.480163 C 0 2.607712 0.268446 -0.406364 C 0 2.316963 -1.176457 -0.534991 C 0 3.524131 -0.779673 0.218596 C 0 -3.149865 -0.081357 -0.831513 C 0 -1.214036 1.894108 -0.441667 C 0 -2.437433 2.218294 -0.978510 C 0 -3.418481 1.224032 -1.179239 H 0 -2.399180 -2.549333 -0.077759 H 0 1.361848 -1.401340 1.563183 H 0 -0.246340 -3.176438 0.944327 H 0 1.996039 1.174290 1.490112 H 0 1.418179 2.029434 0.072655 H 0 2.988726 0.815306 -1.264349 H 0 2.217866 -1.803934 -1.409493 H 0 3.528238 -0.859680 1.305120 H 0 4.501816 -0.951332 -0.227319 H 0 -3.898599 -0.852205 -0.983686 H 0 -0.482200 2.677043 -0.287273 H 0 -2.651762 3.246292 -1.249191 H 0 -4.379319 1.489989 -1.605057	515.9064 614.1024 740.5044 783.4692 812.2838 871.8614 954.8889 1000.2683 1053.4883 1100.1904 1181.5275 1217.9521 1280.8977 1368.0662 1458.3857 1491.1429 1622.4153 3060.8903 3133.2918 3158.4795 3182.9582	526.8246 669.2268 750.4616 802.8659 841.2933 896.0780 976.3308 1023.6164 1064.1024 1105.1942 1186.7683 1230.3242 1296.5056 1391.6354 1469.9247 1536.0682 1640.7728 3105.8734 3144.6333 3166.9607 3195.0150	559.1623 715.2419 768.8851 811.4183 869.8906 947.2929 987.8167 1045.9925 1075.2123 1161.6369 1192.5037 1246.8590 1358.5689 1420.2382 1484.1304 1571.7890 3021.0712 3121.6262 3155.4374 3179.2035 3200.9908
H abstraction ts1 	C 0 -2.426787 -1.137016 0.044742 C 0 -2.583303 -2.026627 1.140925 C 0 -1.556403 -2.254645 2.024249 C 0 -0.309165 -1.598320 1.855899 C 0 -0.149910 -0.742145 0.804946 C 0 -1.167871 -0.468851 -0.134574 C 0 -3.469926 -0.881988 -0.883187 C 0 -1.009507 0.419754 -1.230633 C 0 -2.043434 0.640479 -2.107617 C 0 -3.284453 -0.015445 -1.932615 H 0 -3.536741 -2.528122 1.270645 H 0 -1.692579 -2.937560 2.855954 H 0 0.499888 -1.780678 2.555697 H 0 -4.421845 -1.385701 -0.748960	-1567.4694 53.9720 171.4611 279.4625 405.1531 516.5439 553.6947 741.7745 793.1135 870.2391 915.7637 965.5124 1009.2842 1055.1381	15.0781 109.0329 188.2460 343.3363 471.9237 519.6303 623.7349 755.5525 802.4665 892.2884 949.5430 981.0876 1014.2216 1146.2794	39.5874 122.4842 211.3194 384.5244 506.8783 534.4181 656.4363 780.1884 805.8505 908.2123 952.8373 998.2115 1037.1413 1168.8957

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	H 0 -4.090925 0.169292 -2.633368	1292.9832	1310.1168	1372.9712
	C 0 1.658150 2.099621 2.235646	1388.2162	1402.1403	1411.3210
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	H 0 1.923502 2.964523 2.831463	3083.1652	3092.7782	3141.5610
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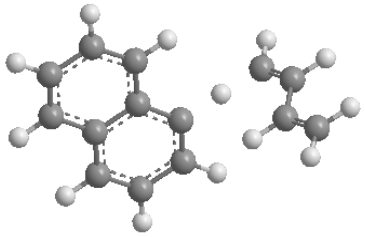
H abstraction ts2 	C 0 -3.305664 -0.345009 -0.377554	-1590.5132	16.6708	36.0458
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	C 0 -2.703413 -2.633296 -0.948317	172.8479	200.9571	246.9359
	C 0 -1.365756 -2.228082 -1.194022	261.5813	373.5996	391.6835
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