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A Unified Mechanism on the Formation of Acenes, Helicenes, and Phenacenes in the Gas Phase

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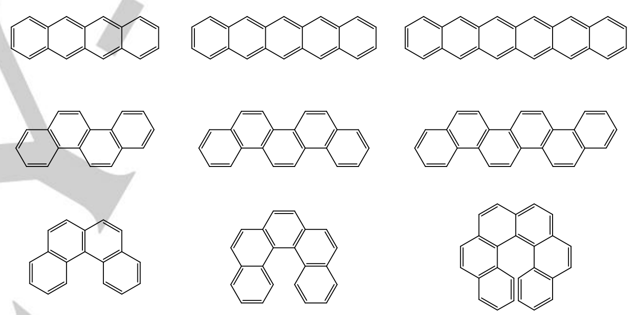
Abstract: A unified low temperature reaction mechanism on the formation of acenes, phenacenes, and helicenes – polycyclic aromatic hydrocarbons (PAHs) that are distinct via the linear, zig-zag, and ortho-condensed arrangements of fused benzene rings - is revealed. This mechanism is mediated through a barrierless, vinylacetylene mediated gas phase chemistry utilizing tetracene, [4]phenacene, and [4]helicene as benchmarks contesting established paradigms that molecular mass growth processes to PAHs transpire at elevated temperatures. This mechanism opens up an isomer-selective route to aromatic structures involving submerged reaction barriers, resonantly stabilized free radical intermediates, and systematic ring annulation potentially yielding molecular wires along with racemic mixtures of helicenes in deep space. Any enantiomeric excess generated by preferential destruction of one enantiomer might be transferred to ice-coated carbonaceous grains and ultimately to biorelevant molecules formed on these icy grains via interaction with ionizing radiation thus providing a unique perception on the *Origins of Life* at the most fundamental level.

Introduction

Tetracene (naphthacene; $C_{18}H_{12}$),[1] [4]phenacene (chrysene; $C_{18}H_{12}$),[2] and [4]helicene (benzo[*c*]phenanthrene; $C_{18}H_{12}$)[3] isolated nearly a century ago are the simplest representatives of three key classes of polycyclic aromatic hydrocarbons (PAHs) - acenes, phenacenes, and helicenes - structural isomers of aromatic systems differentiated by linear, zig-zag, and ortho-condensed arrangements of fused benzene rings. These species received considerable attention as molecular tracers in untangling the underlying molecular mass growth processes leading to PAHs in combustion systems and in the interstellar medium (ISM) at the most fundamental, microscopic level (Scheme 1). Although the presence of PAHs[4] along with their methylated and hetero-atom substituted counterparts[5] have been firmly established in carbonaceous chondrites such as Allende and Murchison with PAHs possibly accounting for up to 20% of the cosmic carbon budget,[6] the underlying mechanisms to their formation beyond anthracene ($C_{14}H_{10}$) and phenanthrene ($C_{14}H_{10}$)[7] in deep space and in combustion systems have remained largely elusive.



Scheme 1. Representatives of key classes of PAHs differing by the linear, zig-zag, and ortho-condensed arrangements of fused benzene rings: acenes (i), phenacenes (ii), and helicenes (iii).

Recent laser desorption – laser multiphoton ionization mass spectrometry (L^2MS) along with D/H and $^{13}C/^{12}C$ isotopic analyses of meteoritic PAHs revealed that these meteoritic PAHs are likely synthesized in circumstellar envelopes of carbon-rich Asymptotic Giant Branch Stars (AGB) and planetary nebulae as the descendants of AGB stars via extensive molecular mass growth processes.[4a, 4c, 8] However, contemporary astrochemical models of PAH formation as derived from combustion chemistry reaction networks[9] predict time scales for the injection of PAHs from carbon stars into the interstellar medium of some 10^9 years, which is much longer than the predicted lifetimes of PAHs of only a few 10^8 years.[10] These models rely on the much discussed Hydrogen-Abstraction/aCetylene-Addition (HACA) mechanism, which involves repetitive sequences of atomic hydrogen abstractions from an aromatic hydrocarbon like benzene followed by consecutive addition of one or two acetylene molecule(s) prior to cyclization and aromatization.[11] Interstellar PAHs can be rapidly destroyed by photolysis,[12] galactic cosmic rays,[13] and interstellar shocks,[10] but - along with their derivatives – they are still present as evidenced from the diffuse interstellar bands (DIBs)[14] - discrete absorption features overlaid on the interstellar extinction curve from the blue part of the visible (400 nm) to the

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Supporting information for this article is given via a link at the end of the document.

near-infrared (1.2 mm) - and from unidentified infrared (UIR) emission bands[15] in the 3–14 mm wavelength range. Thus, the spectroscopic observation of PAHs infers a critical, hitherto unexplained route to their rapid chemical growth in the cold interstellar medium at temperatures down to 10 K.

Here, we reveal an isomer-selective, versatile reaction mechanism involving vinylacetylene mediated gas phase formation of acenes, helicenes, and phenacenes with the simplest 18-*π*-electron tetracene, [4]phenacene, and [4]helicene isomers acting as critical benchmarks. In strong contrast to the aforementioned routes to PAHs synthesis involving HACA, our mechanistical studies of the elementary reactions of distinct anthracenyl and phenanthrenyl radicals ($[C_{14}H_9]^\bullet$; 177 amu) with vinylacetylene (C_4H_4; 52 amu) display *barrierless* pathways via the initial formation of a long-range van-der-Waals complexes in the entrance channels followed by isomerization through addition of the aromatic radical involving a *submerged barrier* leading to resonantly stabilized free $[C_{18}H_{13}]^\bullet$ radicals (RSFRs) (Reaction (1)). The latter undergo hydrogen migration and ring closure followed by aromatization through atomic hydrogen loss yielding distinct $C_{18}H_{12}$ isomers through targeted, stepwise ring expansion involving free radical reaction intermediates. This pathway represents a versatile reaction mechanism to synthesize acenes, helicenes, and phenacenes in low temperature interstellar environments down to 10 K through elementary gas phase reactions of aryl radicals with vinylacetylene. Considering the low temperature, bimolecular gas phase reactions have to be exoergic and all transition states involved shall be lower than the energy of the separated reactants. Since these requirements are fulfilled, the proposed pathway provides a hitherto ignored low temperature route to complex PAHs via ring annulation. Interstellar PAHs are rapidly destroyed in the interstellar medium by photolysis, cosmic rays, and interstellar shocks leading to life times of only a few 10^8 years.[10] This time scale is much shorter than the time scale for injection of PAHs synthesized in carbon-rich outflows of Asymptotic Giant Branch (AGB) stars of some 10^9 years.[10] Therefore, the presence of PAH-like material in the interstellar medium suggests that a critical synthetic pathway to PAHs at low temperatures is missing. The mechanisms elucidated here might fill the gap and can provide a unique route to PAHs at temperatures as low as 10 K. These mechanisms are of interest in organic chemistry and can be linked to material sciences as they provide insight into reactivity, bond-breaking processes, and synthesis of extended π-conjugated systems involving acyclic precursors (vinylacetylene) with extensive applications as building blocks for molecular wires,[16] carbon nanotubes[17] and graphene[18] along with molecular organic semiconductors for organic field effect transistors[19] and organic light emitting diodes.[20]

(1) $[C_{14}H_9]^\bullet + C_4H_4 \rightarrow [C_{18}H_{13}]^\bullet \rightarrow C_{18}H_{12} + H^\bullet$

Briefly, a high-temperature chemical reactor was utilized to investigate the reaction of distinct anthracenyl and phenanthrenyl radicals ($[C_{14}H_9]^\bullet$) with vinylacetylene (C_4H_4). This reactor [7, 9] consists of a heated silicon carbide (SiC) tube and is incorporated within the source chamber of a molecular beam machine equipped with a Wiley-McLaren reflectron time-of-flight mass spectrometer (Re-TOF-MS) (Figure 1). To generate the radical reactants, thermally labile brominated precursor molecules were pyrolyzed *in situ* via cleavage of a weak carbon-bromine bond. These precursors were 2- and 3-bromophenanthrene along with 1- and 2-bromoanthracene ($C_{14}H_9Br$) seeded in separate experiments in vinylacetylene/helium. The temperature of the reactor was 1400 ± 10 K. At this temperature, each brominated precursor dissociates to the corresponding radical plus atomic bromine *in situ* followed by reaction of the radical with vinylacetylene. The reaction products were expanded, passed through a skimmer downstream the reactor, and entered the main chamber, which houses the Reflectron Wiley–McLaren Time-Of-Flight Mass Spectrometer (Re-TOF-MS). Tunable vacuum ultraviolet (VUV) light from the Advanced Light Source crossed the neutral molecular beam downstream of the skimmer in the extraction region of the Re-TOF-MS. A mass spectrum was collected by measuring the arrival time of the ions, as a function of mass-to-charge (*m/z*) ratios. Finally, photoionization efficiency (PIE) curves reporting the ion counts of well-defined *m/z* ratios versus the VUV energy were recorded by integrating the ion signal at mass-to-charges of interest and normalizing it to the photon flux. VUV single photon ionization represents a fragment-free ionization technique and is dubbed as a *soft ionization* method compared to the harsher conditions of electron impact ionization leading often to excessive fragmentation of the parent ion (Supplementary Information).

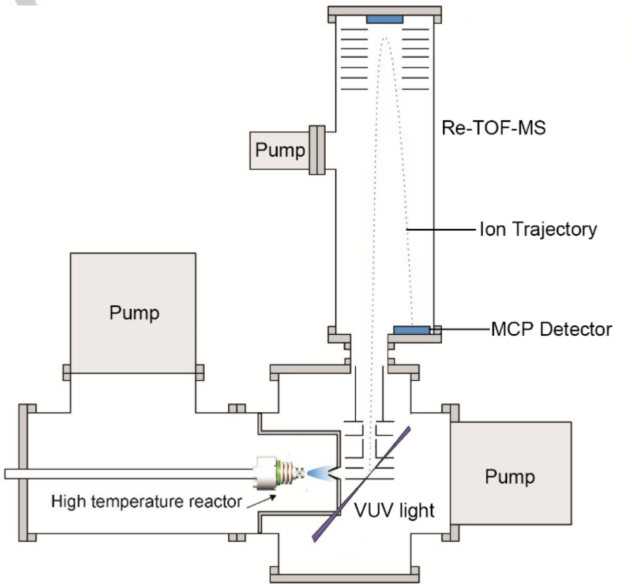

Figure 1. Schematic diagram of the high-temperature reactor along with the molecular beam sampling reflectron time of flight mass spectrometer.[21]

Results and Discussion

Mass Spectra

As a very first step, we analyze the mass spectra of each system qualitatively and extract the molecular formulae of the reaction products. Representative mass spectra recorded at a photoionization energy of 9.50 eV are displayed in Figure 2 for the reactions of 1- and 2-anthracenyl (Figs. 2b, 2d) and 2- and 3-phenanthrenyl (Figs. 2f, 2h) with vinylacetylene. We also conducted ‘blank’ experiments by replacing the vinylacetylene reactant with non-reactive helium carrier gas (Figs. 2a, 2c, 2e, 2g) to guarantee that the newly emerging products (Figs. 2b, 2d, 2f, 2h) are the result of the reaction of the radicals with vinylacetylene. A detailed inspection of these data reveals the formation of molecules with the molecular formulae $C_{16}H_{10}$ (202 amu) and $C_{18}H_{12}$ (228 amu) along with the ^{13}C isotopologues at *m/z* = 203 and 229 in all systems. These ion counts are clearly absent in the control experiments suggesting that molecules detected via *m/z* = 202, 203, 228, and 229 represent reaction products in all $C_{14}H_9$ - C_4H_4 systems. Considering the molecular weight of the reactants and the products, the $C_{18}H_{12}$ isomers along with atomic hydrogen are the result of the reaction of the aromatic radicals with vinylacetylene through reaction (1). The signal for $C_{16}H_{10}$ (202 amu) can be attributed to the reaction of the anthracenyl/phenanthrenyl radicals with acetylene (C_2H_2; 26 amu) and might be linked to the formation of ethynyl-substituted anthracenes and phenanthrenes (Supplementary Figures 1-4). The ion counts at mass-to-charge ratios (*m/z*) of 259 ($C_{13}{}^{13}CH_9{}^{81}Br^+$), 258 ($C_{14}H_9{}^{81}Br^+$), 257 ($C_{13}{}^{13}CH_9{}^{79}Br^+$), 256 ($C_{14}H_9{}^{79}Br^+$), 179 ($C_{13}{}^{13}CH_{10}{}^+$), 178 ($C_{14}H_{10}{}^+$), 177 ($C_{14}H_9{}^+$/$C_{14}{}^{13}CH_8{}^+$), and 176 ($C_{14}H_8{}^+$) are detectable in the control experiments as well and hence cannot be associated with the reaction of anthracenyl/phenanthrenyl radicals with vinylacetylene (Supplementary Figures. 1-4).

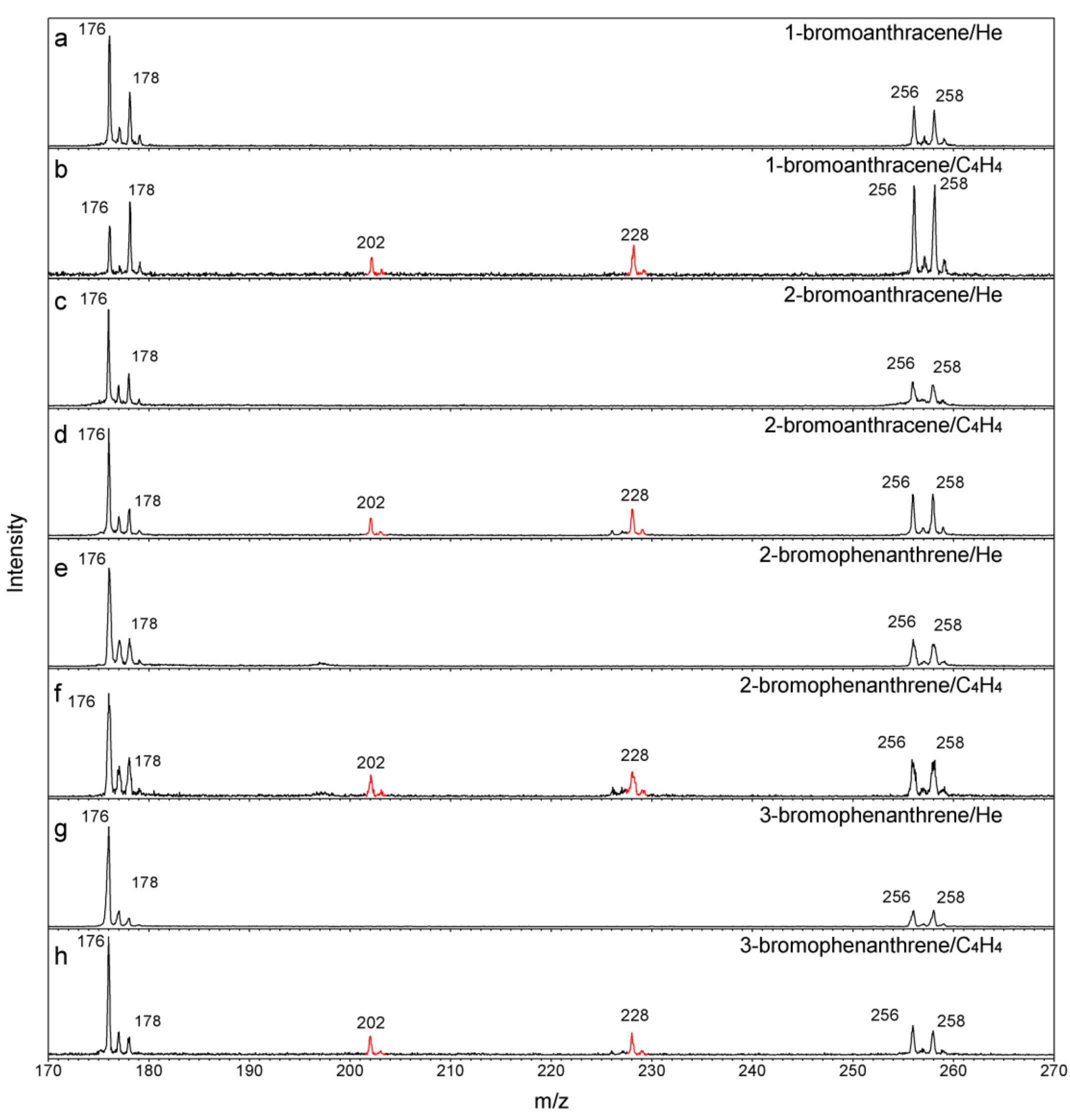

Figure 2. Comparison of mass spectra recorded at a photoionization energy of 9.50 eV. (a) 1-bromoanthracene – vinylacetylene, (b) 1-bromoanthracene – helium, (c) 2-bromoanthracene – vinylacetylene, (d) 2-bromoanthracene – helium, (e) 2-bromophenanthrene – vinylacetylene, (f) 2-bromophenanthrene – helium, (g) 3-bromophenanthrene – vinylacetylene and (h) 3-bromophenanthrene – helium systems. The ion peaks of the newly formed $C_{16}H_{10}$ (*m/z* = 202) and $C_{18}H_{12}$ (*m/z* = 228) species along with the ^{13}C-substituted counterparts (*m/z* = 203 and 229) are highlighted in red.

Photoionization Efficiency (PIE) Curves

The analysis of the mass spectra provided compelling evidence that $C_{18}H_{12}$ isomer(s) are formed via the reaction of anthracenyl/phenanthrenyl radicals with vinylacetylene. The primary goal of this study is, however, to elucidate which $C_{18}H_{12}$ isomer(s) is/are formed. This requires a detailed inspection of the corresponding photoionization efficiency (PIE) curves at *m/z* = 228 ($C_{18}H_{12}^+$). Here, each PIE curve reports the number of ions detected at a well-defined *m/z* ratio such as *m/z* = 228 as a function of the photon energy from 7.20 eV to 10.00 eV (Figure 3). It is important to highlight that the PIE curves of distinct $C_{18}H_{12}$ isomers are very different and hence unique. This is evident from distinct PIE curves of the $C_{18}H_{12}$ isomers - tetracene (naphthacene), [4]phenacene (chrysene), [4]helicene (benzo[*c*]phenanthrene), benz[*a*]anthracene, triphenylene – recorded in separate calibration experiments (Supplementary Figure 5). Therefore, the PIE calibration curves can be utilized to discriminate between multiple $C_{18}H_{12}$ isomers. More than one $C_{18}H_{12}$ isomer might be formed in each reaction investigated, and therefore each experimental PIE curve at *m/z* = 228 represents the sum, i.e. a linear combination, of the calibrated PIE curves of the individual isomers. Consequently, the experimental PIE curves have to be fit with a linear combination of the PIE calibration curves of distinct isomers.

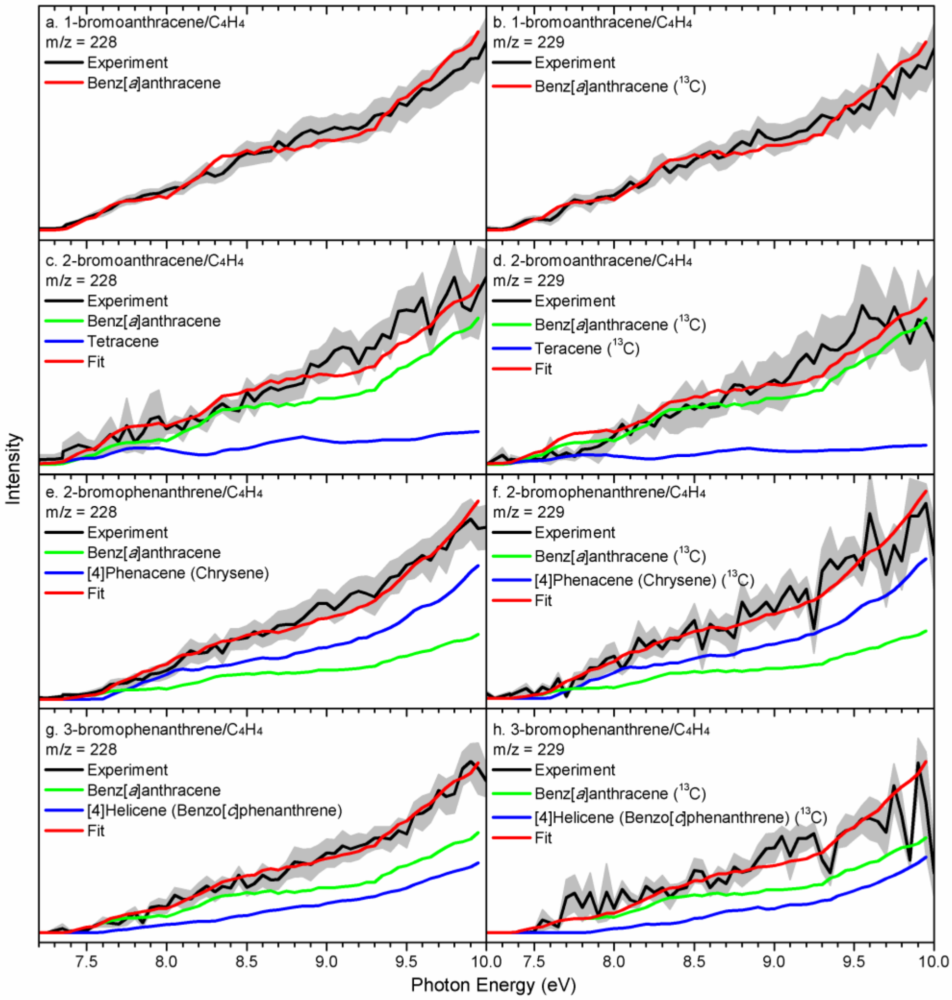

Figure 3. Photoionization efficiency (PIE) curves for *m/z* = 228 and 229. (a) and (b) 1-bromoanthracene – vinylacetylene; (c) and (d) 2-bromoanthracene – vinylacetylene; (e) and (f) 2-bromophenanthrene – vinylacetylene; (g) and (h) 3-bromophenanthrene – vinylacetylene. Black lines: experimentally derived PIE curves; colored lines: reference PIE curves. In case of multiple contributions to one PIE curve, the red line shows the 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.

Discussion

In the 1-anthracenyl-vinylacetylene system, the experimental PIE curve can be fit within the error limits with a single reference PIE curve of benz[*a*]anthracene (Figs. 3a and b). Both PIE curves depict an onset of the ion signal at 7.35 ± 0.05 eV, which agrees nicely with the adiabatic ionization energy of benz[*a*]anthracene of 7.41 ± 0.02 eV.[22] The remaining three systems of 2-anthracenyl, 2-phenanthrenyl, and 3-phenanthrenyl with vinylacetylene require a linear combination of two reference curves of benz[*a*]anthracene/tetracene, [4]phenacene/benz[*a*]anthracene, and [4]helicene/benz[*a*]anthracene, respectively (Figs. 3c-h;). Corresponding PIE curves of *m/z* = 229 ($^{13}CC_{17}H_{12}^{+}$) match these findings and reveal that ion signal at *m/z* = 229 originates solely from the aforementioned ^{13}C-isotoplogue PAHs. Therefore, we can conclude that our studies provide compelling evidence on the formation of four distinct $C_{18}H_{12}$ isomers of PAHs with benz[*a*]anthracene being identified in all four systems; tetracene, [4]phenacene, and [4]helicene represent distinct reaction products (Fig. 4).

The experimental data provide persuasive evidence on the formation of the simplest representatives of three key classes of PAHs, i.e. acenes, phenacenes, and helicenes, formed through the elementary reactions of anthracenyl and phenanthrenyl radicals with vinylacetylene in the gas phase. These representatives are: tetracene, [4]phenacene, and [4]helicene, respectively, along with benz[*a*]anthracene. Our goal is not only to identify the PAH isomers formed, but also to elucidate the underlying reaction mechanisms. In case of polyatomic complex systems, it is useful to combine the experimental results with electronic structure calculations to untangle the synthetic routes (Fig. 4). Our computations reveal that for each reaction, the radical reactant approaches the vinylacetylene molecule resulting in the formation of weakly stabilized van-der-Waals complex (**1.1-1.4**) bound by 8-12 kJ mol^{-1} with rather long carbon-carbon distances between 413 pm and 526 pm. The complexes isomerize via addition of the radical center to the terminal sp^2 carbon of the vinylic group in vinylacetylene resulting in the formation of distinct $C_{18}H_{13}$ intermediates (**2.1** -**2.4**). These processes involve barriers located 4 to 9 kJ mol^{-1} *above* the van-der-Waals complexes, but below the energy of the separated reactants. In this case, a barrier to addition does exist, but since the transition state is lower in energy than the reactants, this barrier is *submerged* with respect to the reactants and hence is called a *submerged barrier*. Hereafter, these intermediates isomerize via hydrogen shifts from the aromatic ring from the carbon atom adjacent to the former radical center to the vinylacetylene moiety forming a –CH_2-C**H**H-CCH side chain with the migrated hydrogen atom denoted in bold. Eventually, the newly formed intermediates (**3.1**-**3.4)** undergo facile ring closure yielding PAH-type radicals which carry four six-membered rings (**4.1-4.4**). A comparison of the molecular structures of these intermediates with the detected reaction products benz[*a*]anthracene (Fig. 4a), tetracene/benz[*a*] anthracene (Fig. 4b), [4]phenacene/benz[*a*]anthracene (Fig. 4c), and [4]helicene/benz[*a*]anthracene (Fig. 4d) suggests that in each radical intermediate, a hydrogen atom has to migrate from the CH_2 moiety of the newly formed ring to the neighboring bare carbon atom forming intermediates **5.1**-**5.4**. The latter eject atomic hydrogen accompanied by aromatization and formation of the closed shell PAH. The overall reactions are exoergic and all transition states are below the energy of the separated reactants. Benz[*a*]anthracene is formed in all systems, whereas tetracene, [4]phenacene, and [4]helicene are unique to the reactions of 2-anthracenyl, 2-, and 3-phenanthrenyl with vinylacetylene, respectively.

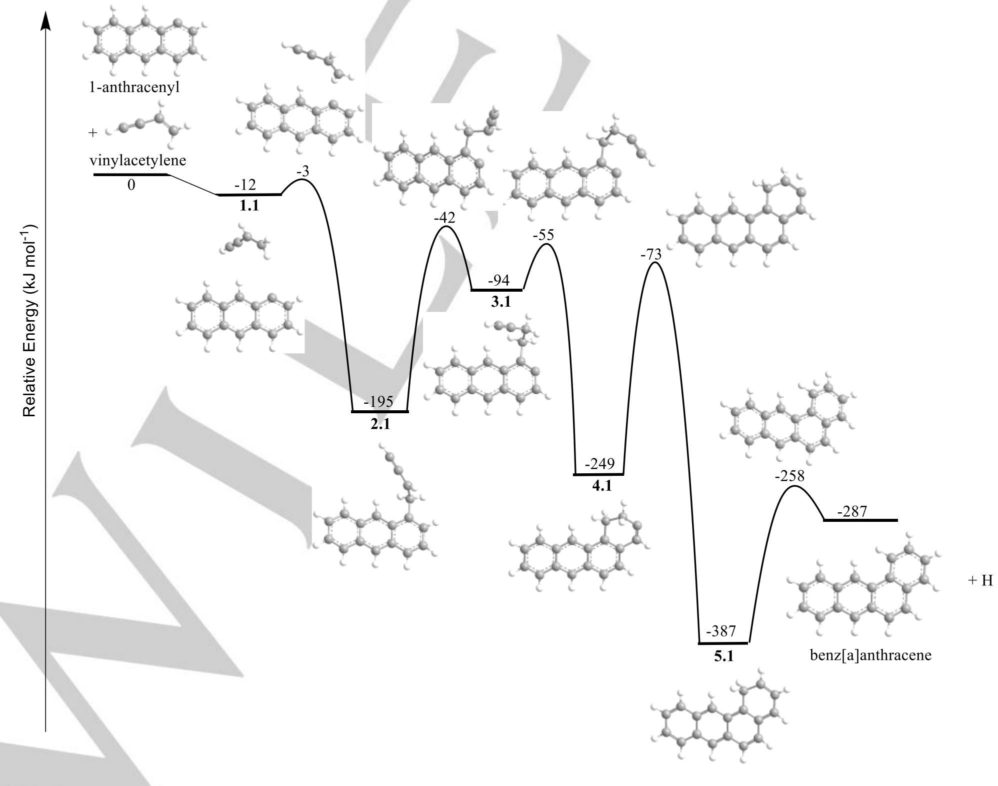

Figure 4(a)

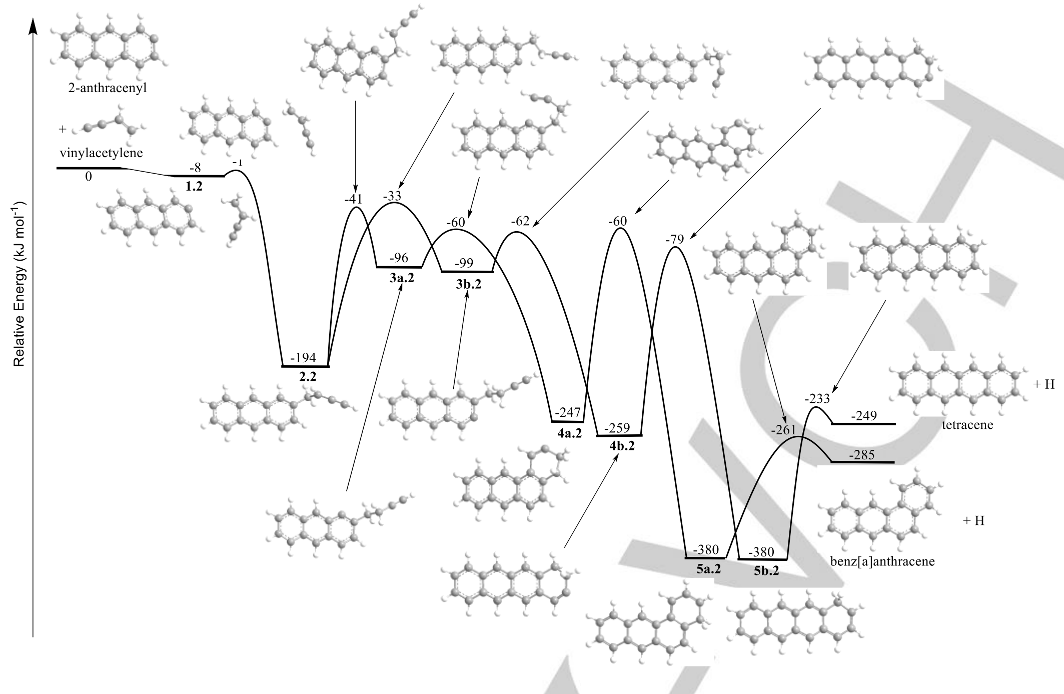

Figure 4(b)

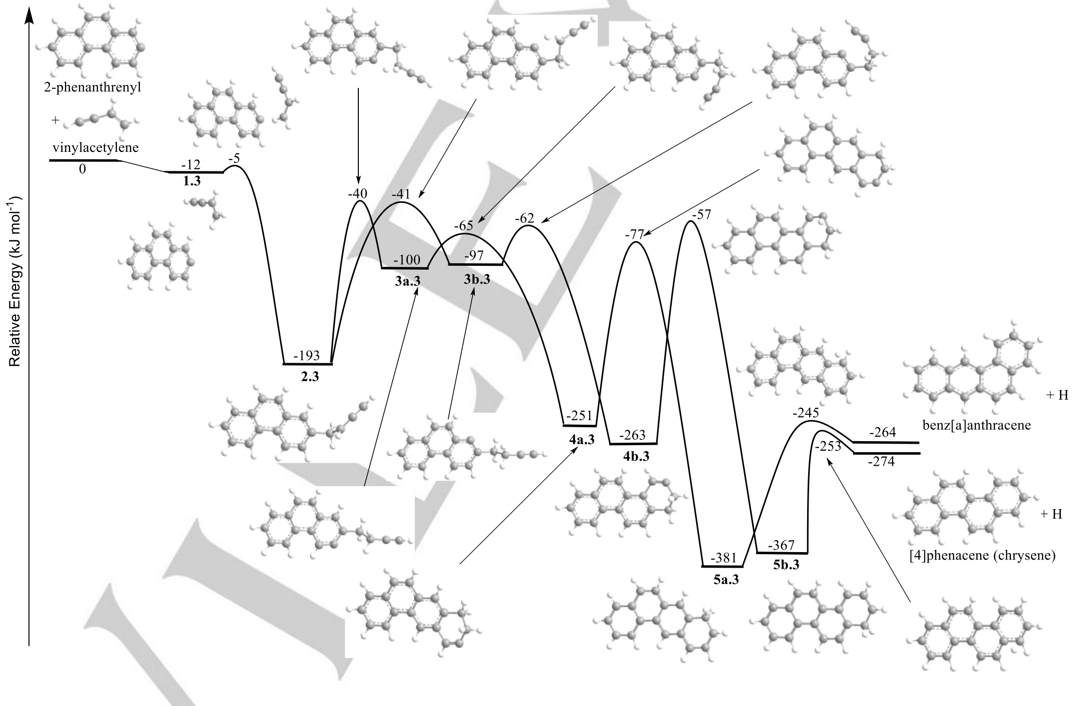

Figure 4(c)

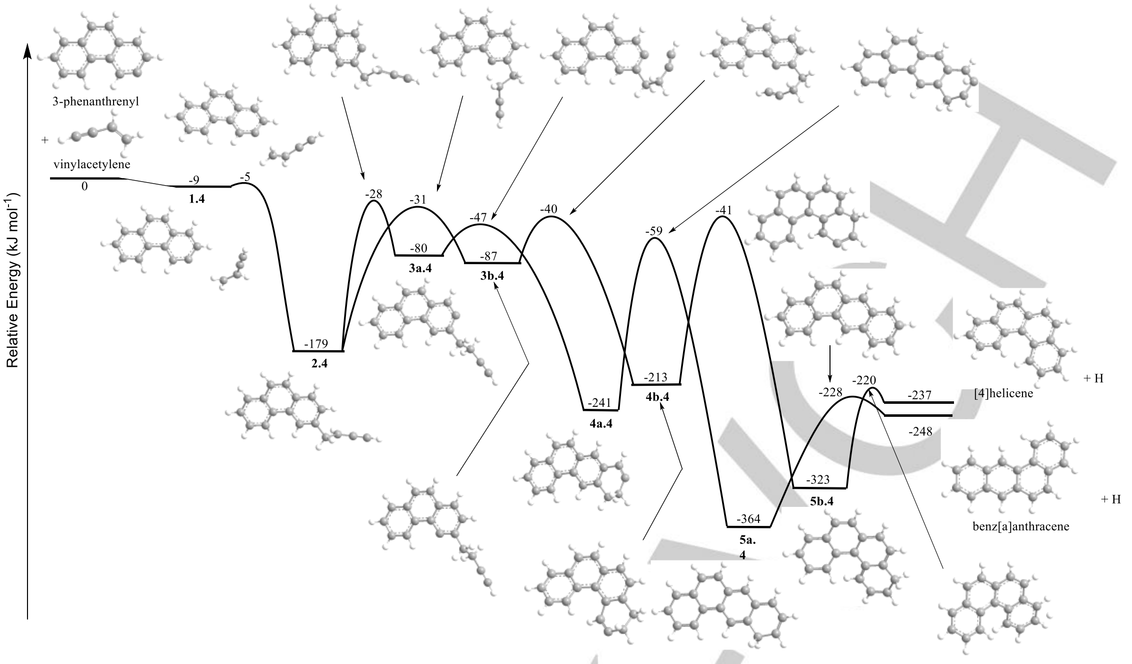

Figure 4(d)

Figure 4. Potential energy surfaces (PESs) of the 1-anthracenyl (a), 2-anthracenyl (b), 2-phenanthrenyl (c), and 3-phenanthrenyl (d) leading to the formation of benz[*a*]anthracene, tetracene, [4]phenacene, and [4]helicene. Relative energies with respect to the reactants are given in kJ mol^{-1}.

Conclusion

In conclusion, our combined experimental and computational study provides compelling evidence of an isomer-selective, unified mechanism to the simplest 18-π-aromatic acenes, phenacenes, and helicenes - tetracene, [4]phenacene, and [4]helicene – via vinylacetylene mediated gas phase reactions involving ring annulation of anthracenyl and phenanthrenyl radicals. These de facto barrierless routes are initiated through the formation of long-range van-der-Waals complexes, which can isomerize through addition of the radical reactant via transition states located below the energy of the separated reactants (submerged barrier). This submerged barrier represents a crucial prerequisite for a bimolecular reaction to proceed at low temperatures since any transition state located above the energy of the separated reactants cannot be overcome at low temperatures of 10 K. Since all reactions investigated are barrierless and exoergic, these elementary reactions may also contribute to the formation of PAHs in cold molecular clouds such as Taurus Molecular Cloud - 1 (TMC-1) at temperatures as low as 10 K thus supplying a hitherto elusive low temperature molecular mass growth process to complex PAHs carrying four six-membered rings as detected along with benz[*a*]anthracene in carbonaceous chondrites like Murchison, Orgueil, and A-881458.[23] Here, the hydrogen abstraction – vinylacetylene addition (HAVA) pathway signifies a versatile reaction mechanism to generate even more complex acenes, helicenes, and phenacenes through barrierless, stepwise ring expansion via elementary gas phase reactions of an aryl radical, which can be formed inside molecular clouds from the corresponding aromatic precursor via photolysis by the internal ultraviolet field, with vinylacetylene. In circumstellar envelopes of carbon stars with temperatures of up to a few 1,000 K and even in combustion flames, molecular mass growth processes could also be triggered by hydrogen abstraction from phenanthrene and anthracene followed by formation of tetracene, [4]phenacene, and/or [4]helicene as identified as products of incomplete combustion of coal,[24] wood,[25] and (bio)diesel.[26] This proposes HAVA as a *facile key mechanism* propelling molecular mass growth processes of PAHs via de facto barrier-less, successive ring expansions involving elementary reactions of aryl radical with vinylacetylene as a molecular building block.

In cold molecular clouds such as the Taurus Molecular Cloud 1 (TMC-1), these processes may lead ultimately to molecular wires[16] and possibly racemic mixtures of helicenes depicting non-superimposable, clockwise and counterclockwise helices.[27] Should a preferential destruction of the minus (M) and plus (P) enantiomer, such as via photodissociation through circularly polarized light, exist, the resulting enantiomeric excess might be incorporated into carbonaceous grains, which can then become coated with nanometer thick icy layers of water (H_2O), ammonia (NH_3), methane (CH_4), carbon monoxide (CO), carbon dioxide (CO_2), and methanol (CH_3OH) in cold molecular clouds. Upon interaction of those ices with ionizing radiation, the grains might transmit their enantiomer excess to the newly formed complex organic molecules (COMs) – among them biorelevant molecules such as amino acids,[28] dipeptides,[29] and even carbon hydrates[30] thus connecting helicene templates to the *Origins of Life* ultimately changing our hypothesis on the interstellar carbon chemistry and the progression of carbonaceous matter in the universe on the most fundamental level.

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Keywords: Hydrogen Abstraction/Vinylacetylene Addition (HAVA) • polycyclic aromatic hydrocarbons • gas-phase chemistry • mass spectrometry • interstellar medium

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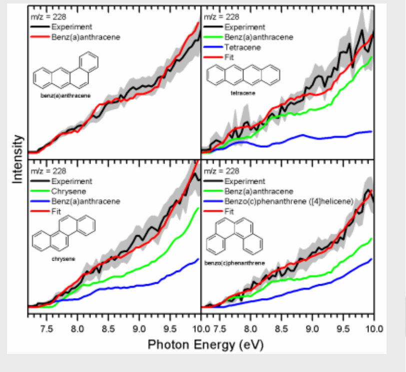
RESEARCH ARTICLE

Acenes, helicenes, and phenacenes can be formed through molecular mass growth processes via ring annulation reactions at low temperatures.



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A Unified Mechanism on the Formation of Acenes, Helicenes, and Phenacenes in the Gas Phase

Supplementary Information

A Unified Mechanism on the Formation of Acenes, Helicenes, and Phenacenes in the Gas Phase

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METHODS

Experimental: The experiments were conducted at the Advanced Light Source (ALS) at the Chemical Dynamics Beamline (9.0.2.) exploiting a high-temperature chemical reactor consisting of a resistively-heated silicon carbide (SiC) tube of 20 mm heating length and 1 mm inner diameter.[1] This device is situated inside the source chamber of a molecular beam apparatus equipped with a Wiley-McLaren reflectron time-of-flight mass spectrometer (Re-TOF-MS) and designed to study the outcome of elementary chemical reactions leading to PAH growth *in situ* through the reaction of aromatic radicals. In detail, the brominated precursors ($C_{14}H_9Br$) [2- and 3-bromophenanthrene, 1- and 2-bromoanthracene; > 97%; TCI America] were kept each in separate experiments in a stainless-steel filter in the entrance of the reactor. The filter was heated up to 473 ± 5 K and monitored by a Type-K thermocouple, to vaporize the precursors. The radical reactants were generated *in situ* via pyrolysis of the brominated precursors seeded in vinylacetylene/helium (5% C_4H_4 seeded in 95% He; Applied Gas) carrier gas at a pressure of 300 Torr. The temperature of the SiC tube was examined using a Type-C thermocouple to be 1400 ± 10 K. At this temperature, each brominated precursor dissociates to the corresponding radical plus atomic bromine *in situ* followed by the reaction of the aromatic radical with vinylacetylene. The reaction products were expanded, passed through a 2 mm skimmer located 10 mm downstream the reactor, and entered the main chamber, which houses the Re-TOF-MS. The products within the supersonic molecular beam were then photoionized in the extraction region of the mass spectrometer by utilizing quasi-continuous tunable synchrotron vacuum ultraviolet (VUV) light. VUV single photon ionization represents a fragment-free ionization technique and is dubbed as a *soft ionization* method compared to the harsher conditions of electron impact ionization leading often to excessive fragmentation of the parent ion. The ions formed via soft photoionization were extracted and introduced onto a microchannel plate detector through an ion lens. Under our experimental condition, the residence time in the reactor tube are few tens of µs.[2] Control experiments were also conducted by expanding neat helium carrier gas with each brominated precursor into the resistively-heated silicon carbide tube. No signals at *m/z* = 228 or 229 were observed in these control experiments. Finally, reference PIE curves of helium-seeded tetracene (naphthacene), [4]phenacene (chrysene), [4]helicene (benzo[*c*]phenanthrene), benz[*a*]anthracene, and triphenylene purchased from Sigma-Aldrich (98%) were recorded in the present work in the same experimental setup (Supplementary Figure 5).

Photoionization efficiency (PIE) curves, which report the ion counts as a function of photon energy from 7.20 eV to 10.00 eV with an interval of 0.05 eV at a well-defined mass-to-charge ratio (*m/z*), were prepared by integrating the signal collected at a specific *m/z* for the species of interest and normalized to the photon flux. PIE analysis is exploited to unambiguously identifying decomposition intermediates including radicals and closed-shell products.[3] If only one species contributes to the signal at a selected *m/z*, this species can be identified just based on the comparison between the experimentally recorded PIE and literature data. However, if several species contribute to the PIE, it has to be fit by a linear combination of multiple isomers which can contribute to the specific *m/z* as expressed in E1.

$$S(E) = \sum a_i \, \sigma_i(E) \qquad \text{(E1)}$$

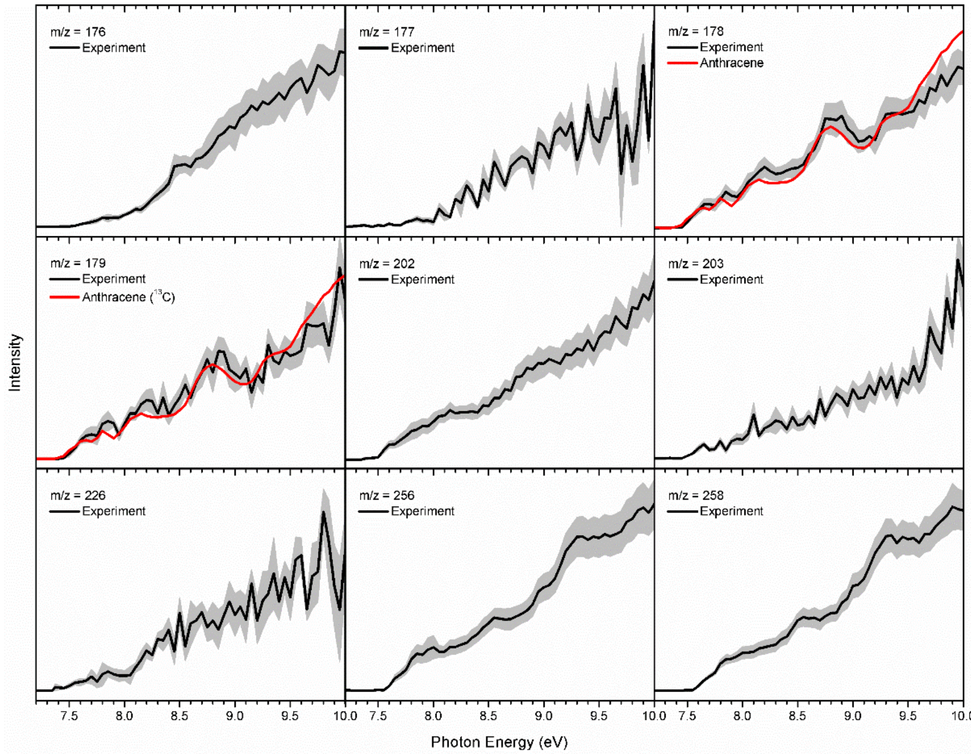
Here, $S(E)$ is the integrated ion intensity normalized by photon flux; $\sigma_i(E)$ stands for the photoionization cross section of species i; and a_i is the coefficient for the linear fit. In this work, the PIE scans in all the four reaction systems were recorded three times and averaged; the experimental uncertainties were derived within one sigma as shown in the shaded areas in Fig. 3 and Supplementary Figs. 1-4.

Theoretical Calculations: The energies and molecular parameters of the local minima and transition states involved in the reactions were computed at the G3(MP2,CC)//B3LYP/6-311G(d,p) level of theory.[4] This computational scheme includes geometry optimization and vibrational frequencies calculations at the density functional B3LYP level of theory with the 6-311G(d,p) basis set. This is followed by the model chemistry G3(MP2,CC) single-point energy calculations at the optimized geometries where the total energy of each species is computed as

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

where ΔE_{MP2} is a basis set correction, ΔE_{MP2} = E[MP2/G3Large] – E[MP2/6-311G**], and E(ZPE) is the zero-point energy. Restricted RHF-RCCSD(T) and RMP2 energies were used for open-shell species; RHF-RCCSD(T) stands for partially spin-adapted open-shell coupled cluster singles and doubles theory augmented with a perturbation correction for triple excitations starting from molecular orbitals obtained from restricted open shell Hartree−Fock calculations. For coupled cluster calculations, the degree of a multireference character of wave functions was monitored through T1 diagnostics. The theoretical method employed normally provides a chemical accuracy of 3–6 kJ mol^{-1} for the relative energies and 0.01–0.02 Å for bond lengths as well as 1–2° for bond angles.[4c] The GAUSSIAN 09[5] and MOLPRO 2010 program packages[6] were used for the B3LYP and G3(MP2,CC) calculations, respectively.

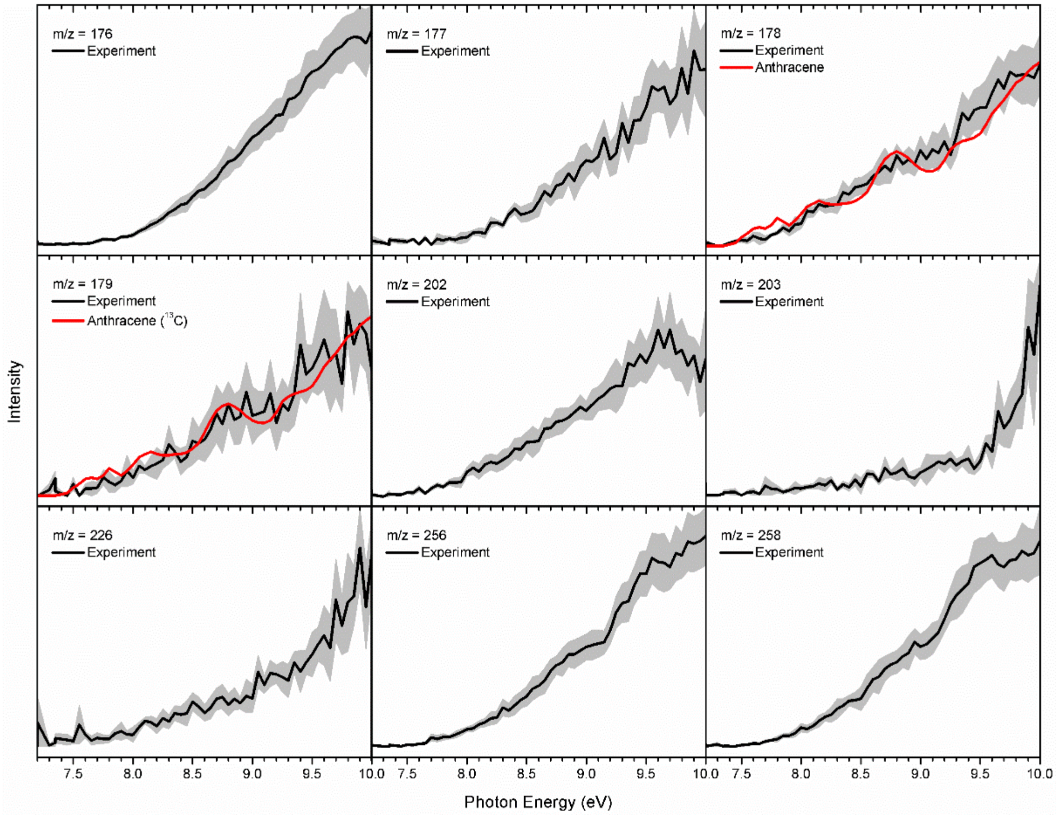
Supplementary Data Analysis: The ion counts at mass-to-charge ratios (*m/z*) of 259 ($C_{13}{}^{13}CH_9{}^{81}Br^+$), 258 ($C_{14}H_9{}^{81}Br^+$), 257 ($C_{13}{}^{13}CH_9{}^{79}Br^+$), 256 ($C_{14}H_9{}^{79}Br^+$), 179 ($C_{13}{}^{13}CH_{10}{}^+$), 178 ($C_{14}H_{10}{}^+$), 177 ($C_{14}H_9{}^+$/$C_{14}{}^{13}CH_8{}^+$), and 176 ($C_{14}H_8{}^+$) are detectable in the control experiments as well and hence cannot be associated with the reaction of anthracenyl/phenanthrenyl radicals with vinylacetylene. These ion counts can be linked to the non-pyrolyzed bromo-substituted anthracene/ phenanthrene precursors (*m/z* = 256 - 259), whereas signal at *m/z* = 178 and 179 is reflective of anthracene/phenanthrene and ^{13}C-anthracene/phenanthrene generated through hydrogen abstraction by the corresponding radicals or hydrogen atom addition to this radical. Finally, signal at *m/z* = 176 and 177 is likely connected with distinct anthracyne/phenanthryne isomers (*m/z* = 176) along with the unreacted anthracenyl/phenanthrenyl radicals ($[C_{14}H_9]^+$; *m/z* = 177) and/or ^{13}C isotopologues anthracyne/phenanthryne isomers (Supplementary Figures 1-4).



Supplementary Figure 1. Photoionization efficiency (PIE) curves of distinct ions detected in 1-bromoanthracene - vinylacetylene system. Source data are provided as a Source Data file.

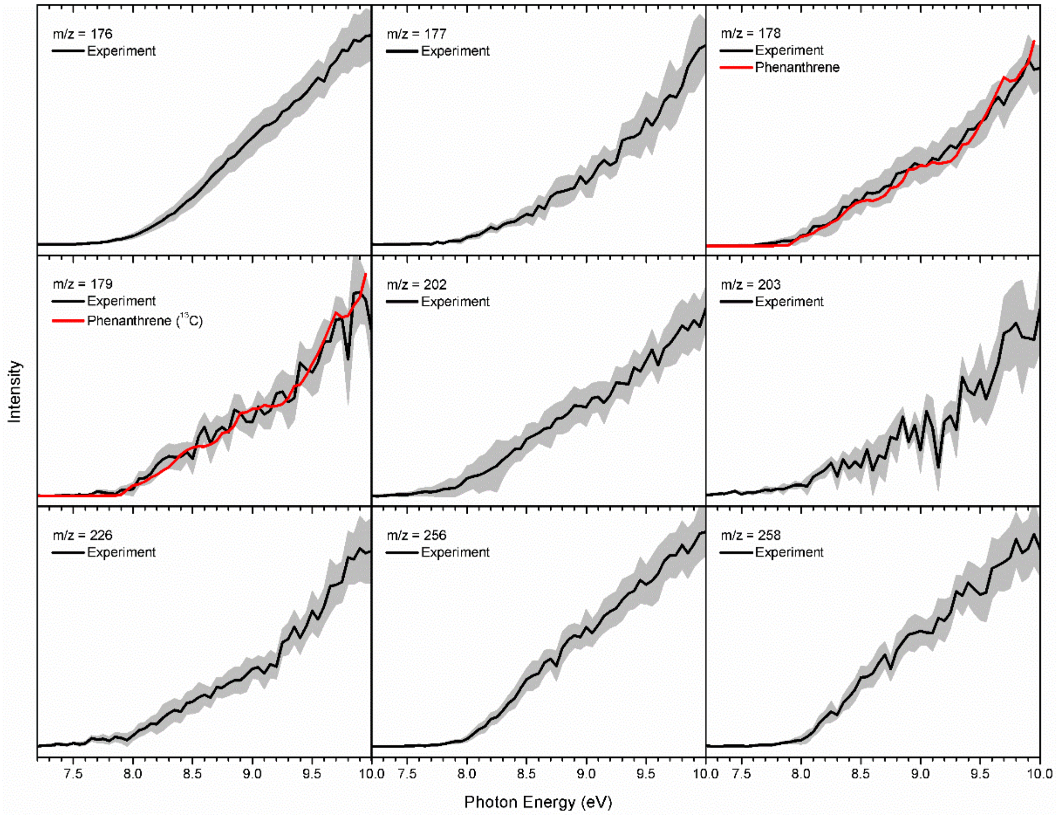
Signal at *m/z* = 202 and 203 can be associated with $C_{16}H_{10}$ molecule(s). After scaling, the curves of *m/z* = 202 and 203 overlap below 9.5 eV indicating that the signal at *m/z* = 203 can be attributed, but not only to the ^{13}C-counterpart of that at *m/z* = 202. Due to the lack of calibrated PIE curves, we could not identify the products at *m/z* = 202, 203 and 226 ($C_{18}H_{10}$). Signal at *m/z* = 177 can be connected to the 1-anthracenyl radical. *m/z* = 176 and *m/z* = 178 originate from the hydrogen atom loss from and hydrogen atom addition to 1-anthracenyl leading to anthracyne isomers and anthracene, respectively. *m/z* = 178 and 179 can be both fit with the reference PIE curve of anthracene, verifying they are both attributed to anthracene with *m/z* = 179 corresponding to the ^{13}C-substituted anthracene. Signals at *m/z* = 256 and 258 are attributed to the precursor 1-bromoanthracene ($C_{14}H_9{}^{79}Br$ and $C_{14}H_9{}^{81}Br$).

It should be noted however that under the conditions of our experiment two-step formation of the four-ring PAH products involving first the production of C_4H_3-substituted three-ring PAH molecules followed by their H-assisted isomerization to the more stable four-ring products is also likely. We compared the direct and two-step mechanisms for the prototype C_6H_5 + C_4H_4 reaction and discussed the conditions where each of them prevails in the recent theoretical and experimental works[7]. The theoretical results in particular showed that the direct mechanism is dominant at low temperatures and pressures.



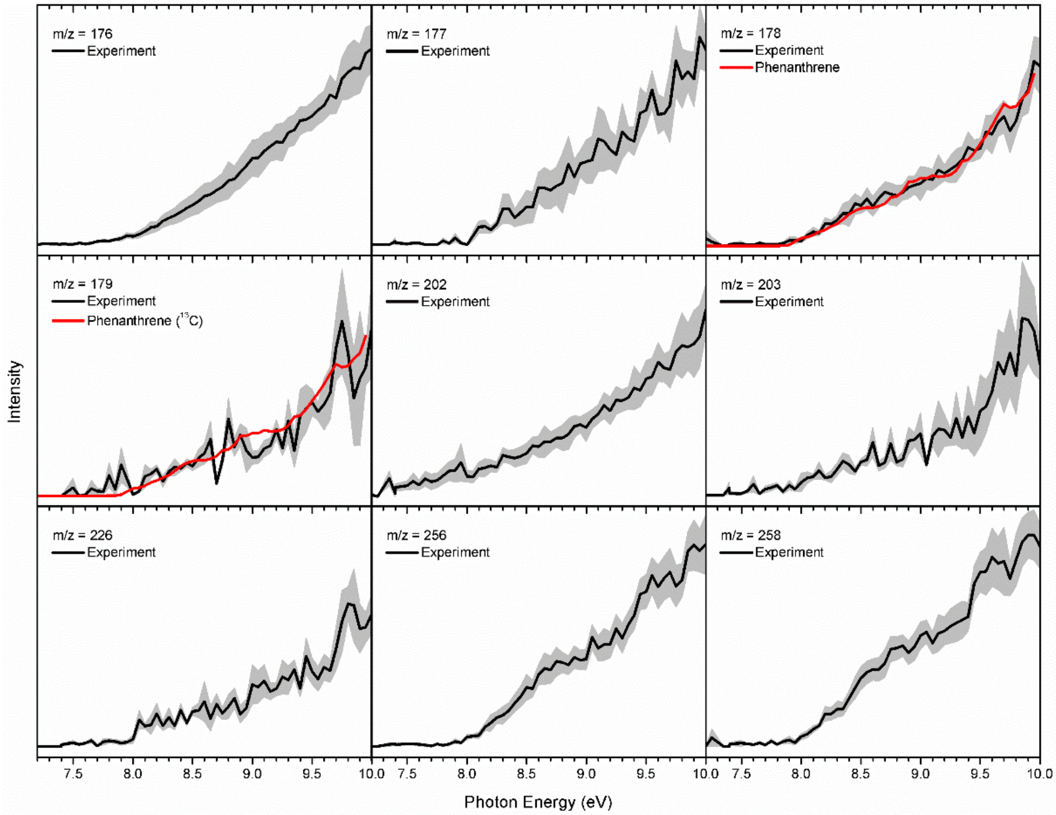
Supplementary Figure 2. Photoionization efficiency (PIE) curves of distinct ions detected in 2-bromoanthracene - vinylacetylene system. Source data are provided as a Source Data file.

Signal at *m/z* = 202 can be associated with $C_{16}H_{10}$ molecule(s). After scaling, the curves of *m/z* = 202 and 203 can be well overlapped in the photon energy range below 9.5 eV, meaning that the signal at *m/z* = 203 can be attributed, but not only to the ^{13}C-counterpart of that at *m/z* = 202. Due to the lack of calibrated PIE curves, it we could not identify the products at *m/z* = 202, 203 and 226 ($C_{18}H_{10}$). Signal at *m/z* = 177 can be connected to the 2-anthracenyl radical. *m/z* = 176 and *m/z* = 178 originate from the hydrogen atom loss from and hydrogen atom addition to 2-anthracenyl leading to anthracyne isomers and anthracene, respectively. *m/z* = 178 and 179 can be both fit with the reference PIE curve of anthracene, verifying they are both attributed to anthracene with *m/z* = 179 corresponding to the ^{13}C-substituted anthracene. Signals at *m/z* = 256 and 258 are attributed to the precursor 2-bromoanthracene ($C_{14}H_9{}^{79}Br$ and $C_{14}H_9{}^{81}Br$).



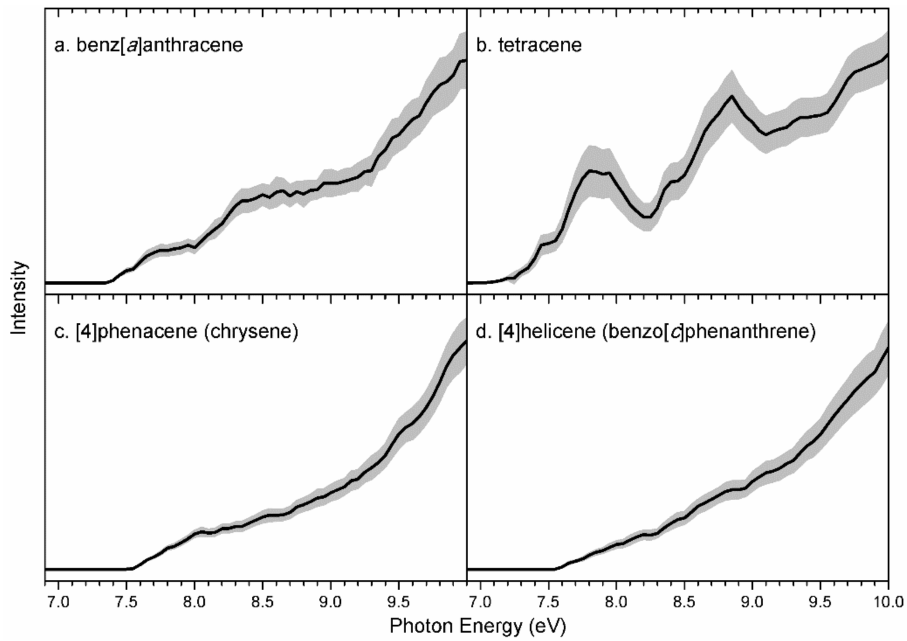
Supplementary Figure 3. Photoionization efficiency (PIE) curves of distinct ions detected in 2-bromophenanthrene - vinylacetylene system. Source data are provided as a Source Data file.

Signal at *m/z* = 202 and 203 can be associated with $C_{16}H_{10}$ molecule(s) and the ^{13}C-isotopially substituted counterpart(s) $^{13}CC_{15}H_{10}$, respectively. After scaling, both data sets are superimposable verifying that signals at *m/z* = 202 and 203 originate from the same (isotopically substituted) isomer. However, due to the lack of calibrated PIE curves, we could not identify the products, as well as for the signal at *m/z* = 226 ($C_{18}H_{10}$). Signal at *m/z* = 177 can be connected to the 2-phenanthrenyl radical. *m/z* = 176 and *m/z* = 178 originate from the hydrogen atom loss from and hydrogen atom addition to 2-phenanthrenyl leading to phenanthryne isomers and phenanthrene, respectively. *m/z* = 178 and 179 can be both fit with the reference PIE curve of phenanthrene, verifying they are both attributed to phenanthrene with *m/z* = 179 corresponding to the ^{13}C-substituted phenanthrene. Signals at *m/z* = 256 and 258 are attributed to the precursor 2-bromophenanthrene ($C_{14}H_9{}^{79}Br$ and $C_{14}H_9{}^{81}Br$).



Supplementary Figure 4. Photoionization efficiency (PIE) curves of distinct ions detected in 3-bromophenanthrene - vinylacetylene system. Source data are provided as a Source Data file.

Signal at *m/z* = 202 can be associated with $C_{16}H_{10}$ molecule(s). After scaling, both data sets are superimposable in the photon energy range below 9.5 eV verifying that signals at *m/z* = 203 are partially attributed to the ^{13}C-isotopially substituted counterpart(s) ($^{13}CC_{15}H_{10}$) of *m/z* = 202. However, due to the lack of calibrated PIE curves, we could not identify the molecules, as well as for the signal at *m/z* = 226 ($C_{18}H_{10}$). Signal at *m/z* = 177 can be connected to the 3-phenanthrenyl radical. *m/z* = 176 and *m/z* = 178 origin from the hydrogen atom loss from and hydrogen atom addition to 3-phenanthrenyl leading to phenanthryne isomers and phenanthrene, respectively. *m/z* = 178 and 179 can be both fit with the reference PIE curve of phenanthrene, verifying they are both attributed to phenanthrene with *m/z* = 179 corresponding to the ^{13}C-substituted phenanthrene. Signals at *m/z* = 256 and 258 are attributed to the precursor 3-bromophenanthrene ($C_{14}H_9{}^{79}Br$ and $C_{14}H_9{}^{81}Br$).



Supplementary Figure 5. Calibration PIE curves of benz[*a*]anthracene, tetracene, [4]phenacene (chrysene) and [4]helicene (benzo[*c*]phenanthrene). The measured onsets of the PIE curves for these four isomers are determined to be 7.35 ± 0.05 eV, 7.00 ± 0.05 eV, 7.55 ± 0.05 eV and 7.55 ± 0.05 eV, respectively, corresponding well the literature reported values of 7.41 ± 0.02 eV[8], 7.04 ± 0.04 eV[9], 7.60 ± 0.03 eV[10] and 7.60 ± 0.02 eV[8].

Supplementary Table 1: Optimized Cartesian Coordinates (Å) and Vibrational Frequencies (cm^{-1}) of the Reactants, Intermediates, Transition States, and Products Involved in the Reactions Considered

Reactant (1-anthracenyl)

$C_{14}H_9$, C_s, $^2A'$

6	0	3.618626	0.739137	0.000004
6	0	2.429169	1.411600	0.000026
6	0	1.186007	0.707100	0.000007
6	0	1.211164	-0.735790	0.000000
6	0	2.477518	-1.397797	-0.000011
6	0	3.643274	-0.685214	-0.000012
6	0	-0.045435	1.370671	0.000002
6	0	0.003462	-1.440482	-0.000007
6	0	-1.225523	-0.774661	-0.000006
6	0	-1.258611	0.676410	-0.000007
6	0	-2.528910	1.335107	-0.000015
6	0	-3.700551	0.631211	-0.000015
6	0	-3.690317	-0.804632	0.000033
6	0	-2.484733	-1.406365	0.000012
1	0	-2.545058	2.419556	-0.000046
1	0	-0.059969	2.456474	-0.000011
1	0	4.554216	1.286844	0.000001
1	0	2.409467	2.496338	0.000025
1	0	2.494188	-2.482516	-0.000017
1	0	4.597138	-1.200358	0.000000
1	0	0.014438	-2.524649	-0.000022
1	0	-4.653217	1.149896	-0.000028
1	0	-4.622040	-1.359359	0.000028

Frequencies

90.6392	122.5246	233.1080
235.2381	265.8430	390.5159
394.9010	400.3608	474.8621
486.1455	511.6743	525.8118
573.6034	616.9427	638.3191
654.9615	724.0718	754.6845
762.4421	769.0248	779.5202
822.0907	854.3457	871.0158
900.1155	901.1429	910.4832
925.1426	971.0449	974.2732
997.3066	1023.4786	1030.8615
1112.5486	1161.9566	1173.4246
1177.3530	1193.0816	1241.7229
1285.4974	1290.8113	1324.0954
1360.1523	1379.7689	1399.4863
1424.4397	1446.6047	1481.0632

1500.7185	1547.2841	1585.8313
1621.9930	1659.4666	1669.8804
3155.2569	3159.4558	3160.0305
3164.9269	3170.1384	3176.2430
3178.0365	3182.7464	3189.5209

Reactant (2-anthracenyl)

$C_{14}H_9$, C_s, $^2A'$

6	0	-3.729426	-0.658472	0.000002
6	0	-2.547620	-1.356369	0.000020
6	0	-1.286785	-0.679702	-0.000001
6	0	-1.258281	0.765119	-0.000002
6	0	-2.510584	1.475543	0.000001
6	0	-3.640847	0.742917	-0.000001
6	0	-0.075983	-1.379564	-0.000007
6	0	-0.026338	1.424061	-0.000005
6	0	1.182982	0.720625	-0.000005
6	0	1.157690	-0.721240	-0.000011
6	0	2.399431	-1.428104	-0.000003
1	0	2.377912	-2.512878	-0.000018
6	0	3.589742	-0.757266	-0.000001
6	0	3.614771	0.667092	0.000012
6	0	2.449821	1.381384	0.000007
1	0	-0.094267	-2.465114	-0.000015
1	0	-4.685674	-1.168567	0.000002
1	0	-2.554861	-2.441974	0.000010
1	0	-2.509948	2.560753	-0.000024
1	0	-0.006999	2.509438	-0.000013
1	0	4.524941	-1.305570	0.000010
1	0	4.569053	1.181607	0.000012
1	0	2.468402	2.466158	0.000011

Frequencies

93.1612	122.6188	237.1269
238.0585	273.5236	379.3238
396.1798	398.8128	464.7045
481.5999	505.1470	533.5882
578.1967	608.4031	639.0054
657.8644	724.2437	750.6996
760.4001	774.0982	787.7957
819.6467	833.9788	860.2623
894.0569	900.7900	910.0882
924.5289	964.7888	971.9467
996.6732	1028.1217	1037.6036
1124.2375	1156.1218	1166.3103
1187.4484	1201.6241	1261.3949

1283.8477	1287.6202	1303.7062
1364.0302	1369.9982	1411.1592
1422.6911	1450.2299	1470.7883
1503.8813	1565.3970	1588.3219
1611.0233	1642.0870	1669.0531
3155.5033	3157.8796	3158.9454
3160.1650	3161.4977	3164.9512
3177.0329	3181.4681	3189.1167

Reactant (2-phenanthrenyl)

$\mathbf{C_{14}H_9}$, C_s, $^2A'$

6	0	3.541405	-0.318861	0.000026
6	0	2.898093	0.877300	0.000071
6	0	1.475929	0.863586	0.000045
6	0	0.783310	-0.383282	-0.000008
6	0	1.541423	-1.577387	-0.000089
6	0	2.928489	-1.561442	-0.000071
6	0	0.737049	2.091406	0.000034
6	0	-0.674146	-0.378862	0.000006
6	0	-1.364312	0.867257	-0.000044
6	0	-0.619528	2.091796	-0.000036
6	0	-2.777129	0.884016	-0.000068
6	0	-3.502912	-0.286694	-0.000019
6	0	-2.828139	-1.519193	0.000073
6	0	-1.448746	-1.560862	0.000087
1	0	-3.284749	1.843044	-0.000119
1	0	1.289456	3.024977	0.000071
1	0	3.424836	1.826035	0.000119
1	0	1.040721	-2.537382	-0.000198
1	0	3.494527	-2.485857	-0.000142
1	0	-1.168519	3.027719	-0.000075
1	0	-4.586583	-0.259879	-0.000038
1	0	-3.393395	-2.444389	0.000144
1	0	-0.961007	-2.526935	0.000192

Frequencies

93.1803	103.3939	227.2987
250.1073	251.7323	391.2264
413.7291	430.3000	447.4041
502.0381	503.1264	535.1764
552.1006	588.4556	626.5861
709.1281	716.7153	725.6625
751.3157	762.7878	806.1086
816.5269	831.0258	869.5320
880.1141	885.0573	942.0704
959.0294	979.3952	993.2079

1009.1544	1059.6505	1066.0941
1116.0812	1156.9712	1175.5666
1181.9529	1203.7568	1236.7112
1258.3335	1289.9183	1308.6882
1347.9748	1371.1689	1394.2518
1442.6966	1456.5422	1474.4373
1522.6916	1536.4821	1590.9117
1620.8333	1648.9947	1659.4053
3156.7900	3160.1727	3161.4162
3169.4250	3171.8602	3176.8397
3184.9913	3191.1969	3204.1872

Reactant (3-phenanthrenyl)

$C_{14}H_9$, C_s, $^2A'$

6	0	3.603294	-0.430782	0.000033
6	0	2.900492	0.762669	0.000106
6	0	1.486179	0.785210	0.000064
6	0	0.748458	-0.435318	-0.000023
6	0	1.480636	-1.654782	-0.000163
6	0	2.838560	-1.586368	-0.000110
6	0	0.781946	2.034784	0.000051
6	0	-0.706018	-0.388382	0.000003
6	0	-1.356583	0.878871	-0.000067
6	0	-0.573690	2.079755	-0.000055
6	0	-2.768431	0.935951	-0.000093
6	0	-3.527304	-0.213805	-0.000015
6	0	-2.890207	-1.466596	0.000114
6	0	-1.512824	-1.548286	0.000123
1	0	-3.248537	1.908976	-0.000167
1	0	1.362462	2.951243	0.000112
1	0	4.686806	-0.449660	0.000074
1	0	3.437136	1.706591	0.000193
1	0	0.971709	-2.610342	-0.000353
1	0	-1.092884	3.032242	-0.000122
1	0	-4.609727	-0.155263	-0.000030
1	0	-3.483094	-2.374219	0.000226
1	0	-1.050930	-2.527099	0.000267

Frequencies

97.7131	100.0124	235.3648
240.0173	250.4867	395.9023
409.4307	429.2292	448.4269
498.8516	507.2381	546.3545
557.3191	581.7923	623.0093
706.6508	718.2155	723.1466
750.4307	778.5303	788.3971

826.8569	836.6886	858.1911
879.8162	885.8595	952.5524
957.2451	978.8948	993.6486
1006.5521	1058.9902	1068.9055
1110.7527	1154.8452	1174.0192
1185.7958	1212.5525	1239.2173
1250.2670	1274.8700	1312.2155
1345.6964	1364.8650	1413.5109
1438.1322	1455.6855	1470.9737
1509.0370	1551.3675	1595.1108
1613.9970	1651.0054	1658.5286
3154.3791	3158.4089	3160.9830
3170.1210	3177.4066	3181.2910
3182.9381	3188.0928	3200.5036

Reactant (vinylacetylene)

C_4H_4, C_s, $^1A'$

6	0	-1.906599	-0.171751	0.000027
6	0	-0.735487	0.110234	0.000110
6	0	0.635836	0.488515	-0.000075
6	0	1.659608	-0.371378	-0.000031
1	0	-2.936433	-0.432155	-0.000368
1	0	0.832476	1.557921	0.000038
1	0	2.682906	-0.016333	0.000060
1	0	1.500909	-1.443157	0.000077

Frequencies

224.2974	316.4152	557.6924
647.5379	680.1508	703.4557
892.2485	954.6944	1010.0445
1111.4702	1321.0081	1443.5272
1668.6642	2205.5052	3136.4367
3147.7814	3236.6393	3476.4475

1.1

$C_{18}H_{13}$, C_1, ^2A

6	0	-2.898968	-3.062990	-0.213731
6	0	-3.246798	-1.741463	-0.189401
6	0	-2.251405	-0.721366	-0.092540
6	0	-0.865452	-1.115492	-0.019259
6	0	-0.546431	-2.507975	-0.048420
6	0	-1.530568	-3.451590	-0.142822
6	0	-2.578221	0.638919	-0.066873
6	0	0.123737	-0.131326	0.077386
6	0	-0.206520	1.226371	0.101136
6	0	-1.599361	1.631687	0.027184

6	0	-1.911008	3.027914	0.054438
6	0	-0.933882	3.978999	0.147586
6	0	0.449121	3.600413	0.221856
6	0	0.722770	2.281292	0.193795
6	0	4.391227	0.461783	-1.119892
6	0	4.683074	-0.754570	-0.647203
6	0	4.089209	-1.331575	0.510113
6	0	3.605414	-1.850163	1.484462
1	0	-2.953417	3.322881	-0.001299
1	0	-3.622382	0.932379	-0.122242
1	0	-3.665579	-3.826118	-0.287928
1	0	-4.289190	-1.445322	-0.244219
1	0	0.497093	-2.799599	0.004338
1	0	-1.274935	-4.504974	-0.165276
1	0	1.165382	-0.425166	0.139545
1	0	-1.192190	5.032340	0.167075
1	0	1.221162	4.358198	0.297460
1	0	3.661985	1.102040	-0.637214
1	0	4.879392	0.841265	-2.009316
1	0	5.419013	-1.369708	-1.159139
1	0	3.178039	-2.291414	2.351333

Frequencies

10.6090	12.8016	18.4681
27.2841	36.7295	50.0925
91.1195	125.2840	226.3766
233.5953	236.4242	266.8251
321.4703	391.3334	395.4316
400.5826	474.5322	486.3766
511.7760	525.6551	559.3831
573.4943	617.2100	638.1807
650.9372	654.7208	681.4533
704.4633	723.1818	755.1226
762.1297	769.6616	778.7394
822.3597	855.6164	870.2972
892.3384	899.5250	900.8336
913.8954	925.3998	964.2521
970.9112	975.2549	999.1547
1010.0513	1023.8983	1031.0920
1111.9250	1112.8691	1162.5875
1173.9880	1176.6340	1193.0175
1244.0563	1285.7553	1294.1856
1321.6652	1324.3147	1360.4707
1380.1723	1399.4277	1424.6643
1445.4210	1446.5754	1481.0447
1501.2966	1546.9256	1586.4615

1621.6874	1658.8822	1667.4847
1669.2450	2201.9594	3137.1485
3145.3661	3152.8702	3157.8592
3158.6183	3164.6581	3168.4022
3176.2626	3180.5361	3181.1914
3187.9254	3234.7954	3475.1197

1.2

$C_{18}H_{13}$, C_1, ^2A

6	0	-5.420679	0.468390	0.165568
6	0	-4.318340	1.236325	-0.085619
6	0	-3.009806	0.663235	-0.093319
6	0	-2.873910	-0.748306	0.170018
6	0	-4.052708	-1.513064	0.428049
6	0	-5.286488	-0.925413	0.426022
6	0	-1.862627	1.422930	-0.347014
6	0	-1.598333	-1.321368	0.163342
6	0	-0.449480	-0.565599	-0.091865
6	0	-0.589007	0.849016	-0.353264
6	0	0.600144	1.617764	-0.613431
6	0	1.777853	0.963875	-0.599255
6	0	1.974922	-0.405135	-0.356538
6	0	0.853891	-1.155838	-0.102494
6	0	5.473471	1.089639	1.431252
6	0	6.261697	0.109968	0.976531
6	0	6.060395	-0.582498	-0.250280
6	0	5.921932	-1.190859	-1.281189
1	0	0.516814	2.681581	-0.811352
1	0	-1.965242	2.485525	-0.544454
1	0	-6.407579	0.917279	0.168140
1	0	-4.420750	2.298126	-0.283947
1	0	-3.948695	-2.574828	0.625945
1	0	-6.172796	-1.517853	0.623027
1	0	-1.496846	-2.384212	0.360736
1	0	2.964119	-0.848071	-0.369764
1	0	0.944575	-2.219657	0.094379
1	0	4.605115	1.427079	0.877687
1	0	5.683813	1.574701	2.376712
1	0	7.123804	-0.203045	1.560490
1	0	5.796104	-1.714993	-2.196676

Frequencies

9.0194	12.0242	13.6868
24.1688	33.4672	48.5881
95.4733	123.3762	227.8985
238.1967	239.2068	273.8981

319.6133	378.8068	396.4283
399.0606	463.0452	479.6628
506.5518	533.2696	559.8251
578.6015	608.5587	639.2855
647.7094	657.8558	681.4730
703.7874	724.0517	750.3020
760.3607	774.1305	792.7943
819.4780	830.2648	858.3501
892.6319	893.5502	898.4537
907.0326	924.5905	963.8329
969.0975	972.5275	996.1664
1009.6652	1028.3697	1037.5820
1112.5655	1125.6702	1156.4806
1168.1546	1186.8507	1201.9003
1261.7811	1283.8232	1288.1088
1303.8435	1322.2334	1364.0261
1369.7463	1410.8508	1422.2950
1446.1046	1450.5691	1471.2137
1504.2080	1564.9974	1588.1174
1610.1532	1641.4594	1668.4056
1668.5693	2202.6744	3136.1862
3146.2619	3154.8343	3157.0086
3157.9982	3159.4189	3160.3929
3164.0530	3176.2364	3182.2679
3188.4293	3235.6921	3475.8815

1.3

$C_{18}H_{13}$, C_1, ^2A

6	0	-1.031739	2.848462	-0.232658
6	0	-1.316712	1.539261	-0.457455
6	0	-0.246356	0.605703	-0.366330
6	0	1.066364	1.065913	-0.051064
6	0	1.263578	2.449755	0.165074
6	0	0.218732	3.358243	0.077772
6	0	-0.482277	-0.790486	-0.589351
6	0	2.150172	0.095235	0.035878
6	0	1.867693	-1.281907	-0.194932
6	0	0.529728	-1.690488	-0.506766
6	0	2.910231	-2.232150	-0.113402
6	0	4.199642	-1.850888	0.185972
6	0	4.484703	-0.494146	0.414487
6	0	3.483022	0.452426	0.340573
1	0	-2.313493	1.186309	-0.701454
1	0	2.249901	2.825969	0.405898
1	0	0.387137	4.415663	0.246636
1	0	-1.491726	-1.110640	-0.823272

1	0	0.340523	-2.745390	-0.676381
1	0	2.675412	-3.276297	-0.292318
1	0	4.990123	-2.590301	0.245244
1	0	5.497414	-0.187109	0.650386
1	0	3.737166	1.488624	0.521954
6	0	-4.331565	-0.630279	1.942989
6	0	-4.986214	-1.222103	0.938690
6	0	-4.773814	-0.941437	-0.440337
6	0	-4.625314	-0.734268	-1.618376
1	0	-3.573882	0.123542	1.765693
1	0	-4.543195	-0.893249	2.972175
1	0	-5.739758	-1.975012	1.156273
1	0	-4.494852	-0.543178	-2.655419

Frequencies

8.2643	10.6004	15.6024
22.1734	29.2421	39.3402
94.8406	105.9924	228.0230
228.7349	250.5388	250.9069
319.0512	393.7777	413.7411
432.3417	447.2096	502.3031
504.1698	537.7777	551.8139
559.1166	589.0904	626.2265
647.4083	685.3990	703.4378
711.3797	716.8667	725.4812
753.6052	763.5113	813.0050
821.2837	831.0136	875.4414
885.2434	888.6852	891.5763
942.2664	959.0764	963.2440
985.3480	993.8161	1008.9132
1009.3703	1059.9532	1065.9765
1111.6708	1116.0757	1156.7315
1176.5103	1182.2362	1204.5158
1237.7103	1258.9951	1290.8698
1308.2033	1321.7987	1347.2808
1370.6125	1395.1061	1442.5084
1445.6910	1456.6729	1474.5877
1522.2047	1536.1092	1590.4913
1619.7897	1648.6242	1658.9762
1668.6535	2200.5296	3136.9039
3148.2678	3157.2969	3159.6054
3161.1937	3167.8022	3170.2645
3178.7473	3182.9243	3188.5527
3201.5371	3237.2501	3474.5447

1.4

$C_{18}H_{13}$, C_1, ^2A

6	0	-1.865767	0.681311	-0.372939
6	0	-0.899671	1.615926	-0.038225
6	0	0.468270	1.266050	0.046990
6	0	0.885453	-0.072815	-0.212802
6	0	-0.114059	-1.025342	-0.554890
6	0	-1.405474	-0.603547	-0.613590
6	0	1.448030	2.254076	0.395487
6	0	2.297699	-0.409880	-0.119730
6	0	3.229973	0.609015	0.230073
6	0	2.764994	1.941163	0.482910
6	0	4.603776	0.292441	0.323329
6	0	5.057904	-0.985593	0.081589
6	0	4.142336	-1.994251	-0.263873
6	0	2.795575	-1.709831	-0.361258
1	0	-2.915071	0.944962	-0.438536
1	0	-1.189195	2.642334	0.165657
1	0	0.146332	-2.055411	-0.763658
1	0	1.109713	3.266407	0.589507
1	0	3.494347	2.699336	0.747723
1	0	5.300906	1.079732	0.590760
1	0	6.114923	-1.214089	0.156748
1	0	4.494632	-3.001505	-0.455259
1	0	2.114779	-2.507449	-0.629321
6	0	-4.977762	-1.692676	1.153733
6	0	-5.980558	-0.867050	0.836750
6	0	-5.944795	0.074030	-0.230146
6	0	-5.954820	0.882269	-1.123918
1	0	-4.044454	-1.696255	0.602993
1	0	-5.072865	-2.384913	1.981527
1	0	-6.901338	-0.891109	1.414499
1	0	-5.959329	1.586172	-1.919588

Frequencies

4.6409	10.1763	10.9051
24.7249	33.8871	45.0621
98.1236	102.6151	227.9384
235.1494	241.3728	250.2819
319.0947	396.6290	409.6617
429.5241	448.5303	499.4912
507.4968	546.9709	557.6317
559.5153	581.7763	622.5836
645.0244	681.2071	703.4415
706.5056	718.3434	723.0773
752.3610	781.5161	792.0535
826.4858	839.5601	857.7558

879.7717	885.9392	892.1753
955.5142	960.8496	964.8991
979.9241	993.2691	1006.3267
1009.4738	1059.3147	1069.1791
1112.0129	1112.4743	1157.0756
1174.4013	1185.8777	1212.8428
1239.5793	1250.3398	1275.9989
1312.1843	1322.0831	1345.5640
1364.5631	1414.2569	1438.1173
1446.0635	1456.3331	1470.9485
1509.2572	1551.2587	1594.4544
1613.1204	1650.7963	1658.3327
1668.2784	2201.9897	3135.3426
3144.9621	3153.8097	3157.4791
3159.7516	3169.1955	3176.4340
3178.9034	3180.4691	3185.8788
3198.9567	3234.4567	3476.0495

Barrier[1.1→2.1]

$C_{18}H_{13}$, C_1, ^2A

6	0	-4.235652	0.975647	0.043479
6	0	-3.716173	-0.288526	0.045081
6	0	-2.303979	-0.502316	0.018283
6	0	-1.432715	0.646536	-0.011281
6	0	-2.018412	1.949738	-0.011397
6	0	-3.375320	2.110380	0.015204
6	0	-1.742316	-1.783316	0.019315
6	0	-0.046914	0.457705	-0.038083
6	0	0.513657	-0.822920	-0.034965
6	0	-0.359610	-1.983673	-0.006509
6	0	0.226404	-3.288348	-0.007593
6	0	1.581139	-3.460756	-0.035511
6	0	2.457515	-2.326538	-0.061867
6	0	1.900338	-1.095872	-0.060519
6	0	3.693603	0.662395	-0.181472
6	0	3.433826	1.760885	0.567222
6	0	2.821537	2.937251	0.073244
6	0	2.302936	3.954072	-0.319445
1	0	-0.433756	-4.148894	0.013730
1	0	-2.399117	-2.648052	0.040188
1	0	-5.309684	1.122685	0.064122
1	0	-4.371375	-1.153184	0.067081
1	0	-1.359414	2.811119	-0.031359
1	0	-3.806600	3.105097	0.015406
1	0	0.606134	1.321190	-0.062157
1	0	2.008583	-4.457830	-0.036940

1	0	3.531792	-2.478805	-0.084073
1	0	3.523896	0.657326	-1.250194
1	0	4.263767	-0.154092	0.238933
1	0	3.686990	1.758921	1.623996
1	0	1.859594	4.850448	-0.677861

Frequencies

-162.7119	12.3555	35.5872
47.6360	85.7129	88.5466
124.9910	190.5296	227.8507
236.0505	245.1472	266.6781
375.9337	392.6699	392.6743
404.2046	477.5918	489.3493
513.9736	527.6642	556.7719
576.7321	594.0944	627.1536
632.5989	655.8763	675.3707
729.4068	729.8196	755.0699
756.8935	770.8176	780.8348
817.1978	853.6549	872.1687
873.6503	896.5255	899.3438
915.5915	925.3464	928.9948
970.6704	973.7997	977.8726
997.0755	1027.1176	1035.9064
1110.6598	1116.3668	1161.7135
1175.9295	1178.7394	1192.9356
1244.6443	1286.0556	1294.6630
1296.1963	1326.1714	1361.0624
1382.2453	1399.2383	1424.6735
1431.9829	1447.2988	1480.7226
1501.6231	1545.6920	1582.5038
1586.0379	1621.3485	1656.9007
1668.8037	2176.5517	3143.6706
3151.5708	3152.8015	3158.3657
3159.5482	3162.3895	3164.5957
3176.5563	3179.3091	3188.2047
3195.8456	3255.7960	3474.6756

Barrier[1.2→2.2]

$C_{18}H_{13}$, C_1, ^2A

6	0	5.231146	-0.758888	-0.076304
6	0	4.033245	-1.416410	-0.104096
6	0	2.799430	-0.698323	-0.052020
6	0	2.842307	0.740981	0.031057
6	0	4.116145	1.387212	0.057470
6	0	5.273535	0.662367	0.005731
6	0	1.557675	-1.342528	-0.078488

6	0	1.641100	1.455173	0.082608
6	0	0.398415	0.814171	0.056503
6	0	0.358370	-0.627822	-0.026698
6	0	-0.926141	-1.276291	-0.052505
6	0	-2.027916	-0.499458	0.001744
6	0	-2.041885	0.903410	0.085096
6	0	-0.829948	1.545837	0.109854
6	0	-4.415027	-1.573642	-0.090848
6	0	-5.246690	-0.745338	0.573089
6	0	-5.939875	0.337200	-0.023862
6	0	-6.541496	1.268035	-0.500420
1	0	-0.970402	-2.359433	-0.115777
1	0	1.525692	-2.426033	-0.140556
1	0	6.159666	-1.317241	-0.116637
1	0	4.000719	-2.499176	-0.166236
1	0	4.146688	2.470068	0.119553
1	0	6.233451	1.165864	0.026628
1	0	1.674265	2.538712	0.144438
1	0	-2.974774	1.454121	0.125866
1	0	-0.786579	2.628995	0.171469
1	0	-4.283411	-1.502610	-1.162673
1	0	-3.954032	-2.411179	0.415781
1	0	-5.393483	-0.877434	1.641854
1	0	-7.072151	2.081222	-0.931177

Frequencies

-103.1078	12.2580	24.6664
32.2581	71.0196	96.0372
123.7285	173.7647	227.4353
239.8297	243.6249	275.2853
359.8683	380.2880	393.8843
398.8848	466.6416	480.5936
506.4862	528.8004	558.4564
580.3672	607.3623	630.8662
639.3124	651.8914	677.8240
718.0377	730.9992	750.7503
760.9470	775.0800	794.2920
819.3151	834.7241	859.9244
871.1027	895.4054	899.9981
908.6724	922.5785	930.4916
968.7043	972.0729	985.1449
995.6929	1028.4686	1038.5332
1112.7417	1126.5626	1156.7788
1168.7526	1187.4774	1202.6057
1265.4176	1284.0103	1288.2738
1304.6514	1305.8085	1365.7509

1370.2166	1411.0212	1422.3735
1435.7888	1452.7579	1470.6971
1504.8128	1567.2658	1588.1754
1602.6022	1612.1914	1642.0690
1668.5182	2184.2542	3141.5405
3149.5330	3153.9634	3156.1568
3156.2674	3158.3912	3158.8475
3163.5512	3175.9755	3180.0972
3188.2115	3249.2279	3475.4627

Barrier[1.3→2.3]

$C_{18}H_{13}$, C_1, ^2A

6	0	1.886506	-1.088916	-0.013089
6	0	1.485392	0.209051	0.042833
6	0	0.090587	0.480483	0.040728
6	0	-0.838563	-0.600245	-0.015036
6	0	-0.333353	-1.919844	-0.068646
6	0	1.029223	-2.178956	-0.068203
6	0	-0.387449	1.830450	0.095514
6	0	-2.265572	-0.303590	-0.015385
6	0	-2.691565	1.054653	0.039707
6	0	-1.716263	2.103669	0.094850
6	0	-4.072298	1.354414	0.039371
6	0	-5.018283	0.354395	-0.013195
6	0	-4.604652	-0.987252	-0.067355
6	0	-3.261472	-1.304755	-0.068196
6	0	4.491285	-1.371255	-0.129382
6	0	5.012850	-0.338299	0.562814
6	0	5.316607	0.926956	0.001118
6	0	5.583669	2.015770	-0.444731
1	0	-4.377422	2.394874	0.081909
1	0	0.341553	2.632592	0.137488
1	0	2.192950	1.030991	0.086684
1	0	-1.015243	-2.759982	-0.111574
1	0	1.394242	-3.199343	-0.111616
1	0	-2.066536	3.129822	0.136534
1	0	-6.074492	0.598418	-0.012745
1	0	-5.343825	-1.779366	-0.108722
1	0	-2.977216	-2.348144	-0.110906
1	0	4.339212	-1.315587	-1.199390
1	0	4.327385	-2.327138	0.350481
1	0	5.197180	-0.446240	1.628416
1	0	5.822320	2.968739	-0.848873

Frequencies

-107.6322	15.8389	24.4313

33.0263	74.3720	95.0339
109.9616	172.2801	227.2723
227.9433	252.3914	256.2989
360.1322	394.0890	410.2633
432.8660	448.5613	502.6707
505.4677	538.8590	553.3825
558.5465	590.3880	619.2662
631.6576	677.5451	710.9604
711.8463	717.9773	726.0312
754.1569	765.3796	812.5443
818.8581	820.8245	875.3953
883.0308	887.9297	895.0380
922.7861	939.5437	958.7142
981.1567	984.5040	992.7991
1007.3237	1058.6825	1065.4201
1112.7070	1116.0793	1159.1637
1176.1836	1182.6174	1204.4015
1237.0563	1259.1768	1292.4810
1306.0483	1310.9461	1350.2688
1370.8584	1394.5960	1435.9168
1443.0471	1456.7237	1475.2816
1522.0607	1536.3346	1590.9348
1608.8013	1621.4859	1648.7397
1658.8473	2183.8777	3142.3332
3156.0728	3156.5750	3159.0593
3160.3847	3163.2563	3169.4711
3177.2347	3182.8171	3188.3628
3201.7919	3248.8507	3475.8330

Barrier[1.4→2.4]

$C_{18}H_{13}$, C_1, ^2A

6	0	1.979786	1.091919	-0.095368
6	0	0.901191	1.959200	-0.098879
6	0	-0.429291	1.480252	-0.061271
6	0	-0.684894	0.078168	-0.017385
6	0	0.433096	-0.800625	-0.013036
6	0	1.683799	-0.262461	-0.050474
6	0	-1.531186	2.398335	-0.067025
6	0	-2.061092	-0.393272	0.020631
6	0	-3.119635	0.560355	0.013052
6	0	-2.814490	1.960218	-0.031578
6	0	-4.459407	0.113096	0.049624
6	0	-4.760809	-1.230528	0.092546
6	0	-3.720551	-2.175383	0.100242
6	0	-2.404069	-1.763230	0.065119
6	0	3.794956	-1.808112	0.038817

6	0	4.791078	-1.145718	-0.583829
6	0	5.676900	-0.246618	0.060731
6	0	6.445145	0.526137	0.578592
1	0	-5.253683	0.852338	0.043238
1	0	-1.313961	3.460749	-0.100667
1	0	3.000595	1.455544	-0.123815
1	0	1.067722	3.031762	-0.131453
1	0	0.290160	-1.873884	0.021166
1	0	-3.637791	2.666688	-0.036392
1	0	-5.793463	-1.559209	0.120280
1	0	-3.952203	-3.233957	0.134072
1	0	-1.625038	-2.514624	0.072190
1	0	3.658653	-1.746317	1.110613
1	0	3.185128	-2.518575	-0.503487
1	0	4.930050	-1.270756	-1.654468
1	0	7.120665	1.199848	1.045680

Frequencies

-105.0053	12.4337	25.8408
33.7886	68.7142	99.6190
102.8574	170.9317	227.4014
237.2921	242.8195	256.4875
359.8529	398.1173	409.8767
429.4270	448.4727	500.4594
501.6892	547.1388	551.1762
558.9581	584.6855	625.3535
631.0541	677.6458	709.6181
716.6593	718.4366	720.0241
752.7884	784.7203	791.9777
814.5084	839.5016	858.8589
879.2381	885.6023	895.1752
918.7181	954.7646	961.0107
979.5186	984.4386	992.6352
1003.9139	1059.6876	1069.4407
1112.1614	1113.1527	1157.1452
1174.1366	1185.5580	1213.4417
1239.2759	1250.8932	1279.2225
1305.6310	1311.8934	1349.3998
1364.4053	1413.1527	1435.9257
1439.2407	1455.6712	1471.7336
1511.0455	1551.4747	1595.1957
1606.1144	1613.4174	1650.7037
1658.3852	2183.8733	3140.7955
3151.8949	3155.5597	3156.8028
3159.2560	3168.0492	3173.5626
3175.9402	3178.8283	3184.7295

3198.0326	3248.4654	3475.9485

2.1

$C_{18}H_{13}$, C_1, ^2A

6	0	-4.304008	0.791439	0.101026
6	0	-3.685468	-0.420411	0.231556
6	0	-2.268141	-0.537659	0.099583
6	0	-1.498347	0.648226	-0.175598
6	0	-2.184715	1.894391	-0.302602
6	0	-3.543288	1.964812	-0.169098
6	0	-1.599647	-1.758316	0.227956
6	0	-0.108492	0.548346	-0.308944
6	0	0.564292	-0.672651	-0.184154
6	0	-0.211692	-1.859756	0.095304
6	0	0.458382	-3.113802	0.229393
6	0	1.812735	-3.195924	0.090014
6	0	2.576558	-2.029968	-0.194113
6	0	1.993808	-0.796372	-0.330349
6	0	2.853548	0.418034	-0.629207
6	0	3.017029	1.349709	0.545952
6	0	2.982043	2.717258	0.437273
6	0	2.939541	3.933053	0.326201
1	0	-0.132509	-3.998331	0.442323
1	0	-2.173851	-2.656105	0.436150
1	0	-5.380742	0.867348	0.203117
1	0	-4.263509	-1.315135	0.438091
1	0	-1.603360	2.787491	-0.506231
1	0	-4.051720	2.917301	-0.267785
1	0	0.449963	1.455140	-0.505545
1	0	2.318394	-4.149710	0.190145
1	0	3.651414	-2.125043	-0.310471
1	0	2.456578	0.975016	-1.482850
1	0	3.845843	0.060711	-0.936043
1	0	3.205188	0.907658	1.519564
1	0	2.913487	4.991221	0.238382

Frequencies

24.1781	45.3535	74.3970
92.6094	133.2618	174.2883
214.2199	223.9321	261.8858
301.7272	330.4682	387.8027
393.9583	416.0829	439.2001
450.7237	479.9224	484.2190
508.2559	543.5271	570.5849
581.2280	601.0143	628.8188
645.2567	649.4363	657.6547

736.5783	746.6621	765.8943
776.5603	800.1925	808.3201
855.8046	866.0816	889.7429
895.2295	906.4957	918.0960
928.5466	970.8141	983.2901
996.0861	1008.5573	1029.0800
1042.3092	1083.0659	1137.9567
1156.0043	1165.4345	1184.7125
1192.5150	1199.7599	1220.4671
1276.1793	1289.4488	1299.8787
1305.3173	1339.6401	1375.8272
1394.5115	1410.8303	1418.3102
1429.8132	1462.2027	1476.5864
1489.0863	1510.7392	1583.8370
1598.4631	1625.6463	1662.6167
1669.4379	2015.7696	2992.8330
3058.2607	3154.3338	3154.8248
3156.3206	3158.4154	3163.5829
3164.7467	3175.9257	3183.9581
3187.6180	3190.0984	3468.1690

2.2

$C_{18}H_{13}$, C_1, ^2A

6	0	-5.055171	-0.910944	-0.246457
6	0	-3.829782	-1.504383	-0.125307
6	0	-2.639989	-0.720498	-0.024456
6	0	-2.756781	0.716937	-0.052829
6	0	-4.056554	1.294969	-0.180308
6	0	-5.170304	0.508090	-0.274312
6	0	-1.371816	-1.298401	0.100307
6	0	-1.597996	1.494973	0.045423
6	0	-0.332633	0.916105	0.169705
6	0	-0.214889	-0.520295	0.197987
6	0	1.085763	-1.098468	0.327576
6	0	2.211961	-0.326533	0.425617
6	0	2.083218	1.098917	0.391469
6	0	0.861668	1.694490	0.271739
6	0	3.592838	-0.942597	0.562156
6	0	4.469373	-0.665906	-0.631812
6	0	5.698725	-0.063587	-0.550329
6	0	6.792849	0.473991	-0.466322
1	0	1.166027	-2.181299	0.351933
1	0	-1.284986	-2.380617	0.121486
1	0	-5.949634	-1.518954	-0.322370
1	0	-3.741551	-2.585654	-0.104169
1	0	-4.143178	2.376387	-0.200911

1	0	-6.150728	0.960759	-0.370823
1	0	-1.684853	2.577170	0.024989
1	0	2.979443	1.705937	0.462338
1	0	0.779288	2.776312	0.252471
1	0	4.083011	-0.566404	1.464910
1	0	3.483342	-2.027198	0.689350
1	0	4.095690	-0.956886	-1.609087
1	0	7.745253	0.939297	-0.399199

Frequencies

23.0093	24.9439	66.8030
106.2083	136.7792	160.0455
212.5669	221.2757	256.8152
304.5587	335.2172	385.4177
390.5751	410.3873	433.6032
447.0949	480.1607	485.4589
498.5206	539.3026	546.9483
596.2458	616.9654	633.7211
646.6007	653.5526	674.7342
753.8002	758.2006	766.8583
778.6970	784.8910	822.1061
840.1177	853.5059	879.5926
881.0078	906.0865	919.1049
923.4195	970.3708	975.8094
982.8715	995.9975	1026.9855
1029.5282	1135.3487	1142.4958
1159.9835	1174.8126	1179.7320
1189.6621	1203.1661	1212.5389
1290.2120	1292.4036	1294.0014
1298.5353	1333.3360	1374.2496
1394.5495	1400.9723	1416.6249
1435.0769	1466.6764	1474.6229
1492.6355	1515.5404	1576.8041
1594.3262	1627.6691	1667.3937
1673.4407	2013.8572	3002.7934
3062.3250	3151.2262	3151.8387
3154.7596	3156.5480	3158.0046
3159.6619	3163.1190	3175.4376
3177.7724	3187.6778	3468.0642

2.3

$C_{18}H_{13}$, C_1, ^2A

6	0	2.078835	-0.740191	-0.466305
6	0	1.476333	0.504589	-0.485119
6	0	0.083915	0.660311	-0.323930
6	0	-0.737630	-0.487157	-0.129888

6	0	-0.103661	-1.747561	-0.111855
6	0	1.261581	-1.871041	-0.274982
6	0	-0.514619	1.963810	-0.353177
6	0	-2.173524	-0.313434	0.037342
6	0	-2.720147	1.001409	0.001332
6	0	-1.852166	2.125764	-0.197912
6	0	-4.111582	1.183271	0.162376
6	0	-4.952266	0.108488	0.354794
6	0	-4.418743	-1.190750	0.391776
6	0	-3.062162	-1.393339	0.236616
6	0	3.584151	-0.881092	-0.623964
6	0	4.333035	-0.464470	0.615770
6	0	5.342239	0.463982	0.616537
6	0	6.240065	1.292812	0.605271
1	0	-4.510486	2.191903	0.131403
1	0	0.130754	2.823051	-0.502129
1	0	2.083195	1.394021	-0.625708
1	0	-0.689643	-2.646824	0.028143
1	0	1.713458	-2.857726	-0.261039
1	0	-2.292607	3.117049	-0.221761
1	0	-6.018401	0.262091	0.476957
1	0	-5.075288	-2.040170	0.543249
1	0	-2.681656	-2.405970	0.271059
1	0	3.932481	-0.288750	-1.473546
1	0	3.817587	-1.929070	-0.854101
1	0	4.046868	-0.923743	1.557227
1	0	7.021815	2.011737	0.602164

Frequencies

9.8314	20.2235	59.3217
95.2208	129.0258	161.1233
212.2206	225.1143	229.7712
307.9111	352.9758	388.0443
400.6054	405.0906	442.1007
449.5562	464.5803	505.0011
515.5738	542.4237	544.7680
563.8599	590.2600	621.8730
647.0507	654.3108	704.1170
732.1984	735.8419	757.1342
786.3564	798.3867	825.3343
837.3534	870.9792	878.3453
883.9336	913.2570	949.0620
954.5617	964.4245	980.8495
992.5996	1017.1794	1025.6913
1061.8415	1121.1228	1143.2486
1170.0345	1175.1754	1181.9131

1190.6237	1192.7454	1226.5203
1252.0016	1272.1775	1298.2321
1307.0896	1328.6371	1367.7892
1373.5751	1400.2453	1423.6701
1450.9626	1462.9773	1476.2213
1497.6244	1528.3220	1564.7274
1606.0014	1643.5851	1657.2483
1661.4693	2013.8291	2997.9735
3074.2526	3152.3538	3155.8074
3158.3572	3159.0112	3160.4214
3169.7565	3177.1188	3183.5521
3190.3799	3203.0981	3469.1831

2.4

$\mathbf{C_{18}H_{13}}$, C_1, ^2A

6	0	2.011990	1.303005	0.345369
6	0	0.911233	2.109002	0.172703
6	0	-0.388248	1.563013	0.068226
6	0	-0.557567	0.152716	0.144943
6	0	0.596223	-0.644011	0.325216
6	0	1.862584	-0.098354	0.428007
6	0	-1.530077	2.409355	-0.112478
6	0	-1.897927	-0.405965	0.037710
6	0	-3.002963	0.475830	-0.141318
6	0	-2.779585	1.889943	-0.212894
6	0	-4.308395	-0.054492	-0.246245
6	0	-4.533300	-1.411904	-0.178417
6	0	-3.447604	-2.286509	-0.002007
6	0	-2.163360	-1.792452	0.103022
6	0	3.086308	-0.979170	0.617259
6	0	4.016111	-0.941272	-0.567482
6	0	5.349790	-0.634379	-0.477949
6	0	6.536752	-0.358877	-0.386560
1	0	-5.137881	0.631724	-0.382290
1	0	-1.372955	3.481493	-0.167560
1	0	3.002372	1.739384	0.418246
1	0	1.028866	3.186172	0.114103
1	0	0.497513	-1.720708	0.390802
1	0	-3.637273	2.540157	-0.349678
1	0	-5.540282	-1.804919	-0.260302
1	0	-3.618451	-3.355795	0.052134
1	0	-1.348951	-2.492272	0.238309
1	0	3.632586	-0.675403	1.514750
1	0	2.754669	-2.012037	0.785637
1	0	3.598498	-1.168598	-1.543821
1	0	7.569500	-0.122076	-0.312971

Frequencies

19.5487	23.8666	63.9684
100.3530	127.3446	152.5588
210.9558	219.1093	241.1611
316.9660	328.7704	389.4491
403.4799	425.3523	437.9209
445.8010	469.5420	471.6434
522.9856	532.7390	556.3236
565.6391	613.7019	638.7316
643.8357	648.5201	713.4914
728.8354	731.4962	756.6362
782.6379	798.1576	814.1525
855.8464	867.6400	879.1503
889.9381	895.4272	913.0510
954.8680	971.0894	981.4643
992.5906	1022.6376	1046.1117
1061.4599	1118.6210	1142.8985
1171.2036	1174.6244	1183.7181
1188.0453	1205.8236	1225.7529
1242.9798	1265.2396	1294.6681
1305.2820	1322.1829	1367.4603
1379.5803	1400.4496	1435.9832
1454.0768	1459.2995	1472.5130
1487.0347	1542.8016	1553.3393
1603.8689	1646.8957	1658.3877
1659.8261	2013.9492	3000.5302
3063.6975	3151.8573	3156.2514
3158.9030	3160.1322	3169.0925
3175.7768	3176.6411	3178.6244
3186.1469	3200.9650	3468.4175

Barrier[2.1→3.1]

$C_{18}H_{13}$, C_1, ^2A

6	0	4.841695	-0.537818	0.180782
6	0	4.053894	0.578436	0.220787
6	0	2.633475	0.479237	0.108333
6	0	2.042265	-0.825860	-0.048665
6	0	2.902175	-1.965356	-0.085355
6	0	4.257701	-1.827120	0.025639
6	0	1.800341	1.602326	0.146218
6	0	0.650791	-0.935499	-0.159527
6	0	-0.181074	0.186656	-0.122656
6	0	0.410726	1.498235	0.035782
6	0	-0.430735	2.656591	0.078293
6	0	-1.793912	2.552227	-0.028482

6	0	-2.332770	1.259658	-0.181281
6	0	-1.609550	0.109918	-0.235389
6	0	-2.447492	-1.141430	-0.392347
6	0	-4.926872	-1.141730	0.220157
6	0	-5.802957	-1.544461	0.946305
6	0	-3.889548	-0.630451	-0.614292
1	0	5.918678	-0.448191	0.267052
1	0	4.497344	1.561617	0.339293
1	0	2.456884	-2.947744	-0.203537
1	0	4.898358	-2.701277	-0.004022
1	0	2.247036	2.584783	0.265852
1	0	0.213380	-1.921341	-0.275368
1	0	0.036038	3.629084	0.200371
1	0	-2.427076	3.431450	0.007538
1	0	-2.393602	-1.765375	0.504906
1	0	-2.116878	-1.761554	-1.232028
1	0	-6.574271	-1.906385	1.580558
1	0	-4.176650	-0.591437	-1.666746
1	0	-3.648156	0.595011	-0.349680

Frequencies

-1637.1158	34.9953	71.5629
89.3091	103.6695	164.4740
183.6222	215.6766	257.9076
283.2743	294.0677	360.5799
394.7430	403.0738	436.7053
463.3389	478.9514	515.7772
529.8101	552.6523	562.1015
590.8450	602.2450	623.3906
638.1051	668.3249	678.2749
741.4786	744.0818	756.2397
774.0936	796.2926	799.0663
841.6821	855.4533	870.5568
893.3195	907.1181	923.7409
953.7773	962.9161	970.3497
996.0252	1000.8354	1019.6140
1029.4844	1074.4425	1135.2622
1156.5730	1161.4648	1182.8339
1190.2067	1191.5819	1225.2238
1272.7645	1284.7352	1293.3309
1297.7350	1341.1643	1356.0282
1368.3758	1381.9396	1411.7166
1423.5243	1449.2290	1470.5181
1485.6092	1506.9243	1571.5998
1588.2876	1607.4759	1645.9363
1667.8592	1671.5983	2169.2285

3029.5084	3060.1276	3084.5647
3153.2663	3156.6391	3158.1036
3162.2888	3168.6521	3175.5753
3177.7580	3187.8373	3475.2985

Barrier[2.2→3a.2]

$C_{18}H_{13}$, C_1, ^2A

6	0	4.380838	-1.794755	0.072056
6	0	3.029129	-1.968121	0.177483
6	0	2.136532	-0.856144	0.093226
6	0	2.691759	0.460308	-0.106253
6	0	4.109680	0.595527	-0.211397
6	0	4.928786	-0.495320	-0.125064
6	0	0.749143	-1.004754	0.197237
6	0	1.829669	1.559443	-0.190749
6	0	0.443467	1.420440	-0.086035
6	0	-0.109893	0.093413	0.113893
6	0	-1.519196	0.027395	0.209623
6	0	-2.360521	1.091816	0.134780
6	0	-1.803095	2.391668	-0.064457
6	0	-0.447470	2.539065	-0.169447
6	0	-4.640070	-1.650067	-0.161395
6	0	-3.826396	0.734997	0.259053
6	0	-5.285839	-2.408382	-0.843417
6	0	-3.841541	-0.767195	0.623177
1	0	-0.017209	3.523758	-0.319286
1	0	-4.352486	0.907825	-0.684457
1	0	0.327418	-1.993149	0.345209
1	0	5.046084	-2.648305	0.138111
1	0	2.610703	-2.957850	0.327445
1	0	4.526129	1.586148	-0.361783
1	0	6.003464	-0.377470	-0.206254
1	0	2.250711	2.549082	-0.342320
1	0	-2.455289	3.257035	-0.130387
1	0	-4.334721	1.333670	1.021894
1	0	-5.861513	-3.072679	-1.439667
1	0	-3.938637	-0.951438	1.694783
1	0	-2.594550	-0.972634	0.422825

Frequencies

-1646.7040	36.9422	65.9677
80.5445	112.8369	166.5683
179.7517	213.4396	255.8642
285.9372	306.7097	367.0411
387.3403	409.4242	430.4173
457.0501	477.6482	518.2960

522.9646	537.0671	566.0700
598.7336	604.2298	623.4084
636.3972	667.4125	673.0720
745.1440	755.4890	767.8912
775.1324	785.6029	804.8947
848.4135	855.4590	874.5980
896.0237	906.3312	921.1930
934.5886	968.3418	971.4224
996.1253	1001.3132	1019.7811
1029.1581	1073.9971	1127.8691
1158.9925	1173.2587	1182.4320
1186.7508	1200.8267	1225.4839
1267.1790	1287.0454	1290.5943
1296.7427	1330.6161	1355.0359
1362.3887	1377.7991	1402.0730
1424.8765	1456.0604	1481.1543
1488.8566	1508.2247	1556.1567
1586.5873	1622.4255	1658.4347
1668.9264	1671.2832	2168.2750
3032.3537	3062.8507	3084.8043
3151.6226	3153.9013	3157.9931
3162.6728	3169.6714	3173.0831
3175.9301	3188.0621	3474.7323

Barrier[2.2→3b.2]

$C_{18}H_{13}$, C_1, ^2A

6	0	5.121220	-0.705143	-0.175717
6	0	3.935693	-1.384488	-0.147844
6	0	2.691130	-0.687875	-0.064899
6	0	2.709443	0.753142	-0.010747
6	0	3.970763	1.422862	-0.042533
6	0	5.139027	0.718030	-0.122275
6	0	1.462139	-1.354487	-0.034256
6	0	1.496723	1.445476	0.071152
6	0	0.268733	0.779450	0.101882
6	0	0.247070	-0.666309	0.046716
6	0	-1.008015	-1.355295	0.078084
6	0	-2.180442	-0.655349	0.157464
6	0	-2.118414	0.758604	0.210783
6	0	-0.980249	1.487248	0.190559
6	0	-3.603616	-1.178616	0.182393
6	0	-5.654225	0.296009	-0.201095
6	0	-6.629535	0.543138	-0.868020
6	0	-4.481170	0.033678	0.565260
1	0	-1.004669	-2.441214	0.040026
1	0	1.450836	-2.439506	-0.075129

1	0	6.058193	-1.246938	-0.239017
1	0	3.921092	-2.468698	-0.188328
1	0	3.983254	2.507082	-0.002108
1	0	6.089295	1.239470	-0.145767
1	0	1.509589	2.530395	0.112095
1	0	-0.973598	2.571630	0.237514
1	0	-3.891465	-1.549180	-0.805599
1	0	-3.731979	-2.005297	0.886779
1	0	-7.492077	0.754882	-1.450612
1	0	-3.584475	0.927189	0.368269
1	0	-4.651648	0.119738	1.640434

Frequencies

-1652.1454	28.5400	73.0101
80.6031	122.9283	164.2772
181.1959	211.5780	262.2085
303.8453	306.0492	310.3534
379.7253	412.3119	434.3443
471.0580	481.0833	497.6839
533.1805	536.1028	547.2948
606.8282	621.4634	624.4440
642.1782	667.9472	692.0255
739.9727	753.6999	761.3494
776.7575	777.1112	829.5335
843.6048	844.8284	855.1366
879.3872	909.3863	914.3853
921.3719	948.8339	959.4897
970.4060	995.7599	1023.7007
1028.8838	1074.8856	1142.3309
1156.6590	1167.3823	1187.6936
1189.5216	1201.3857	1252.1576
1271.8109	1281.9462	1286.3359
1299.7704	1304.7815	1363.7270
1368.7761	1375.7893	1413.5205
1423.1155	1440.6221	1473.4351
1480.8869	1504.9137	1578.9373
1591.1288	1623.2412	1648.4491
1665.7325	1669.1982	2168.9595
3040.3980	3068.8432	3084.5683
3147.1422	3155.3289	3156.7888
3158.5024	3159.7847	3163.6018
3176.0131	3188.2347	3474.5915

Barrier[2.3→3a.3]

$C_{18}H_{13}$, C_1, ^2A

6	0	-2.105884	0.785355	-0.163793

6	0	-1.097730	1.718386	-0.035275
6	0	0.257217	1.310845	0.012606
6	0	0.602514	-0.072425	-0.072057
6	0	-0.449853	-1.017680	-0.208840
6	0	-1.734619	-0.558673	-0.244950
6	0	1.298791	2.288330	0.145308
6	0	2.004852	-0.459793	-0.018556
6	0	2.999379	0.551561	0.114043
6	0	2.605337	1.927286	0.193416
6	0	4.363120	0.186206	0.166177
6	0	4.749884	-1.133967	0.091539
6	0	3.773323	-2.136030	-0.038324
6	0	2.434920	-1.803845	-0.091577
6	0	-3.605674	0.998110	-0.213964
6	0	-4.197996	-0.376802	-0.597924
6	0	-5.273259	-0.896959	0.180134
6	0	-6.160287	-1.358135	0.856643
1	0	5.106862	0.969849	0.267100
1	0	1.015672	3.333854	0.207424
1	0	-1.324650	2.779144	0.029231
1	0	-0.236031	-2.076607	-0.281457
1	0	3.380454	2.679706	0.294161
1	0	5.799872	-1.400301	0.132977
1	0	4.071475	-3.176760	-0.096649
1	0	1.707538	-2.599120	-0.190569
1	0	-3.892832	1.771084	-0.932775
1	0	-3.983367	1.311132	0.763438
1	0	-4.359962	-0.492212	-1.671527
1	0	-3.122829	-1.051442	-0.416876
1	0	-6.946413	-1.758930	1.447881

Frequencies

-1659.8223	31.3595	66.2648
81.5836	110.8300	163.4599
184.4562	209.7350	244.4047
296.6711	303.4721	335.4230
391.5330	420.1386	432.3160
462.1416	481.7319	518.3919
531.4427	548.4132	553.2026
591.9137	611.3078	623.1449
626.5361	668.3133	712.5461
715.5192	734.0511	756.4640
784.3601	789.7890	819.9712
841.0777	863.6036	877.6529
880.6823	896.5060	930.7945
952.9990	955.5055	978.7008

992.2647	1009.7460	1022.9699
1060.8912	1074.6784	1121.6531
1167.3027	1174.6417	1187.3174
1187.7591	1213.3591	1237.5986
1259.5147	1263.7875	1277.3745
1298.0173	1313.2107	1360.9332
1363.6894	1370.4956	1405.4192
1441.0474	1459.6117	1468.3601
1482.3262	1515.6159	1551.9368
1602.3885	1628.4896	1650.7064
1657.6221	1664.6704	2168.2717
3038.8916	3067.9027	3084.0208
3144.7191	3155.9687	3158.9539
3168.6398	3175.2586	3179.7386
3185.9549	3199.7924	3475.4595

Barrier[2.3→3b.3]

$C_{18}H_{13}$, C_1, ^2A

6	0	2.067821	-1.130290	0.151170
6	0	1.564988	0.141592	0.226390
6	0	0.210078	0.481543	0.170077
6	0	-0.717338	-0.598201	0.016142
6	0	-0.203609	-1.915630	-0.064027
6	0	1.149695	-2.187675	0.000204
6	0	-0.262943	1.831181	0.257421
6	0	-2.139574	-0.293298	-0.049742
6	0	-2.562916	1.064393	0.042592
6	0	-1.590085	2.106345	0.196672
6	0	-3.940768	1.370989	-0.019837
6	0	-4.885375	0.379402	-0.168911
6	0	-4.473904	-0.961031	-0.260971
6	0	-3.133979	-1.286045	-0.202633
6	0	3.578713	-1.201563	0.225134
6	0	4.030091	0.234399	0.576999
6	0	5.034734	0.848994	-0.226292
6	0	5.859376	1.388048	-0.923868
1	0	-4.244679	2.410151	0.052016
1	0	0.466478	2.624634	0.371704
1	0	-0.886986	-2.746854	-0.178344
1	0	1.498006	-3.214043	-0.064033
1	0	-1.941550	3.130656	0.263088
1	0	-5.939198	0.629167	-0.215429
1	0	-5.212457	-1.746001	-0.378802
1	0	-2.849961	-2.327648	-0.277015
1	0	4.001266	-1.510275	-0.735268
1	0	3.924254	-1.921433	0.973604

1	0	2.889612	0.789324	0.397454
1	0	4.193785	0.385956	1.645682
1	0	6.591403	1.857444	-1.533783

Frequencies

-1652.2240	30.6599	73.6897
75.1508	102.5550	171.3072
179.1319	214.1251	230.9131
276.0316	298.2433	381.7254
395.4553	412.0944	457.8629
467.2387	486.3402	511.0075
519.8024	553.1832	560.2461
568.9631	607.8644	614.4307
623.7891	667.6784	692.9186
717.0155	756.9716	758.8968
779.5971	798.6462	823.9234
833.8820	849.5173	876.5718
877.9660	929.9952	946.0068
960.7992	982.3407	991.3447
992.9556	1011.3207	1021.0864
1061.3719	1074.4500	1109.2813
1164.3724	1175.5276	1185.1794
1186.6873	1212.5561	1229.9331
1243.9410	1283.1384	1291.4495
1292.8557	1324.9947	1355.0686
1358.3932	1367.6858	1398.9756
1430.5191	1457.6263	1481.3233
1487.5999	1521.3576	1555.2273
1591.2520	1636.5104	1652.5455
1655.0618	1662.2880	2167.9190
3035.2994	3065.5965	3084.1219
3154.0088	3158.0503	3161.9487
3168.7900	3183.2102	3184.3799
3190.9038	3204.3734	3475.3380

Barrier[2.4→3a.4]

$C_{18}H_{13}$, C_1, ^2A

6	0	2.052875	0.920699	0.203993
6	0	1.073975	1.866264	0.129555
6	0	-0.275207	1.426812	0.054095
6	0	-0.569735	0.029216	0.063721
6	0	0.501755	-0.892157	0.147247
6	0	1.810608	-0.454734	0.216852
6	0	-1.342242	2.380006	-0.028903
6	0	-1.962778	-0.394404	-0.010973
6	0	-2.987357	0.592337	-0.091268

6	0	-2.637148	1.982048	-0.098103
6	0	-4.340120	0.190801	-0.163630
6	0	-4.688996	-1.141787	-0.158232
6	0	-3.683526	-2.120041	-0.079888
6	0	-2.355297	-1.752063	-0.008491
6	0	3.077911	-1.284282	0.289433
6	0	5.386708	-0.314782	-0.217357
6	0	6.371337	-0.322137	-0.915600
6	0	4.208971	-0.273594	0.584914
1	0	-5.106004	0.957056	-0.224148
1	0	-1.088912	3.434884	-0.034823
1	0	1.287311	2.930413	0.124396
1	0	0.300848	-1.956951	0.159884
1	0	-3.435412	2.714202	-0.160257
1	0	-5.730894	-1.435782	-0.214310
1	0	-3.950912	-3.170740	-0.075788
1	0	-1.606509	-2.531133	0.049837
1	0	3.024978	-2.059672	1.059323
1	0	3.263577	-1.788505	-0.663138
1	0	7.240779	-0.335269	-1.525602
1	0	4.427571	-0.170091	1.649674
1	0	3.523170	0.782380	0.350758

Frequencies

-1651.7038	29.8635	68.0358
82.8044	114.6228	157.8022
175.2173	214.5689	254.8334
280.0254	309.8601	342.2464
398.6291	413.8923	433.4894
463.2496	473.0112	516.2132
527.9668	538.8684	556.5485
589.3343	610.2472	623.5628
647.2102	668.4024	714.4018
725.6193	736.7787	753.9645
776.4280	793.1496	815.0975
838.9178	874.2892	878.9556
885.9269	888.3297	900.6767
953.9407	955.1722	977.9009
992.1213	1021.7689	1026.7736
1060.6718	1074.8875	1124.5281
1171.9964	1181.6272	1187.0382
1188.9120	1207.1877	1235.4110
1252.2904	1261.3109	1284.9197
1300.3614	1307.3234	1361.4739
1362.6774	1373.1261	1405.4327
1444.7721	1455.2196	1468.6125

1482.6600	1522.8415	1545.5548
1599.9027	1629.5910	1649.3206
1658.3156	1664.8112	2168.5655
3038.0769	3067.2494	3083.7175
3155.5254	3158.1975	3159.4151
3167.8669	3173.5687	3175.7291
3185.0174	3199.9317	3475.3904

Barrier[2.4→3b.4]

$C_{18}H_{13}$, C_1, ^2A

6	0	1.655652	2.603279	0.002188
6	0	0.319456	2.926112	-0.119224
6	0	-0.693434	1.936921	-0.105221
6	0	-0.336269	0.559380	0.036870
6	0	1.032812	0.302729	0.154703
6	0	2.025134	1.250734	0.145994
6	0	-2.079003	2.284966	-0.228834
6	0	-1.371799	-0.454733	0.049602
6	0	-2.731698	-0.055956	-0.073483
6	0	-3.050179	1.335632	-0.212011
6	0	-3.742707	-1.042803	-0.058867
6	0	-3.428246	-2.378666	0.070791
6	0	-2.083536	-2.773518	0.189381
6	0	-1.077807	-1.829026	0.178512
6	0	3.422398	0.680762	0.280418
6	0	3.910530	-1.787228	-0.170397
6	0	4.467149	-2.617235	-0.847670
6	0	3.215397	-0.815051	0.606404
1	0	-4.777687	-0.730691	-0.152798
1	0	-2.337920	3.333307	-0.336662
1	0	2.411251	3.382664	-0.009778
1	0	0.022361	3.964041	-0.227319
1	0	-4.093713	1.617455	-0.305648
1	0	-4.214323	-3.125253	0.080001
1	0	-1.836326	-3.824479	0.288187
1	0	-0.044078	-2.140670	0.266278
1	0	3.980139	0.794453	-0.653608
1	0	4.001391	1.182177	1.062212
1	0	4.965342	-3.345239	-1.439310
1	0	1.958872	-0.833695	0.357448
1	0	3.241589	-1.031861	1.676065

Frequencies

-1658.6694	33.7802	67.3508
81.6424	107.1489	160.4185
177.4347	210.9929	251.0930

277.8362	301.9719	384.1850
405.3788	416.6391	424.7725
459.5969	488.2460	516.2952
524.5472	542.9066	553.9538
572.9943	604.5431	622.9934
649.1437	668.5743	701.4027
716.0653	744.2571	757.3601
795.2868	800.3102	808.1821
841.0342	853.2051	883.8264
897.1558	909.9314	955.5969
958.2945	962.0001	978.4276
994.3971	1020.4161	1044.1957
1066.3416	1076.3445	1116.2585
1163.2570	1172.5951	1179.4088
1185.5480	1206.3050	1229.4370
1241.8537	1254.7495	1288.3945
1292.7568	1325.5951	1356.5983
1359.3054	1363.4797	1424.3259
1427.0535	1452.6125	1480.8008
1484.0457	1533.5757	1537.6986
1588.1291	1636.3497	1649.7456
1655.6468	1674.3019	2167.2333
3034.8046	3064.8611	3083.9454
3152.3492	3154.7285	3158.4670
3168.7576	3171.3211	3174.4856
3182.1324	3192.3489	3475.1654

3.1

$C_{18}H_{13}$, C_1, ^2A

6	0	-4.368422	0.331430	0.125754
6	0	-3.574177	-0.753618	0.369747
6	0	-2.164217	-0.694583	0.147829
6	0	-1.590537	0.532237	-0.341379
6	0	-2.456757	1.642763	-0.580863
6	0	-3.801514	1.546352	-0.355494
6	0	-1.319263	-1.780130	0.390260
6	0	-0.210619	0.605404	-0.563896
6	0	0.639304	-0.480023	-0.328936
6	0	0.060352	-1.712328	0.168592
6	0	0.897147	-2.841635	0.428300
6	0	2.249080	-2.779943	0.207162
6	0	2.748168	-1.568131	-0.284101
6	0	2.070967	-0.432902	-0.570552
6	0	2.792190	0.783438	-1.116340
6	0	2.565402	2.363116	0.858001
6	0	1.817912	2.955232	1.589051

6	0	3.479884	1.659319	-0.036140
1	0	0.442309	-3.752096	0.805670
1	0	-1.744534	-2.707111	0.762751
1	0	-5.437308	0.274563	0.298079
1	0	-4.003512	-1.679786	0.737513
1	0	-2.024324	2.568168	-0.946678
1	0	-4.447232	2.397094	-0.542142
1	0	0.198908	1.545328	-0.910033
1	0	2.895796	-3.628009	0.400773
1	0	2.118754	1.403161	-1.711008
1	0	3.576871	0.435386	-1.792800
1	0	1.152428	3.465545	2.240909
1	0	4.114604	2.396128	-0.541647
1	0	4.147836	1.025624	0.556650

Frequencies

29.8656	44.2026	79.5568
94.6011	131.5547	159.2203
217.4285	232.9769	267.9297
301.2097	326.3472	348.6760
392.7119	408.4740	444.8477
477.9266	501.4578	508.0626
516.3021	550.9707	570.7931
624.0000	638.4978	656.0007
665.7622	677.7073	716.5480
738.8062	756.7201	771.4991
790.2733	792.9182	827.6679
845.9671	852.9246	890.9789
902.3152	909.0464	925.1246
957.2539	969.6813	983.1632
995.1393	1011.8576	1028.8071
1042.5872	1125.9741	1155.9374
1161.6843	1169.8143	1191.2603
1204.8341	1231.4623	1256.0015
1284.0503	1300.2195	1309.8307
1345.1344	1357.3524	1367.7013
1376.9808	1411.5708	1424.5594
1442.5080	1470.8204	1474.9302
1496.6728	1504.5714	1567.5456
1587.8292	1614.4646	1639.5581
1668.1797	2221.6842	3020.2504
3048.4167	3057.7177	3095.3518
3154.5111	3157.6412	3159.1433
3162.9997	3175.7248	3179.4996
3187.8971	3195.9900	3478.3376

3a.2

$C_{18}H_{13}$, C_1, ^2A

6	0	-4.940304	-1.364145	-0.126722
6	0	-3.650382	-1.775454	0.060273
6	0	-2.573733	-0.836699	0.069388
6	0	-2.875075	0.561116	-0.123297
6	0	-4.236875	0.946315	-0.315512
6	0	-5.237608	0.015317	-0.317444
6	0	-1.244857	-1.230979	0.258770
6	0	-1.831321	1.493516	-0.115681
6	0	-0.501996	1.109701	0.073252
6	0	-0.204899	-0.297697	0.265611
6	0	1.156360	-0.607340	0.449785
6	0	2.204247	0.244490	0.474896
6	0	1.873049	1.634588	0.281400
6	0	0.583466	2.041419	0.090892
6	0	5.802208	-0.654865	-0.519697
6	0	3.639694	-0.190322	0.659397
6	0	6.949542	-0.971398	-0.353754
6	0	4.403646	-0.272081	-0.687347
1	0	0.360584	3.094305	-0.045071
1	0	3.671817	-1.167385	1.144555
1	0	-1.012599	-2.280164	0.403965
1	0	-5.747424	-2.087940	-0.130999
1	0	-3.422522	-2.826156	0.205694
1	0	-4.462551	1.997616	-0.460562
1	0	-6.266879	0.322416	-0.464539
1	0	-2.061556	2.544936	-0.260295
1	0	2.676703	2.365178	0.300627
1	0	4.158395	0.514158	1.316394
1	0	7.964907	-1.251652	-0.216804
1	0	4.349884	0.695248	-1.198701
1	0	3.900264	-0.993465	-1.339533

Frequencies

28.8584	40.5915	61.2942
94.8454	122.3532	163.2402
190.7610	213.8905	253.4506
295.4432	331.0671	354.7764
386.6480	407.9672	427.6247
463.8581	477.8171	507.7474
529.7604	541.4919	602.1703
626.6669	641.3630	661.5245
665.6896	677.0248	744.6675
754.4029	764.0126	768.8833
775.6809	787.8625	808.9106

848.2791	855.4381	895.6099
906.9362	919.7429	956.2250
960.4203	969.2291	971.7650
996.7607	1007.3131	1028.9352
1031.4863	1128.4483	1157.3590
1170.4108	1182.2915	1189.3274
1206.2674	1239.0567	1282.4043
1288.9861	1289.5299	1300.7262
1320.6564	1357.3107	1366.2427
1375.2736	1400.3164	1425.0407
1446.4025	1477.0160	1490.5440
1497.2601	1501.4908	1548.8062
1586.1284	1626.1947	1662.4225
1671.4132	2221.4711	3024.9805
3044.1521	3055.9264	3099.4122
3148.6899	3154.7434	3159.5823
3164.3902	3174.2189	3175.0422
3177.4963	3189.2424	3477.8693

3b.2

$C_{18}H_{13}$, C_1, ^2A

6	0	-4.975641	-1.270573	-0.171889
6	0	-3.691862	-1.716532	-0.026057
6	0	-2.596906	-0.800580	0.021512
6	0	-2.871972	0.610669	-0.088066
6	0	-4.227725	1.033023	-0.239383
6	0	-5.247011	0.123013	-0.280011
6	0	-1.272793	-1.226810	0.171656
6	0	-1.806840	1.517841	-0.042145
6	0	-0.487068	1.089149	0.108088
6	0	-0.207030	-0.323107	0.218935
6	0	1.146130	-0.761620	0.376114
6	0	2.201370	0.119068	0.429871
6	0	1.852945	1.481910	0.311230
6	0	0.623222	2.004745	0.160048
6	0	3.634363	-0.323058	0.596234
6	0	5.891770	-0.407672	-0.485497
6	0	7.031892	-0.753292	-0.328090
6	0	4.499437	-0.001410	-0.647610
1	0	1.334973	-1.828481	0.461653
1	0	-1.067970	-2.289828	0.254792
1	0	-5.797275	-1.977034	-0.206107
1	0	-3.483655	-2.778185	0.056705
1	0	-4.434007	2.095036	-0.321699
1	0	-6.271648	0.458077	-0.395224
1	0	-2.012955	2.580529	-0.124466

1	0	0.442403	3.072056	0.080363
1	0	4.075930	0.176425	1.464012
1	0	3.669644	-1.397168	0.792056
1	0	8.042238	-1.053930	-0.197411
1	0	4.452593	1.074054	-0.850068
1	0	4.072044	-0.500157	-1.524246

Frequencies

28.4133	44.7937	59.8911
96.2120	122.1873	165.1458
191.2646	214.4773	264.6460
299.9358	325.8754	355.0619
379.2008	405.2365	438.2169
467.2234	470.0781	480.6934
535.9363	545.9878	601.0676
629.8119	642.4472	666.0307
670.4698	677.7228	726.0515
753.6153	762.2585	771.2854
776.0401	788.6662	831.0727
841.8302	853.2565	872.3508
906.2026	913.6150	921.6188
937.3516	967.2777	970.5739
996.4438	1015.8958	1027.7029
1030.7281	1140.9846	1157.6175
1175.5092	1187.3581	1199.0938
1201.9956	1252.1922	1281.7417
1283.6174	1288.5378	1299.3812
1311.6130	1361.7630	1368.7400
1377.2161	1414.3987	1420.4969
1437.0050	1471.6078	1476.6841
1493.3039	1504.2438	1567.6348
1589.0695	1619.6982	1643.9807
1668.5061	2221.6867	3023.5715
3040.9555	3053.1375	3090.1239
3145.1554	3156.4661	3157.2216
3159.3826	3160.3465	3164.4834
3176.7110	3188.8790	3477.9582

3a.3

$C_{18}H_{13}$, C_1, ^2A

6	0	-2.072682	0.031981	0.463015
6	0	-1.233389	1.127685	0.314519
6	0	0.167989	0.995007	0.171702
6	0	0.771993	-0.295126	0.172848
6	0	-0.085152	-1.420699	0.325127
6	0	-1.417573	-1.196821	0.455848

6	0	0.993960	2.158222	0.024197
6	0	2.212819	-0.410510	0.021094
6	0	2.988704	0.775834	-0.123100
6	0	2.339443	2.053506	-0.116234
6	0	4.390225	0.676393	-0.272054
6	0	5.019735	-0.549003	-0.280545
6	0	4.258672	-1.722212	-0.139063
6	0	2.888582	-1.651376	0.008048
6	0	-3.570665	0.159829	0.601315
6	0	-4.323898	-0.403196	-0.629504
6	0	-5.773688	-0.291739	-0.503562
6	0	-6.964131	-0.187103	-0.376978
1	0	4.966905	1.589044	-0.380667
1	0	0.516226	3.132192	0.026804
1	0	-1.661244	2.126860	0.310837
1	0	0.313559	-2.427610	0.338959
1	0	2.951365	2.942415	-0.226990
1	0	6.095882	-0.610579	-0.395572
1	0	4.749747	-2.688704	-0.145430
1	0	2.329196	-2.571999	0.114232
1	0	-3.840720	1.209472	0.738585
1	0	-3.908493	-0.377695	1.491956
1	0	-3.992873	0.126231	-1.529525
1	0	-4.047541	-1.453676	-0.769809
1	0	-8.017661	-0.099989	-0.273420

Frequencies

25.8782	40.0383	57.9460
99.3916	104.8343	161.5148
195.7126	223.0515	235.1714
298.5483	329.5455	358.3144
398.5205	412.9295	439.3187
471.2894	481.4851	507.7680
538.5283	549.0905	566.4182
603.2899	641.2636	665.2155
676.4522	701.9157	712.1750
729.5296	756.4533	772.0765
784.0779	790.4360	820.9956
854.1296	878.1656	878.8432
895.0585	929.7017	956.5286
966.8658	978.7999	993.3042
1006.4142	1016.5385	1026.4744
1060.2455	1122.6154	1169.4959
1179.2170	1181.4658	1191.3294
1222.5236	1238.1008	1265.6008
1266.3643	1285.7378	1308.9186

1312.8895	1355.2290	1364.7869
1375.1806	1402.5985	1438.2882
1457.3336	1467.1382	1477.1977
1495.3394	1504.9677	1550.6033
1595.3374	1622.8665	1651.0590
1658.0434	2221.5602	3024.2242
3045.0850	3053.3265	3091.0913
3143.7943	3158.7187	3161.0548
3170.2145	3177.2126	3178.2143
3186.2680	3198.9203	3477.3879

3b.3

$C_{18}H_{13}$, C_1, ^2A

6	0	-2.065092	-0.222894	0.511834
6	0	-1.260963	0.874364	0.422431
6	0	0.119904	0.913078	0.257286
6	0	0.785204	-0.351292	0.164596
6	0	-0.008922	-1.517771	0.248673
6	0	-1.378209	-1.461680	0.414308
6	0	0.870075	2.132777	0.180643
6	0	2.229957	-0.369044	-0.007203
6	0	2.934349	0.867424	-0.079013
6	0	2.216614	2.105598	0.018990
6	0	4.337072	0.860092	-0.246588
6	0	5.037027	-0.322956	-0.340983
6	0	4.347019	-1.544930	-0.270238
6	0	2.976691	-1.564359	-0.107398
6	0	-3.566869	-0.151914	0.663890
6	0	-4.284414	0.003725	-0.701561
6	0	-5.737417	0.056768	-0.572796
6	0	-6.931027	0.096427	-0.439101
1	0	4.858487	1.810127	-0.300007
1	0	0.334036	3.071425	0.254636
1	0	0.459331	-2.491404	0.187439
1	0	-1.949304	-2.383337	0.481707
1	0	2.780021	3.030891	-0.039340
1	0	6.113399	-0.313334	-0.468989
1	0	4.892904	-2.478742	-0.343777
1	0	2.472767	-2.520826	-0.056276
1	0	-3.837457	0.692955	1.300842
1	0	-3.932462	-1.057052	1.155624
1	0	-3.924757	0.914515	-1.191642
1	0	-4.005927	-0.829450	-1.355997
1	0	-7.987030	0.133741	-0.330839

Frequencies

21.4210	37.7969	56.4243
97.5488	106.5894	160.8734
196.9752	214.1347	226.1030
299.1800	340.8006	360.9177
400.6798	411.3267	463.4702
465.4371	483.5695	498.4005
534.7310	553.3636	560.9940
606.5749	637.8526	665.3871
676.2652	699.9109	719.2109
733.8121	758.2159	768.6574
782.5388	794.6059	827.4069
831.7039	876.4369	879.0286
942.9668	947.3193	959.2363
970.6282	983.7372	993.8919
1005.3283	1008.6290	1030.2076
1061.0969	1110.5097	1166.0094
1166.6852	1185.2419	1187.2375
1223.0020	1239.1284	1250.1823
1284.5308	1291.2501	1308.6211
1323.3585	1351.9839	1365.6375
1366.5308	1389.2787	1431.0317
1456.2001	1476.6229	1487.8141
1498.4238	1507.9334	1547.1928
1586.7407	1639.8987	1653.5388
1655.5610	2221.3270	3025.3058
3050.7430	3055.3590	3096.7613
3149.3826	3160.1715	3164.7455
3170.8962	3184.9336	3189.1635
3192.5116	3205.1170	3477.4273

3a.4

$C_{18}H_{13}$, C_1, ^2A

6	0	-1.771720	1.665480	-0.578681
6	0	-0.637147	2.401037	-0.480736
6	0	0.588351	1.705278	-0.285809
6	0	0.573760	0.283085	-0.201566
6	0	-0.665503	-0.389793	-0.316916
6	0	-1.869402	0.278305	-0.511263
6	0	1.825127	2.418423	-0.176021
6	0	1.833750	-0.421554	-0.002621
6	0	3.039777	0.330397	0.100794
6	0	2.997070	1.759720	0.008530
6	0	4.267849	-0.341501	0.293503
6	0	4.321479	-1.714810	0.384069
6	0	3.135699	-2.462043	0.283394
6	0	1.924288	-1.828586	0.095015

6	0	-3.188786	-0.447683	-0.625163
6	0	-5.391653	-0.878939	0.487709
6	0	-6.439575	-1.456670	0.377023
6	0	-4.108901	-0.190971	0.594402
1	0	5.175412	0.248299	0.369779
1	0	1.804656	3.500830	-0.244104
1	0	-0.634798	3.484290	-0.547521
1	0	-0.696607	-1.471683	-0.260692
1	0	3.929187	2.308912	0.090403
1	0	5.270273	-2.217732	0.532058
1	0	3.170992	-3.543352	0.353812
1	0	1.030632	-2.434486	0.021865
1	0	-3.712305	-0.124902	-1.529558
1	0	-3.013664	-1.521690	-0.722542
1	0	-7.369265	-1.962547	0.287457
1	0	-4.277744	0.886398	0.696194
1	0	-3.596566	-0.511173	1.508143

Frequencies

24.1542	46.5744	58.3270
100.1169	105.3922	164.8158
188.6905	209.0779	248.9084
311.1185	323.9582	359.1065
396.5848	420.6150	433.1540
449.4249	474.6527	518.0537
529.4000	551.3162	565.2404
631.7767	638.2744	666.3493
676.3442	706.0565	717.9281
725.5764	752.3095	770.9775
786.8242	790.9051	811.1581
868.9219	878.6914	880.7738
886.9083	899.0990	955.9374
967.3103	978.7074	993.3849
1008.1453	1016.4826	1039.4871
1060.7488	1124.6579	1170.2032
1180.0558	1182.0421	1197.9850
1216.3508	1235.0750	1256.3144
1273.3748	1288.7339	1304.5424
1314.0389	1356.1695	1369.1779
1375.6606	1400.8762	1441.7561
1448.7973	1466.9214	1476.9392
1495.4662	1519.5163	1536.4166
1591.6637	1627.8742	1648.5067
1659.2785	2221.4257	3024.1248
3045.0601	3053.2723	3090.8369
3157.6437	3159.5754	3161.1112

3168.9416	3174.1277	3177.9671
3186.2770	3200.1549	3477.4992

3b.4

$C_{18}H_{13}$, C_1, ^2A

6	0	-1.713341	1.979595	-0.288014
6	0	-0.476064	2.543832	-0.059575
6	0	0.694929	1.755836	0.016685
6	0	0.588657	0.339445	-0.148248
6	0	-0.698104	-0.137306	-0.371353
6	0	-1.858136	0.575993	-0.457772
6	0	1.988779	2.327883	0.250084
6	0	1.774193	-0.489270	-0.078592
6	0	3.033279	0.127182	0.155170
6	0	3.101849	1.551581	0.316239
6	0	4.190137	-0.680778	0.223406
6	0	4.109484	-2.048399	0.066575
6	0	2.862456	-2.656867	-0.164885
6	0	1.717808	-1.889825	-0.235852
6	0	-3.211075	-0.061145	-0.678938
6	0	-5.194286	-1.091096	0.456570
6	0	-6.274566	-1.582149	0.266714
6	0	-3.879043	-0.489282	0.653069
1	0	5.149276	-0.206011	0.402308
1	0	2.060913	3.403513	0.373862
1	0	-2.595783	2.609808	-0.350835
1	0	-0.387825	3.618339	0.060270
1	0	4.072695	2.002146	0.494078
1	0	5.005479	-2.656272	0.121438
1	0	2.801619	-3.732291	-0.287858
1	0	0.755590	-2.356642	-0.414663
1	0	-3.870568	0.640572	-1.196280
1	0	-3.109332	-0.939733	-1.319394
1	0	-7.230011	-2.018545	0.108791
1	0	-3.970251	0.381926	1.310818
1	0	-3.223530	-1.198184	1.169759

Frequencies

23.0078	48.3624	57.5477
101.7890	115.9913	163.0211
176.8828	212.2801	248.8619
304.4795	321.0691	357.7840
403.2807	426.2687	441.0786
457.5357	472.0565	515.6432
535.0209	555.9607	567.1989
625.2927	640.0444	665.0364

676.0224	706.3623	718.4262
732.0555	759.7588	767.9698
789.5037	798.0429	809.0460
847.1659	886.4264	890.2262
905.5861	952.6193	964.4342
968.6925	979.9940	996.5393
1008.9999	1011.6306	1044.5795
1065.4071	1115.0721	1162.2076
1171.5466	1176.2460	1183.1722
1219.9524	1230.8584	1244.2317
1272.4739	1291.8898	1302.3808
1321.4956	1357.7850	1362.4904
1367.0235	1420.1862	1428.4820
1447.5877	1476.9476	1481.3634
1498.5194	1517.5437	1536.2388
1584.6267	1640.3984	1650.2792
1656.5844	2221.1600	3025.3649
3050.1755	3055.3352	3097.1353
3149.1695	3156.1407	3159.4603
3166.7116	3172.8105	3175.8042
3177.6128	3188.9619	3476.8152

Barrier[3.1→4.1]

$\mathbf{C_{18}H_{13}}$, C_1, ^2A

6	0	4.768517	-0.081278	0.173803
6	0	3.852879	0.933017	0.198766
6	0	2.455549	0.662232	0.078577
6	0	2.023575	-0.702863	-0.069982
6	0	3.014178	-1.732153	-0.092100
6	0	4.342575	-1.432489	0.026215
6	0	1.488372	1.669402	0.096477
6	0	0.657238	-0.982380	-0.188801
6	0	-0.320920	0.020017	-0.164615
6	0	0.122220	1.393797	-0.022326
6	0	-0.837164	2.451349	-0.006117
6	0	-2.174516	2.182625	-0.125011
6	0	-1.744681	-0.241255	-0.281718
6	0	-2.568038	0.842145	-0.270802
6	0	-4.490578	-0.934276	0.407350
6	0	-4.806488	0.217229	0.156447
6	0	-2.300441	-1.645654	-0.456936
6	0	-3.481042	-1.983880	0.497136
1	0	-0.484413	3.472442	0.102111
1	0	1.804609	2.702632	0.204025
1	0	5.826591	0.136303	0.266261
1	0	4.174200	1.963394	0.310692

1	0	2.690757	-2.761888	-0.204765
1	0	5.082864	-2.224491	0.008363
1	0	0.370429	-2.019453	-0.308415
1	0	-2.906216	2.983799	-0.110968
1	0	-5.366752	1.113271	0.023804
1	0	-2.656687	-1.760331	-1.486117
1	0	-1.528289	-2.399175	-0.305346
1	0	-3.125695	-2.056130	1.531145
1	0	-3.888811	-2.963885	0.231036

Frequencies

-375.6197	29.8242	65.9256
99.2131	123.5383	145.2700
205.9056	256.0193	265.5053
301.3014	321.0653	338.9614
387.5297	405.3924	451.6152
475.0396	496.8977	508.7544
518.7510	545.1433	574.9748
624.1108	640.8207	648.4102
654.0391	717.9313	738.2784
744.7419	758.9162	772.9246
793.1220	796.2251	844.4706
849.2410	850.2974	882.1151
903.8743	909.2322	928.6035
957.4404	965.9913	968.2473
994.1907	1007.6400	1027.5147
1028.6689	1122.5394	1154.5467
1162.1970	1186.7348	1190.2470
1196.6494	1219.9334	1241.6136
1283.5181	1297.1811	1306.5476
1325.6470	1353.2325	1372.8254
1379.9521	1410.6575	1424.6340
1444.7076	1468.3166	1475.5253
1483.0455	1503.9973	1571.4586
1588.1134	1599.5661	1638.0625
1667.8084	2069.6074	3026.2083
3032.9837	3062.2893	3109.9127
3148.9394	3155.4323	3157.0416
3161.9358	3167.1991	3175.1045
3187.4717	3189.4275	3436.0556

Barrier[3a.2→4a.2]

$C_{18}H_{13}$, C_1, ^2A

6	0	-4.423220	-1.403783	-0.030397
6	0	-3.100407	-1.724763	-0.150927
6	0	-2.090315	-0.715342	-0.099757

6	0	-2.496235	0.657219	0.082095
6	0	-3.889737	0.947662	0.204018
6	0	-4.823596	-0.048631	0.149755
6	0	-0.730128	-1.015385	-0.221229
6	0	-1.517632	1.654752	0.132276
6	0	-0.156510	1.360858	0.011397
6	0	0.251757	-0.019721	-0.169538
6	0	1.639342	-0.262046	-0.292504
6	0	2.611872	0.688563	-0.242457
6	0	2.179180	2.045956	-0.060833
6	0	0.856281	2.365984	0.060058
6	0	4.087943	0.377427	-0.403545
6	0	4.593657	-0.769141	0.516096
6	0	3.700507	-1.913583	0.368228
6	0	2.607389	-2.378199	0.081527
1	0	-0.430226	-2.047333	-0.364526
1	0	-5.178290	-2.180767	-0.071165
1	0	-2.794987	-2.756876	-0.288413
1	0	-4.193522	1.980273	0.341235
1	0	-5.877735	0.186800	0.243833
1	0	-1.823336	2.687974	0.269081
1	0	2.930470	2.829496	-0.022939
1	0	0.555526	3.398893	0.199334
1	0	4.284135	0.084865	-1.440474
1	0	4.679786	1.275495	-0.206676
1	0	5.625751	-1.020475	0.253340
1	0	4.598927	-0.446332	1.563167
1	0	1.822616	-3.078974	-0.081389

Frequencies

-379.9803	40.9334	57.1378
112.8057	124.5691	129.7323
209.4895	251.1520	253.8747
317.7267	332.7205	361.9962
396.8365	408.9698	427.9215
475.2144	497.5127	505.6920
523.5353	550.2554	584.7774
631.2696	640.8925	642.6924
645.5749	724.8940	744.5097
753.2000	757.8503	770.2496
774.7682	804.5203	825.9053
851.6233	862.8962	887.2893
901.7580	906.0107	924.4191
960.2890	968.7719	987.1945
994.4296	997.1452	1023.0034
1028.2694	1128.8040	1153.0855

1168.2075	1179.9376	1189.8856
1205.4138	1210.5164	1240.8224
1282.5820	1290.3797	1305.0531
1323.6828	1356.0994	1366.3520
1374.2935	1397.9526	1424.4040
1446.2298	1474.7525	1482.9601
1487.8167	1503.4062	1543.7607
1584.7997	1621.1600	1653.0602
1668.4551	2058.1551	3025.8988
3027.6280	3060.4885	3074.2299
3146.8827	3152.3702	3157.5137
3162.3174	3172.9600	3174.3791
3176.0412	3187.9146	3437.2411

Barrier[3b.2→4b.2]

$C_{18}H_{13}$, C_1, ^2A

6	0	4.926225	-0.771115	0.203655
6	0	3.730848	-1.431801	0.146005
6	0	2.499494	-0.716197	0.039096
6	0	2.539690	0.724537	-0.007281
6	0	3.809971	1.374164	0.055435
6	0	4.965954	0.651383	0.157555
6	0	1.260726	-1.364058	-0.022815
6	0	1.338850	1.436331	-0.112179
6	0	0.104117	0.787314	-0.174100
6	0	0.061229	-0.654281	-0.128796
6	0	-1.205803	-1.315533	-0.194470
6	0	-2.386496	-0.622728	-0.306735
6	0	-2.291530	0.793965	-0.346106
6	0	-1.141771	1.498085	-0.273587
6	0	-4.390281	1.702287	0.230735
6	0	-3.719317	-1.328964	-0.431302
6	0	-4.789594	-0.839704	0.585142
6	0	-4.871050	0.616246	0.511251
1	0	-1.217794	-2.402153	-0.166490
1	0	1.231520	-2.449103	0.011079
1	0	5.853238	-1.327460	0.285018
1	0	3.698830	-2.515932	0.180588
1	0	3.840057	2.458282	0.020332
1	0	5.922989	1.158827	0.204449
1	0	1.368986	2.521220	-0.146497
1	0	-1.125035	2.584348	-0.286355
1	0	-4.255930	2.750453	0.097641
1	0	-4.117716	-1.159356	-1.437601
1	0	-3.580401	-2.406873	-0.313897
1	0	-5.750891	-1.311917	0.360392

1	0	-4.515425	-1.139922	1.602327

Frequencies

-369.2775	43.6573	66.7137
112.7314	126.9875	151.3943
211.0945	240.6380	282.0608
303.5823	331.0060	346.3922
382.7079	418.4063	449.1299
470.9729	480.5624	481.5141
528.1951	561.1758	588.8656
626.9396	644.1544	657.4487
673.2698	732.6799	739.4416
752.3564	754.3870	767.0380
776.6860	832.8609	838.2185
850.0423	853.1888	876.2237
899.0056	906.8711	914.4738
926.9854	942.8984	969.1097
994.4498	996.6021	1027.6441
1029.6980	1142.1783	1159.2205
1178.7458	1187.4642	1192.0969
1203.6020	1219.3242	1262.1776
1284.1916	1289.3631	1300.5220
1325.8056	1349.5288	1368.4422
1378.4898	1414.7524	1422.3780
1437.5872	1470.5987	1475.6802
1480.3806	1503.6871	1570.4273
1590.1444	1611.4330	1643.6895
1667.6900	2068.5042	3024.5925
3028.7603	3061.5832	3077.7909
3140.0741	3142.7426	3153.9892
3156.3818	3157.5503	3162.4240
3175.0575	3187.4820	3434.8933

Barrier[3a.3→4a.3]

$C_{18}H_{13}$, C_1, ^2A

6	0	2.338266	0.593779	-0.292486
6	0	1.865095	-0.723350	-0.351304
6	0	3.648485	-2.188536	0.138708
6	0	4.411674	-1.283173	0.434814
6	0	1.370656	1.574749	-0.147250
6	0	0.554800	-1.088656	-0.264995
6	0	-0.442712	-0.085133	-0.129657
6	0	-0.008289	1.268943	-0.067030
6	0	-0.977106	2.315314	0.081293
6	0	-2.303833	2.041578	0.162242
6	0	-1.864035	-0.381221	-0.046166

6	0	-2.787772	0.694014	0.101204
6	0	-2.381345	-1.694993	-0.105696
6	0	-3.736745	-1.940000	-0.022454
6	0	-4.643243	-0.875918	0.124310
6	0	-4.170907	0.416858	0.184042
6	0	3.808568	0.932341	-0.419992
6	0	4.722923	0.138344	0.555418
1	0	-0.624217	3.340377	0.127698
1	0	1.669060	2.619128	-0.099794
1	0	3.235797	-3.157528	-0.019988
1	0	0.275212	-2.135175	-0.299481
1	0	-3.025783	2.843625	0.274404
1	0	-1.707812	-2.534488	-0.220365
1	0	-4.103328	-2.959192	-0.071358
1	0	-5.707204	-1.073562	0.189107
1	0	-4.860743	1.246988	0.296221
1	0	4.138967	0.708582	-1.440004
1	0	3.958315	2.003198	-0.258578
1	0	4.552728	0.462469	1.587994
1	0	5.772141	0.345940	0.324140

Frequencies

-369.2247	48.8796	56.9105
108.0364	126.5607	143.9205
208.5326	235.9907	272.2345
300.1120	342.1870	343.9538
401.1087	425.7563	443.0903
469.4598	488.8423	524.6430
539.2678	550.0645	564.8262
585.7951	650.2269	657.4264
684.3791	716.5108	730.2928
736.0388	755.7211	775.0146
787.9936	820.6456	847.5044
856.2380	869.5627	877.3741
891.1590	896.4045	947.9886
954.4617	975.8188	990.8753
994.6097	1005.1564	1027.2928
1059.7656	1122.5814	1171.4640
1179.6384	1187.1138	1190.3605
1206.4238	1227.1529	1239.7017
1263.1753	1277.7009	1312.0782
1325.4373	1342.2046	1363.9169
1378.6058	1400.4079	1441.5872
1457.3511	1464.4218	1476.8734
1482.0635	1506.6653	1548.6725
1598.6498	1616.7169	1650.2558

1657.2323	2066.6946	3025.2211
3027.6202	3060.5442	3075.9957
3137.1357	3154.7439	3157.8218
3164.7474	3169.4389	3174.3145
3183.6969	3197.4640	3434.7248

Barrier[3b.3→4b.3]

$C_{18}H_{13}$, C_1, ^2A

6	0	2.325502	-0.886376	-0.271981
6	0	1.711869	0.341355	-0.310026
6	0	0.334250	0.560988	-0.219022
6	0	-0.515793	-0.583422	-0.082468
6	0	0.097248	-1.854128	-0.043764
6	0	1.466739	-2.002634	-0.135622
6	0	-0.246523	1.872487	-0.266987
6	0	-1.955612	-0.387211	0.011294
6	0	-2.480573	0.935934	-0.037274
6	0	-1.588358	2.049493	-0.179667
6	0	-3.875910	1.136533	0.053635
6	0	-4.741135	0.072684	0.188916
6	0	-4.229210	-1.234892	0.237139
6	0	-2.869555	-1.455993	0.150097
6	0	4.184603	1.189386	0.468120
6	0	3.312201	1.995701	0.180511
6	0	3.824521	-1.068757	-0.401973
6	0	4.650741	-0.189166	0.577844
1	0	-4.258093	2.151387	0.014701
1	0	0.412410	2.724307	-0.382685
1	0	-0.509447	-2.743723	0.062908
1	0	1.898470	-2.999054	-0.105749
1	0	-2.013916	3.046806	-0.218425
1	0	-5.809829	0.241151	0.257608
1	0	-4.904935	-2.076156	0.343276
1	0	-2.505878	-2.474546	0.189914
1	0	2.809186	2.923364	0.039012
1	0	4.085081	-2.118701	-0.243340
1	0	4.131755	-0.810398	-1.420775
1	0	5.715472	-0.279735	0.342236
1	0	4.519697	-0.536589	1.608680

Frequencies

-382.4300	38.1296	62.9800
101.1435	125.4528	137.6969
212.3314	224.0078	244.8834
315.0979	337.5763	379.7373
401.6398	423.1942	459.2506

467.4755	500.0606	512.4080
529.3412	552.4314	565.5843
585.8981	642.9705	646.1013
682.0425	704.1206	720.3792
752.5094	757.6096	771.8221
783.9957	824.5844	826.6982
844.3756	876.6473	878.0298
896.9247	940.3100	957.2151
973.6515	985.9808	990.9588
991.6608	1003.2959	1024.5119
1060.8293	1109.1934	1166.8758
1167.3890	1186.1793	1188.2533
1210.4471	1224.8192	1239.1728
1250.7190	1284.5435	1316.3139
1324.4498	1347.5722	1359.3183
1369.2099	1390.8807	1424.9983
1455.4383	1475.0835	1482.6914
1486.5080	1512.2818	1550.3703
1587.2609	1631.3220	1650.3685
1654.4991	2055.3712	3025.8518
3027.6596	3060.3215	3074.9694
3145.8690	3157.2589	3161.5754
3168.1588	3182.7060	3189.0630
3190.5776	3203.7547	3437.0644

Barrier[3a.4→4a.4]

$C_{18}H_{13}$, C_1, ^2A

6	0	4.708115	-0.068874	0.483534
6	0	4.529847	1.113519	0.239215
6	0	2.258906	0.799783	-0.319476
6	0	1.979205	-0.572658	-0.330397
6	0	1.312697	1.771635	-0.206569
6	0	0.642897	-0.934823	-0.231202
6	0	-0.399445	0.016036	-0.126564
6	0	-0.055076	1.397291	-0.116647
6	0	-1.082548	2.389346	-0.009486
6	0	-2.389943	2.037321	0.083797
6	0	-1.802856	-0.361192	-0.025887
6	0	-2.790173	0.661357	0.078724
6	0	-2.244080	-1.704027	-0.027282
6	0	-3.582903	-2.024505	0.069616
6	0	-4.551323	-1.011446	0.172694
6	0	-4.154825	0.307704	0.176475
6	0	3.069809	-1.612654	-0.484191
6	0	4.239784	-1.451098	0.527414
1	0	-0.791195	3.434479	-0.004563

1	0	1.570516	2.826736	-0.184402
1	0	4.678144	2.162882	0.133342
1	0	0.402309	-1.991730	-0.243130
1	0	-3.160291	2.797231	0.164215
1	0	-1.524635	-2.508706	-0.105880
1	0	-3.887936	-3.064988	0.065676
1	0	-5.601748	-1.268464	0.248366
1	0	-4.891543	1.100552	0.255207
1	0	2.645517	-2.614982	-0.381541
1	0	3.491819	-1.540852	-1.492401
1	0	5.037296	-2.158458	0.280255
1	0	3.903219	-1.689991	1.542253

Frequencies

-367.6305	44.4571	61.5955
113.8892	123.3122	144.7281
205.7185	238.3477	258.4180
321.8353	331.9460	350.9292
401.9651	424.8496	434.1165
467.6625	477.1189	518.4113
535.2450	546.5910	570.9164
628.7400	643.7132	657.8529
684.5744	716.9020	728.1323
740.3460	753.0393	764.0172
791.9291	813.4339	849.4857
862.3787	870.9951	876.9783
881.9039	890.0921	938.4600
953.6755	976.6012	990.3583
992.5737	1016.4739	1032.3434
1060.6580	1124.3128	1171.3361
1182.3910	1190.0949	1194.7571
1205.4488	1220.3941	1236.1558
1257.9422	1285.5242	1307.6934
1325.6823	1345.2224	1367.0099
1375.9433	1401.5036	1443.5397
1450.2528	1465.4965	1476.6538
1482.2476	1517.7639	1538.3120
1594.4958	1621.2336	1648.3043
1657.9960	2067.7743	3024.7706
3027.4694	3060.4702	3075.5548
3142.1330	3154.8024	3157.9619
3165.1043	3169.7221	3174.2242
3183.9674	3198.0467	3435.3995

Barrier[3b.4→4b.4]

$C_{18}H_{13}$, C_1, ^2A

6	0	1.341732	-0.280949	-0.055478
6	0	2.581457	0.408966	0.070331
6	0	1.375644	-1.676435	-0.268635
6	0	0.099854	0.475968	-0.010808
6	0	3.788345	-0.325186	0.054313
6	0	2.591144	1.839337	0.168485
6	0	2.569453	-2.370046	-0.294789
6	0	0.164913	1.904440	0.009085
6	0	3.787758	-1.693254	-0.114845
6	0	1.438932	2.553725	0.108137
6	0	-1.182915	-0.091293	0.007613
6	0	-1.032828	2.647955	-0.061853
6	0	-2.362736	0.610779	-0.068477
6	0	-2.257565	2.023654	-0.127412
6	0	-1.704370	-2.200601	0.817136
6	0	-2.826667	-2.227559	0.326340
6	0	-3.755504	-0.002644	-0.018701
6	0	-3.848771	-1.491143	-0.417447
1	0	0.447188	-2.200313	-0.449169
1	0	4.724781	0.212188	0.163403
1	0	3.547462	2.343181	0.262032
1	0	2.566444	-3.440483	-0.467900
1	0	4.722352	-2.242506	-0.130164
1	0	1.460613	3.638171	0.145019
1	0	-0.974672	3.731249	-0.069032
1	0	-3.164309	2.617894	-0.196978
1	0	-0.848146	-2.495669	1.378765
1	0	-4.142790	0.105177	1.001833
1	0	-4.422123	0.576900	-0.665084
1	0	-3.666736	-1.614055	-1.491187
1	0	-4.857334	-1.866039	-0.219509

Frequencies

-440.7086	52.5865	71.1126
104.4113	121.8881	176.4113
201.5795	242.0969	268.4237
289.5272	335.0178	374.6189
403.0362	428.2938	439.9085
466.6841	474.1286	520.3917
530.9782	563.0270	577.7305
607.3147	635.9767	671.9781
687.6991	706.7815	721.5228
757.5189	758.9835	775.4422
797.2661	811.6493	841.9961
852.7616	875.5023	891.5665
897.0179	955.1999	957.2746

969.8057	980.8249	1002.4490
1004.1986	1026.6460	1041.8524
1065.5513	1113.0286	1166.0490
1172.3370	1177.8829	1184.5300
1197.0758	1227.2623	1232.8743
1244.2052	1268.5634	1303.5107
1335.2630	1354.4475	1355.6125
1372.1036	1405.7794	1424.9431
1448.5466	1470.6543	1477.2230
1480.2373	1523.5252	1533.9419
1582.5179	1634.5254	1648.2825
1655.3402	2028.6001	3011.7935
3024.1197	3054.6746	3061.6359
3144.0145	3153.4370	3157.5199
3167.9632	3169.9264	3173.8381
3184.0739	3209.0760	3424.6802

4.1

$C_{18}H_{13}$, C_1, ^2A

6	0	4.749936	-0.035405	0.051134
6	0	3.820266	0.966034	0.084780
6	0	2.423655	0.671453	0.042967
6	0	2.006930	-0.705090	-0.034719
6	0	3.012127	-1.720177	-0.067711
6	0	4.339593	-1.397208	-0.026284
6	0	1.442669	1.665963	0.071158
6	0	0.641738	-1.008109	-0.073375
6	0	-0.349938	-0.016459	-0.040086
6	0	0.079101	1.364601	0.026614
6	0	-0.906608	2.395365	0.032864
6	0	-2.232510	2.089279	-0.026951
6	0	-1.756833	-0.307730	-0.082026
6	0	-2.672201	0.732562	-0.086766
6	0	-4.523700	-0.797928	0.075523
6	0	-4.122477	0.439276	-0.147580
6	0	-2.267755	-1.731750	-0.230499
6	0	-3.666876	-1.958085	0.399615
1	0	-0.579478	3.428664	0.079982
1	0	1.746900	2.707024	0.124502
1	0	5.807560	0.200808	0.083326
1	0	4.130386	2.004217	0.143478
1	0	2.700140	-2.757856	-0.126642
1	0	5.090980	-2.178429	-0.051878
1	0	0.361543	-2.052239	-0.135425
1	0	-2.977843	2.877641	-0.027400
1	0	-4.808640	1.260526	-0.333244

1	0	-2.323845	-1.966375	-1.302338
1	0	-1.576748	-2.451658	0.210353
1	0	-3.589556	-2.052053	1.491669
1	0	-4.084101	-2.899809	0.031671

Frequencies

61.3539	77.4859	131.3577
146.7276	162.2317	228.1865
268.8032	299.1290	304.9336
361.7243	380.3499	415.3406
440.8654	459.4920	476.7945
517.2748	530.0655	539.4319
570.1450	617.2724	634.7563
640.0802	693.4469	719.3942
751.2434	762.6852	776.2301
783.3346	796.7100	805.5264
849.0943	853.5275	870.3707
891.6858	906.4888	916.9415
928.9030	956.4681	968.5436
971.6804	995.1549	1000.5927
1019.2491	1028.7378	1097.1144
1154.3622	1164.6717	1178.2761
1186.4603	1197.7320	1201.6304
1220.3796	1232.3180	1277.0330
1293.7654	1303.3737	1321.4211
1337.4987	1358.9953	1377.0247
1390.8165	1416.2365	1426.8744
1456.4017	1465.4953	1475.6822
1487.2480	1511.9590	1569.8755
1587.4677	1619.8827	1641.4634
1667.9569	1694.6369	2990.4656
3000.4913	3058.9499	3087.8741
3146.7292	3153.8535	3156.7723
3158.6705	3161.7109	3174.9980
3176.4557	3185.4446	3187.8999

4a.2

$C_{18}H_{13}$, C_1, ^2A

6	0	4.398137	-1.366995	-0.019219
6	0	3.076168	-1.711698	0.021265
6	0	2.055451	-0.712098	0.019379
6	0	2.448922	0.672845	-0.029500
6	0	3.841228	0.990074	-0.071271
6	0	4.786174	0.002896	-0.065807
6	0	0.695223	-1.037225	0.062551
6	0	1.453289	1.652066	-0.039209

6	0	0.093570	1.327422	0.004125
6	0	-0.307287	-0.060266	0.065691
6	0	-1.715163	-0.372791	0.120745
6	0	-2.654774	0.645590	0.088869
6	0	-2.236311	2.001291	0.019197
6	0	-0.912415	2.336207	-0.017774
6	0	-4.131136	0.319434	0.216843
6	0	-4.512389	-1.025244	-0.446467
6	0	-3.473828	-2.010582	-0.072348
6	0	-2.204027	-1.771167	0.201870
1	0	0.429077	-2.086656	0.086229
1	0	5.161923	-2.136465	-0.016056
1	0	2.780522	-2.755150	0.057070
1	0	4.134947	2.034018	-0.108032
1	0	5.839782	0.256634	-0.097762
1	0	1.740587	2.698263	-0.084692
1	0	-2.992421	2.779643	0.000026
1	0	-0.607349	3.375862	-0.069134
1	0	-4.378551	0.259350	1.285666
1	0	-4.738104	1.126609	-0.202732
1	0	-5.511429	-1.331577	-0.123591
1	0	-4.546344	-0.929997	-1.540709
1	0	-1.517632	-2.569090	0.460086

Frequencies

62.8998	76.2999	130.1321
151.5634	165.4206	233.6017
263.4483	304.1606	324.0395
348.9191	373.9975	419.2833
449.0016	466.2809	476.2885
518.2509	526.0013	546.1420
557.6623	606.1345	632.7388
640.1165	696.7670	739.5776
749.3797	757.8867	770.6381
774.1612	801.8738	813.2749
831.3165	854.4795	879.3528
890.7617	901.5933	905.5352
930.1623	967.1256	970.3345
980.5730	984.5159	995.6064
1018.6455	1028.6496	1094.4476
1154.5774	1162.8903	1169.5531
1186.5345	1198.1324	1199.3775
1220.7274	1246.3365	1262.8960
1291.6047	1306.2797	1323.8695
1341.3182	1359.3068	1372.3248
1387.5353	1411.3201	1426.2286

1456.6048	1465.0093	1474.6300
1487.0411	1514.2885	1563.8222
1587.7610	1620.9847	1649.0315
1668.3400	1684.3224	2989.6867
2999.1873	3059.3394	3063.5994
3153.7502	3156.0919	3157.1718
3161.5544	3168.8714	3174.8595
3175.3059	3187.2414	3188.8016

4b.2

$C_{18}H_{13}$, C_1, ^2A

6	0	4.898951	-0.767251	0.082012
6	0	3.707037	-1.437548	0.056837
6	0	2.467578	-0.731156	0.017350
6	0	2.494318	0.710369	0.004152
6	0	3.760261	1.370091	0.031526
6	0	4.925660	0.655644	0.069082
6	0	1.230807	-1.388638	-0.009286
6	0	1.284296	1.413462	-0.034686
6	0	0.052076	0.755229	-0.062415
6	0	0.026076	-0.685951	-0.049321
6	0	-1.243817	-1.344285	-0.089158
6	0	-2.418578	-0.651639	-0.132438
6	0	-2.391160	0.794259	-0.113432
6	0	-1.190201	1.455983	-0.089966
6	0	-3.680956	1.510903	-0.067051
6	0	-3.755225	-1.346564	-0.292760
6	0	-4.913399	-0.626293	0.447998
6	0	-4.778087	0.825682	0.203569
1	0	-1.256462	-2.430452	-0.101514
1	0	1.210715	-2.474366	-0.000659
1	0	5.832803	-1.317256	0.112176
1	0	3.685507	-2.522417	0.066613
1	0	3.779845	2.454963	0.021683
1	0	5.879643	1.170462	0.089424
1	0	1.304690	2.499087	-0.042337
1	0	-1.173924	2.541551	-0.073745
1	0	-3.679121	2.589272	-0.199806
1	0	-4.005258	-1.360690	-1.361228
1	0	-3.688549	-2.387829	0.033607
1	0	-5.874058	-1.014331	0.096243
1	0	-4.869657	-0.821784	1.527470

Frequencies

54.6827	83.1873	130.9824
162.9738	178.3750	212.4788

297.7671	308.0178	311.1957
331.8621	382.0617	408.4198
449.9552	480.0192	484.6343
487.0762	514.3770	548.3070
588.4893	605.0275	642.7841
663.4368	726.7779	743.1887
754.2599	756.3179	769.7093
778.6907	783.4796	825.5680
852.7773	854.1800	872.5600
891.6354	895.3556	918.2747
919.2365	923.6004	940.0484
969.2557	976.5639	994.5650
1021.0610	1030.2054	1138.6535
1146.3434	1164.4472	1177.6651
1190.4494	1201.1366	1207.6384
1210.3365	1252.2432	1287.3252
1294.1662	1297.5720	1311.0258
1319.8460	1349.1669	1372.7923
1383.0311	1415.8589	1439.5751
1466.5098	1475.5487	1479.4214
1479.6563	1505.3860	1573.2814
1594.2779	1627.3812	1662.0173
1672.0144	1683.1042	3001.9680
3009.7596	3055.0659	3069.8016
3143.3107	3149.6572	3154.4061
3155.4468	3157.7308	3158.7563
3162.9240	3175.3706	3187.7492

4a.3

$\mathbf{C_{18}H_{13}}$, C_1, ^2A

6	0	-2.383558	0.606083	0.137294
6	0	-1.964049	-0.755232	0.163313
6	0	-3.000907	-1.809130	0.186460
6	0	-4.250156	-1.468533	-0.075326
6	0	-1.425904	1.589440	0.051776
6	0	-0.614749	-1.062560	0.125936
6	0	0.380964	-0.064872	0.049235
6	0	-0.043080	1.291744	0.003458
6	0	0.929549	2.338122	-0.084956
6	0	2.258531	2.061386	-0.124738
6	0	1.804705	-0.364057	0.007354
6	0	2.735928	0.711346	-0.079932
6	0	2.317252	-1.680223	0.050260
6	0	3.674336	-1.926949	0.009113
6	0	4.588094	-0.862514	-0.077667
6	0	4.120787	0.432531	-0.120988

6	0	-3.856988	0.924833	0.293327
6	0	-4.780389	-0.121777	-0.383932
1	0	0.580453	3.364999	-0.118781
1	0	-1.727884	2.632764	0.029794
1	0	-2.695415	-2.836194	0.366015
1	0	-0.331705	-2.107858	0.145379
1	0	2.986335	2.863265	-0.191082
1	0	1.639245	-2.521147	0.117860
1	0	4.036548	-2.948267	0.044223
1	0	5.653234	-1.061681	-0.109896
1	0	4.815668	1.263362	-0.187598
1	0	-4.091861	0.933879	1.365482
1	0	-4.078022	1.924584	-0.090063
1	0	-4.801634	0.019815	-1.472789
1	0	-5.807153	0.007698	-0.029289

Frequencies

62.5347	69.3882	130.3033
162.4936	172.8623	210.3778
265.1478	304.2037	328.9066
356.2866	378.9829	424.1345
437.8356	456.5011	495.2235
505.6761	537.0466	545.2611
561.9391	592.9621	648.6775
658.6915	715.9925	735.6546
745.7769	756.5119	774.0882
778.4188	793.9649	823.6136
827.3396	877.2114	889.6865
894.1793	894.9731	906.3870
919.3385	955.4766	967.0039
976.5978	991.6124	1005.2895
1021.8505	1059.3124	1117.2289
1152.5395	1173.9161	1178.7512
1186.2278	1201.1460	1209.5863
1228.0748	1244.3167	1251.9869
1269.7093	1299.5491	1316.4544
1321.7673	1347.4544	1365.6240
1391.4690	1416.1856	1453.3105
1461.5731	1468.3168	1477.5258
1493.6438	1524.6710	1545.5372
1600.7917	1645.2892	1653.5256
1659.0109	1684.2467	2998.9847
3007.6838	3056.8689	3068.7182
3142.7771	3148.1661	3155.9969
3159.1698	3169.0246	3175.1726
3179.2928	3186.1104	3200.9943

4b.3

$C_{18}H_{13}$, C_1, ^2A

6	0	2.366785	-0.891488	-0.119764
6	0	1.815614	0.393189	-0.166136
6	0	0.400954	0.569108	-0.103162
6	0	-0.452353	-0.573581	-0.019769
6	0	0.144468	-1.848971	0.021962
6	0	1.515190	-1.999482	-0.022801
6	0	-0.197847	1.874353	-0.108297
6	0	-1.898186	-0.392015	0.026885
6	0	-2.435018	0.925208	0.005910
6	0	-1.543286	2.042733	-0.056721
6	0	-3.834157	1.114943	0.050357
6	0	-4.694775	0.041143	0.112672
6	0	-4.172385	-1.263134	0.132205
6	0	-2.808528	-1.471377	0.090693
6	0	4.030291	1.334652	0.017651
6	0	2.755725	1.538616	-0.262340
6	0	3.865609	-1.079651	-0.254922
6	0	4.677112	0.061366	0.403471
1	0	-4.221476	2.128423	0.033747
1	0	0.437327	2.749055	-0.141560
1	0	-0.470932	-2.735342	0.096521
1	0	1.944390	-2.995766	0.012317
1	0	-1.967882	3.041253	-0.059950
1	0	-5.766854	0.198376	0.145685
1	0	-4.843891	-2.113107	0.179614
1	0	-2.441777	-2.489196	0.104894
1	0	2.388082	2.520282	-0.536166
1	0	4.167705	-2.044250	0.162245
1	0	4.114693	-1.102423	-1.324365
1	0	5.721276	0.012126	0.081610
1	0	4.676279	-0.032860	1.498103

Frequencies

50.5994	73.0669	123.4771
141.5097	185.4868	215.5161
253.5217	291.4363	320.7626
359.8049	387.4402	413.9113
469.7941	486.7514	489.1098
499.6501	533.9613	536.0887
573.9517	577.4456	616.3093
647.4382	685.5364	720.5798
739.4937	759.3840	772.8936
786.0837	816.3841	828.3474

843.3398	860.0180	876.2778
878.0805	887.7470	920.1467
944.2850	959.1130	972.9967
980.6875	991.7109	1018.9331
1024.9493	1059.2449	1087.5357
1156.3644	1169.4076	1180.2542
1194.4321	1200.6684	1206.2470
1225.2743	1245.3003	1256.0550
1268.9235	1289.4750	1323.4789
1333.2373	1351.3888	1364.2989
1372.0681	1402.0391	1444.4762
1461.4783	1466.8275	1475.2527
1489.0501	1527.1674	1566.9982
1601.8129	1622.0089	1650.2063
1657.4922	1685.9439	2993.3920
3002.5455	3058.8669	3065.5766
3158.4203	3159.2711	3163.5233
3169.3764	3170.7237	3184.4078
3192.5301	3206.2668	3207.8730

4a.4

$C_{18}H_{13}$, C_1, ^2A

6	0	4.675631	0.136151	0.178206
6	0	3.800578	1.093499	-0.072134
6	0	2.364925	0.742409	-0.102487
6	0	2.001076	-0.634587	-0.138457
6	0	1.370599	1.700791	-0.057719
6	0	0.668442	-0.982818	-0.103430
6	0	-0.368245	-0.020576	-0.046108
6	0	0.003057	1.352105	-0.032045
6	0	-1.012133	2.362602	0.015267
6	0	-2.328676	2.034240	0.046481
6	0	-1.777738	-0.374356	-0.007877
6	0	-2.752163	0.665354	0.036369
6	0	-2.238773	-1.710826	-0.012777
6	0	-3.585479	-2.009082	0.022426
6	0	-4.541322	-0.979395	0.064332
6	0	-4.125209	0.333822	0.071253
6	0	3.091854	-1.674133	-0.306409
6	0	4.408462	-1.298744	0.423233
1	0	-0.703709	3.402794	0.025424
1	0	1.640442	2.752237	-0.030018
1	0	4.085091	2.133722	-0.203346
1	0	0.417228	-2.036357	-0.132503
1	0	-3.088480	2.807973	0.080952
1	0	-1.528371	-2.526734	-0.043319

1	0	-3.907150	-3.044520	0.017911
1	0	-5.598136	-1.219386	0.091628
1	0	-4.852641	1.138365	0.104161
1	0	2.744886	-2.655570	0.027996
1	0	3.317002	-1.762070	-1.377170
1	0	5.222663	-1.935851	0.065495
1	0	4.321853	-1.473334	1.504040

Frequencies

63.8134	68.8320	128.8109
162.1896	175.4394	208.8773
271.6155	303.8461	324.8264
348.6475	393.9943	412.6624
440.5942	451.7508	491.8773
518.4727	539.1756	553.9920
566.8416	571.4073	653.4744
657.5316	716.8370	734.3604
752.8331	756.6627	758.6344
786.7004	796.0212	817.1502
835.8537	877.0086	880.6296
889.5598	897.5893	907.7540
929.7180	955.4122	974.2577
977.9634	991.6009	996.6453
1021.3991	1059.8289	1116.9082
1153.3216	1174.4992	1177.9825
1186.1880	1205.0127	1205.9175
1225.9652	1242.8532	1247.6432
1276.2920	1300.2108	1318.3800
1323.2601	1348.2430	1367.9165
1384.9670	1419.3762	1455.3272
1461.6393	1467.4692	1477.0238
1491.3941	1523.7901	1548.7343
1602.0522	1643.1834	1655.6433
1657.7591	1685.0941	2998.6579
3007.0588	3056.7877	3067.5348
3144.5005	3153.8979	3157.2074
3159.3160	3168.1621	3174.7933
3175.9078	3185.2322	3200.6647

4b.4

$C_{18}H_{13}$, C_1, ^2A

6	0	-1.315024	-0.286384	0.020871
6	0	-2.520398	0.466044	-0.125409
6	0	-1.451485	-1.667155	0.302878
6	0	-0.030496	0.410674	-0.031221
6	0	-3.767806	-0.194919	-0.124742

6	0	-2.466652	1.896348	-0.190861
6	0	-2.686137	-2.287387	0.327827
6	0	-0.048459	1.836750	0.050931
6	0	-3.856604	-1.554769	0.080929
6	0	-1.289231	2.549475	-0.046851
6	0	1.241571	-0.230265	-0.159250
6	0	1.156778	2.549654	0.195435
6	0	2.423974	0.504732	0.025772
6	0	2.365051	1.890023	0.228953
6	0	1.411471	-1.646591	-0.583126
6	0	2.555478	-2.253980	-0.325487
6	0	3.775442	-0.174094	-0.105942
6	0	3.749750	-1.659780	0.315701
1	0	-0.578183	-2.251547	0.550076
1	0	-4.666306	0.397766	-0.262106
1	0	-3.396224	2.444532	-0.301318
1	0	-2.747137	-3.345540	0.556220
1	0	-4.822193	-2.047522	0.087169
1	0	-1.256615	3.633734	-0.027772
1	0	1.118155	3.630207	0.282171
1	0	3.286155	2.447385	0.365086
1	0	0.610344	-2.132049	-1.126524
1	0	4.091070	-0.119761	-1.156748
1	0	4.523785	0.369820	0.477581
1	0	3.678646	-1.760874	1.407381
1	0	4.675177	-2.156408	0.010338

Frequencies

73.7367	78.9769	121.5612
148.6465	196.8688	234.7094
263.1894	313.1817	315.4395
376.7394	398.9598	427.6737
433.6204	479.9453	490.5716
513.9837	531.1947	553.7898
565.9516	587.4050	629.1661
665.7452	690.3377	719.1719
748.7683	756.6539	771.9627
804.7847	807.8323	818.1282
851.7703	862.6322	867.9709
893.3117	913.3256	956.9658
960.5185	970.6060	977.8376
983.6718	1001.6300	1005.5870
1016.9465	1067.4976	1106.6028
1151.7162	1167.7119	1174.5718
1184.2790	1189.7341	1197.9652
1226.4940	1238.2811	1243.1174

1251.5944	1293.1978	1319.5514
1325.8213	1344.2038	1352.7974
1366.1069	1411.8015	1437.9385
1451.0037	1463.7995	1471.9685
1481.4738	1532.0117	1555.5640
1589.7005	1624.2836	1647.8967
1660.2611	1680.8060	2992.3681
3001.4041	3058.8698	3062.7730
3156.0336	3157.8460	3160.1324
3170.1629	3174.1417	3174.8434
3178.1592	3186.5893	3222.0688

Barrier[4.1→5.1]

$C_{18}H_{13}$, C_1, ^2A

6	0	4.755689	-0.035292	-0.038093
6	0	3.822710	0.965656	-0.071087
6	0	2.429048	0.668241	-0.038880
6	0	2.014650	-0.708148	0.027443
6	0	3.019474	-1.721534	0.060278
6	0	4.348064	-1.396338	0.028587
6	0	1.443750	1.664484	-0.065536
6	0	0.647230	-1.012276	0.055619
6	0	-0.343399	-0.019759	0.022940
6	0	0.084598	1.362434	-0.030073
6	0	-0.907481	2.393764	-0.030736
6	0	-2.229480	2.088303	0.019379
6	0	-1.746407	-0.314316	0.059300
6	0	-2.680739	0.726342	0.069947
6	0	-4.541962	-0.799327	-0.277036
6	0	-4.088080	0.421195	0.190853
6	0	-2.227311	-1.755620	0.173833
6	0	-3.663643	-1.898175	-0.296294
1	0	-0.579325	3.427421	-0.063642
1	0	1.748631	2.705709	-0.111094
1	0	5.812805	0.203871	-0.062978
1	0	4.131677	2.004569	-0.121994
1	0	2.708847	-2.760064	0.110615
1	0	5.100114	-2.176897	0.053506
1	0	0.365820	-2.056900	0.106980
1	0	-2.976439	2.874866	0.023221
1	0	-4.765479	1.182473	0.563657
1	0	-1.611079	-2.420178	-0.438855
1	0	-2.097893	-2.111256	1.207048
1	0	-4.734029	-1.883410	0.467663
1	0	-3.923919	-2.767999	-0.896783

Frequencies

-1643.8525	57.1720	80.7083
105.9184	154.9935	161.3069
219.5075	267.7021	298.6101
324.1772	359.3968	403.3565
446.6373	467.6932	477.4557
496.0821	512.2430	528.5442
545.9427	566.5931	619.8648
634.6789	645.5988	690.1686
719.9341	739.8293	744.8183
755.1274	770.3375	782.3300
794.9945	820.0929	849.1579
852.8327	883.1384	901.1773
907.2736	927.1337	968.1234
971.9516	975.8200	981.7923
994.9070	1031.3602	1082.6861
1100.0576	1152.7672	1164.4003
1190.7047	1194.6843	1204.3534
1212.1131	1228.8029	1234.4164
1286.7930	1291.1317	1306.2018
1322.9482	1346.2045	1354.0373
1379.2151	1392.2105	1417.2539
1424.9933	1441.5327	1453.0802
1461.9642	1487.1194	1510.5030
1555.7675	1585.8347	1622.4082
1641.5033	1664.1696	2082.3500
2972.2157	3046.1768	3116.1840
3153.9770	3155.3399	3157.0944
3159.4481	3162.0675	3175.3233
3177.6783	3183.4424	3188.2144

Barrier[4a.2→5a.2]

$C_{18}H_{13}$, C_1, ^2A

6	0	-4.391828	-1.374944	0.015153
6	0	-3.065312	-1.714436	-0.002555
6	0	-2.053225	-0.711358	-0.006982
6	0	-2.451497	0.669921	0.014769
6	0	-3.842778	0.983411	0.034290
6	0	-4.785149	-0.009050	0.033077
6	0	-0.684994	-1.031126	-0.027935
6	0	-1.455427	1.654022	0.028935
6	0	-0.097264	1.329990	0.005425
6	0	0.306493	-0.054734	-0.046395
6	0	1.729986	-0.377991	-0.102885
6	0	2.668760	0.674640	-0.049651
6	0	2.240252	2.014939	0.032696

6	0	0.907192	2.342602	0.050302
6	0	4.143972	0.367259	-0.215304
6	0	4.466560	-1.032043	0.253393
6	0	3.546429	-2.087630	0.127877
6	0	2.213305	-1.706888	-0.245404
1	0	-0.409339	-2.078551	-0.015958
1	0	-5.151483	-2.148386	0.015774
1	0	-2.764558	-2.756814	-0.016548
1	0	-4.141328	2.026446	0.050471
1	0	-5.839877	0.241478	0.047239
1	0	-1.745825	2.699607	0.066138
1	0	2.987515	2.801752	0.059996
1	0	0.598060	3.380916	0.102087
1	0	4.409533	0.444364	-1.282659
1	0	4.756614	1.111220	0.302787
1	0	5.482989	-1.237939	0.585252
1	0	3.899725	-1.616908	1.285107
1	0	1.545128	-2.486688	-0.592515

Frequencies

-1456.4172	65.3963	70.1406
127.8317	134.5823	167.9121
224.9997	269.5621	306.3887
320.8989	353.6614	404.5472
435.7741	456.3936	478.0148
499.5738	521.5916	525.9183
546.7904	564.6275	614.2343
633.4967	641.9358	702.5123
723.9781	730.6368	751.9691
756.4438	773.0323	793.6029
801.1112	809.3599	858.2320
863.9518	898.1729	902.9333
910.0896	933.2012	948.2806
966.5335	970.3261	976.1153
996.7908	1032.7154	1065.3583
1104.2006	1159.8081	1166.2729
1184.8494	1185.7362	1199.2689
1222.4116	1229.0933	1247.8126
1269.1448	1288.4584	1295.2774
1306.2518	1354.8627	1357.0258
1371.5225	1384.8774	1415.9788
1420.6658	1443.2766	1453.3819
1457.9013	1478.5261	1514.6536
1531.5918	1584.4380	1592.4980
1635.8169	1663.7489	2124.4975
2952.9828	3051.2879	3117.1067

3154.4588	3156.4193	3158.5500
3162.3704	3163.2809	3175.8025
3176.1953	3186.1670	3188.7427

Barrier[4b.2→5b.2]

$C_{18}H_{13}$, C_1, ^2A

6	0	4.902507	-0.749532	-0.091532
6	0	3.712519	-1.425719	-0.069263
6	0	2.471551	-0.725753	-0.023454
6	0	2.491213	0.715423	-0.000259
6	0	3.753519	1.381341	-0.025005
6	0	4.922761	0.672389	-0.069055
6	0	1.235695	-1.389860	0.000731
6	0	1.277639	1.412366	0.045550
6	0	0.046431	0.748222	0.068343
6	0	0.029607	-0.694803	0.045167
6	0	-1.238273	-1.361675	0.084205
6	0	-2.413345	-0.675005	0.134952
6	0	-2.406130	0.777557	0.116367
6	0	-1.194439	1.442138	0.095448
6	0	-3.686985	1.456806	0.119985
6	0	-3.751059	-1.379257	0.313556
6	0	-4.833567	-0.610132	-0.422516
6	0	-4.753941	0.796133	-0.449135
1	0	-1.243350	-2.447924	0.100868
1	0	1.221746	-2.475657	-0.013804
1	0	5.838528	-1.295470	-0.126862
1	0	3.696241	-2.510588	-0.086579
1	0	3.767998	2.466173	-0.008162
1	0	5.874162	1.191999	-0.087477
1	0	1.292415	2.497933	0.060503
1	0	-1.184000	2.527671	0.081541
1	0	-3.747745	2.490855	0.441902
1	0	-3.699611	-2.416776	-0.025654
1	0	-3.989278	-1.412216	1.385846
1	0	-5.483067	-1.123243	-1.127900
1	0	-5.738263	0.163410	0.161262

Frequencies

-1686.0193	53.9798	83.0137
128.1090	163.9279	182.5640
212.6420	304.2931	309.2776
319.3321	330.8711	396.2796
439.3305	471.4363	478.1219
484.1202	494.8752	535.5244
550.7056	588.2283	608.6998

642.6290	659.8562	716.5311
742.4987	748.0505	754.6161
760.8285	768.7028	776.9150
780.5724	832.8827	851.8699
857.9085	866.3214	887.2465
911.8189	914.0345	926.2597
931.0344	968.4605	987.2489
994.0948	1031.2016	1076.1032
1138.9817	1146.3626	1164.4139
1188.3814	1190.9983	1194.9875
1211.0027	1213.9978	1275.2611
1290.0898	1296.7905	1298.0982
1299.7677	1312.8815	1356.2965
1375.5860	1394.8994	1413.4903
1429.2503	1437.9517	1456.0239
1476.5192	1491.6198	1505.6389
1558.3344	1588.0314	1623.8100
1648.4674	1665.7114	2086.2740
2990.7219	3071.0891	3131.3846
3148.7141	3154.6487	3156.2092
3158.0140	3159.1534	3161.5751
3163.4274	3175.6664	3188.0662

Barrier[4a.3→5a.3]

$C_{18}H_{13}$, C_1, ^2A

6	0	2.376138	0.620051	0.126976
6	0	1.971182	-0.752800	0.126271
6	0	3.010596	-1.769914	0.167309
6	0	4.222236	-1.447501	-0.395552
6	0	1.415978	1.599840	0.064824
6	0	0.612987	-1.058826	0.092082
6	0	-0.384024	-0.066446	0.047279
6	0	0.033018	1.295456	0.022027
6	0	-0.943959	2.337184	-0.038016
6	0	-2.273108	2.055159	-0.072185
6	0	-1.808683	-0.370172	0.013819
6	0	-2.744681	0.702659	-0.047706
6	0	-2.315167	-1.688467	0.038368
6	0	-3.671877	-1.940211	0.002909
6	0	-4.590442	-0.878535	-0.059103
6	0	-4.128675	0.419159	-0.083385
6	0	3.855719	0.947415	0.283569
6	0	4.686807	-0.115698	-0.411400
1	0	-0.600422	3.366368	-0.055459
1	0	1.711129	2.645416	0.065900
1	0	2.779622	-2.766085	0.528854

1	0	0.335837	-2.105753	0.088609
1	0	-3.004477	2.855170	-0.118149
1	0	-1.633138	-2.527427	0.086581
1	0	-4.029465	-2.963546	0.022973
1	0	-5.654962	-1.081555	-0.087395
1	0	-4.827338	1.248120	-0.130783
1	0	4.083059	1.941319	-0.110392
1	0	4.101291	0.975135	1.354585
1	0	5.338764	-1.090536	0.210145
1	0	5.455828	0.173257	-1.123993

Frequencies

-1702.0470	63.8285	68.5675
124.3172	163.9716	179.5080
205.4396	279.6200	304.0093
326.9698	359.2034	412.1427
433.6105	455.0989	460.6241
502.1154	534.0336	536.0025
556.5631	559.5010	589.0528
646.2568	658.3716	718.7207
723.3599	736.2205	756.7143
765.3405	768.5233	791.9541
796.0433	820.2323	823.7571
877.8203	887.0004	892.7347
900.5097	923.3904	955.9211
974.5829	978.2464	991.7658
994.0148	1059.3001	1079.1189
1121.5185	1151.5574	1173.9455
1184.7327	1187.1544	1208.6048
1211.3895	1226.2576	1244.1588
1261.9690	1282.7505	1298.4902
1305.6860	1315.2918	1358.4812
1376.2505	1388.9892	1418.7109
1437.1311	1454.2625	1460.5160
1462.2000	1498.4934	1525.2447
1543.6059	1596.0756	1635.3957
1644.9854	1656.5104	2085.2169
2986.6330	3067.3269	3130.9075
3147.0898	3156.0015	3159.2618
3162.1863	3169.3320	3175.2797
3180.6329	3186.5870	3201.7675

Barrier[4b.3→5b.3]

$C_{18}H_{13}$, C_1, ^2A

6	0	2.362980	-0.913762	-0.078220
6	0	1.825172	0.392478	-0.118473

6	0	0.394228	0.565338	-0.060371
6	0	-0.460428	-0.571474	-0.009889
6	0	0.133037	-1.853247	0.032078
6	0	1.505971	-2.012950	0.004544
6	0	-0.190790	1.870207	-0.033222
6	0	-1.904704	-0.387036	0.010243
6	0	-2.435512	0.934060	0.009364
6	0	-1.538965	2.046401	-0.003018
6	0	-3.835560	1.128585	0.028693
6	0	-4.700358	0.057501	0.045364
6	0	-4.183593	-1.250092	0.043527
6	0	-2.820707	-1.464050	0.027309
6	0	4.103674	1.381266	0.179489
6	0	2.744453	1.487107	-0.245931
6	0	3.859707	-1.111808	-0.236216
6	0	4.616459	0.078581	0.302571
1	0	-4.218560	2.143756	0.028996
1	0	0.456611	2.736742	-0.016851
1	0	-0.487842	-2.736823	0.091763
1	0	1.926235	-3.013404	0.028865
1	0	-1.957260	3.047287	0.018726
1	0	-5.772332	0.218070	0.058571
1	0	-4.859917	-2.097445	0.053832
1	0	-2.458801	-2.483719	0.021819
1	0	2.405094	2.438349	-0.637549
1	0	4.181365	-2.041201	0.242007
1	0	4.096935	-1.215979	-1.307385
1	0	5.617929	-0.077828	0.698811
1	0	4.220158	0.819549	1.331344

Frequencies

-1507.5402	49.3443	75.4120
117.4314	137.5321	184.8998
211.9898	266.6032	292.2479
308.2841	378.3427	409.2743
447.4029	476.2417	483.3506
507.5457	512.5224	535.0892
548.8829	570.2123	574.6709
623.0152	656.9898	677.1947
704.0920	732.8070	747.3914
757.7046	770.6294	788.7927
823.7460	829.8035	839.5972
877.4420	880.5450	889.2771
931.0993	941.8305	956.6999
963.5426	979.3140	993.6388
1006.3799	1057.8436	1070.0894

1092.0179	1160.1727	1176.9569
1185.9713	1195.2672	1214.6183
1220.7060	1224.5375	1247.2154
1259.4077	1275.2937	1284.0642
1307.6578	1346.0708	1355.1771
1366.4945	1378.9243	1407.7742
1432.4154	1436.8674	1455.8596
1460.9273	1483.4779	1525.3933
1559.6430	1586.7757	1602.3393
1641.7807	1654.9814	2125.9863
2959.1990	3058.8655	3123.3999
3158.5277	3160.3709	3164.8597
3170.2271	3171.6508	3185.0607
3193.1829	3204.5574	3208.4844

Barrier[4a.4→5a.4]
$C_{18}H_{13}$, C_1, ^2A

6	0	4.770226	0.095271	0.296773
6	0	3.777406	1.038338	-0.113070
6	0	2.380247	0.715029	-0.105805
6	0	1.990780	-0.663990	-0.144749
6	0	1.373314	1.684148	-0.067395
6	0	0.658960	-1.001301	-0.107862
6	0	-0.371512	-0.028930	-0.046211
6	0	0.010844	1.345146	-0.039692
6	0	-1.000355	2.362805	0.001812
6	0	-2.317521	2.041966	0.036614
6	0	-1.780960	-0.372330	-0.003279
6	0	-2.749281	0.674533	0.035914
6	0	-2.250807	-1.706406	0.002280
6	0	-3.599305	-1.995421	0.041618
6	0	-4.547896	-0.959083	0.077631
6	0	-4.123274	0.352151	0.075103
6	0	3.075951	-1.711046	-0.325952
6	0	4.373917	-1.255708	0.305254
1	0	-0.685155	3.400851	0.005359
1	0	1.653016	2.733006	-0.044660
1	0	4.079721	2.049718	-0.367468
1	0	0.397569	-2.051987	-0.147994
1	0	-3.073199	2.819772	0.067493
1	0	-1.546029	-2.527246	-0.022255
1	0	-3.927911	-3.028587	0.045240
1	0	-5.606197	-1.191716	0.108161
1	0	-4.845782	1.161163	0.103766
1	0	2.757628	-2.679812	0.068054
1	0	3.255357	-1.854681	-1.403182

1	0	5.056445	-2.016524	0.679506
1	0	4.460130	-0.504998	1.394079

Frequencies

-1535.1086	59.2185	70.4051
120.4771	163.4348	174.7755
199.2882	274.1322	304.8170
329.4530	350.7639	411.0548
436.1967	451.4158	488.0829
495.1308	517.2267	536.1278
545.3248	559.7685	597.3691
645.1188	649.3256	712.0385
719.2800	739.3030	750.3532
755.8506	771.3444	793.8976
797.1796	821.9796	830.1179
876.7665	883.0853	890.6305
897.9210	937.8897	955.7163
964.0009	979.8096	992.9206
994.1458	1057.9582	1067.6374
1123.2603	1158.4826	1174.1957
1184.1509	1192.1897	1196.2592
1221.6598	1225.6207	1246.8988
1263.4250	1290.1408	1301.7418
1314.4752	1323.5730	1348.3610
1367.1373	1384.9051	1427.3546
1433.5191	1452.9000	1455.0909
1463.6374	1480.3946	1517.5840
1547.8460	1594.2340	1618.5319
1650.0501	1653.5998	2128.3761
2967.3056	3063.8007	3121.3735
3148.2522	3156.3485	3159.2532
3160.9810	3169.5517	3175.7091
3177.4228	3186.4695	3201.9749

Barrier[4b.4→5b.4]

$C_{18}H_{13}$, C_1, ^2A

6	0	1.307706	-0.280045	-0.017822
6	0	2.516290	0.474337	0.113293
6	0	1.443529	-1.668516	-0.270888
6	0	0.029004	0.417965	0.031257
6	0	3.763756	-0.187636	0.117285
6	0	2.463292	1.902694	0.173603
6	0	2.677137	-2.287678	-0.290824
6	0	0.045071	1.840216	-0.046248
6	0	3.850317	-1.550110	-0.065311
6	0	1.283138	2.555893	0.043518

6	0	-1.252133	-0.237554	0.148951
6	0	-1.162827	2.554538	-0.198693
6	0	-2.437349	0.515568	-0.039038
6	0	-2.374376	1.897635	-0.237072
6	0	-1.427908	-1.609967	0.553691
6	0	-2.576339	-2.364516	0.180273
6	0	-3.792740	-0.151472	0.128080
6	0	-3.718653	-1.628217	-0.168596
1	0	0.566653	-2.258529	-0.492042
1	0	4.662920	0.406553	0.243038
1	0	3.393443	2.451638	0.275104
1	0	2.736818	-3.350346	-0.497214
1	0	4.815448	-2.043783	-0.067903
1	0	1.249573	3.640047	0.024831
1	0	-1.122458	3.634756	-0.287186
1	0	-3.293704	2.459880	-0.365505
1	0	-0.668598	-2.084564	1.161489
1	0	-4.124318	-0.032428	1.172435
1	0	-4.543742	0.347025	-0.491423
1	0	-2.891725	-2.197702	-1.051698
1	0	-4.601814	-2.131357	-0.556682

Frequencies

-1493.9697	70.7016	78.0149
123.6808	130.7219	191.8711
252.8163	259.0671	303.3714
326.4422	377.5522	423.0284
430.1684	465.2315	480.7900
504.6157	519.9272	531.2719
565.9128	575.9973	607.5168
630.5068	670.7723	682.2326
722.2111	735.0385	746.3002
761.5650	779.4193	800.3674
817.4354	826.4838	834.6089
852.9741	890.7114	917.8530
935.2355	955.3704	969.0709
973.4918	982.4805	1001.5098
1006.6146	1061.1142	1081.3731
1099.1765	1157.4692	1173.8904
1184.1464	1188.9813	1195.2922
1216.2919	1225.0665	1238.5385
1251.6927	1257.5477	1287.8468
1313.4577	1339.6323	1354.0094
1364.7474	1374.3800	1405.3925
1426.9969	1435.6733	1451.3741
1457.0783	1479.9812	1528.9453

1546.0134	1579.8553	1606.1667
1647.2359	1656.8927	2118.0690
2957.9640	3057.0928	3127.5770
3156.3383	3158.2749	3160.6665
3171.2225	3175.6367	3178.7769
3181.5655	3187.0759	3216.0233

5.1

$C_{18}H_{13}$, C_s, $^2A''$

6	0	-4.764452	-0.041163	-0.000095
6	0	-3.832093	0.962236	-0.000097
6	0	-2.438809	0.666462	-0.000014
6	0	-2.022025	-0.710206	0.000045
6	0	-3.024309	-1.725438	0.000037
6	0	-4.354557	-1.401989	-0.000026
6	0	-1.453888	1.666540	0.000008
6	0	-0.652315	-1.012334	0.000086
6	0	0.333893	-0.016113	0.000071
6	0	-0.095988	1.365211	0.000053
6	0	0.899749	2.396856	0.000079
6	0	2.220473	2.091294	0.000042
6	0	1.735823	-0.315013	0.000026
6	0	2.676708	0.725409	-0.000028
6	0	3.685460	-1.939924	0.000006
6	0	4.546503	-0.884220	-0.000100
6	0	4.070462	0.443778	-0.000100
6	0	2.199999	-1.754444	0.000055
1	0	0.571934	3.431184	0.000137
1	0	-1.761669	2.707984	-0.000009
1	0	-5.822004	0.197515	-0.000152
1	0	-4.143250	2.001822	-0.000152
1	0	-2.711474	-2.764560	0.000089
1	0	-5.104772	-2.184775	-0.000022
1	0	-0.365508	-2.056912	0.000139
1	0	2.966381	2.879213	0.000087
1	0	4.061264	-2.957391	-0.000117
1	0	5.616989	-1.061505	-0.000194
1	0	4.770942	1.270858	-0.000245
1	0	1.768664	-2.282488	0.867287
1	0	1.768704	-2.282586	-0.867137

Frequencies

64.1710	83.9605	131.9170
158.3927	164.2088	227.8302
269.9654	298.9875	323.5749
358.9791	403.6433	451.2516

478.0181	481.3125	484.8803
527.4937	533.3781	546.7851
570.0078	627.1370	633.0329
644.9989	678.7203	718.9379
744.3841	754.7322	763.5721
772.1369	790.8389	795.2324
828.6341	850.6534	868.5681
881.5142	904.5155	916.5421
944.1923	945.1023	966.3596
969.1504	978.7328	990.9031
993.4975	1032.6989	1075.5181
1125.6913	1152.3511	1163.0328
1182.6231	1192.1147	1198.8611
1207.0590	1224.1402	1235.9754
1286.2608	1296.9193	1302.2241
1336.4473	1355.9253	1382.5092
1405.9084	1416.4765	1420.2772
1444.4007	1446.6778	1452.2696
1483.8668	1510.5258	1556.8562
1581.4955	1586.7452	1624.9511
1642.4495	1662.8650	2932.5768
2937.2338	3152.5356	3155.5601
3156.1072	3157.1256	3160.9191
3171.8690	3174.3983	3175.4449
3183.0111	3184.2000	3187.5376

5a.2

$C_{18}H_{13}$, C_s, $^2A''$

6	0	4.393269	-1.389076	-0.000117
6	0	3.065717	-1.722050	-0.000107
6	0	2.057081	-0.713971	-0.000056
6	0	2.461852	0.665411	-0.000014
6	0	3.855379	0.972312	-0.000025
6	0	4.792930	-0.024032	-0.000075
6	0	0.688866	-1.027232	-0.000046
6	0	1.469610	1.651637	0.000036
6	0	0.109516	1.334071	0.000046
6	0	-0.303728	-0.048876	0.000004
6	0	-1.731894	-0.363863	0.000015
6	0	-2.660363	0.692052	0.000064
6	0	-2.216431	2.035438	0.000104
6	0	-0.886681	2.356586	0.000096
6	0	-4.151680	0.430268	0.000075
6	0	-4.534824	-1.015129	0.000034
6	0	-2.208556	-1.702888	-0.000023
6	0	-3.592085	-1.996046	-0.000012

1	0	0.420154	-2.076181	-0.000079
1	0	5.149588	-2.165869	-0.000156
1	0	2.760207	-2.763348	-0.000139
1	0	4.158716	2.014147	0.000007
1	0	5.848956	0.221658	-0.000083
1	0	1.763333	2.697009	0.000068
1	0	-2.959910	2.827034	0.000142
1	0	-0.569006	3.393596	0.000128
1	0	-4.608511	0.935034	0.867659
1	0	-4.608532	0.935088	-0.867467
1	0	-5.591051	-1.261055	0.000041
1	0	-1.511000	-2.528261	-0.000061
1	0	-3.900813	-3.036529	-0.000042

Frequencies

60.4218	67.5495	112.9500
141.0507	162.9049	217.0088
273.6505	304.6844	319.1999
351.0002	400.9817	448.2771
469.5902	476.0066	482.1614
525.1362	531.8401	548.2882
567.2450	627.8316	635.1657
643.1521	667.1631	729.1008
733.2076	749.6966	754.8857
767.9457	794.0456	801.9713
807.1093	853.6639	881.3500
885.0921	902.0972	914.4979
936.5675	951.0691	964.8489
967.4431	969.0979	988.8348
994.7088	1031.6810	1073.1065
1124.3154	1160.0029	1167.5373
1182.4001	1185.0062	1198.7545
1201.8195	1219.1808	1242.2096
1284.0897	1289.6888	1300.0840
1316.9668	1358.1221	1379.6025
1393.1148	1419.1785	1429.6318
1441.8041	1448.5774	1457.7304
1488.5119	1514.9929	1538.3806
1587.9372	1591.1485	1609.1886
1641.0128	1665.6298	2937.3482
2941.2155	3149.9708	3154.1689
3154.4155	3156.5307	3161.1143
3173.8131	3174.6641	3174.8641
3183.8373	3187.5567	3214.1764

5b.2

$C_{18}H_{13}$, C_s, $^2A''$

6	0	4.922371	-0.731338	-0.000006
6	0	3.735282	-1.413630	0.000008
6	0	2.489967	-0.720507	0.000002
6	0	2.501728	0.721489	-0.000018
6	0	3.761110	1.393708	-0.000032
6	0	4.934904	0.690737	-0.000026
6	0	1.257285	-1.391626	0.000016
6	0	1.284329	1.412172	-0.000024
6	0	0.054879	0.740506	-0.000010
6	0	0.046241	-0.703587	0.000011
6	0	-1.217937	-1.374136	0.000026
6	0	-2.404905	-0.703061	0.000021
6	0	-2.404302	0.748625	-0.000002
6	0	-1.187256	1.422010	-0.000016
6	0	-3.645465	1.447982	-0.000013
6	0	-3.723109	-1.458858	0.000042
6	0	-4.878543	0.766127	-0.000004
6	0	-4.949051	-0.597592	0.000020
1	0	-1.214827	-2.461083	0.000042
1	0	1.249884	-2.477567	0.000031
1	0	5.861668	-1.272810	-0.000002
1	0	3.725141	-2.498732	0.000023
1	0	3.769551	2.478778	-0.000047
1	0	5.883770	1.215332	-0.000036
1	0	1.292712	2.497944	-0.000039
1	0	-1.185809	2.507757	-0.000033
1	0	-3.629189	2.531970	-0.000030
1	0	-3.755567	-2.132642	-0.869129
1	0	-3.755567	-2.132592	0.869252
1	0	-5.795375	1.346808	-0.000016
1	0	-5.911564	-1.097296	0.000026

Frequencies

44.5833	65.8176	106.0859
161.6047	170.9488	201.2713
303.0064	312.0689	315.2954
321.4442	399.9777	446.0977
469.2427	481.3483	487.3921
497.9062	535.3868	547.9221
608.8148	612.4659	642.4314
655.9998	671.4142	735.6427
745.4172	753.3208	767.6267
774.5186	782.1540	792.1965
849.1574	859.0063	860.7568
878.3735	899.9180	904.5712

909.3727	936.8462	952.2829
954.7388	966.9974	968.5121
992.5753	1031.0492	1076.9745
1146.4205	1156.7070	1164.5708
1184.2287	1190.5795	1198.2437
1209.1003	1213.8919	1284.7826
1292.3664	1303.1086	1305.4027
1313.3418	1349.2581	1376.9361
1403.8125	1412.3886	1422.7828
1439.0092	1447.0474	1466.9077
1492.9767	1506.7685	1549.1553
1568.1988	1585.2361	1621.7590
1641.5880	1663.5626	2971.5340
2977.0165	3142.4993	3153.9147
3154.2029	3155.3855	3157.4655
3158.8983	3162.7404	3171.7281
3175.1914	3182.1609	3187.6685

5a.3

$C_{18}H_{13}$, C_s, $^2A''$

6	0	-4.785853	-0.127040	0.000232
6	0	-2.369003	0.654071	0.000090
6	0	-1.976726	-0.721948	0.000160
6	0	-2.978607	-1.743886	0.000302
6	0	-4.347456	-1.422831	0.000335
6	0	-1.391618	1.621345	-0.000027
6	0	-0.612605	-1.038466	0.000095
6	0	0.392002	-0.059947	-0.000023
6	0	-0.012703	1.308084	-0.000057
6	0	0.975302	2.341169	-0.000142
6	0	2.302311	2.047416	-0.000177
6	0	1.815884	-0.375877	-0.000087
6	0	2.761683	0.689618	-0.000148
6	0	2.310070	-1.698314	-0.000087
6	0	3.665497	-1.961952	-0.000134
6	0	4.593838	-0.907629	-0.000181
6	0	4.143337	0.394713	-0.000191
6	0	-3.838379	1.033382	0.000035
1	0	0.641494	3.373694	-0.000174
1	0	-1.676842	2.670137	-0.000070
1	0	-5.847876	0.092241	0.000272
1	0	-2.664620	-2.781294	0.000392
1	0	-5.073652	-2.229525	0.000471
1	0	-0.345744	-2.088222	0.000173
1	0	3.041855	2.841189	-0.000224
1	0	1.619776	-2.532004	-0.000064

1	0	4.013626	-2.988756	-0.000137
1	0	5.657117	-1.119052	-0.000212
1	0	4.850049	1.218200	-0.000233
1	0	-4.048492	1.676138	0.868912
1	0	-4.048532	1.675809	-0.869074

Frequencies

58.2790	68.0790	103.0700
161.8676	172.0659	193.0342
277.3538	301.4887	328.7514
355.5519	410.2154	437.7498
452.0908	485.5369	496.0824
531.8009	533.6901	560.8523
567.0208	603.1785	650.5745
658.0242	665.1074	718.9711
734.9940	755.9300	773.8078
777.5939	778.2217	793.6344
821.5648	874.8388	878.8150
889.2522	893.1515	906.3562
942.0542	949.6771	955.2262
968.3167	974.2023	990.9625
996.4541	1059.7821	1081.8097
1127.9989	1162.4514	1173.9151
1180.5195	1187.4050	1205.9096
1213.0104	1230.8283	1248.5124
1266.4082	1297.3822	1314.2005
1316.0352	1343.7897	1371.9727
1385.6812	1419.3172	1440.7257
1446.8904	1454.0524	1461.5386
1498.8410	1521.4832	1545.2148
1564.9647	1594.6140	1631.3406
1644.1687	1655.3262	2962.1242
2965.1226	3142.4750	3153.7239
3155.8202	3159.0107	3168.7367
3171.3876	3175.2266	3178.0078
3182.4594	3185.8135	3200.4954

5b.3

$C_{18}H_{13}$, C_s, $^2A''$

6	0	-2.350974	-0.927768	0.000071
6	0	-1.825640	0.381740	-0.000025
6	0	-0.390986	0.562640	0.000037
6	0	0.471832	-0.568909	0.000057
6	0	-0.109982	-1.857338	0.000183
6	0	-1.478215	-2.021931	0.000205
6	0	0.197396	1.868247	0.000129

6	0	1.915887	-0.380103	-0.000013
6	0	2.445037	0.940937	0.000089
6	0	1.544638	2.049383	0.000188
6	0	3.844749	1.138637	0.000069
6	0	4.711997	0.069466	-0.000078
6	0	4.197388	-1.239009	-0.000233
6	0	2.834848	-1.455276	-0.000202
6	0	-4.691756	0.046101	-0.000080
6	0	-4.132849	1.290271	-0.000195
6	0	-2.737101	1.485008	-0.000185
6	0	-3.844153	-1.184824	0.000017
1	0	4.225417	2.154786	0.000160
1	0	-0.440443	2.741159	0.000206
1	0	0.517987	-2.737731	0.000324
1	0	-1.892770	-3.025645	0.000323
1	0	1.958921	3.052247	0.000299
1	0	5.783823	0.232051	-0.000092
1	0	4.875112	-2.085388	-0.000390
1	0	2.475492	-2.475731	-0.000375
1	0	-5.769101	-0.077078	-0.000079
1	0	-4.776236	2.164471	-0.000300
1	0	-2.365128	2.498866	-0.000343
1	0	-4.102848	-1.812856	-0.868064
1	0	-4.102921	-1.812786	0.868127

Frequencies

42.5667	67.9478	96.8323
127.7846	183.9568	195.9714
266.0296	290.0070	301.1674
375.4007	407.4617	453.0783
477.6905	482.9975	496.8497
524.9835	529.3702	554.6028
564.4615	576.9693	629.6253
660.3533	666.9361	689.7241
709.0553	752.9592	767.7416
770.1507	787.0014	818.8718
830.1521	857.6650	874.6254
884.4752	888.3652	929.1121
950.1870	950.6232	955.5356
964.7044	968.6805	991.5446
1020.6782	1057.5885	1081.2897
1111.0330	1163.1342	1177.1608
1182.5254	1199.6333	1204.0559
1210.3065	1224.4641	1250.8690
1258.4393	1279.3171	1301.6653
1314.8171	1352.8838	1373.1895

1385.9677	1418.0097	1429.7424
1444.8206	1458.2032	1460.4472
1488.9631	1523.8440	1560.9695
1572.3647	1598.1678	1613.2540
1644.8952	1656.1100	2946.3038
2947.9225	3152.4462	3153.8063
3158.9772	3163.8230	3169.3465
3175.9604	3184.3479	3192.9976
3199.6408	3209.3691	3222.3590

5a.4

$C_{18}H_{13}$, C_s, $^2A''$

6	0	4.756594	0.060481	0.000082
6	0	3.758948	1.050014	0.000060
6	0	2.369905	0.701371	0.000039
6	0	1.981627	-0.675155	0.000058
6	0	4.451373	-1.273688	0.000091
6	0	1.365334	1.672194	-0.000003
6	0	0.643225	-1.003184	0.000033
6	0	-0.384783	-0.032415	0.000001
6	0	0.002163	1.340224	-0.000022
6	0	-1.006927	2.361235	-0.000060
6	0	-2.325521	2.044961	-0.000076
6	0	-1.797678	-0.371231	-0.000021
6	0	-2.762687	0.678656	-0.000060
6	0	-2.272342	-1.702944	-0.000013
6	0	-3.622848	-1.987486	-0.000035
6	0	-4.568384	-0.948213	-0.000067
6	0	-4.138376	0.361515	-0.000079
6	0	3.036921	-1.766580	0.000066
1	0	-0.688846	3.398558	-0.000075
1	0	1.646977	2.720892	-0.000017
1	0	5.797820	0.367091	0.000102
1	0	4.032887	2.098621	0.000055
1	0	5.241409	-2.016534	0.000112
1	0	0.379671	-2.054669	0.000050
1	0	-3.079105	2.825559	-0.000103
1	0	-1.569826	-2.526250	0.000010
1	0	-3.954672	-3.019723	-0.000027
1	0	-5.628074	-1.176731	-0.000083
1	0	-4.858317	1.173466	-0.000106
1	0	2.880381	-2.424414	0.869085
1	0	2.880422	-2.424399	-0.868970

Frequencies

55.2506	71.2487	105.6279

161.2118	164.4789	199.8565
271.8183	306.4996	329.2217
350.6861	413.8522	435.2306
451.4923	483.5528	497.9403
532.8372	540.2239	556.0046
567.5121	604.0279	651.4932
657.2947	664.3998	718.4386
735.3703	754.7940	757.5660
781.4954	788.7829	792.0180
820.8737	874.2671	879.7950
884.2011	894.3521	907.2607
945.1842	952.9658	955.7369
968.4397	977.8182	990.7518
991.4147	1059.2738	1084.0220
1127.2137	1166.8494	1171.9873
1183.3779	1188.2717	1199.2577
1203.8451	1228.4794	1247.6990
1270.1718	1299.2113	1310.5439
1326.2028	1342.2091	1369.2753
1389.2351	1421.3829	1445.6011
1449.2631	1454.3934	1462.3116
1484.0784	1531.0795	1542.6529
1564.7191	1596.8151	1627.5964
1651.7188	1654.8669	2960.3072
2963.3180	3152.7536	3153.7684
3156.8808	3159.2028	3166.8723
3171.1434	3172.4452	3175.5928
3182.8983	3185.0788	3200.2075

5b.4

$C_{18}H_{13}$, C_1, ^2A

6	0	-1.317900	-0.284739	0.056219
6	0	-2.521340	0.451452	-0.178954
6	0	-1.464881	-1.642923	0.436087
6	0	-0.037430	0.409470	-0.002344
6	0	-3.767895	-0.212742	-0.171115
6	0	-2.466611	1.871606	-0.342978
6	0	-2.698244	-2.262264	0.467920
6	0	-0.059632	1.832013	-0.009054
6	0	-3.861976	-1.553797	0.128364
6	0	-1.293543	2.535152	-0.201180
6	0	1.252234	-0.247886	-0.051650
6	0	1.138928	2.560765	0.155160
6	0	2.422097	0.516139	0.193810
6	0	2.341591	1.907897	0.309873
6	0	3.830907	-1.562445	-0.156264

6	0	1.423980	-1.606784	-0.468677
6	0	2.695683	-2.216139	-0.529228
6	0	3.781942	-0.142332	0.306774
1	0	-0.598951	-2.202101	0.757711
1	0	-4.661939	0.366155	-0.378601
1	0	-3.391343	2.409179	-0.523899
1	0	-2.766735	-3.299818	0.775396
1	0	-4.826527	-2.048433	0.139265
1	0	-1.260687	3.618346	-0.252225
1	0	1.094659	3.644307	0.168863
1	0	3.250409	2.478392	0.474947
1	0	4.795320	-2.057086	-0.188856
1	0	0.578232	-2.153017	-0.855807
1	0	2.759383	-3.236507	-0.893809
1	0	4.525758	0.455859	-0.238516
1	0	4.114966	-0.089929	1.358953

Frequencies

71.1922	78.5857	108.5869
125.5761	190.7622	242.1849
255.4690	296.0040	326.6983
371.9079	429.1422	434.1483
450.3267	491.8168	509.8968
519.2587	536.0931	555.3495
576.9308	606.2830	638.9155
674.7288	685.5106	693.4812
731.1506	753.0768	758.4751
787.6872	800.0661	820.5592
832.9000	849.9772	859.8330
888.0821	929.7133	942.2792
958.6036	964.9762	969.8489
972.9674	980.6288	998.2526
1004.3532	1059.6940	1099.6454
1115.7824	1162.6131	1172.4448
1179.5239	1184.5331	1197.6747
1201.5928	1215.3356	1240.8819
1251.2744	1263.0592	1292.2904
1319.8769	1346.4420	1366.6485
1385.4202	1412.8638	1422.8546
1444.8343	1451.4954	1453.0099
1484.7999	1532.3907	1544.5623
1570.3206	1589.0610	1610.6661
1647.2389	1657.0061	2914.8586
2982.3357	3152.9464	3154.4698
3157.2982	3159.6872	3169.1395
3174.7593	3176.5512	3178.1999

3186.0998	3210.7947	3231.7827

Barrier[5.1→Product (benz[a]anthracene)]
$C_{18}H_{13}$, C_1, ^2A

6	0	4.765809	-0.020448	-0.012125
6	0	3.827300	0.976842	-0.013095
6	0	2.436147	0.669522	-0.011200
6	0	2.031306	-0.707934	-0.009072
6	0	3.037837	-1.716569	-0.006472
6	0	4.366301	-1.383781	-0.008445
6	0	1.441330	1.658844	-0.005641
6	0	0.660766	-1.019523	-0.009415
6	0	-0.326636	-0.038575	-0.014068
6	0	0.086503	1.342193	-0.002934
6	0	-0.913087	2.376694	0.020862
6	0	-2.232773	2.079819	0.033155
6	0	-1.752788	-0.345800	-0.019228
6	0	-2.694171	0.715695	0.010864
6	0	-3.622974	-1.929160	-0.101919
6	0	-4.536636	-0.875328	-0.064644
6	0	-4.075068	0.427999	-0.001664
6	0	-2.250995	-1.676628	-0.031305
1	0	-0.580200	3.409217	0.033340
1	0	1.737220	2.703515	0.001125
1	0	5.821700	0.225570	-0.013361
1	0	4.130970	2.018527	-0.014559
1	0	2.731844	-2.757600	-0.002880
1	0	5.122097	-2.161025	-0.006774
1	0	0.388115	-2.067587	0.001632
1	0	-2.975194	2.870546	0.054853
1	0	-3.972441	-2.953209	-0.161940
1	0	-5.601346	-1.076141	-0.095568
1	0	-4.777959	1.254111	0.022504
1	0	-1.569856	-2.502029	-0.186988
1	0	-1.943983	-2.167066	1.846697

Frequencies

-633.9300	66.1618	72.2154
141.9498	163.5654	184.7823
258.8260	268.0685	303.3531
308.3759	350.0481	364.0385
403.1935	454.2686	458.8380
477.5504	497.7465	523.4863
539.4268	558.9632	583.3058
587.6099	636.4653	661.8738
698.4532	733.8711	753.1455

766.1215	772.6382	773.7821
799.0604	804.2857	825.1986
857.3392	886.0579	892.1774
896.3771	907.1921	919.9035
968.1679	970.5498	985.1426
996.0405	996.2977	999.6250
1034.3223	1063.2493	1118.3406
1152.7487	1167.9596	1176.1488
1186.0002	1196.9451	1220.4329
1237.9222	1258.6818	1289.2408
1302.1729	1321.0873	1343.6977
1365.3282	1385.6176	1416.7586
1439.8548	1448.3895	1469.4961
1481.9280	1512.2579	1532.2530
1577.6138	1596.0242	1620.5717
1637.1078	1659.4533	1667.9149
3154.5695	3157.5671	3158.7262
3162.3314	3162.7260	3174.5365
3175.5150	3177.3857	3181.8519
3188.3058	3189.5202	3204.8324

Barrier[5a.2→Product (benz[a]anthracene)]

$C_{18}H_{13}$, C_1, ^2A

6	0	-4.400293	-1.368729	0.033495
6	0	-3.074815	-1.713142	0.032441
6	0	-2.059567	-0.713567	0.011530
6	0	-2.452315	0.667146	-0.008252
6	0	-3.840977	0.986782	-0.006473
6	0	-4.787978	-0.002005	0.013773
6	0	-0.691631	-1.037012	0.009619
6	0	-1.448836	1.646711	-0.027570
6	0	-0.096280	1.317481	-0.028237
6	0	0.304476	-0.066345	-0.010239
6	0	1.733349	-0.386747	-0.012954
6	0	2.678508	0.671705	-0.020434
6	0	2.230188	2.035304	-0.037621
6	0	0.911461	2.343119	-0.043993
6	0	4.068876	0.372447	0.008684
6	0	4.510249	-0.948883	-0.071594
6	0	2.219566	-1.710585	-0.026643
6	0	3.578127	-1.986282	-0.067018
1	0	-5.162843	-2.139180	0.049532
1	0	-2.778150	-2.756803	0.047728
1	0	-4.135441	2.030985	-0.021362
1	0	-5.841684	0.253172	0.015046
1	0	-0.429435	-2.087801	0.026528

1	0	-1.734745	2.694065	-0.041396
1	0	2.978152	2.820979	-0.040251
1	0	0.587683	3.378440	-0.058183
1	0	4.773606	1.186129	-0.118750
1	0	4.438738	0.696017	1.883962
1	0	5.571712	-1.163601	-0.107104
1	0	1.525196	-2.540560	-0.024421
1	0	3.914563	-3.016228	-0.102402

Frequencies

-675.9664	66.0985	70.2289
142.8351	164.4634	184.9606
255.2531	280.3963	297.1083
307.7378	348.9379	379.8958
402.4583	455.3975	460.8329
476.6742	498.1899	523.6831
540.4421	562.2662	575.4778
587.5002	636.6398	662.3903
699.1188	734.9864	754.7314
759.1346	771.3309	771.7813
804.6940	807.6194	822.1843
856.8898	885.2690	888.9149
894.6961	906.7974	919.8253
967.2437	970.1169	982.0907
996.2104	996.3582	1005.5825
1034.2381	1063.1388	1116.9840
1153.0824	1167.2806	1176.7807
1186.3818	1196.8721	1218.1798
1240.3470	1255.1470	1288.6149
1302.3163	1320.4703	1340.5942
1366.2610	1384.9889	1417.2749
1440.9644	1448.7027	1467.9201
1480.7995	1512.5425	1533.6058
1581.2279	1596.3730	1617.8438
1634.8878	1654.6088	1667.8344
3155.1105	3157.5272	3159.7164
3162.2989	3166.4494	3172.9325
3175.4869	3178.0420	3180.2435
3188.2864	3190.4640	3203.2042

Barrier[5b.2→Product (tetracene)]

$C_{18}H_{13}$, C_1, ^2A

6	0	4.908533	0.730772	-0.018015
6	0	3.728909	1.415298	-0.036682
6	0	2.474527	0.724523	-0.021634
6	0	2.484165	-0.724027	0.014297

6	0	3.748012	-1.397825	0.032867
6	0	4.918155	-0.697336	0.017416
6	0	1.256090	1.396157	-0.039670
6	0	1.275189	-1.411784	0.029730
6	0	0.038064	-0.740307	0.011869
6	0	0.028723	0.708701	-0.023837
6	0	-1.211331	1.380699	-0.037204
6	0	-2.415742	0.694345	-0.020762
6	0	-2.408438	-0.754298	0.004127
6	0	-1.192253	-1.427184	0.024230
6	0	-3.662540	-1.445527	-0.011890
6	0	-3.687249	1.372329	-0.023869
6	0	-4.846268	-0.763215	-0.069615
6	0	-4.861762	0.657412	-0.095032
1	0	5.850444	1.267468	-0.029715
1	0	3.720958	2.499929	-0.063111
1	0	3.754737	-2.482459	0.059803
1	0	5.867255	-1.221154	0.032088
1	0	1.249171	2.481512	-0.065228
1	0	1.282607	-2.497135	0.056184
1	0	-1.217972	2.466198	-0.051842
1	0	-1.186651	-2.512621	0.045216
1	0	-3.653795	-2.530218	0.007857
1	0	-3.825521	1.889274	1.967643
1	0	-3.695497	2.450551	-0.132413
1	0	-5.785012	-1.304546	-0.098987
1	0	-5.809430	1.180796	-0.145443

Frequencies

-552.2041	56.2617	87.2795
148.9004	162.6610	184.6268
239.4983	274.3318	302.1729
310.7182	318.9475	341.1803
389.8781	448.4938	475.6485
481.2296	498.9777	505.2825
520.4308	560.6560	567.9435
618.2536	633.6734	644.5994
730.9613	748.3766	756.6004
758.3864	763.1999	772.5568
780.2848	787.9574	847.7258
862.1408	864.9707	867.3588
892.5349	910.4693	915.9320
917.8775	944.5362	972.3417
973.8476	993.6071	996.3318
1022.4620	1027.7450	1141.3392
1148.7894	1151.1249	1183.4760

1188.8399	1202.1163	1220.2035
1222.8688	1290.4376	1298.8484
1314.6758	1316.9505	1358.9615
1369.4014	1404.3227	1415.2815
1416.7437	1427.9492	1477.2322
1478.5602	1501.2940	1545.5398
1561.4391	1580.7179	1601.3570
1644.8156	1648.4487	1672.5402
3155.9129	3157.7292	3158.5189
3160.2224	3161.3246	3162.8095
3164.7303	3171.3559	3176.9130
3180.8350	3188.8098	3192.0498

Barrier[5a.3→Product (benz[a]anthracene)]
$C_{18}H_{13}$, C_1, ^2A

6	0	-4.723368	-0.065344	-0.084503
6	0	-2.383791	0.638559	-0.016793
6	0	-1.980999	-0.737348	-0.001860
6	0	-2.986296	-1.747477	-0.016879
6	0	-4.318770	-1.418986	-0.066841
6	0	-1.393270	1.625526	-0.030897
6	0	-0.610836	-1.049315	0.008025
6	0	0.377548	-0.069563	-0.003718
6	0	-0.035863	1.309149	-0.027092
6	0	0.960973	2.345778	-0.043358
6	0	2.281748	2.051821	-0.036859
6	0	1.808739	-0.378062	0.004286
6	0	2.747584	0.689942	-0.012853
6	0	2.308148	-1.695824	0.029064
6	0	3.666675	-1.953669	0.036304
6	0	4.587743	-0.896640	0.018819
6	0	4.128316	0.404748	-0.005352
6	0	-3.784921	0.948195	-0.008445
1	0	0.625724	3.377409	-0.060289
1	0	-1.688586	2.670232	-0.038180
1	0	-5.778065	0.179696	-0.130088
1	0	-2.678645	-2.787867	-0.004347
1	0	-5.069553	-2.200334	-0.097980
1	0	-0.339306	-2.097720	0.021614
1	0	3.021773	2.845118	-0.048842
1	0	1.622883	-2.533506	0.043617
1	0	4.018907	-2.978796	0.055977
1	0	5.652272	-1.101115	0.024666
1	0	4.830384	1.231987	-0.018597
1	0	-4.025822	1.403903	1.931721
1	0	-4.088134	1.982063	-0.125566

Frequencies

-607.3426	65.7410	67.9187
143.8822	164.3939	181.5367
243.4283	282.5622	287.9059
303.3685	352.8035	362.6748
404.1042	433.4223	455.0179
497.9103	499.1761	523.3755
540.4522	553.2140	576.6472
586.2237	635.0303	663.0968
699.3160	735.1550	753.5394
759.2649	774.0300	779.1884
795.2632	803.2780	821.6553
867.9244	879.9269	888.4163
892.3093	907.5640	919.7754
955.1493	973.2670	982.4866
993.2039	994.6921	1000.0479
1037.9661	1063.5739	1120.7119
1149.5201	1168.3663	1177.7331
1186.8313	1195.7792	1221.0263
1240.8164	1260.6892	1285.5509
1302.1962	1322.3062	1346.2516
1368.0037	1384.4007	1402.7652
1440.3464	1451.4096	1469.2363
1485.7483	1511.4170	1535.0762
1571.7282	1594.1923	1619.4587
1645.5240	1658.4187	1660.7630
3155.9934	3158.8718	3160.3773
3160.8198	3169.9154	3170.3914
3177.0080	3179.3037	3180.3931
3187.0947	3191.5953	3200.8388

Barrier[5b.3→Product ([4]phenacene (chrysene))]

$C_{18}H_{13}$, C_1, ^2A

6	0	2.368203	-0.917039	-0.021205
6	0	1.830620	0.399817	-0.009100
6	0	0.390496	0.577409	0.002261
6	0	-0.459356	-0.554661	-0.016635
6	0	0.131811	-1.854475	-0.039117
6	0	1.483119	-2.028278	-0.037243
6	0	-0.200204	1.879028	0.033701
6	0	-1.900544	-0.378269	-0.010207
6	0	-2.440264	0.940153	0.019716
6	0	-1.549577	2.052867	0.042906
6	0	-3.842253	1.127477	0.027166
6	0	-4.700606	0.052705	0.005500

6	0	-4.176339	-1.252911	-0.024514
6	0	-2.813746	-1.460582	-0.032030
6	0	4.638890	-0.014885	-0.084559
6	0	4.109385	1.281169	-0.075406
6	0	2.743301	1.484490	-0.027509
6	0	3.782132	-1.106528	-0.001937
1	0	-4.230147	2.140525	0.050408
1	0	0.434688	2.754109	0.055140
1	0	-0.502407	-2.730168	-0.053669
1	0	1.903297	-3.028374	-0.042951
1	0	-1.969663	3.052859	0.068827
1	0	-5.773585	0.206893	0.011403
1	0	-4.848734	-2.103261	-0.041839
1	0	-2.448814	-2.478501	-0.055443
1	0	5.710777	-0.167994	-0.126334
1	0	4.776120	2.135241	-0.112831
1	0	2.376129	2.501638	-0.023703
1	0	4.033892	-1.536364	1.888218
1	0	4.168042	-2.111515	-0.127956

Frequencies

-664.1910	45.9120	71.8537
127.3126	174.0059	185.5730
225.8989	272.6205	287.1787
294.1170	357.8142	391.1271
400.8876	452.5933	485.7720
487.0845	495.7069	522.4832
544.2281	569.3310	576.1702
579.4241	585.3074	683.1265
691.6021	694.9080	739.9569
754.5307	777.6908	781.0210
798.7432	830.6566	837.6457
863.5698	875.3016	885.3858
891.2730	893.7804	950.0542
959.1132	966.4070	976.3818
993.9958	1001.3504	1035.0733
1057.7045	1062.9139	1099.7473
1155.8878	1170.8193	1176.6716
1186.6765	1205.1429	1211.6480
1246.7485	1256.6727	1272.5669
1283.2118	1321.2110	1351.1333
1375.4346	1386.3198	1392.2807
1450.6736	1458.5912	1461.6518
1481.7805	1519.4218	1552.2178
1557.4179	1601.9031	1620.8231
1637.3695	1650.9270	1659.1415

3160.3035	3165.0310	3165.9990
3167.7238	3170.7335	3174.0710
3185.7379	3189.4806	3195.1072
3196.2379	3212.2978	3213.4717

Barrier[5a.4→Product (benz[a]anthracene)]

$C_{18}H_{13}$, C_1, ^2A

6	0	4.727841	0.047224	-0.078309
6	0	3.770246	1.029575	-0.020609
6	0	2.383599	0.700818	0.001668
6	0	1.996796	-0.679630	-0.013352
6	0	4.356525	-1.315948	-0.096688
6	0	1.375976	1.675849	0.019240
6	0	0.635227	-1.010818	-0.018259
6	0	-0.368290	-0.044499	-0.006555
6	0	0.024591	1.340217	0.015104
6	0	-0.988300	2.362272	0.030703
6	0	-2.304087	2.048336	0.025483
6	0	-1.793927	-0.374365	-0.012162
6	0	-2.749096	0.679317	0.004230
6	0	-2.273450	-1.699854	-0.032368
6	0	-3.627831	-1.978126	-0.036132
6	0	-4.564839	-0.935122	-0.019877
6	0	-4.125230	0.373218	-0.000035
6	0	3.024631	-1.681317	-0.013032
1	0	-0.668563	3.398842	0.047123
1	0	1.657349	2.724388	0.032986
1	0	5.777899	0.314079	-0.115439
1	0	4.057344	2.075738	-0.007659
1	0	5.122211	-2.081124	-0.148469
1	0	0.377799	-2.062772	-0.023994
1	0	-3.056221	2.830167	0.037699
1	0	-1.575768	-2.527166	-0.044744
1	0	-3.964522	-3.008532	-0.051398
1	0	-5.626137	-1.155826	-0.022690
1	0	-4.839799	1.189679	0.012930
1	0	2.999518	-2.200978	1.921197
1	0	2.736600	-2.719385	-0.131857

Frequencies

-614.9423	65.9907	68.3341
144.4517	164.0904	181.4065
249.7067	267.2801	301.5716
309.1188	338.5590	367.1025
406.7725	432.8356	455.2443
497.7425	499.3358	524.5326

540.7273	551.0334	578.3428
587.3342	634.6782	663.2093
699.2051	735.2208	752.4185
759.3158	772.8060	781.6845
794.6500	803.6449	821.6190
870.0182	880.3607	887.8999
890.5301	907.4944	920.1169
955.5683	973.7026	982.5828
993.3556	995.4364	1001.5086
1037.5532	1063.7525	1120.7901
1149.7576	1167.3618	1179.0221
1186.9359	1195.9904	1218.4381
1239.3442	1260.5541	1288.9362
1302.9361	1321.6776	1346.2389
1370.9964	1382.1443	1402.4135
1439.8624	1451.6309	1469.5421
1485.2621	1512.5966	1533.6513
1573.3383	1594.9185	1617.4404
1645.1700	1659.4696	1661.6137
3155.2466	3158.2680	3160.6186
3161.7472	3169.6633	3170.3450
3176.7466	3179.0096	3180.7195
3187.1226	3191.4886	3201.7632

Barrier[5b.4→Product ([4]helicene)]
$C_{18}H_{13}$, C_1, ^2A

6	0	-1.319008	-0.281341	0.055658
6	0	-2.516218	0.467454	-0.176511
6	0	-1.478414	-1.638270	0.439650
6	0	-0.035493	0.399278	-0.011932
6	0	-3.770326	-0.186332	-0.168122
6	0	-2.446178	1.883302	-0.339675
6	0	-2.716882	-2.244069	0.473915
6	0	-0.040267	1.814982	-0.017627
6	0	-3.875237	-1.524855	0.131576
6	0	-1.261898	2.533363	-0.200561
6	0	1.253734	-0.270012	-0.075244
6	0	1.174929	2.541830	0.159032
6	0	2.442094	0.488218	0.160130
6	0	2.365041	1.899983	0.309361
6	0	3.823181	-1.498551	-0.195100
6	0	1.424941	-1.620751	-0.477568
6	0	2.672830	-2.213566	-0.542304
6	0	3.708145	-0.166839	0.185895
1	0	-0.619821	-2.204030	0.768402
1	0	-4.659054	0.400742	-0.374983

1	0	-3.364052	2.432949	-0.518618
1	0	-2.796486	-3.278881	0.787593
1	0	-4.843783	-2.011441	0.143895
1	0	-1.217276	3.616157	-0.248425
1	0	1.124301	3.624768	0.195733
1	0	3.277279	2.457236	0.492778
1	0	4.797459	-1.971327	-0.232021
1	0	0.569870	-2.188538	-0.811315
1	0	2.757960	-3.237639	-0.887873
1	0	4.597345	0.443943	0.290886
1	0	3.946412	-0.386896	2.130509

Frequencies

-632.3006	78.9257	83.5231
126.2557	172.4769	200.9969
257.2137	272.6702	277.3966
325.8698	342.6530	382.2233
429.0157	440.6880	447.9896
489.9082	520.3890	524.4399
531.4756	551.5865	587.1372
595.6161	632.2121	684.4855
690.7008	705.9765	756.5468
761.6351	767.9350	778.3114
815.7599	821.2620	827.1259
853.6897	865.0457	885.3947
903.1902	964.0438	966.1404
970.6607	981.5616	984.8475
999.2579	1006.4045	1014.1833
1056.9227	1070.9959	1126.6027
1149.3698	1168.3808	1176.5747
1182.2264	1189.9820	1215.6966
1235.2425	1237.0495	1254.6683
1275.5210	1324.6264	1348.2723
1363.5661	1384.0112	1395.9531
1444.7937	1447.4260	1453.7568
1479.5987	1531.3171	1532.7200
1554.3676	1591.6082	1622.4276
1632.0886	1647.6774	1663.1665
3158.6627	3160.6091	3162.1857
3167.3042	3170.7617	3174.4250
3178.2578	3180.6159	3187.2551
3191.1706	3212.5471	3230.0063

Product (benz[a]anthracene)

$C_{18}H_{12}$, C_s, $^1A'$

6	0	4.750909	-0.011143	-0.000021

6	0	3.806427	0.980219	-0.000066
6	0	2.416871	0.664448	-0.000032
6	0	2.020388	-0.715163	0.000048
6	0	3.033152	-1.717683	0.000103
6	0	4.359532	-1.377054	0.000064
6	0	1.415650	1.646798	-0.000069
6	0	0.651529	-1.034592	0.000063
6	0	-0.342246	-0.061162	-0.000011
6	0	0.062454	1.321403	-0.000051
6	0	-0.942618	2.351657	-0.000027
6	0	-2.260875	2.049095	0.000067
6	0	-1.772069	-0.378503	-0.000024
6	0	-2.717818	0.683441	0.000070
6	0	-2.263217	-1.699541	-0.000145
6	0	-3.620119	-1.966591	-0.000113
6	0	-4.548007	-0.915479	0.000033
6	0	-4.096482	0.389028	0.000113
1	0	-0.614108	3.385729	-0.000072
1	0	1.704334	2.693574	-0.000098
1	0	5.805409	0.240957	-0.000054
1	0	4.103463	2.023876	-0.000119
1	0	2.733355	-2.760629	0.000172
1	0	5.120221	-2.149583	0.000089
1	0	0.385963	-2.084737	0.000177
1	0	-3.006667	2.837149	0.000127
1	0	-1.572346	-2.532705	-0.000291
1	0	-3.965653	-2.994218	-0.000215
1	0	-5.611211	-1.126771	0.000068
1	0	-4.803521	1.212285	0.000202

Frequencies

66.9441	70.5933	145.3996
165.1442	187.1886	270.9426
290.2912	307.4310	359.3514
399.2444	430.4008	454.7955
476.8307	498.2616	522.8199
540.8750	549.8414	578.0624
587.7182	636.7060	663.6738
700.0824	734.8948	751.9587
760.2287	771.8906	773.8297
794.7018	804.7732	821.0431
856.7780	879.7818	888.4322
889.9263	906.4712	920.0196
954.5847	968.3015	982.0403
992.5044	995.6999	999.8229
1034.0774	1063.7901	1122.8912

1156.0649	1168.3480	1179.0007
1187.4805	1197.5257	1222.4932
1241.0162	1261.9221	1288.9485
1302.4486	1322.5947	1346.0884
1369.2939	1386.0206	1417.1925
1442.0701	1452.1765	1473.5902
1487.0809	1513.8151	1535.5351
1587.6016	1599.3727	1631.1361
1650.3023	1661.5476	1669.3935
3153.6239	3156.4162	3157.2866
3159.6436	3161.3762	3169.3926
3174.6870	3175.8605	3178.8033
3186.5355	3187.6510	3200.7646

Product (tetracene)

$C_{18}H_{12}$, D_{2h}, ^1A_g

6	0	-4.880868	-0.714593	-0.000023
6	0	-3.706308	-1.407180	0.000024
6	0	-2.446436	-0.724867	0.000019
6	0	-2.446440	0.724861	0.000010
6	0	-3.706314	1.407167	-0.000030
6	0	-4.880870	0.714573	-0.000054
6	0	-1.233635	-1.404483	0.000037
6	0	-1.233647	1.404489	0.000016
6	0	-0.000062	0.725101	0.000023
6	0	-0.000050	-0.725083	0.000028
6	0	1.233759	-1.404441	0.000019
6	0	2.446373	-0.724997	-0.000006
6	0	2.446336	0.725071	0.000011
6	0	1.233736	1.404468	0.000016
6	0	3.706460	1.407245	0.000022
6	0	3.706409	-1.407274	-0.000034
6	0	4.880796	0.714650	-0.000011
6	0	4.880794	-0.714697	-0.000042
1	0	1.234104	-2.490225	0.000030
1	0	-1.234085	-2.490237	0.000056
1	0	-5.826446	-1.244987	-0.000042
1	0	-3.705841	-2.492205	0.000055
1	0	-3.705849	2.492192	-0.000039
1	0	-5.826449	1.244966	-0.000093
1	0	-1.234102	2.490244	0.000011
1	0	1.234114	2.490253	0.000048
1	0	3.705692	2.492303	0.000045
1	0	3.705635	-2.492305	-0.000149
1	0	5.826529	1.244779	-0.000015
1	0	5.826508	-1.244839	-0.000061

Frequencies

56.6677	89.8687	150.2349
163.3029	191.7672	271.6842
305.0880	317.8380	318.2151
383.1829	448.2711	474.2910
478.2506	483.7332	505.6366
518.9333	562.7261	567.2160
618.6343	634.6984	645.0686
734.0461	745.3839	757.2624
758.0488	762.7706	769.4186
778.2442	788.4091	844.2708
854.6964	864.8384	867.8053
892.0771	910.6425	916.2646
917.0998	945.2665	972.0444
973.5429	995.7186	995.9254
1020.5165	1022.5671	1147.0034
1150.1731	1151.9345	1186.1990
1189.2929	1204.2186	1223.4379
1224.2577	1291.1088	1298.7581
1315.6568	1318.2211	1359.8793
1367.7136	1411.6615	1418.0693
1424.1335	1432.3510	1479.5855
1482.1677	1501.4907	1557.3290
1577.9723	1583.4680	1608.9739
1648.6058	1663.3022	1677.4485
3154.4942	3156.2684	3156.9190
3158.6473	3159.6685	3159.7479
3163.3338	3164.4089	3176.3438
3176.4538	3188.2354	3188.5552

Product ([4]phenacene (chrysene))

$C_{18}H_{12}$, C_{2h}, ^1A_g

6	0	-2.399469	0.945998	-0.000147
6	0	-1.868084	-0.376375	0.000009
6	0	-0.428723	-0.562644	-0.000088
6	0	0.428589	0.563210	-0.000092
6	0	-0.153475	1.868929	-0.000279
6	0	-1.501791	2.052722	-0.000350
6	0	0.153254	-1.868693	-0.000262
6	0	1.868386	0.376576	0.000025
6	0	2.399479	-0.945842	-0.000140
6	0	1.501339	-2.052644	-0.000330
6	0	3.800225	-1.142656	-0.000095
6	0	4.666047	-0.073675	0.000155
6	0	4.150607	1.235814	0.000398

6	0	2.789444	1.452782	0.000334
6	0	-3.800480	1.142339	-0.000083
6	0	-4.666001	0.073393	0.000179
6	0	-4.150243	-1.236322	0.000397
6	0	-2.789160	-1.452804	0.000296
1	0	4.181243	-2.158668	-0.000247
1	0	-0.488341	-2.739211	-0.000415
1	0	0.487710	2.739746	-0.000477
1	0	-1.915108	3.055976	-0.000554
1	0	1.914616	-3.055909	-0.000520
1	0	5.738023	-0.235290	0.000192
1	0	4.828818	2.081839	0.000659
1	0	2.431550	2.473459	0.000597
1	0	-4.181091	2.158445	-0.000211
1	0	-5.737963	0.234485	0.000254
1	0	-4.828442	-2.082226	0.000645
1	0	-2.430684	-2.473292	0.000524

Frequencies

46.2440	75.3345	130.6381
176.0140	186.9401	234.7647
291.5277	293.9840	383.7838
390.4963	438.2359	483.8995
485.7740	487.6976	520.3514
544.8448	563.5937	577.1572
579.6728	586.3287	685.4355
691.4652	695.5061	742.1617
752.0434	774.2768	782.4887
791.1596	827.2408	836.5131
864.4452	872.8276	879.1657
890.9320	893.4056	946.9371
954.8610	962.1241	974.4133
992.4923	994.0718	1037.9732
1057.2755	1061.9305	1102.0977
1161.1974	1173.4631	1177.6178
1187.2618	1205.5238	1213.7956
1249.6799	1257.0681	1275.7585
1284.4912	1323.0628	1354.2059
1381.8564	1387.0999	1394.8475
1456.0603	1462.6471	1463.4650
1484.9744	1521.1376	1556.1350
1559.4560	1606.3056	1638.1869
1648.3628	1658.3456	1660.2696
3159.2455	3159.8381	3163.6207
3164.6463	3169.5769	3170.5141
3184.8973	3185.6694	3194.4362

3194.7278	3211.6467	3211.9500

Product ([4]helicene)

$\mathbf{C_{18}H_{12}}$, C_1, ^1A

6	0	1.287798	-0.279763	-0.055558
6	0	2.479862	0.474641	0.186309
6	0	1.458297	-1.636123	-0.437541
6	0	0.000000	0.394822	0.000001
6	0	3.737249	-0.173348	0.190672
6	0	2.402436	1.890118	0.345549
6	0	2.699936	-2.235833	-0.460493
6	0	0.000000	1.810257	0.000001
6	0	3.851727	-1.511323	-0.107120
6	0	1.216409	2.534176	0.192107
6	0	-1.287801	-0.279762	0.055558
6	0	-1.216410	2.534176	-0.192107
6	0	-2.479863	0.474641	-0.186309
6	0	-2.402437	1.890118	-0.345550
6	0	-3.737250	-0.173349	-0.190669
6	0	-3.851725	-1.511324	0.107122
6	0	-1.458296	-1.636123	0.437539
6	0	-2.699934	-2.235835	0.460492
1	0	0.606017	-2.206526	-0.773883
1	0	4.620964	0.418455	0.405657
1	0	3.315994	2.444306	0.532582
1	0	2.787296	-3.270312	-0.773394
1	0	4.822638	-1.993393	-0.109682
1	0	1.166478	3.616973	0.236133
1	0	-1.166477	3.616972	-0.236135
1	0	-3.315994	2.444307	-0.532587
1	0	-4.620967	0.418451	-0.405652
1	0	-4.822636	-1.993394	0.109685
1	0	-0.606012	-2.206522	0.773878
1	0	-2.787295	-3.270315	0.773390

Frequencies

80.2218	83.8854	127.2909
175.4361	208.1735	258.9348
279.5112	323.3194	378.6828
418.8939	439.1411	440.4948
478.8886	519.6121	524.8564
526.6732	553.1130	588.0844
590.4840	632.3869	686.3076
690.1395	706.5668	756.2354
761.7342	769.4997	769.7281
811.1795	817.7191	827.1338

853.0495	865.7599	883.2607
889.2281	962.5368	965.5920
970.0986	978.8107	981.4595
993.6113	1006.5654	1015.0728
1055.8073	1072.1108	1130.0846
1153.7919	1168.4216	1178.9412
1182.1761	1190.3732	1217.8357
1235.8625	1239.1172	1254.4738
1279.2140	1325.6934	1352.1847
1368.0771	1385.4001	1397.3935
1449.5856	1449.7109	1456.2259
1484.2627	1532.2685	1534.2562
1557.8431	1596.8717	1638.1958
1647.5165	1648.6777	1667.3128
3157.3345	3158.6187	3159.9734
3161.1871	3169.7735	3170.3106
3177.0321	3179.2489	3186.4399
3187.0759	3213.2433	3231.1046

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