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Authors
Zhao, Long
Prendergast, Matthew B
Kaiser, Ralf I
et al.

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Synthesis of Polycyclic Aromatic Hydrocarbons via Phenyl Addition – Dehydrocyclization: The Third Way

Long Zhao,[a] Matthew Prendergast,[a] Ralf I. Kaiser,[a]* Bo Xu,[b] Utuq Ablikim,[b] Musahid Ahmed,[b]* Bing-Jian Sun,[c] Yue-Lin Chen,[c] Agnes H.H. Chang,[c]* Rana K. Mohamed,[a,d] Felix R. Fischer[d,e,f]*

Abstract: Polycyclic Aromatic Hydrocarbons (PAHs) represent the link between resonance-stabilized free radicals and carbonaceous nanoparticles generated in incomplete combustion processes and in circumstellar envelopes of carbon rich Asymptotic Giant Branch (AGB) stars. Although these PAHs resemble building blocks of complex carbonaceous nanostructures, their fundamental formation mechanisms have remained elusive. By exploring these reaction mechanisms of the phenyl radical with biphenyl/naphthalene theoretically and experimentally, we provide compelling evidence on a novel Phenyl-Addition/dehydroCyclization (PAC) pathway leading to prototype PAHs: triphenylene and fluoranthene. PAC operates efficiently at high temperatures leading through rapid molecular mass growth processes to complex aromatic structures, which are difficult to synthesize via traditional pathways such as Hydrogen-Abstraction/Acetylene-Addition. The elucidation of the fundamental reactions leading to PAHs is necessary to facilitate an understanding of the origin and evolution of the molecular universe and, in particular, of carbon in our Galaxy.

Introduction

[a] Dr. L. Zhao, Dr. M. Prendergast, Dr. R. K. Mohamed, Prof. R. I. Kaiser
Department of Chemistry
University of Hawaii at Manoa
Honolulu, Hawaii, 96822 (USA)
E-mail: ralfk@hawaii.edu
[b] Dr. B. Xu, Dr. U. Ablikim, Dr. M. Ahmed
Chemical Sciences Division
Lawrence Berkeley National Laboratory
Berkeley, CA 94720 (USA)
E-mail: mahmed@lbl.gov
[c] Dr. B. J. Sun, Dr. Y. L. Chen, Prof. A. H. H. Chang
Department of Chemistry
National Dong Hwa University
Shoufeng, Hualien 974 (Taiwan, ROC)
Email: hhchang@gms.ndhu.edu.tw
[d] Dr. R. K. Mohamed, Prof. Felix R. Fischer
Department of Chemistry
University of California Berkeley
Berkeley, CA 94720 (USA)
Email: ffischer@berkeley.edu
[e] Prof. Felix R. Fischer
Materials Sciences Division
Lawrence Berkeley National Laboratory
Berkeley, CA 94720 (USA)
[f] Prof. Felix R. Fischer
Kavli Energy Nano Sciences Institute at the University of California Berkeley and the Lawrence Berkeley National Laboratory
Berkeley, CA 94720 (USA)

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For decades, polycyclic aromatic hydrocarbons (PAHs) – organic molecules featuring laterally fused benzene rings[1] - have been at the center of attention as prospective candidates to untangle the molecular carriers of the unidentified infrared (UIR) emissions[2] and of the diffuse interstellar bands (DIBs).[2] These surveys propose that PAHs may encompass up to 20% of the galactic carbon budget[3] and act as a link between resonantly stabilized free radicals (RSFRs)[4] and carbonaceous nanoparticles in interstellar and circumstellar environments.[5] The detection of PAHs in carbonaceous chondrites such as Murchison along with $^{13}C/^{12}C$ isotopic analyses advocates an extraterrestrial origin of PAHs[1, 6] with fundamental astrochemical models of PAH synthesis borrowed from the combustion community.[7] The Hydrogen-Abstraction/Acetylene-Addition (HACA) mechanism has been suggested to be important in the formation of PAHs in outflows of carbon-rich asymptotic giant branch (AGB) stars[8] and in the combustion of fossil fuel.[9] A repetitive sequence of an abstraction of a hydrogen atom from the aromatic hydrocarbon followed by an addition of acetylene (C_2H_2) prior to cyclization and aromatization lead to PAHs carrying up to four fused benzene rings - naphthalene ($C_{10}H_8$),[7a] phenanthrene ($C_{14}H_{10}$),[7c, 10] and pyrene ($C_{16}H_{10}$)[11] – can be synthesized at high temperatures involving HACA. Recently, the the Hydrogen-Abstraction/Vinylacetylene-Addition (HAVA) mechanism has been invoked since naphthalene ($C_{10}H_8$),[12] phenanthrene ($C_{14}H_{10}$), and anthracene ($C_{14}H_{10}$)[13] were shown to be synthesized via barrier-less collisions of phenyl ($C_6H_5^•$) and naphthyl ($C_{10}H_7^•$) radicals with vinylacetylene (C_4H_4) via ring annulation at temperatures as low as 10 K.

Despite their potential in synthesizing PAHs in extreme environments, both the HAVA and HACA mechanisms have come under scrutiny, since flame data and recent models infer that a stepwise addition of acetylene is too slow to reproduce the quantified mass fractions of PAHs in combustion flames and in circumstellar environments.[14] Koshi et al.[15] along with Li et al.[16] postulated that a overlooked Phenyl-Addition/dehydroCyclization (PAC) mechanism may result in a rapid synthesis of PAHs. This hypothetical PAC route involves an addition of phenyl to an aromatic hydrocarbon. This is followed by hydrogen loss and successive dehydrogenation succeeded by cyclization along with another hydrogen atom loss accompanied by aromatization (Fig. 1). However, the validity of PAC has remained uncharted, since not a single experimental study could substantiate to what extent PAHs can form since all mechanisms – HACA, HAVA, and PAC – operate simultaneously in combustion environments. This complexity requires a systematic elucidation of the fundamental elementary reactions[17] involved in the PAC route.

Here, we reveal the facile gas phase synthesis of two prototype PAHs – fluoranthene ($C_{16}H_{10}$) and triphenylene ($C_{18}H_{12}$) – via

Phenyl-Addition/ dehydroCyclization (PAC) in high temperature environments (Fig. 1). This is achieved by first disentangling the previously elusive chemistry of the elementary reactions of phenyl ($C_6H_5^•$) with biphenyl (C_6H_5-C_6H_5) and naphthalene ($C_{10}H_8$) forming triphenylene ($C_{18}H_{12}$) and fluoranthene ($C_{16}H_{10}$), respectively. Then, we trace the reactivity of a prototype radical intermediate in PAC – 2-(1-naphthyl)phenyl ($C_{16}H_{11}^•$) – and provide critical evidence on the role of key hydrocarbon radicals. These findings suggest PAC as a *third way* – besides HACA and HAVA – to efficiently synthesize PAHs serving as building blocks of two- and three-dimensional aromatic structures in combustion flames and in circumstellar envelopes. Briefly, a high temperature chemical reactor was used to form fluoranthene ($C_{16}H_{10}$) and triphenylene ($C_{18}H_{12}$) via the reactions of the phenyl radical with naphthalene ($C_{10}H_8$) and biphenyl (C_6H_5-C_6H_5), respectively; second, ring closure of the 2-(1-naphthyl) phenyl radical ($C_{16}H_{11}^•$) followed by hydrogen loss and aromatization to fluoranthene ($C_{16}H_{10}$) highlights the key role of aromatic radical intermediates in the PAC mechanism. All products were detected isomer-specifically through fragment-free photoionization in a molecular beam via tunable vacuum ultraviolet light in tandem with the identification of the ionized molecules in a reflectron time-of-flight mass spectrometer (SI).

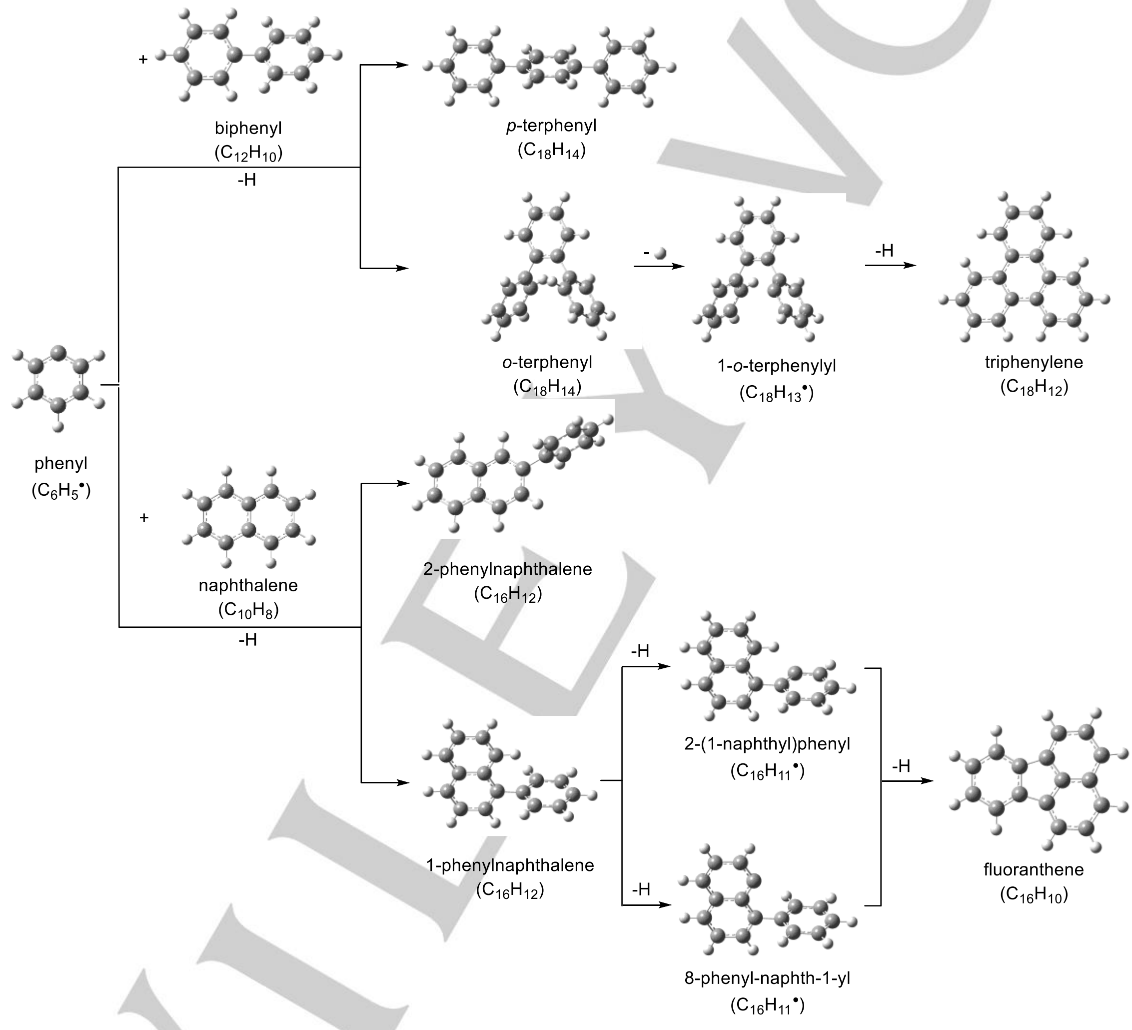


Figure 1. Postulated reactions leading to PAH formation via the Phenyl Addition/dehydro-Cyclization (PAC) mechanism. Carbon and hydrogen atoms are color coded gray and white, respectively.

Results and Discussion

Mass Spectra

Representative mass spectra recorded at a photoionization energy of 9.50 eV for the reactions of biphenyl and naphthalene with the phenyl radical are displayed in Fig. 2. A comparison of these data with reference spectra obtained for biphenyl and naphthalene seeded in non-reactive helium gas provides evidence on the synthesis of molecules with the molecular formula $C_{18}H_{12}$ (228 amu) and $C_{18}H_{14}$ (230 amu) (Fig. 2a) as well as of $C_{16}H_{10}$ (202 amu) and $C_{16}H_{12}$ (204 amu) (Fig. 2c); these species are absent in the control experiments (Figs. 2b and 2d).

The following analysis allows us to gauge the reactivity of the 2-(1-naphthyl)phenyl radical intermediate ($C_{16}H_{11}$) (Figs. 2e,f). At 600K, the 1-(2-bromophenyl)naphthalene precursor molecule is assigned through the molecular ion peaks at *m/z* = 282 ($C_{16}H_{11}{}^{79}Br$), 283 ($^{13}CC_{15}H_{11}{}^{79}Br$), 284 ($C_{16}H_{11}{}^{81}Br$), and 285 ($^{13}CC_{15}H_{11}{}^{81}Br$) (Fig. 2f). When the temperature is increased to 1300K, new ion counts arise at *m/z* = 202 ($C_{16}H_{10}{}^{+}$), 203 ($C_{16}H_{11}{}^{+}$/$^{13}CC_{15}H_{10}{}^{+}$), and 204 ($C_{16}H_{12}{}^{+}$) (Fig. 2e). To further identify the nature of the *isomers* formed in these systems, photoionization efficiency (PIE) curves, which record the intensities of an ion at a well-defined mass-to-charge ratio versus the photon energy, were collected between 7.5 to 10.0 eV. The experimentally recorded PIE curves are fit with a linear combination of known PIE calibration curves of distinct structural isomers to identify which molecule(s) is(are) synthesized.

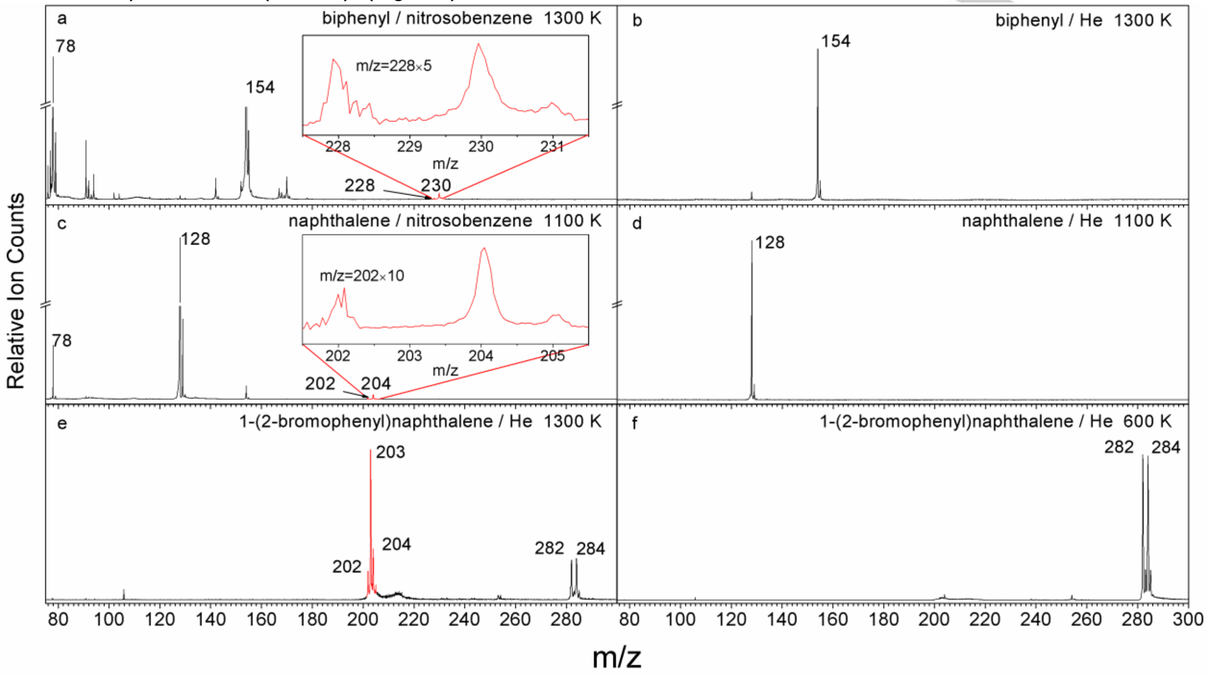


Figure 2. Comparison of photoionization mass spectra recorded at a photoionization energy of 9.50 eV. (a) biphenyl ($C_{12}H_{10}$)-nitrosobenzene (C_6H_5NO); the insert highlights the ion signals at m/z = 228; (b) biphenyl ($C_{12}H_{10}$)-helium (He); (c) naphthalene ($C_{10}H_8$)-nitrosobenzene (C_6H_5NO); the insert highlights the ion signals at m/z = 202 (d) naphthalene ($C_{10}H_8$)-helium; pyrolysis of 1-(2-bromophenyl) naphthalene at 1300K (e) and 600K (f). Mass peaks of the newly formed species of interest are highlighted in red. The inserts magnify sections of the mass spectra.

Photoionization Efficiency (PIE) Curves

In the biphenyl – phenyl system, accounting for the molecular weight of the reactants ($C_{12}H_{10}$, 154 amu; $C_6H_5{}^{\bullet}$, 77 amu) and the products ($C_{18}H_{14}$, 230 amu; H, 1 amu), molecules with the formula $C_{18}H_{14}$ can be linked to reaction products of the elementary reaction of biphenyl with the phenyl radical (Figs. 2a,b) with ion count at *m/z* = 231 connected to ^{13}C-substituted counterpart of *m/z* = 230 ($^{13}CC_{17}H_{14}$) (reaction (1a)). Ion counts at *m/z* = 230 and 231 are absent in the control experiment suggesting that signals at these mass-to-charge ratios originate from *reaction* between the phenyl radical and biphenyl. Ion counts at *m/z* = 77 ($C_6H_5{}^{+}$), 78 ($C_6H_6{}^{+}$/$C_5{}^{13}CH_5{}^{+}$), and 79 ($C_5{}^{13}CH_6{}^{+}$) are also observable; they are attributed to phenyl ($C_6H_5{}^{\bullet}$), benzene (C_6H_6), and ^{13}C-benzene ($C_5{}^{13}CH_6$). Signal is also detectable at *m/z* = 228, which can be associated with two subsequent hydrogen atom losses and dehydrogenation from $C_{18}H_{14}$ via $C_{18}H_{13}{}^{\bullet}$ to $C_{18}H_{12}$ (reaction (1b)). To summarize, the analysis of the mass spectra alone reveals that the reaction of the biphenyl ($C_{12}H_{10}$) with phenyl ($C_6H_5{}^{\bullet}$) synthesizes hydrocarbon molecule(s) with the molecular formulae $C_{18}H_{12}$ and $C_{18}H_{14}$. To identify the structural isomers formed, the PIE curves recorded at *m/z* = 228, 230 and 231 are analyzed (Figs. 3a-c). For *m/z* = 230 and 231, the experimental PIE curves depict onsets of the ion counts at 7.85 ± 0.05 eV, which agree very well with the adiabatic ionization energy of *p*-terphenyl of 7.80 ± 0.03 eV.[18] After scaling, both PIE graphs at *m/z* = 230 and 231 are identical and can be replicated with the PIE curve of the *p*-terphenyl isomer (SI) (Figs. 3b and 3c) amplifying that signal at *m/z* = 231 originates from ^{13}C-labeled *p*-terphenyl ($^{13}CC_{17}H_{14}$). Most important, after scaling, the PIE curve at *m/z* = 228 does not overlap with the PIE curve at *m/z* = 230 suggesting that signal at *m/z* = 228 does not originate from fragments of *m/z* = 230. Here, the PIE curve at *m/z* = 228 can be reproduced with a PIE curve of triphenylene ($C_{18}H_{12}$) (SI) (Fig. 3a). The experimentally determined onset of ion counts at *m/z* = 228 at 7.85 ± 0.05 eV corresponds to the adiabatic ionization energy of triphenylene of 7.89 ± 0.04 eV.[19] Consequently, our investigations reveal that in the phenyl – biphenyl system, molecular mass growth processes account for the formation of *p*-terphenyl ($C_{18}H_{14}$) and of triphenylene ($C_{18}H_{12}$) formed via reactions (1a) and (1b), respectively.

(1a) $C_6H_5{}^{\bullet} + C_{12}H_{10} \rightarrow C_{18}H_{14} + H^{\bullet}$

(1b) $C_{18}H_{14} \rightarrow C_{18}H_{13}{}^{\bullet} + H^{\bullet} \rightarrow C_{18}H_{12} + 2H^{\bullet}$

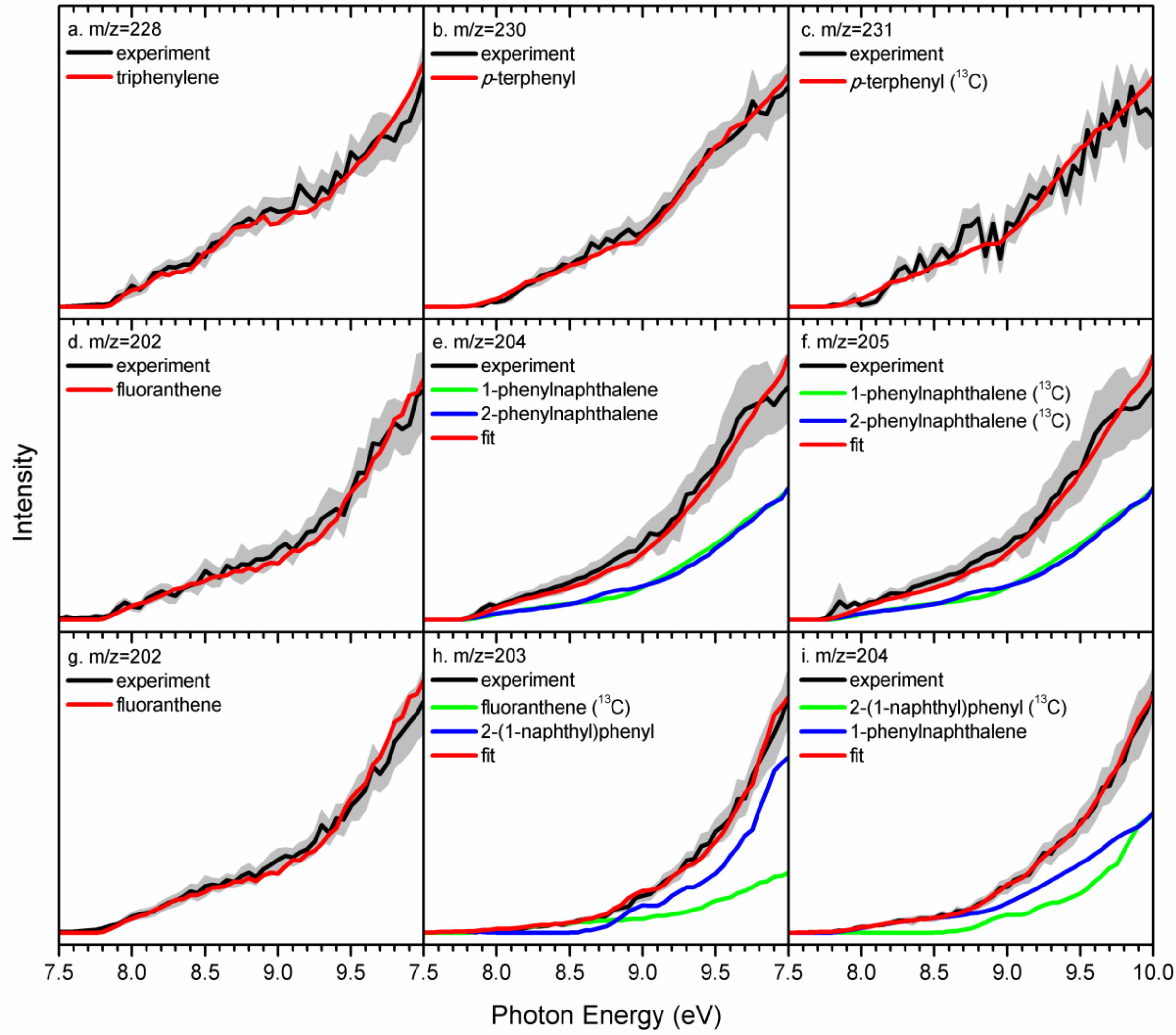


Figure 3. Photoionization efficiency (PIE) curves: (a)-(c): phenyl ($C_6H_5^•$) - biphenyl ($C_{12}H_{10}$); (d)-(f): phenyl ($C_6H_5^•$) - naphthalene ($C_{10}H_8$); (g)-(i): 1-(2-bromophenyl)naphthalene (1300K). Black: experimental PIE curves; blue/green/red: reference PIE curves; the red line resembles the overall fit.

In the naphthalene – phenyl system, considering the molecular weight of the reactants ($C_{10}H_8$, 128 amu; $C_6H_5^•$, 77 amu) and the products ($C_{16}H_{12}$, 204 amu; H, 1 amu), molecules with the formula $C_{16}H_{12}$ are identified (Figs. 2c,d) with ion count at m/z = 205 correlated with the ^{13}C-substituted counterpart of m/z = 204 ($^{13}CC_{15}H_{12}$) (reaction (2a)). Since the ion counts at m/z = 204 and 205 cannot be detected in the control experiment, signals at both mass-to-charge ratios are linked to the *reaction* between the phenyl radical and naphthalene. Signal can be monitored at m/z = 202 as well. This is linked to two successive atomic hydrogen atom losses and dehydrogenation from $C_{16}H_{12}$ yielding ultimately $C_{16}H_{10}$ (reaction (2b)). Ion counts at m/z = 77 ($C_6H_5^+$), 78 ($C_6H_6^+/C_5{}^{13}CH_5^+$), 79 ($C_5{}^{13}CH_6^+$), 128 ($C_{10}H_8^+$), and 129 ($^{13}CC_9H_8^+$) can also be detected. The corresponding neutrals are phenyl ($C_6H_5^•$), benzene (C_6H_6), ^{13}C-benzene ($^{13}CC_5H_6$), naphthalene ($C_{10}H_8$), and ^{13}C- naphthalene ($^{13}CC_9H_8$). Thus, the mass spectra reveal that the reaction of naphthalene ($C_{10}H_8$) with phenyl ($C_6H_5^•$) synthesizes hydrocarbon molecules with the molecular formulae $C_{16}H_{12}$ and $C_{16}H_{10}$. To assign the isomers, the PIE curves at m/z = 202, 204 and 205 are examined (Figs. 3d-f). At m/z = 204 and 205, both PIE graphs are superimposable after scaling and can be fit with a linear combination of the reference PIE graphs of 1- and 2-phenylnaphthalene (SI). Hence signal at m/z = 205 originates from $^{13}CC_{15}H_{12}$. The PIE calibration curves for 1- and 2-phenylnaphthalene isomers are nearly superimposable, and hence it is not feasible to determine accurate branching ratios of these isomers in the phenyl-naphthalene system. On the other hand, the PIE curves at m/z = 202 and 204 are distinct; data at m/z = 202 can be replicated with the PIE graph of fluoranthene ($C_{16}H_{10}$) (SI). The experimental onset of the ion counts at m/z = 202 at 7.85 ± 0.05 eV correlates nicely with the adiabatic ionization energy of fluoranthene of 7.90 ± 0.10 eV.[20] Altogether, the experiments propose that in the phenyl – naphthalene system, 1- and/or 2-phenylnaphthalene ($C_{16}H_{12}$) along with fluoranthene ($C_{16}H_{10}$) are formed.

(2a) $$C_6H_5^• + C_{10}H_8 \rightarrow C_{16}H_{12} + H^•$$

(2b) $$C_{16}H_{12} \rightarrow C_{16}H_{11}^• + H^• \rightarrow C_{16}H_{10} + 2H^•$$

Considering the 1-(2-bromophenyl)naphthalene system, signal at *m/z* = 282 ($C_{16}H_{11}{}^{79}Br$), 283 (${}^{13}CC_{15}H_{11}{}^{79}Br$), 284 ($C_{16}H_{11}{}^{81}Br$), and 285 (${}^{13}CC_{15}H_{11}{}^{81}Br$) is associated with the precursor molecules and their ${}^{13}C$ substituted counterparts. A detailed analysis of the PIE graphs in the 1300K experiment (Figs. 3g-i) reveals that ion counts at *m/z* = 202 are associated with fluoranthene ($C_{16}H_{10}$); the reference curves match the experimental data exceptionally well and reveal an onset of 7.80 ± 0.05 eV, which correlates nicely with the adiabatic ionization energy of fluoranthene of 7.90 ± 0.10 eV.[20] The PIE graph at *m/z* = 203 ($C_{16}H_{11}{}^{+}$/${}^{13}CC_{15}H_{10}{}^{+}$) can be replicated by a linear combination of the reference curves of ${}^{13}C$-fluoranthene and the 2-(1-naphthyl)phenyl radical. Finally, the signal at *m/z* = 204 can be explained by 1-phenylnaphthalene formed, e.g., by hydrogen abstraction of the 2-(1-naphthyl) phenyl radical. In summary, our investigations reveal that the 2-(1-naphthyl)phenyl radical – a key intermediate in the PAC mechanism – undergoes isomerization via ring closure followed by atomic hydrogen loss yielding eventually fluoranthene ($C_{16}H_{10}$) (reaction (3), Fig. 1).

(3) $$C_{16}H_{11}{}^{\bullet} \rightarrow C_{16}H_{10} + H^{\bullet}$$

Reaction Mechanisms

Formation of Triphenylene

The present study reveals that two prototype PAHs carrying three and four benzene rings – triphenylene ($C_{18}H_{12}$) and fluoranthene ($C_{16}H_{10}$) – are synthesized within the phenyl–naphthalene and phenyl–biphenyl systems, respectively, in the gas phase. To elucidate the underlying reaction mechanisms, we combined these findings with electronic structure calculations. Considering the reaction of the phenyl radical with biphenyl (reaction (1a)), the phenyl radical can add to the ortho (*o*-), meta (*m*-), and/or para (*p*-) position of the phenyl moiety of the biphenyl molecule through barrier up to 27 kJ mol^{-1} (Figs. 4a/4b). The resulting doublet radical intermediates **i1** to **i3** undergo hydrogen atom loss forming *o*-, *m*-, and *p*-terphenyl. Secondary reactions of atomic hydrogen and/or phenyl radicals with *o*-terphenyl lead via hydrogen abstraction to the 1-*o*-terphenylyl (**i4**) radical, which can undergo facile cyclization to the doublet intermediate radical **i5**. Accompanied by aromatization, the latter undergoes unimolecular decomposition via atomic hydrogen loss forming triphenylene in overall exoergic reactions. Considering the heights of the barriers along with the overall reaction energies, the reaction of phenyl with *o*-terphenyl is favorable both kinetically and thermodynamically. These computations assist in rationalizing our experimental observations of the formation of *p*-terphenyl ($C_{18}H_{14}$) and triphenylene ($C_{18}H_{12}$). The initial replacement of a hydrogen atom by a phenyl group in the biphenyl reactant represents a prototype of an aromatic radical substitution reaction (S_R); this reaction favors the addition of the radical reactant to the *o*- and *p*-position of the phenyl moiety[21] followed by atomic hydrogen loss leading to *o*- and *p*-terphenyl, but not to *m*-terphenyl. The *p*-terphenyl was observed experimentally; the absence of *o*-terphenyl, but the identification of triphenylene suggests an efficient conversion via dehydrogenation and cyclization of *o*-terphenyl to triphenylene (Fig. 1) thus demonstrating the unique capability of PAC to synthesize triphenylene.

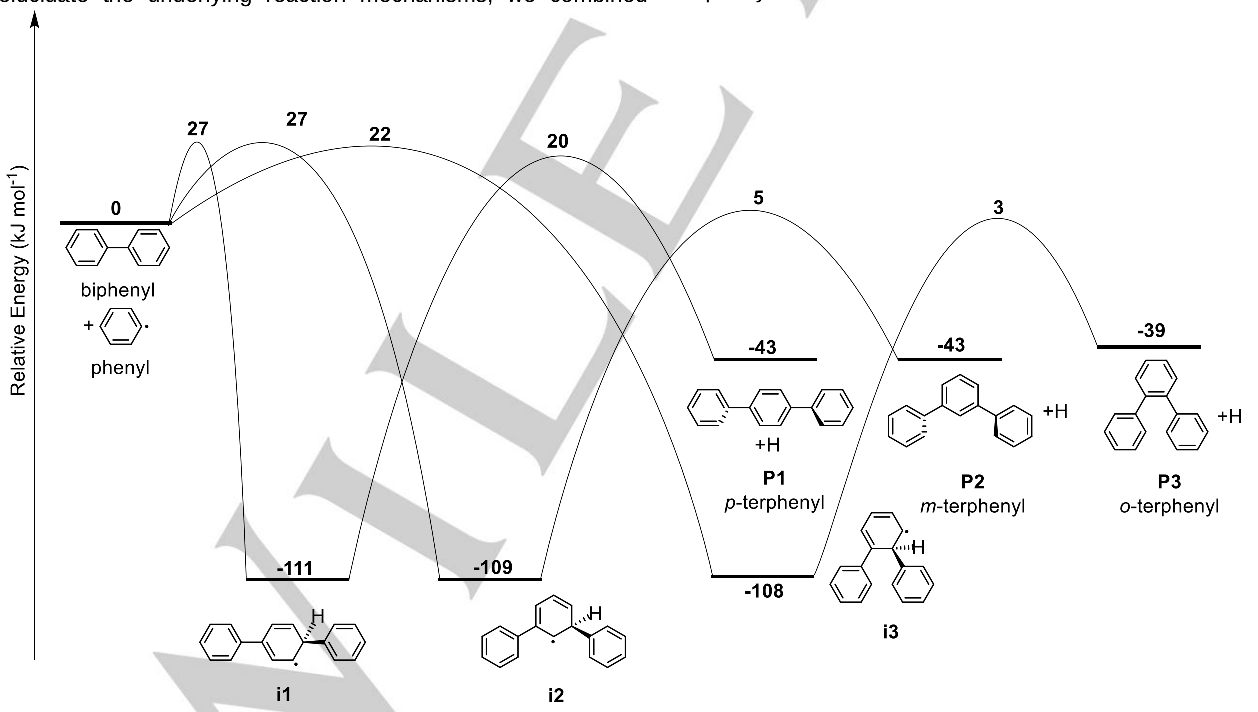


Figure 4a. Potential energy surface (PES) for the reaction of phenyl ($C_6H_5{}^{\bullet}$) with biphenyl ($C_{12}H_{10}$).

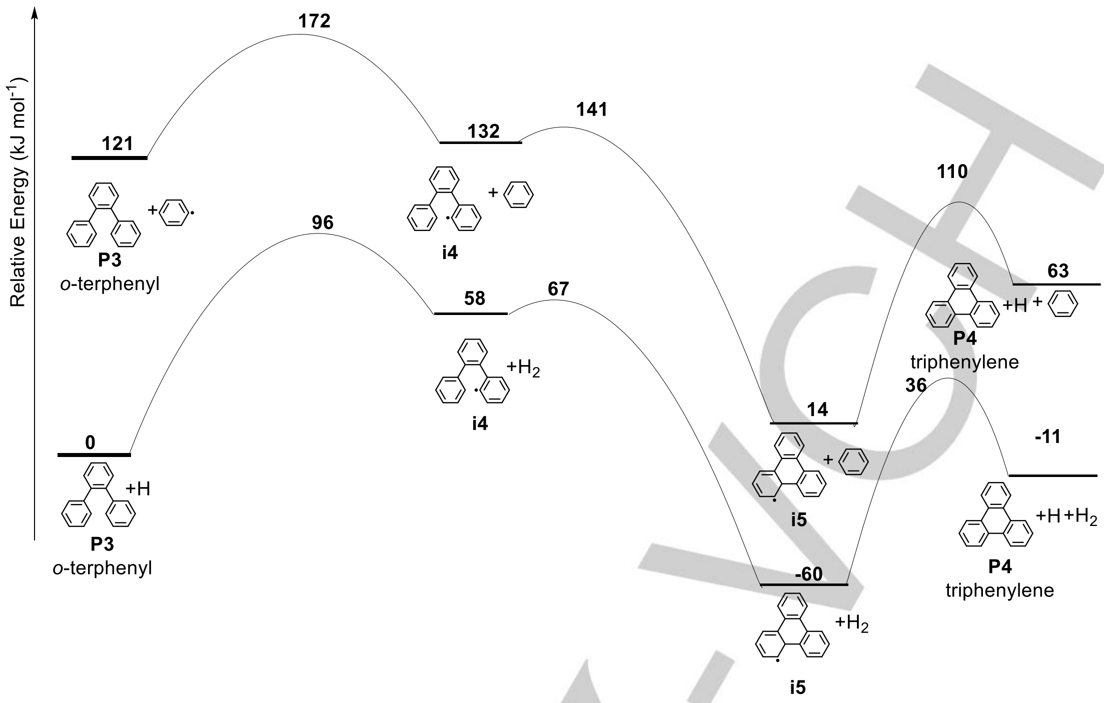


Figure 4b. Potential energy surface (PES) for the formation of triphenylene ($C_{18}H_{12}$) via hydrogen atom abstraction, cyclization, and hydrogen atom elimination.

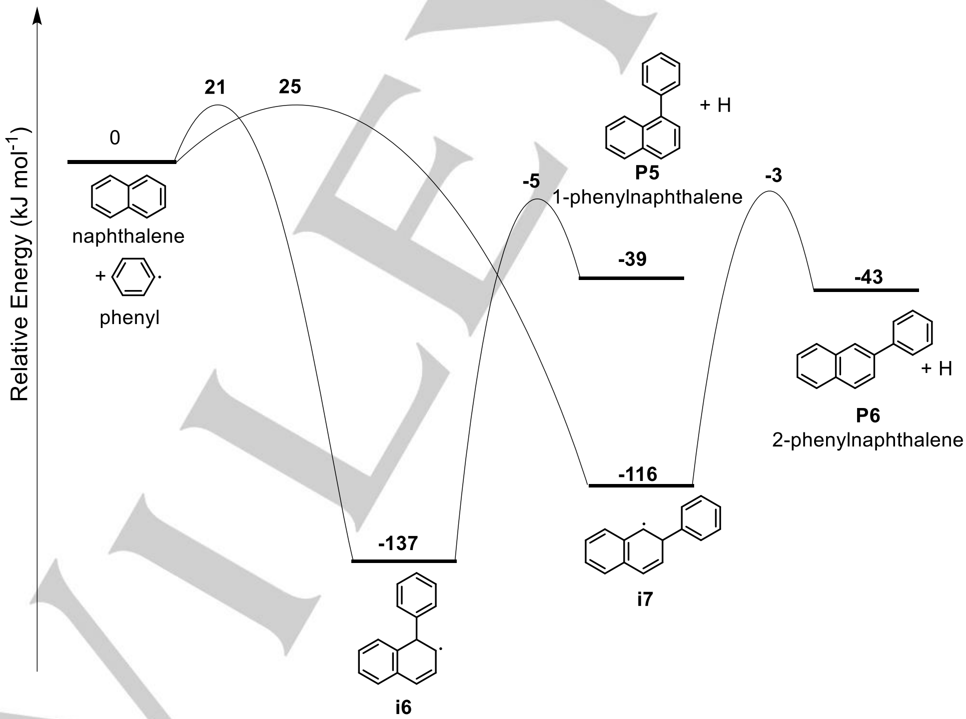


Figure 5a. Potential energy surface (PES) for the reaction of phenyl ($C_6H_5^{\cdot}$) with naphthalene ($C_{10}H_8$).

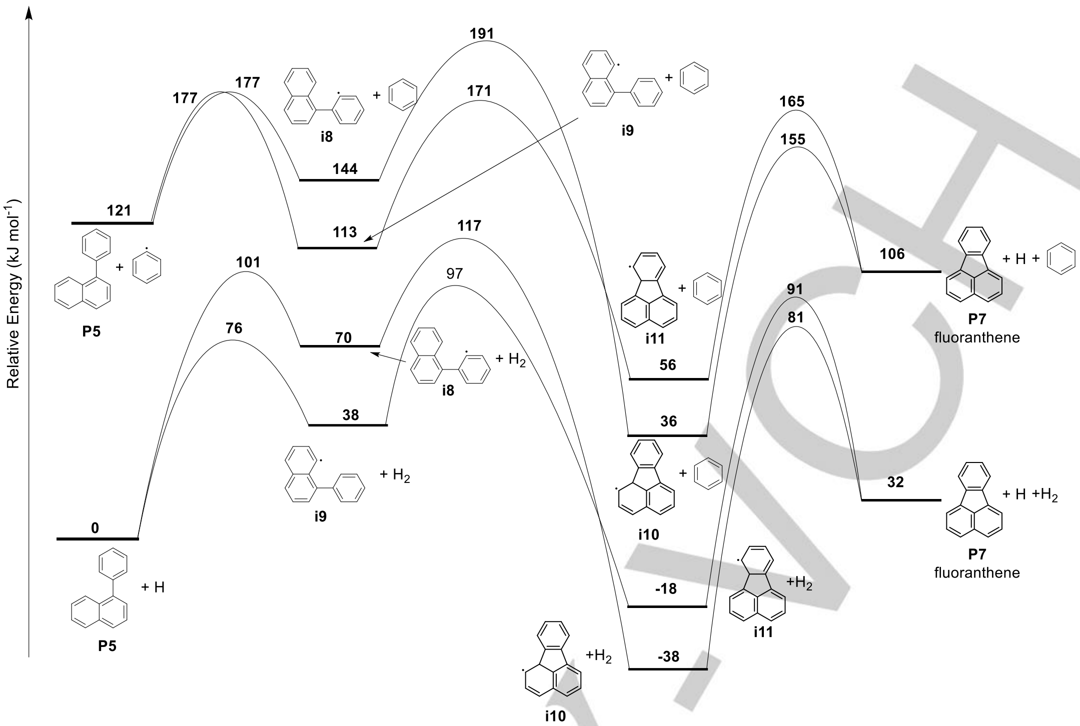


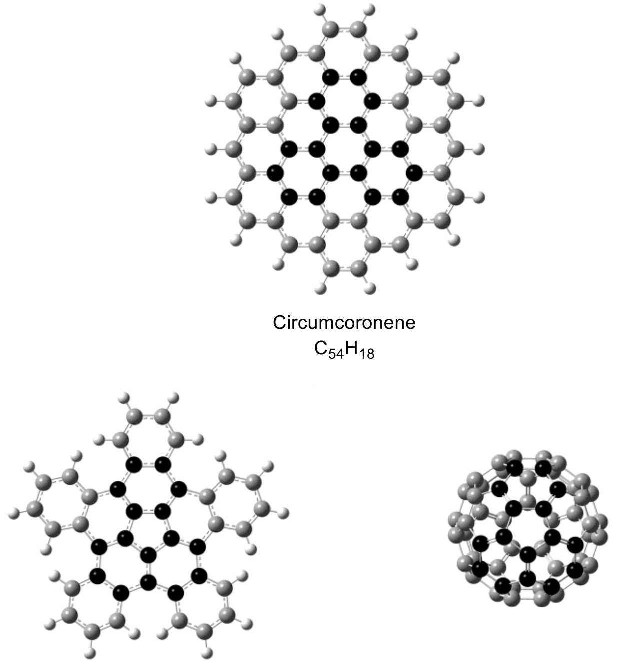
Figure 5b. Potential energy surface (PES) for the formation of fluoranthene ($C_{16}H_{10}$) via hydrogen atom abstraction, cyclization, and hydrogen atom elimination.

Formation of Fluoranthene

In the phenyl – naphthalene system (Fig. 5a), the phenyl radical adds to the C1 or C2 carbon atom of naphthalene yielding **i6** and **i7** doublet radical intermediates. These emit atomic hydrogen yielding 1-/2-phenylnaphthalene, respectively, in overall exoergic reactions. Secondary reaction of atomic hydrogen and/or phenyl radicals can abstract atomic hydrogen from 1-phenylnaphthalene. The hydrogen abstractions at the ortho positions of the phenyl and at the C8 carbon atom of the naphthalene moieties are critical to highlight. These abstractions lead to 2-(1-naphthyl)phenyl (**i8**) and 8-phenyl-naphth-1-yl (**i9**). Both the 2-(1-naphthyl)phenyl and 8-phenyl-naphth-1-yl radicals undergo cyclization to 1- and 7-H-fluoranthenyl **i10** and **i11**, respectively. Unimolecular decomposition of these intermediates via atomic hydrogen loss accompanied by aromatization forms fluoranthene (Fig. 5b). These predictions correlate well with our experimental findings and rationalize the identification of fluoranthene via PAC.

Conclusion

To conclude, our experimental data identified fluoranthene ($C_{16}H_{10}$) and triphenylene ($C_{18}H_{12}$) as key reaction products in the phenyl–biphenyl and phenyl-naphthalene systems with electronic structure calculations revealing the critical involvement of the previously elusive PAC mechanism. Since the initial addition of the phenyl radical to benzene and naphthalene along with the hydrogen abstraction from *o*-terphenyl and 1-phenylnaphthalene involve barriers of at least 21 kJ mol^{-1}, high temperature conditions in combustion processes and circumstellar envelopes of carbon stars, are essential to an efficient mass growth processes to PAHs via PAC. The 18π aromatic triphenylene ($C_{18}H_{12}$) – a benchmark of a fully benzenoid PAH – and fluoranthene ($C_{16}H_{10}$) – a prototype of a non-alternant PAH – represent key molecular building blocks in molecular mass growth processes of two- and three-dimensional PAHs. These pathways may be involved in the formation of 2D and 3D nanostructures with buckminsterfullerene (C_{60}) detected in hydrocarbon flames[22] and toward the planetary nebula TC 1 (Scheme 1).[23] Overall, our findings establish a rigorous framework promoting PAC as a *third way* to synthesize PAHs via efficient molecular mass growth processes. In particular, the incorporation of a five-membered ring in PAHs such as fluoranthene, which has a dipole moment of 0.34 Debye, could aid in the detection of an individual PAH in the gas phase interstellar medium via its rotational spectrum exploiting the Atacama Large Millimeter/ submillimeter Array (ALMA) thus transforming how we think about the origin and evolution of carbonaceous matter in the Universe.[24]



Circumcoronene
$C_{54}H_{18}$

pentabenzocorannulene
$C_{40}H_{20}$

buckminsterfullerene
(C_{60})

Scheme 1. Fluoranthene ($C_{16}H_{10}$) and triphenylene ($C_{18}H_{12}$) as molecular building blocks in two- and three-dimensional PAHs and fullerenes: circumcoronene ($C_{54}H_{18}$), pentabenzocorannulene ($C_{40}H_{20}$), and buckminsterfullerene (C_{60}).

Method

Experimental: The experiments were carried out at the Chemical Dynamics Beamline (9.0.2) of the Advanced Light Source utilizing a resistively-heated silicon-carbide (SiC) chemical reactor interfaced to a molecular beam apparatus operated with a Wiley-McLaren reflectron time-of-flight mass spectrometer (Re-TOF-MS).[7a, 7b, 11-13, 25] The chemical reactor mimics the high temperature conditions present in combustion flames and in circumstellar envelopes of carbon stars. Phenyl radicals ($C_6H_5^{\bullet}$) were prepared *in situ* via pyrolysis of the nitrosobenzene precursor (C_6H_5NO; Sigma-Aldrich) with the biphenyl and naphthalene reactants provided by Sigma-Aldrich. The reactants were seeded in helium carrier gas (0.394 ± 0.005 atm). In the pyrolysis experiments, custom synthesized 1-(2-bromophenyl)naphthalene alone was seeded in the helium carrier gas at 0.394 ± 0.005 atm (Supplementary Information). The temperature of the SiC tube was monitored using a Type-C thermocouple and was maintained at 1300 ± 10 K (nitrosobenzene/biphenyl; 1-(2-bromophenyl)naphthalene) and 1100 ± 10 K (nitrosobenzene/naphthalene). The products formed in the reactor were expanded supersonically and passed through a 2 mm diameter skimmer located 10 mm downstream of the pyrolytic reactor and enter into the main chamber, which houses the Re-TOF-MS. The quasi-continuous tunable vacuum ultraviolet (VUV) light from the Advanced Light Source intercepted the neutral molecular beam perpendicularly in the extraction region of a Wiley–McLaren RE-TOF-MS. VUV single photon ionization is essentially a fragment-free ionization technique and hence is characterized as a *soft ionization* method compared to electron impact ionization, the latter leading to excessive fragmentation of the parent ion[26]. The ions formed via photoionization are extracted and eventually detected by a microchannel plate detector. Photoionization efficiency (PIE) curves, which report ion counts as a function of photon energy with a step interval of 0.05 eV at a well-defined mass-to-charge ratio (*m/z*), were produced by integrating the signal recorded at the specific *m/z* for the species of interest. Reference (blank) experiments were also conducted by expanding helium carrier gas into the resistively-heated SiC tube without seeding the reactants in nitrosobenzene. To identify the products of interest observed in this work, PIE calibration curves for 1-phenylnaphthalene, 2-phenylnaphthalene, fluoranthene, *o*-terphenyl, *m*-terphenyl, *p*-terphenyl, and triphenylene (Sigma Aldrich) were collected (Supplementary information). It is important to note that in blank experiments of nitrosobenzene seeded in helium carrier gas conducted at identical temperatures and pressures as the current experiments, naphthalene, triphenylene, or fluoranthene are not formed.[7a]

Computational: The synthetic routes to triphenylene and fluoranthene are explored via electronic structure calculations. Along these routes, reactants, intermediates, products, and the transition states connecting these species are identified and characterized. Geometries and harmonic frequencies are optimized via density functional theory at the B3LYP[27]/cc-pVTZ level. The energies are refined by the coupled cluster[28] CCSD(T)/cc-pVDZ with B3LYP/cc-pVTZ zero-point energy corrections. B3LYP/cc-pVTZ//CCSD(T)/ cc-pVTZ level of calculation are expected to have an accuracy within 9 kJ mol^{-1}.[29] The GAUSSIAN09 program[30] is used in these electronic structure calculations.

Acknowledgements

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Keywords: Phenyl-Addition/dehydroCyclization (PAC) • polycyclic aromatic hydrocarbons • gas-phase chemistry • mass spectrometry • interstellar medium

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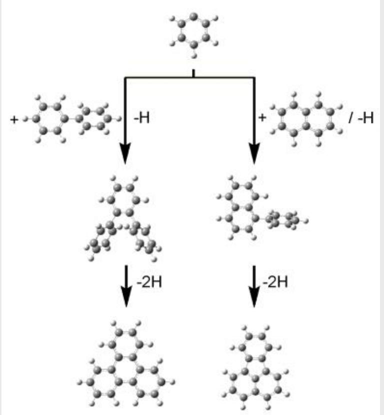
Entry for the Table of Contents

Layout 1:

RESEARCH ARTICLE

The triphenylene and fluoranthene molecules – potential precursors to two- and three-dimensional graphitic nano sheets in the interstellar medium – can be formed through rapid molecular mass growth processes via the reactions of phenyl radical with biphenyl and naphthalene at high temperatures.



Long Zhao,[a] Matthew Prendergast,[a] Ralf I. Kaiser,[a] Bo Xu,[b] Utuq Ablikim,[b] Musahid Ahmed,[b]* Bing-Jian Sun,[c] Yue-Lin Chen,[c] Agnes H.H. Chang[c]*, Rana K. Mohamed,[a,d] Felix R. Fischer[d,e,f]**

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Synthesis of Polycyclic Aromatic Hydrocarbons via Phenyl Addition – Dehydrocyclization: The Third Way

Supplementary Information

Synthesis of Polycyclic Aromatic Hydrocarbons via Phenyl Addition – Dehydrocyclization: The Third Way

Long Zhao,[1] Matthew Prendergast,[1] Ralf I. Kaiser[1*]

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

Bo Xu,[2] Utuq Ablikim,[2] Musahid Ahmed[2*]

[2] *Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA*

Bing-Jian Sun, Yue-Lin Chen, Agnes H.H. Chang[3*]

[3] *Department of Chemistry, National Dong Hwa University, Shoufeng, Hualien 974, Taiwan, ROC*

Rana K Mohamed,[1,4] Felix R. Fischer[4-6*]

[4] *Department of Chemistry, University of California, Berkeley, CA 94720, USA*
[5] *Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA*
[6] *Kavli Energy Nano Sciences Institute at the University of California Berkeley and the Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA*

[*] Corresponding author:
Ralf I. Kaiser <ralfk@hawaii.edu>
Musahid Ahmed <mahmed@lbl.gov>
Agnes H.H. Chang <hhchang@gms.ndhu.edu.tw>
Felix R. Fischer <ffischer@berkeley.edu>

Synthesis of 1-(2-bromophenyl)naphthalene

Materials and General Methods. Unless otherwise stated, all manipulations of air and/or moisture sensitive compounds were carried out in oven-dried glassware, under an atmosphere of nitrogen gas. All solvents and reagents were purchased from Alfa Aesar, Spectrum Chemicals, Acros Organics, TCI America, and Sigma-Aldrich and were used as received unless otherwise noted. Organic solvents were dried by passing through a column of alumina and were degassed by vigorous bubbling of nitrogen or argon through the solvent for 20 min. Flash column chromatography was performed on SiliCycle silica gel (particle size 40–63 μm). Thin layer chromatography was carried out using SiliCycle silica gel 60 Å F-254 precoated plates (0.25 mm thick) and visualized by UV absorption. All ^{1}H and ^{13}C NMR spectra were recorded on Bruker AVB-400 and AVQ-400 MHz spectrometers, and are referenced to residual solvent peaks ($CDCl_3$ ^{1}H NMR = 7.26 ppm, ^{13}C NMR = 77.16 ppm). ESI mass spectrometry was performed on a Finnigan LTQFT (Thermo) spectrometer in positive ionization mod**e.**

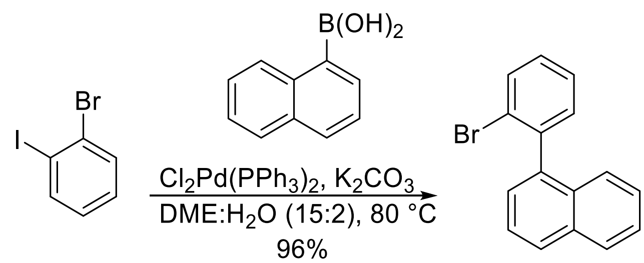


Figure S2. The synthesis of 1-(2-bromophenyl)naphthalene.

Procedure for 1-(2-bromophenyl)naphthalene: 2.0 g (7.07 mmol) of 1-bromo-2-iodobenzene, 1.34 g (7.78 mmol) of naphthalen-1-ylboronic acid, 2.44 g (17.67 mmol) K_2CO_3 , 74.43 mg (0.11 mmol) of $Cl_2Pd(PPh_3)_2$ in a 30 ml mixture of DME:H_2O (15:2) were stirred at 80°C for four hours. After cooling, the product was extracted with diethyl ether (3 × 15 ml) and dried with sodium sulfate. After the solvent was removed, the residue was purified by silica gel column chromatography (hexane), yielding 1.92g (96%) of 1-(2-bromophenyl)naphthalene as a colorless solid. ^{1}H NMR (400 MHz, in $CDCl_3$): δ 7.92(d, J = 8.2 Hz, 2H), 7.75 (dd, J = 7.91 Hz, J = 1.03 Hz, 1H), 7.58 – 7.29 (m, 8H). ^{13}C NMR (101 MHz, in $CDCl_3$): δ 141.5, 139.2, 133.6, 132.8, 132.3, 131.7, 129.9, 129.5, 128.5, 128.2, 127.4, 126.9, 126.7, 126.5, 125.4, 124.5. HRMS (EI+) calcd. for $C_{16}H_{11}Br$ 282.0044, found 282.0048.

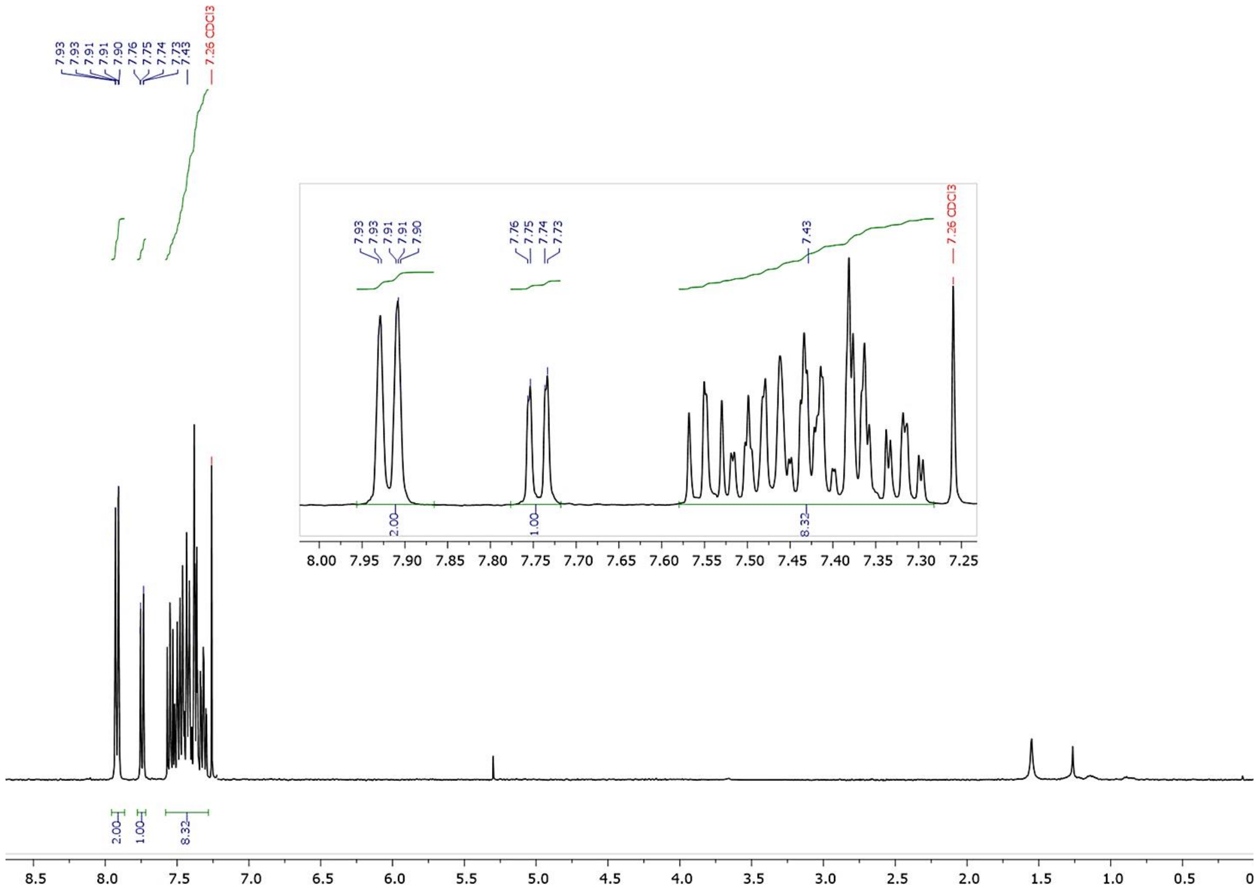


Figure S3. ^{1}H NMR spectrum of 1-(2-bromophenyl)naphthalene.

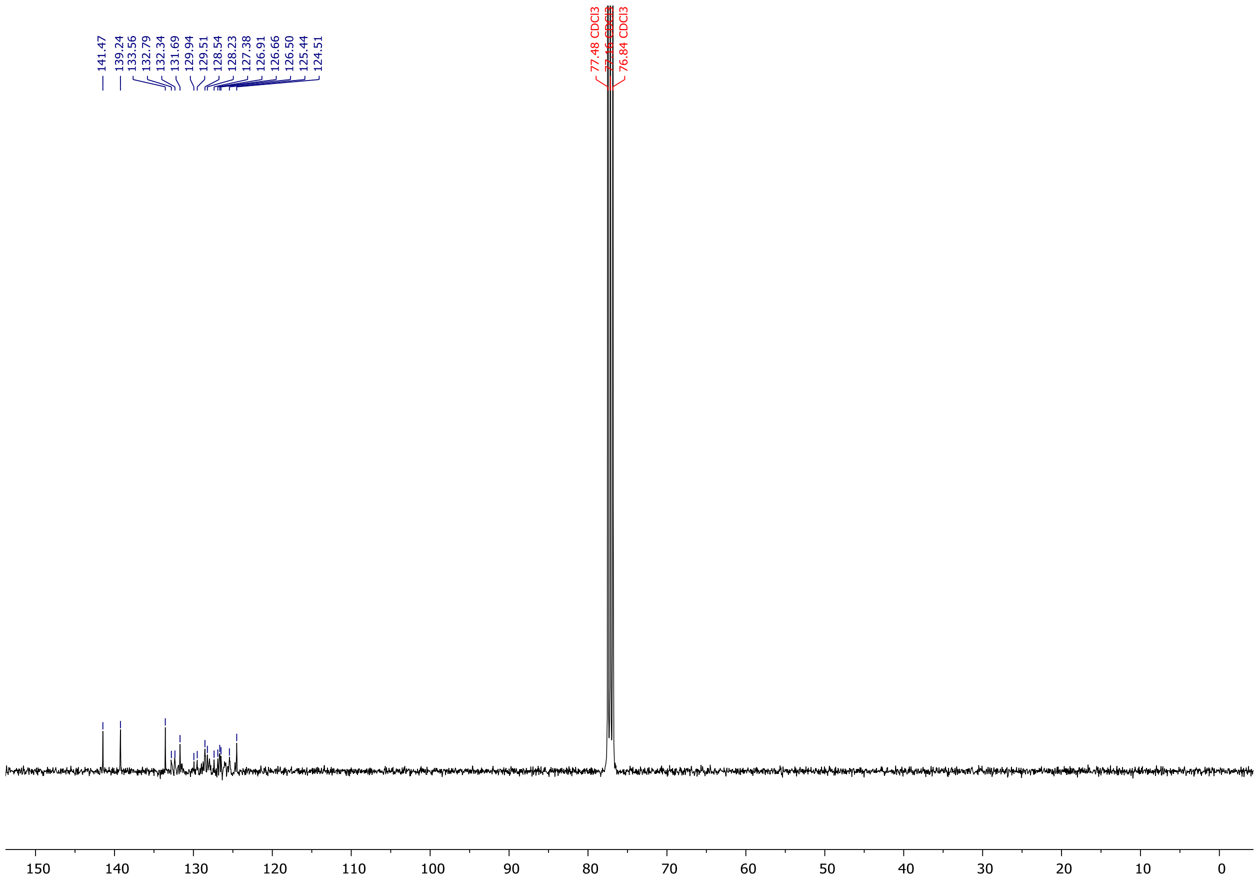


Figure S4. ^{13}C NMR spectrum of 1-(2-bromophenyl)naphthalene.

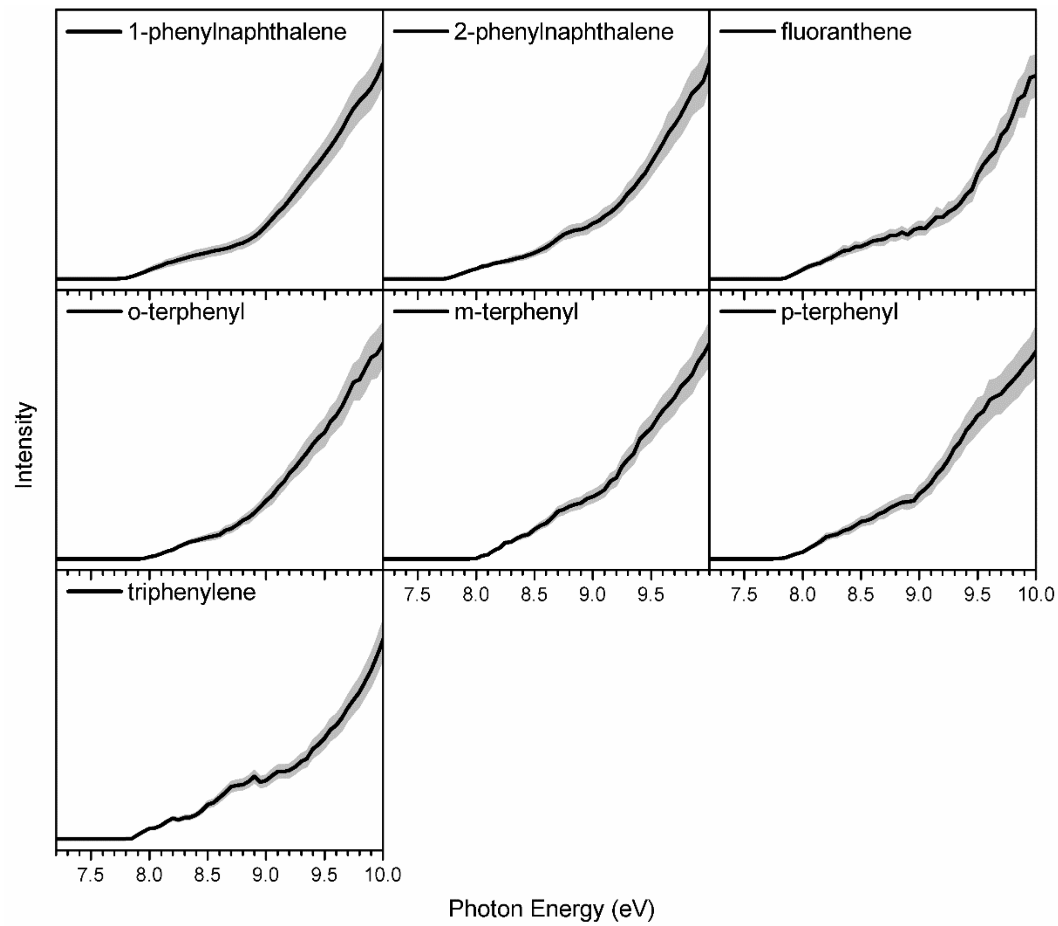


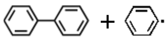
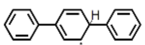
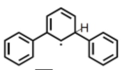
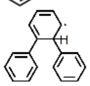
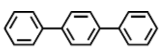
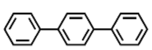
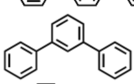
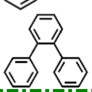
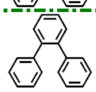
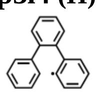
Figure S5. Calibration photoionization efficiency (PIE) curves recorded for helium-seeded 1-phenylnaphthalene, 2-phenylnaphthalene, fluoranthene, *o*-terphenyl, *m*-terphenyl, *p*-terphenyl and triphenylene at identical physical conditions (pressure, temperature) as the real experiments.

These PIE calibration curves were newly recorded and are shown as black lines along with the error limits (grey area). The adiabatic ionization energies of these isomers were determined to be 7.75 ± 0.05, 7.70 ± 0.05, 7.80 ± 0.05, 7.95 ± 0.05 eV, 8.00 ± 0.05 eV, 7.80 ± 0.05 eV and 7.85 ± 0.05 eV, respectively, and are in excellent agreement with literature values of 7.75 eV,[7] 7.90 ± 0.10 eV,[8] 7.99 ± 0.01 eV,[9] 8.01 ± 0.01 eV,[9] 7.80 ± 0.03 eV,[10] and 7.89 ± 0.04 eV[11]. 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.

Table S1. Experiment conditions of the experiments.

Reaction	Temperature (K)	Pressure (atm)	Heating length (mm)	Inner diameter of the tube (mm)
Biphenyl / nitrosobenzene	1300 ± 10	0.394 ± 0.005	20	2
1-(2-Bromophenyl)naphthalene pyrolysis	1300 ± 10	0.394 ± 0.005	20	2
Naphthalene / nitrosobenzene	1100 ± 10	0.394 ± 0.005	20	2

Table S2. The CCSD(T)/cc-pVDZ energies on the B3LYP/cc-pVTZ optimized geometries of relevant reactants, intermediates, transition states and products on their adiabatic singlet or doublet ground state potential energy surfaces.

	B3LYP/ cc-pVTZ + E_{zpc} [a]	**E_{zpc} [b]**	**CCSD(T)/cc-pVDZ**	**E^c (kJ/mol)**
	-694.841940	0.268593	-692.879086	0
tsi1	-694.831530	0.268777	-692.869142	27
tsi2	-694.830513	0.268698	-692.869009	27
tsi3	-694.830653	0.268960	-692.870947	22
i1 	-694.872055	0.271169	-692.924032	-111
i2 	-694.866879	0.270570	-692.922434	-109
i3 	-694.868276	0.270924	-692.922554	-108
tsi1p1	-694.829240	0.263908	-692.866755	20
tsi2p2	-694.827982	0.263848	-692.872553	5
tsi3p3	-694.823732	0.263820	-692.873105	3
p1  **+ H**	-694.839788	0.262110	-692.888981	-43
p1'  **+ H**	-694.839831	0.262102	-692.888954	-43
p2  **+ H**	-694.839408	0.262012	-692.889123	-44
p3  **+ H**	-694.833183	0.261860	-692.887213	-39
p3  **+ H**	-694.833183	0.261860	-692.887213	0
tsp3i4 (H)	-694.815507	0.259667	-692.848384	96
i4  **+ H_2**	-694.825652	0.258790	-692.862287	58
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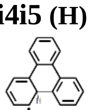
i5  **+ H_2**	-694.863946	0.260012	-692.908436	-60
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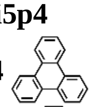
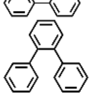
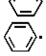
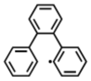
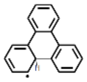
p4  **+ H + H_2**	-694.841292	0.251109	-692.880777	-11
p3  + 	-925.887893	0.349103	-923.282577	121
tsp3i4 	-925.873370	0.344141	-923.258289	172

i4  + 	-925.888709	0.349100	-923.278432	132
tsi4i5 	-925.883319	0.348449	-923.274392	141
i5  + 	-925.927003	0.350322	-923.324582	14
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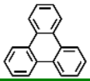
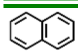
p4  **+ H +** 	-925.904349	0.341419	-923.296923	63
 + 	-617.435192	0.234463	-615.685395	0
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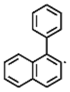
i6 	-617.471509	0.237091	-615.740050	-137
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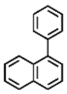
p5  **+ H**	-617.428559	0.228029	-615.693804	-39
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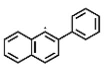
i7 	-617.465453	0.236878	-615.732144	-116
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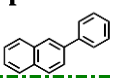
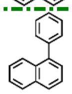
p6  **+ H**	-617.432888	0.227980	-615.695420	-43
p5  **+ H**	-617.428559	0.228029	-615.693804	0
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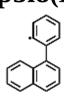
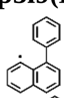
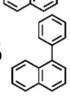
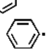
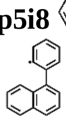
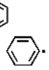
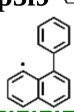
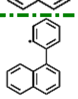
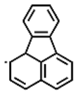
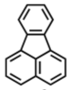
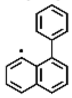
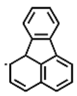
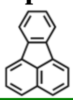
i8  **+ H_2**	-617.421067	0.224996	-615.664243	70
tsp5i9(H)	-617.408895	0.225943	-615.662622	76
i9  **+ H_2**	-617.422301	0.224968	-615.676171	38
p5  + 	-848.483269	0.315272	-846.089167	121
tsp5i8 	-848.468946	0.310426	-846.063092	177
i8  + 	-848.484124	0.315306	-846.080388	144
tsp5i9 	-848.465205	0.310419	-846.062988	177
i9  + 	-848.485358	0.315278	-846.092317	113
i8 	-616.251137	0.214927	-614.500789	0
tsi8i10	-616.229692	0.213276	-614.481360	47

i10 	-616.283290	0.215106	-614.542125	-108
tsi10p7	-616.239333	0.207922	-614.489802	11
p7  **+ H**	-616.247762	0.206308	-614.506544	-38
i9 	-616.252371	0.214899	-614.512718	-32
tsi9i11	-616.233601	0.213639	-614.489079	27
i11 	-616.278252	0.214770	-614.533992	-88
tsi11p7	-616.238721	0.207979	-614.485517	21
p7  **+ H**	-616.247762	0.206308	-614.506544	-38

[a] B3LYP/cc-pVTZ energy with zero-point energy correction in hartree.

[b] zero-point energy by B3LYP/cc-pVTZ in hartree.

[c] relative energy by CCSD(T)/cc-pVDZ with B3LYP/cc-pVTZ zero-point energy correction.

Table S3. Coordinates of relevant reactants, intermediates and products in the biphenyl ($C_{12}H_{10}$) - phenyl ($C_6H_5^{\bullet}$) system.

biphenyl		phenyl	
C	-0.401663; 1.131029; -2.849995	C	0.000000; 1.221238; 0.769133
C	-0.401074; 1.130701; -1.461548	C	0.000000; 1.209128; -0.629799
C	0.000000; 0.000000; -0.741140	C	0.000000; 0.000000; -1.318515
C	0.401074; -1.130701; -1.461548	C	0.000000; -1.209128; -0.629799
C	0.401663; -1.131029; -2.849995	C	0.000000; -1.221238; 0.769133
C	0.000000; 0.000000; -3.551196	C	0.000000; 0.000000; 1.391403
H	-0.724520; 2.014386; -3.385092	H	0.000000; 2.153163; 1.318818
H	-0.738908; 2.009071; -0.928177	H	0.000000; 2.145567; -1.173412
H	0.738908; -2.009071; -0.928177	H	0.000000; 0.000000; -2.400146
H	0.724520; -2.014386; -3.385092	H	0.000000; -2.145567; -1.173412
H	0.000000; 0.000000; -4.632911	H	0.000000; -2.153163; 1.318818
C	0.000000; 0.000000; 0.741140		
C	0.401074; 1.130701; 1.461548		
C	-0.401074; -1.130701; 1.461548		
C	0.401663; 1.131029; 2.849995		
H	0.738908; 2.009071; 0.928177		
C	-0.401663; -1.131029; 2.849995		
H	-0.738908; -2.009071; 0.928177		
C	0.000000; 0.000000; 3.551196		
H	0.724520; 2.014386; 3.385092		
H	-0.724520; -2.014386; 3.385092		
H	0.000000; 0.000000; 4.632911		
i1		**i2**	
C	4.660616; 1.426712; 0.284173	C	-4.40781; -0.561817; 1.172172
C	3.318839; 1.157142; 0.498834	C	-3.210045; 0.132842; 1.064994
C	2.727042; -0.037311; 0.04249	C	-2.410817; 0.018962; -0.077481
C	3.562205; -0.944578; -0.639115	C	-2.857664; -0.807696; -1.113468
C	4.904349; -0.67348; -0.849286	C	-4.055789; -1.501657; -1.008225
C	5.465736; 0.51434; -0.390808	C	-4.836348; -1.382926; 0.135811
H	5.079835; 2.359189; 0.639007	H	-5.004352; -0.46548; 2.069833
H	2.712537; 1.897291; 1.001081	H	-2.878909; 0.754265; 1.886276
H	3.16121; -1.887984; -0.980975	H	-2.269934; -0.88935; -2.017856
H	5.519205; -1.397883; -1.367313	H	-4.384457; -2.129751; -1.82583
H	6.513405; 0.725379; -0.556528	H	-5.770202; -1.922768; 0.217608
C	1.314705; -0.32249; 0.265576	C	-1.123733; 0.754157; -0.184079
C	0.591282; -1.232946; -0.566082	C	-0.021305; 0.158123; -0.730523
C	0.579896; 0.296627; 1.32419	C	-1.030291; 2.089482; 0.297288
C	-0.719839; -1.510968; -0.38186	C	1.30979; 0.840718; -0.881685
H	1.100897; -1.692924; -1.401886	H	-0.073959; -0.870729; -1.061575
C	-0.727876; 0.040057; 1.556455	C	0.190659; 2.792458; 0.22047
H	1.096312; 0.973439; 1.99128	H	-1.905927; 2.575845; 0.701332
C	-1.542014; -0.906242; 0.720584	C	1.305403; 2.235376; -0.321823

H	-1.228508; -2.186751; -1.057467	H	0.233874; 3.805505; 0.601252
H	-1.233781; 0.520683; 2.384063	H	2.233062; 2.790375; -0.369126
H	-1.887117; -1.722806; 1.375148	H	1.52735; 0.91472; -1.961158
C	-2.820652; -0.250239; 0.188838	C	2.452033; -0.003392; -0.305111
C	-2.74818; 0.838262; -0.681705	C	3.481561; -0.466705; -1.120535
C	-4.075818; -0.725207; 0.56153	C	2.47917; -0.321589; 1.053554
C	-3.903958; 1.435513; -1.166413	C	4.517702; -1.232486; -0.594951
H	-1.779211; 1.217541; -0.97949	H	3.473627; -0.22778; -2.1772
C	-5.236336; -0.129037; 0.077907	C	3.510976; -1.085766; 1.581451
H	-4.147812; -1.569495; 1.236535	H	1.684929; 0.032033; 1.698239
C	-5.153275; 0.953526; -0.78787	C	4.534903; -1.54428; 0.758092
H	-3.830679; 2.27863; -1.840848	H	5.309028; -1.584425; -1.243776
H	-6.20294; -0.511596; 0.378441	H	3.516799; -1.325179; 2.636786
H	-6.053686; 1.419216; -1.165669	H	5.338704; -2.140113; 1.169496
i3		***p*-terphenyl (D_2, P1)**	
C	-3.663173; -0.644102; 0.907197	C	-0.001319; 1.195498; -0.692982
C	-2.61939; 0.265879; 0.895028	C	0.000000; 0.000000; -1.419085
C	-1.626329; 0.233494; -0.102093	C	0.001319; -1.195498; -0.692982
C	-1.73031; -0.778235; -1.071969	C	-0.001319; -1.195498; 0.692982
C	-2.779248; -1.686129; -1.062245	C	0.000000; 0.000000; 1.419085
C	-3.754712; -1.626103; -0.07482	C	0.001319; 1.195498; 0.692982
H	-4.404122; -0.59475; 1.694412	H	0.012949; 2.139714; -1.220795
H	-2.556176; 0.996583; 1.688752	H	-0.012949; -2.139714; -1.220795
H	-0.991807; -0.851334; -1.856317	H	0.012949; -2.139714; 1.220795
H	-2.832651; -2.445567; -1.831277	H	-0.012949; 2.139714; 1.220795
H	-4.568719; -2.338175; -0.063781	C	0.000000; 0.000000; 2.899875
C	-0.537162; 1.216231; -0.128929	C	0.755352; 0.932215; 3.620461
C	0.761874; 0.864711; -0.837548	C	-0.755352; -0.932215; 3.620461
C	-0.679035; 2.460745; 0.450229	C	0.756259; 0.932108; 5.008806
C	1.744688; 2.006158; -0.889828	H	1.367195; 1.647446; 3.087316
C	0.313772; 3.443931; 0.405982	C	-0.756259; -0.932108; 5.008806
H	-1.616034; 2.709898; 0.929758	H	-1.367195; -1.647446; 3.087316
C	1.527166; 3.195847; -0.283875	C	0.000000; 0.000000; 5.710205
H	2.668394; 1.817962; -1.421401	H	1.355675; 1.656997; 5.543743
H	0.140765; 4.403763; 0.871427	H	-1.355675; -1.656997; 5.543743
H	2.280017; 3.972234; -0.334121	H	0.000000; 0.000000; 6.791920
H	0.526925; 0.594361; -1.877183	C	0.000000; 0.000000; -2.899875
C	1.464848; -0.365562; -0.243391	C	0.755352; -0.932215; -3.620461
C	1.647907; -0.486809; 1.133807	C	-0.755352; 0.932215; -3.620461
C	1.98559; -1.354193; -1.075508	C	0.756259; -0.932108; -5.008806
C	2.327186; -1.575485; 1.664736	H	1.367195; -1.647446; -3.087316
H	1.253185; 0.274838; 1.793272	C	-0.756259; 0.932108; -5.008806
C	2.669; -2.444321; -0.547832	H	-1.367195; 1.647446; -3.087316
H	1.853011; -1.274419; -2.148065	C	0.000000; 0.000000; -5.710205
C	2.840734; -2.558849; 0.825781	H	1.355675; -1.656997; -5.543743
H	2.45605; -1.656659; 2.736119	H	-1.355675; 1.656997; -5.543743

H	3.062336; -3.204489; -1.21001	H	0.000000; 0.000000; -6.791920
H	3.368394; -3.407501; 1.240076		
***p*-terphenyl (C_{2h}, P1)**		***m*-terphenyl (P2)**	
C	0.000000; 1.195528; 0.692941	C	0.064517; -0.030412; 0.000000
C	0.000000; 0.000000; 1.419372	C	0.729897; -0.158053; 1.222050
C	0.000000; -1.195528; 0.692941	C	2.103027; -0.423644; 1.204887
C	0.000000; -1.195528; -0.692941	C	2.778553; -0.555585; 0.000000
C	0.000000; 0.000000; -1.419372	C	2.103027; -0.423644; -1.204887
C	0.000000; 1.195528; -0.692941	C	0.729897; -0.158053; -1.222050
H	0.034462; 2.139483; 1.220196	H	-0.987202; 0.221216; 0.000000
H	-0.034462; -2.139483; 1.220196	H	2.635945; -0.552217; 2.137015
H	-0.034462; -2.139483; -1.220196	H	3.837329; -0.778996; 0.000000
H	0.034462; 2.139483; -1.220196	H	2.635945; -0.552217; -2.137015
C	0.000000; 0.000000; -2.900092	C	0.000322; -0.004472; -2.503810
C	-0.741598; 0.943153; -3.620898	C	0.582306; 0.665435; -3.585809
C	0.741598; -0.943153; -3.620898	C	-1.287976; -0.525214; -2.668248
C	-0.742169; 0.943274; -5.009201	C	-0.098454; 0.810491; -4.787109
H	-1.343084; 1.667192; -3.087940	H	1.567628; 1.098064; -3.475832
C	0.742169; -0.943274; -5.009201	C	-1.969225; -0.381658; -3.869519
H	1.343084; -1.667192; -3.087940	H	-1.749847; -1.068733; -1.855033
C	0.000000; 0.000000; -5.710487	C	-1.377697; 0.287158; -4.934887
H	-1.330452; 1.677081; -5.544304	H	0.368539; 1.340579; -5.606728
H	1.330452; -1.677081; -5.544304	H	-2.961271; -0.800445; -3.976041
H	0.000000; 0.000000; -6.792189	H	-1.908461; 0.399383; -5.870742
C	0.000000; 0.000000; 2.900092	C	0.000322; -0.004472; 2.503810
C	0.741598; -0.943153; 3.620898	C	-1.287976; -0.525214; 2.668248
C	-0.741598; 0.943153; 3.620898	C	0.582306; 0.665435; 3.585809
C	0.742169; -0.943274; 5.009201	C	-1.969225; -0.381658; 3.869519
H	1.343084; -1.667192; 3.087940	H	-1.749847; -1.068733; 1.855033
C	-0.742169; 0.943274; 5.009201	C	-0.098454; 0.810491; 4.787109
H	-1.343084; 1.667192; 3.087940	H	1.567628; 1.098064; 3.475832
C	0.000000; 0.000000; 5.710487	C	-1.377697; 0.287158; 4.934887
H	1.330452; -1.677081; 5.544304	H	-2.961271; -0.800445; 3.976041
H	-1.330452; 1.677081; 5.544304	H	0.368539; 1.340579; 5.606728
H	0.000000; 0.000000; 6.792189	H	-1.908461; 0.399383; 5.870742
***o*-terphenyl (P3)**		**i4**	
C	-0.029430; 0.704710; 1.199074	C	-0.588382; 1.259342; -0.013139
C	0.029430; -0.704710; 1.199074	C	0.817546; 1.14985; 0.021287
C	0.070388; -1.374862; 2.427175	C	1.583177; 2.32111; 0.040564
C	0.038615; -0.693062; 3.634193	C	0.99568; 3.576896; 0.03163
C	-0.038615; 0.693062; 3.634193	C	-0.388034; 3.684952; 0.010565
C	-0.070388; 1.374862; 2.427175	C	-1.162606; 2.53417; -0.010825
H	0.097653; -2.456353; 2.425493	H	2.659986; 2.239777; 0.099533
H	0.064269; -1.242017; 4.566029	H	1.615588; 4.463126; 0.054933
H	-0.064269; 1.242017; 4.566029	H	-0.863201; 4.656776; 0.006549
H	-0.097653; 2.456353; 2.425493	H	-2.2406; 2.615782; -0.051208

C	-0.008270; 1.527460; -0.041531	C	-1.499569; 0.084347; -0.086643
C	1.002721; 1.381364; -0.996030	C	-2.502105; -0.092747; 0.87103
C	-0.976025; 2.515021; -0.249364	C	-1.425117; -0.825794; -1.145751
C	1.042956; 2.194500; -2.120348	C	-3.395961; -1.152657; 0.780284
H	1.767691; 0.631340; -0.850806	H	-2.57018; 0.598563; 1.700703
C	-0.940511; 3.325290; -1.377684	C	-2.321555; -1.881014; -1.240611
H	-1.770955; 2.638898; 0.474521	H	-0.66402; -0.698804; -1.903517
C	0.070388; 3.168554; -2.317858	C	-3.309258; -2.050687; -0.276389
H	1.838518; 2.068623; -2.842874	H	-4.158944; -1.276992; 1.537465
H	-1.704876; 4.077541; -1.522028	H	-2.250958; -2.570422; -2.071607
H	0.101271; 3.799458; -3.196098	H	-4.006121; -2.874936; -0.349754
C	0.008270; -1.527460; -0.041531	C	1.517717; -0.156964; 0.092469
C	0.976025; -2.515021; -0.249364	C	2.715865; -0.401271; -0.603646
C	-1.002721; -1.381364; -0.996030	C	1.080736; -1.208563; 0.869394
C	0.940511; -3.325290; -1.377684	C	3.380455; -1.616703; -0.488051
H	1.770955; -2.638898; 0.474521	H	3.113271; 0.367281; -1.254779
C	-1.042956; -2.194500; -2.120348	C	1.687405; -2.424011; 1.025578
H	-1.767691; -0.631340; -0.850806	C	2.879561; -2.629527; 0.322892
C	-0.070388; -3.168554; -2.317858	H	4.295549; -1.775725; -1.042634
H	1.704876; -4.077541; -1.522028	H	1.273461; -3.195625; 1.661498
H	-1.838518; -2.068623; -2.842874	H	3.402831; -3.573182; 0.40899
H	-0.101271; -3.799458; -3.196098		
i5		**triphenylene (P4)**	
C	-1.204529; 0.861705; -0.004233	C	0.707680; 1.252902; 0.000000
C	-1.362988; -0.542399; 0.105518	C	-0.707680; 1.252902; 0.000000
C	-2.655381; -1.065694; 0.215532	C	-1.378272; 2.491214; 0.000000
C	-3.772656; -0.247209; 0.181233	C	-0.697568; 3.688465; 0.000000
C	-3.61866; 1.12952; 0.032853	C	0.697568; 3.688465; 0.000000
C	-2.349765; 1.672214; -0.052739	C	1.378272; 2.491214; 0.000000
H	-2.79182; -2.130722; 0.338208	H	-2.456541; 2.519524; 0.000000
H	-4.76003; -0.678462; 0.276822	H	-1.245409; 4.621173; 0.000000
H	-4.485578; 1.776241; 0.011164	H	1.245409; 4.621173; 0.000000
H	-2.234127; 2.745333; -0.116479	H	2.456541; 2.519524; 0.000000
C	0.137236; 1.420047; -0.024431	C	1.438885; -0.013583; 0.000000
C	0.459593; 2.62592; -0.607294	C	2.846591; -0.051989; 0.000000
C	1.190956; 0.601301; 0.686185	C	0.731205; -1.239320; 0.000000
C	1.759077; 3.137804; -0.589064	C	3.543088; -1.240121; 0.000000
H	-0.31181; 3.184042; -1.122283	H	3.410242; 0.867665; 0.000000
C	2.558714; 1.213515; 0.635812	C	1.468319; -2.439225; 0.000000
C	2.797509; 2.408945; 0.046602	C	2.845520; -2.448344; 0.000000
H	1.977052; 4.078853; -1.073333	H	4.624758; -1.232031; 0.000000
H	3.361609; 0.692228; 1.138056	H	0.953701; -3.387189; 0.000000
H	3.799734; 2.818691; 0.055523	H	3.379349; -3.389142; 0.000000
C	-0.17127; -1.409144; 0.02045	C	-1.438885; -0.013583; 0.000000
C	-0.268829; -2.756652; -0.346234	C	-2.846591; -0.051989; 0.000000
C	1.105749; -0.866629; 0.256159	C	-0.731205; -1.239320; 0.000000

C	0.856829; -3.557905; -0.455938	C	-3.543088; -1.240121; 0.000000
H	-1.236119; -3.180191; -0.575542	H	-3.410242; 0.867665; 0.000000
C	2.229523; -1.676169; 0.130198	C	-1.468319; -2.439225; 0.000000
C	2.112594; -3.016699; -0.217367	C	-2.845520; -2.448344; 0.000000
H	0.753807; -4.595587; -0.743841	H	-4.624758; -1.232031; 0.000000
H	3.213746; -1.261778; 0.291462	H	-0.953701; -3.387189; 0.000000
H	2.999947; -3.628071; -0.313108	H	-3.379349; -3.389142; 0.000000
H	0.891373; 0.584607; 1.753898		

Table S4. Coordinates of relevant reactants, intermediates and products in the naphthalene ($C_{10}H_8$) - phenyl ($C_6H_5^{\bullet}$) system.

naphthalene		i6	
C	0.000000; 2.423896; 0.705848	C	3.230301; -1.785215; 0.344279
C	0.000000; 1.240661; 1.396932	C	3.26188; -0.42499; 0.579152
C	0.000000; 0.000000; 0.713987	C	2.194027; 0.408507; 0.189884
C	0.000000; 0.000000; -0.713987	C	1.069611; -0.174843; -0.442463
C	0.000000; 1.240661; -1.396932	C	1.05971; -1.546479; -0.671595
C	0.000000; 2.423896; -0.705848	C	2.124553; -2.352597; -0.288628
H	0.000000; -1.239240; 2.479812	H	3.10563; 2.242863; 0.905605
H	0.000000; 3.364555; 1.240263	H	4.061; -2.407762; 0.649139
H	0.000000; 1.239240; 2.479812	H	4.119187; 0.02264; 1.066389
C	0.000000; -1.240661; 1.396932	C	2.238811; 1.819701; 0.416596
C	0.000000; -1.240661; -1.396932	C	-0.111697; 0.679142; -0.889608
H	0.000000; 1.239240; -2.479812	H	0.19903; -1.995554; -1.151308
H	0.000000; 3.364555; -1.240263	H	2.092073; -3.41685; -0.479028
C	0.000000; -2.423896; -0.705848	C	0.076989; 2.144456; -0.612946
C	0.000000; -2.423896; 0.705848	C	1.185419; 2.645859; 0.006796
H	0.000000; -1.239240; -2.479812	H	-0.203048; 0.559667; -1.978461
H	0.000000; -3.364555; -1.240263	H	-0.724938; 2.80328; -0.918487
H	0.000000; -3.364555; 1.240263	H	1.253509; 3.711843; 0.18584
		C	-1.445449; 0.196138; -0.311872
		C	-1.650505; 0.158887; 1.068634
		C	-2.487259; -0.191214; -1.15115
		C	-2.864864; -0.260255; 1.59333
		H	-0.851466; 0.457807; 1.734616
		C	-3.707359; -0.610722; -0.628551
		H	-2.344562; -0.166136; -2.224754
		C	-3.899225; -0.646921; 0.745771
		H	-3.006194; -0.285433; 2.66592
		H	-4.50429; -0.909488; -1.296887
		H	-4.845581; -0.973603; 1.155649
i7		**1-phenylnaphthalene (P5)**	
C	-4.29878; -0.276594; -0.596533	C	3.309639; -1.827228; 0.222462
C	-3.434908; 0.809554; -0.679861	C	3.479399; -0.480289; 0.04446
C	-2.145002; 0.746218; -0.162348	C	2.367077; 0.391884; -0.046361
C	-1.694402; -0.461365; 0.470142	C	1.045556; -0.151147; 0.031741
C	-2.599214; -1.556354; 0.537685	C	0.911165; -1.54832; 0.235927
C	-3.869982; -1.461879; 0.016919	C	2.010205; -2.362908; 0.327642
H	-1.576845; 2.768155; -0.723758	H	3.54492; 2.186061; -0.258619
H	-5.29801; -0.207504; -1.003986	H	4.168935; -2.480791; 0.292344
H	-3.76507; 1.725313; -1.155123	H	4.473995; -0.057518; -0.023241
C	-1.226368; 1.863201; -0.241017	C	2.539992; 1.787916; -0.197667
C	-0.404559; -0.533076; 0.993164	C	-0.074454; 0.735694; -0.063747
H	-2.269992; -2.472941; 1.010687	H	-0.077044; -1.972756; 0.331587

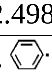
H	-4.542568; -2.307079; 0.081259	H	1.880194; -3.424964; 0.488164
C	0.578815; 0.596453; 0.941179	C	0.152444; 2.089435; -0.192012
C	0.016326; 1.81197; 0.254154	C	1.455152; 2.619255; -0.259253
H	-0.075922; -1.451581; 1.46329	H	-0.694453; 2.758324; -0.268811
H	0.822725; 0.885673; 1.976489	H	1.589718; 3.686846; -0.371497
H	0.672846; 2.668976; 0.171277	C	-1.477911; 0.241945; -0.032149
C	1.912365; 0.159675; 0.323694	C	-2.368152; 0.706289; 0.940357
C	1.977783; -0.234097; -1.013817	C	-1.956161; -0.654076; -0.993994
C	3.079451; 0.140995; 1.083522	C	-3.692851; 0.286229; 0.954954
C	3.182143; -0.635372; -1.575667	H	-2.012455; 1.393119; 1.696962
H	1.078538; -0.224105; -1.61609	C	-3.280914; -1.070905; -0.982832
C	4.288263; -0.26154; 0.523936	H	-1.287622; -1.011519; -1.765687
H	3.044077; 0.444098; 2.123	C	-4.154292; -0.604139; -0.006703
C	4.342729; -0.65088; -0.807858	H	-4.363283; 0.653563; 1.720755
H	3.216236; -0.936825; -2.614431	H	-3.632759; -1.757334; -1.741729
H	5.185011; -0.269655; 1.129568	H	-5.18551; -0.930835; 0.002823
H	5.281017; -0.963988; -1.245942		
2-phenylnaphthalene (P6)		**i8**	
C	4.558982; -0.066477; 0.034751	C	3.330788; -1.803933; 0.203703
C	3.692102; 0.974825; -0.173494	C	3.482574; -0.452707; 0.04391
C	2.292489; 0.769771; -0.140681	C	2.358872; 0.404892; -0.043409
C	1.79059; -0.542093; 0.108992	C	1.043648; -0.155291; 0.024022
C	2.713824; -1.595385; 0.323185	C	0.928818; -1.556022; 0.207681
C	4.064037; -1.364348; 0.286284	C	2.03823; -2.357503; 0.292414
H	1.733161; 2.813511; -0.547438	H	3.519143; 2.211555; -0.243584
H	5.627186; 0.102534; 0.008121	H	4.19841; -2.446802; 0.269611
H	4.069338; 1.971539; -0.365501	H	4.471251; -0.015107; -0.014872
C	1.361937; 1.816204; -0.346727	C	2.518071; 1.803024; -0.189258
C	0.392461; -0.748382; 0.141347	C	-0.08558; 0.722051; -0.06904
H	2.333986; -2.590891; 0.51614	H	-0.05334; -1.997324; 0.286288
H	4.757897; -2.178099; 0.450131	H	1.92055; -3.423632; 0.434036
C	-0.501573; 0.281374; -0.061063	C	0.12911; 2.078262; -0.202571
C	0.014747; 1.582391; -0.306384	C	1.425019; 2.622441; -0.261348
H	0.026318; -1.744069; 0.356966	H	-0.721878; 2.739252; -0.295332
H	-0.674554; 2.395295; -0.489761	H	1.548008; 3.690968; -0.377022
C	-1.964644; 0.050351; -0.022699	C	-1.482846; 0.222739; -0.034863
C	-2.526108; -1.11333; -0.561219	C	-2.475161; 0.868756; 0.727366
C	-2.826524; 0.989104; 0.555679	C	-1.936497; -0.859822; -0.758592
C	-3.896124; -1.332605; -0.518067	C	-3.79376; 0.430668; 0.715938
H	-1.884287; -1.840304; -1.040284	H	-2.193601; 1.712177; 1.344987
C	-4.196902; 0.769877; 0.600438	C	-3.217095; -1.338877; -0.813947
H	-2.417321; 1.887825; 0.997276	C	-4.175669; -0.66584; -0.049794
C	-4.738625; -0.39214; 0.063782	H	-4.52932; 0.947487; 1.317619
H	-4.3075; -2.236111; -0.948548	H	-3.485733; -2.194003; -1.420411
H	-4.841878; 1.506218; 1.061594	H	-5.204619; -1.001588; -0.054582
H	-5.806357; -0.562257; 0.09657		

i9		i10	
C	3.270455; -1.86446; 0.259741	C	-2.107272; 2.400836; -0.313461
C	3.460284; -0.518075; 0.090055	C	-2.911777; 1.263017; -0.099092
C	2.368529; 0.378944; -0.029739	C	-2.296432; -0.017299; 0.097377
C	1.027707; -0.138053; 0.019407	C	-0.911917; -0.023684; 0.263626
C	0.934766; -1.519091; 0.204502	C	-0.087987; 1.207257; 0.462605
C	1.955396; -2.397015; 0.321329	C	-0.741839; 2.403971; -0.158266
H	3.562232; 2.165079; -0.218492	H	-3.990464; -1.33958; -0.153484
H	4.118967; -2.530366; 0.351066	H	-3.983525; 1.331555; -0.227637
H	4.463624; -0.113925; 0.048962	C	-2.916347; -1.276798; -0.033994
C	2.55384; 1.772807; -0.180485	C	-0.12469; -1.158965; 0.122918
C	-0.085553; 0.751419; -0.087018	H	-0.165034; 3.29774; -0.353475
H	1.796084; -3.458522; 0.459501	C	-0.750205; -2.397856; -0.022653
C	0.163807; 2.100929; -0.225276	C	-2.147934; -2.435574; -0.065608
C	1.474934; 2.611133; -0.272319	H	-0.180403; -3.311637; -0.12532
H	-0.669381; 2.783277; -0.324671	H	-2.644345; -3.391057; -0.17356
H	1.623672; 3.676189; -0.390472	C	2.513031; 1.375289; 0.083718
C	-1.478762; 0.244963; -0.046297	C	1.311151; 0.695909; 0.160229
C	-2.445218; 0.894536; 0.729655	C	1.275995; -0.712522; 0.058126
C	-1.87156; -0.872899; -0.790678	C	2.45395; -1.428903; -0.118799
C	-3.757462; 0.442074; 0.763089	C	3.658627; -0.737314; -0.207608
H	-2.157534; 1.74709; 1.330165	C	3.6893; 0.65126; -0.11365
C	-3.184793; -1.323589; -0.759624	H	2.548529; 2.454115; 0.16874
C	-4.133129; -0.669614; 0.018008	H	2.439189; -2.508413; -0.194761
H	-4.485307; 0.954063; 1.378661	H	4.580684; -1.28384; -0.354579
H	-3.468215; -2.184785; -1.350169	H	4.633489; 1.173376; -0.192485
H	-5.155104; -1.023354; 0.043969	H	-2.593737; 3.312303; -0.638847
H	-1.148485; -1.378791; -1.414619	H	-0.078309; 1.4137; 1.5526
i11		**fluoranthene (P7)**	
C	-2.171103; -2.409906; 0.092462	C	0.000000; 2.420049; 2.156911
C	-2.919603; -1.256325; 0.179724	C	0.000000; 1.274613; 2.923832
C	-2.289949; 0.010665; 0.089708	C	0.000000; 0.000000; 2.298836
C	-0.896453; -0.000402; -0.087087	C	0.000000; 0.000000; 0.901141
C	-0.133573; -1.176301; -0.187808	C	0.000000; 1.167991; 0.105743
C	-0.766862; -2.39038; -0.10145	C	0.000000; 2.387952; 0.738907
H	-3.97384; 1.364437; 0.300147	H	0.000000; -1.346736; 4.003981
H	-3.990917; -1.315475; 0.323686	H	0.000000; 1.346736; 4.003981
C	-2.902049; 1.287943; 0.169775	C	0.000000; -1.274613; 2.923832
C	-0.098154; 1.17481; -0.159844	C	0.000000; -1.167991; 0.105743
H	-0.226108; -3.324891; -0.177452	H	0.000000; 3.318850; 0.186674
C	-0.733816; 2.405194; -0.073543	C	0.000000; -2.387952; 0.738907
C	-2.133707; 2.434944; 0.084558	C	0.000000; -2.420049; 2.156911
H	-0.180497; 3.333337; -0.124798	H	0.000000; -3.318850; 0.186674
H	-2.625341; 3.397248; 0.147359	H	0.000000; -3.382828; 2.650918
C	2.49074; -1.422418; 0.12589	C	0.000000; 1.408818; -2.491764
C	1.296945; -0.755451; -0.481347	C	0.000000; 0.711123; -1.294332

C	1.273768; 0.751797; -0.256511	C	0.000000; -0.711123; -1.294332
C	2.454635; 1.433394; -0.039025	C	0.000000; -1.408818; -2.491764
C	3.6319; 0.725717; 0.20127	C	0.000000; -0.696037; -3.690468
C	3.608429; -0.693604; 0.362198	C	0.000000; 0.696037; -3.690468
H	2.478875; -2.493961; 0.275555	H	0.000000; -2.491145; -2.503495
H	2.454464; 2.513388; 0.045054	H	0.000000; -1.230609; -4.630979
H	4.552568; 1.261523; 0.385369	H	0.000000; 1.230609; -4.630979
H	4.504619; -1.186889; 0.71685	H	0.000000; 2.491145; -2.503495
H	-2.669281; -3.367533; 0.170776	H	0.000000; 3.382828; 2.650918
H	1.408556; -0.89924; -1.576383		

Table S5. Coordinates of relevant transition states.

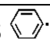
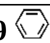
Atom	X	Y	Z	Atom	X	Y	Z
		tsi2				**tsi2p2**	
C	-4.730332	-0.324253	0.259982	C	4.839427	-0.250228	0.547797
C	-3.614261	0.498278	0.185395	C	3.64696	0.459805	0.592068
C	-2.343605	-0.032641	-0.062503	C	2.501044	-0.01788	-0.052668
C	-2.229094	-1.416816	-0.23169	C	2.590452	-1.229689	-0.745895
C	-3.344678	-2.240233	-0.15586	C	3.783163	-1.939018	-0.792348
C	-4.600655	-1.69789	0.090061	C	4.913232	-1.452902	-0.145112
H	-5.704338	0.109882	0.443771	H	5.7106	0.133761	1.061975
H	-3.73153	1.567951	0.296458	H	3.596139	1.383131	1.153411
H	-1.253349	-1.852535	-0.399805	H	1.724408	-1.606924	-1.273014
H	-3.230664	-3.309021	-0.280689	H	3.831387	-2.869685	-1.34216
H	-5.469811	-2.339183	0.149219	H	5.842315	-2.00572	-0.180729
C	-1.151687	0.845593	-0.143371	C	1.227866	0.74179	-0.000253
C	-0.165382	0.623893	-1.097871	C	0.011951	0.083272	0.144915
C	-1.002408	1.934525	0.731438	C	1.221346	2.138841	-0.117897
C	0.999574	1.422564	-1.152408	C	-1.214646	0.785084	0.241282
H	-0.281424	-0.182392	-1.809008	H	-0.002874	-0.994002	0.231434
C	0.097001	2.786571	0.628684	C	0.020566	2.842639	-0.125272
H	-1.747601	2.112571	1.494376	H	2.153779	2.66812	-0.256827
C	1.0768	2.561964	-0.318733	C	-1.184593	2.184667	0.019244
H	0.175391	3.636928	1.293672	H	0.032131	3.916766	-0.255234
H	1.920271	3.232757	-0.406366	H	-2.111026	2.7415	0.029016
H	1.61485	1.382138	-2.040286	H	-1.253284	0.920507	2.011771
C	2.545333	0.066878	-0.305666	C	-2.499682	0.024401	0.155569
C	3.376404	-0.584391	-1.189219	C	-2.724239	-1.110306	0.940213
C	2.596876	-0.110826	1.058293	C	-3.492046	0.412059	-0.747197
C	4.324573	-1.468854	-0.668947	C	-3.902121	-1.834659	0.825088
H	3.309222	-0.425127	-2.259192	H	-1.978616	-1.410545	1.664344
C	3.546539	-0.99843	1.56707	C	-4.674802	-0.30992	-0.860138
H	1.926389	0.421434	1.721132	H	-3.330121	1.272066	-1.382586
C	4.406125	-1.672801	0.704395	C	-4.884495	-1.43639	-0.07555
H	4.995055	-1.99474	-1.3374	H	-4.058185	-2.705784	1.447563
H	3.613833	-1.16055	2.635749	H	-5.428649	0.00632	-1.568961
H	5.140952	-2.358894	1.104076	H	-5.804294	-1.998915	-0.163076
		tsi1				**tsi1p1**	
C	-4.164581	-1.606004	0.879353	C	4.970554	0.993511	-0.823669

C	-2.914231	-1.00452	0.916294	C	3.584536	0.985544	-0.753836
C	-2.598119	0.060802	0.062755	C	2.904443	0.012758	-0.009983
C	-3.585999	0.499741	-0.829057	C	3.667049	-0.950835	0.662226
C	-4.836573	-0.100614	-0.865108	C	5.053306	-0.941844	0.594006
C	-5.13293	-1.157456	-0.011604	C	5.712571	0.030114	-0.149708
H	-4.379892	-2.433457	1.542585	H	5.472142	1.749718	-1.413034
H	-2.162841	-1.381907	1.596521	H	3.021302	1.726375	-1.30488
H	-3.381031	1.337644	-1.481473	H	3.169427	-1.697201	1.26647
H	-5.585144	0.263862	-1.556306	H	5.620192	-1.691247	1.130462
H	-6.107423	-1.626006	-0.040637	H	6.792867	0.037092	-0.203279
C	-1.266489	0.698607	0.103226	C	1.428684	0.000613	0.064726
C	-0.657931	1.190355	-1.06552	C	0.712503	-1.206473	0.095454
C	-0.572151	0.855481	1.315681	C	0.688005	1.192027	0.081532
C	0.587469	1.782575	-1.034694	C	-0.663773	-1.226696	0.168318
H	-1.173613	1.094845	-2.01163	H	1.249293	-2.143298	0.031543
C	0.671755	1.449365	1.36006	C	-0.688806	1.183655	0.158398
H	-1.041447	0.542007	2.238484	H	1.205597	2.140835	0.040839
C	1.317007	1.860124	0.171731	C	-1.41232	-0.02887	0.278529
H	1.028854	2.156684	-1.948528	H	-1.182908	-2.174921	0.192494
H	1.170373	1.582658	2.310519	H	-1.23093	2.119103	0.14957
H	2.17271	2.516994	0.230897	H	-1.488022	-0.059132	2.079612
C	2.888659	0.259576	-0.074034	C	-2.89549	-0.02831	0.104889
C	2.547575	-0.904482	-0.723028	C	-3.701605	0.899896	0.770895
C	4.123783	0.484533	0.490422	C	-3.509471	-0.934219	-0.763072
C	3.513508	-1.908554	-0.813936	C	-5.074822	0.922481	0.574747
H	1.563587	-1.042693	-1.15338	H	-3.248639	1.591636	1.468534
C	5.082826	-0.526707	0.392332	C	-4.886022	-0.916127	-0.956567
H	4.359433	1.412391	0.998546	H	-2.904882	-1.644534	-1.310213
C	4.775076	-1.717249	-0.257876	C	-5.674421	0.012409	-0.289733
H	3.278702	-2.837238	-1.319287	H	-5.679976	1.644942	1.106314
H	6.065706	-0.380972	0.823266	H	-5.339503	-1.624775	-1.636944
H	5.520097	-2.498247	-0.331562	H	-6.745483	0.027595	-0.44039
tsp3i4 				**tsp3i4(H)**			
C	-0.414211	-0.549874	-1.065424	C	-0.70722	1.178563	-0.055701
C	-1.463814	-1.295858	-0.489532	C	0.701171	1.2163	0.002182
C	-1.501204	-2.677987	-0.708181	C	1.337418	2.462808	0.002468
C	-0.532184	-3.325704	-1.459249	C	0.620599	3.649155	-0.035806
C	0.509585	-2.592346	-2.010877	C	-0.766808	3.609984	-0.071602
C	0.559585	-1.221188	-1.81187	C	-1.415268	2.384684	-0.08207

H	-2.295429	-3.253172	-0.251347	H	2.417012	2.492754	0.06446
H	-0.586206	-4.396627	-1.602743	H	1.143007	4.596416	-0.026498
H	1.276365	-3.081334	-2.596508	H	-1.341881	4.525773	-0.098225
H	1.356908	-0.644566	-2.259977	H	-2.494756	2.350127	-0.136281
C	-0.317461	0.933419	-0.96417	C	-1.486284	-0.086971	-0.14331
C	-1.374383	1.758956	-1.373681	C	-1.229049	-1.050461	-1.131677
C	0.835583	1.569172	-0.517659	C	-2.5514	-0.361738	0.697376
C	-1.263914	3.142039	-1.327669	C	-2.004935	-2.197383	-1.235332
H	-2.286316	1.305625	-1.73855	H	-0.416942	-0.886442	-1.827202
C	0.9646	2.943052	-0.45116	C	-3.338466	-1.48798	0.636867
H	1.885054	0.871346	-0.075376	H	-2.855176	0.548889	1.836346
C	-0.097953	3.742438	-0.864935	C	-3.059063	-2.425669	-0.356586
H	-2.093571	3.753921	-1.655942	H	-1.785183	-2.91844	-2.011215
H	1.876726	3.390868	-0.077015	H	-4.147674	-1.644109	1.338814
H	-0.015921	4.820842	-0.824635	H	-3.65836	-3.322956	-0.440271
C	-2.519659	-0.697703	0.372941	C	1.550505	-0.00181	0.105542
C	-3.86984	-0.954819	0.115089	C	2.617443	-0.196252	-0.776979
C	-2.197543	0.084116	1.486463	C	1.343277	-0.949335	1.112489
C	-4.865828	-0.441665	0.937054	C	3.44518	-1.30673	-0.663962
H	-4.140398	-1.550677	-0.746803	H	2.789678	0.523003	-1.567053
C	-3.191198	0.592068	2.312064	C	2.173448	-2.055697	1.230111
H	-1.160292	0.289621	1.710954	H	0.53233	-0.811615	1.81408
C	-4.530165	0.333882	2.039912	C	3.22624	-2.241159	0.340766
H	-5.904439	-0.646659	0.712946	H	4.259967	-1.441662	-1.363128
H	-2.918194	1.189275	3.17204	H	1.999423	-2.773038	2.021215
H	-5.303879	0.732973	2.682064	H	3.870733	-3.105234	0.431656
C	2.996895	0.309122	0.40883	H	-3.0529	1.02467	2.514643
C	4.204136	0.636748	-0.17808				
C	2.905259	-0.552643	1.484858				
C	5.371783	0.074104	0.336931				
H	4.247985	1.313594	-1.022148				
C	4.077227	-1.111214	1.992962				
H	1.946813	-0.796512	1.924621				
C	5.305347	-0.796735	1.419465				
H	6.328888	0.316087	-0.107384				
H	4.029506	-1.790757	2.83433				
H	6.21254	-1.232121	1.816973				
tsi4i5				**tsi5p4**			
C	-0.975532	-1.094790	-0.055403	C	1.066432	-0.980431	-0.016832

C	-1.425398	0.244890	-0.108067	C	1.393668	0.396599	0.006004
C	-2.803532	0.476364	-0.184750	C	2.750683	0.762676	0.058046
C	-3.719246	-0.564571	-0.176605	C	3.758329	-0.177738	0.070275
C	-3.273566	-1.877117	-0.083347	C	3.436412	-1.535081	0.038292
C	-1.911128	-2.131112	-0.025939	C	2.114525	-1.920791	0.001049
H	-3.166703	1.491364	-0.262618	H	3.02339	1.805394	0.10692
H	-4.777405	-0.350214	-0.245001	H	4.791733	0.138523	0.115565
H	-3.979059	-2.696996	-0.072279	H	4.217302	-2.283288	0.058142
H	-1.554337	-3.151692	0.018720	H	1.888309	-2.975719	0.007664
C	0.469809	-1.408283	-0.024879	C	-0.330213	-1.397749	-0.030975
C	1.038042	-2.157426	0.998023	C	-0.704197	-2.739488	-0.193652
C	1.312360	-0.864707	-1.025326	C	-1.35814	-0.423727	0.193536
C	2.412336	-2.387275	1.038716	C	-2.024695	-3.138213	-0.186844
H	0.404015	-2.545098	1.784682	H	0.0547	-3.490101	-0.35176
C	2.690392	-1.143347	-1.002631	C	-2.71422	-0.861005	0.115338
H	0.868286	-0.494858	-1.938524	C	-3.038291	-2.183632	-0.039451
C	3.236435	-1.875800	0.037828	H	-2.273985	-4.18181	-0.321906
H	2.836856	-2.965717	1.848044	H	-3.510622	-0.141544	0.21794
H	3.320140	-0.781330	-1.804278	H	-4.076987	-2.484418	-0.065967
H	4.300511	-2.070642	0.062517	C	0.331125	1.404177	-0.027357
C	-0.473016	1.379435	-0.019938	C	0.619761	2.773259	-0.175016
C	-0.855585	2.646138	0.459386	C	-1.019542	1.011723	0.089736
C	0.861188	1.258143	-0.368848	C	-0.373355	3.729158	-0.178015
C	0.058522	3.688178	0.544266	H	1.641468	3.095522	-0.302646
H	-1.871405	2.811231	0.793116	C	-2.013666	2.00206	0.094269
C	1.799646	2.255595	-0.296549	C	-1.704251	3.340319	-0.03317
C	1.385361	3.505642	0.167011	H	-0.117717	4.773613	-0.295391
H	-0.266300	4.648937	0.920888	H	-3.051241	1.725533	0.196464
H	2.829864	2.083541	-0.583530	H	-2.493803	4.079595	-0.029534
H	2.093015	4.321732	0.240583	H	-1.234739	-0.434008	1.953116
Atom	X	Y	Z	Atom	X	Y	Z
	tsi6				**tsi6p5**		
C	3.097598	-1.759147	0.820987	C	3.345068	-1.7996	0.150088
C	3.01473	-0.414955	1.083309	C	3.48482	-0.453611	-0.066314
C	2.123188	0.413019	0.360916	C	2.358446	0.403407	-0.085857
C	1.295043	-0.176219	-0.637626	C	1.058807	-0.15129	0.113173
C	1.407299	-1.558614	-0.887787	C	0.953092	-1.539378	0.352316
C	2.29008	-2.336273	-0.178018	C	2.06566	-2.344628	0.367311
H	2.683635	2.256765	1.337246	H	3.493597	2.201689	-0.44872

H	3.786046	-2.379712	1.37901	H	4.214601	-2.443041	0.163106
H	3.639199	0.033019	1.846163	H	4.465634	-0.022238	-0.222007
C	2.051291	1.813233	0.578792	C	2.500904	1.796663	-0.299409
C	0.368471	0.655227	-1.352495	C	-0.085089	0.734235	0.125333
H	0.778332	-2.005639	-1.647154	H	1.959049	-3.404669	0.555375
H	2.364806	-3.39588	-0.382642	C	0.117648	2.085636	-0.161349
C	0.406007	2.036959	-1.172416	C	1.401186	2.615878	-0.340193
C	1.220162	2.603277	-0.184196	H	-0.744193	2.734898	-0.231948
H	-0.108409	0.246095	-2.232029	H	1.517381	3.674682	-0.529286
H	-0.22972	2.670636	-1.775276	C	-1.487469	0.211814	0.064147
H	1.205132	3.67443	-0.031338	C	-2.473192	0.665536	0.943242
C	-1.652223	0.134839	-0.356425	C	-1.861437	-0.67886	-0.946969
C	-1.912662	0.650807	0.891594	C	-3.789702	0.238091	0.822057
C	-2.512653	-0.697622	-1.034757	H	-2.197316	1.347	1.736583
C	-3.117437	0.299266	1.503754	C	-3.177441	-1.106748	-1.069212
H	-1.21147	1.309151	1.388705	C	-4.147266	-0.651309	-0.183819
C	-3.716871	-1.039433	-0.413449	H	-4.53507	0.597402	1.51926
H	-2.278715	-1.085437	-2.019216	H	-3.445014	-1.792962	-1.861887
C	-4.013845	-0.542036	0.850973	H	-5.171612	-0.986299	-0.277411
H	-3.353598	0.684487	2.488024	H	-1.118711	-1.027022	-1.651816
H	-4.417557	-1.692188	-0.919386	H	-0.019804	-1.96859	0.540742
H	-4.946741	-0.809685	1.32897	H	-0.00276	0.934129	2.000741
	tsi7				**tsi7p6**		
C	-3.967369	-1.025345	-0.56675	C	3.676245	0.965792	0.31989
C	-3.21879	-0.048162	-1.179388	C	2.740919	-1.575926	-0.36763
C	-2.087709	0.503721	-0.544332	C	4.085633	-1.349155	-0.226681
C	-1.721991	0.031402	0.755221	C	4.559427	-0.066938	0.119832
C	-2.518082	-0.972713	1.361133	H	4.038504	1.950408	0.58786
C	-3.612765	-1.489336	0.715844	H	2.376678	-2.559759	-0.635267
H	-1.604933	1.915487	-2.109639	H	4.790168	-2.15521	-0.382516
H	-4.832673	-1.439459	-1.066643	H	5.622752	0.09983	0.227705
H	-3.492927	0.312155	-2.163227	C	1.803074	-0.531195	-0.170684
C	-1.304701	1.533493	-1.14163	C	2.286378	0.76632	0.180197
C	-0.597726	0.590466	1.396532	C	0.415909	-0.73655	-0.30298
H	-2.244308	-1.330227	2.345829	C	1.339831	1.803862	0.396801
H	-4.208674	-2.257528	1.1905	C	-0.500637	0.310703	-0.183968
C	0.208108	1.530499	0.75473	H	0.06196	-1.72324	-0.571526
C	-0.211736	2.046045	-0.512224	C	0.005487	1.58904	0.239333
H	-0.340528	0.251845	2.391798	H	1.698286	2.778129	0.704999

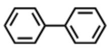
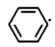
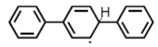
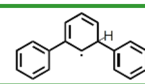
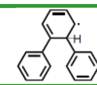
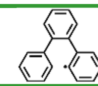
H	0.924671	2.095104	1.333535	H	-0.699055	2.387182	0.426923
H	0.368048	2.831782	-0.976959	C	-1.967699	0.043284	-0.090205
C	2.035344	0.335717	0.155187	C	-2.903557	0.959602	-0.579823
C	1.947897	-0.493709	-0.938902	C	-2.440275	-1.116551	0.528387
C	3.155663	0.437364	0.948297	C	-4.265137	0.722047	-0.459575
C	3.063474	-1.268669	-1.261354	H	-2.558422	1.852616	-1.083458
H	1.046883	-0.545475	-1.537212	C	-3.804191	-1.358306	0.645391
C	4.266792	-0.341424	0.614787	H	-1.736489	-1.825025	0.943061
H	3.190372	1.097157	1.807366	C	-4.722313	-0.440399	0.152424
C	4.21695	-1.190031	-0.486059	H	-4.97119	1.441229	-0.853237
H	3.029335	-1.931489	-2.117162	H	-4.147236	-2.261922	1.131715
H	5.165849	-0.282777	1.215803	H	-5.783855	-0.627002	0.244368
H	5.078749	-1.792486	-0.740543	H	-0.546659	0.728978	-1.944875
tsp5i8 				**tsp5i9** 			
C	4.166897	-1.615288	-1.308322	C	-2.347021	-3.162185	0.11971
C	3.605401	-2.219873	-0.215542	C	-3.394815	-2.288667	0.016594
C	2.52863	-1.618892	0.48103	C	-3.183292	-0.889341	-0.048179
C	2.033762	-0.350576	0.040834	C	-1.845047	-0.366789	0.023981
C	2.629014	0.235419	-1.105664	C	-0.803054	-1.320621	0.100032
C	3.665675	-0.377925	-1.76076	C	-1.025258	-2.666017	0.142546
H	2.310812	-3.213261	1.916852	H	-5.273888	-0.409102	-0.250045
H	4.987937	-2.087302	-1.831337	H	-2.522785	-4.229081	0.16457
H	3.975007	-3.176748	0.131308	H	-4.41213	-2.656526	-0.027476
C	1.926815	-2.254328	1.592592	C	-4.27285	0.000103	-0.197415
C	0.948236	0.252324	0.751714	C	-1.660831	1.051896	-0.01788
H	2.249554	1.178167	-1.471193	H	0.501809	-1.04891	0.033024
H	4.10011	0.088452	-2.635105	H	-0.190012	-3.353917	0.177113
C	0.388126	-0.417635	1.817125	C	-2.760577	1.86723	-0.1854
C	0.873108	-1.669606	2.240302	C	-4.064878	1.349253	-0.280379
H	-0.43364	0.038852	2.351791	H	-2.614603	2.938799	-0.212293
H	0.410053	-2.160331	3.085873	H	-4.899998	2.026328	-0.400728
C	0.415417	1.593063	0.3812	C	-0.3294	1.695096	0.14428
C	-0.90838	1.782401	0.00324	C	0.186926	2.519204	-0.859155
C	1.223074	2.738054	0.449771	C	0.395239	1.558389	1.331
C	-1.437194	3.02106	-0.304969	C	1.395082	3.183359	-0.683856
H	-1.738077	0.74185	-0.119602	H	-0.361771	2.632661	-1.785014
C	0.711839	3.995012	0.153199	C	1.597546	2.228908	1.510516
H	2.256284	2.636019	0.756128	H	0.004193	0.932952	2.122251
C	-0.617786	4.14431	-0.226493	C	2.103393	3.042038	0.503051

H	-2.472465	3.115169	-0.608089	H	1.782062	3.81134	-1.475595
H	1.35465	4.862492	0.22365	H	2.141256	2.114723	2.438823
H	-1.013376	5.124233	-0.460052	H	3.04295	3.559839	0.641771
C	-2.647922	-0.217992	-0.287682	C	1.833017	-1.139047	-0.108378
C	-3.740518	-0.244443	0.557465	C	2.566441	-1.680674	0.929494
C	-2.472508	-1.137193	-1.30402	C	2.409633	-0.748791	-1.300697
C	-4.700482	-1.239629	0.375919	C	3.943489	-1.829145	0.766768
H	-3.852776	0.48833	1.346737	H	2.088032	-1.980869	1.853236
C	-3.436886	-2.128931	-1.477888	C	3.787356	-0.899881	-1.45426
H	-1.605234	-1.094658	-1.950222	H	1.810495	-0.330641	-2.09878
C	-4.546217	-2.177676	-0.639509	C	4.549733	-1.438529	-0.422799
H	-5.565018	-1.280661	1.026279	H	4.538936	-2.24925	1.56747
H	-3.320147	-2.861581	-2.266284	H	4.262266	-0.597644	-2.379022
H	-5.292265	-2.948956	-0.777986	H	5.618198	-1.555438	-0.546757
tsp5i8 (H)				**tsp5i9 (H)**			
C	3.345771	-1.810361	0.277493	C	-3.338304	-1.805667	-0.165891
C	3.504362	-0.468652	0.05539	C	-3.492047	-0.455733	0.001158
C	2.384838	0.389923	-0.069285	C	-2.376048	0.416289	0.056128
C	1.067901	-0.162262	0.021102	C	-1.046706	-0.125456	-0.03974
C	0.944682	-1.552988	0.270437	C	-0.972361	-1.516908	-0.236355
C	2.050546	-2.353925	0.394214	C	-2.041023	-2.352182	-0.305713
H	3.547328	2.186668	-0.334218	H	-3.547661	2.213254	0.261136
H	4.210368	-2.45344	0.373668	H	-4.202135	-2.456171	-0.208439
H	4.495405	-0.039182	-0.021235	H	-4.482315	-0.026636	0.085931
C	2.545655	1.781685	-0.265336	C	-2.543769	1.814263	0.189236
C	-0.05677	0.712788	-0.107486	C	0.073007	0.760599	0.037031
H	-0.039775	-1.983622	0.377334	H	-1.907991	-3.412955	-0.476349
H	1.929126	-3.411091	0.58985	C	-0.156616	2.115564	0.146902
C	0.155993	2.063436	-0.277531	C	-1.458012	2.646166	0.219341
C	1.454164	2.60162	-0.357458	H	0.691106	2.78465	0.209348
H	-0.697231	2.721398	-0.371806	H	-1.591563	3.715379	0.315449
H	1.580143	3.6664	-0.50102	C	1.476186	0.268538	0.025247
C	-1.455828	0.206295	-0.074173	C	2.371629	0.705672	-0.95406
C	-2.387552	0.665714	0.840246	C	1.946962	-0.589746	1.022588
C	-1.930864	-0.727627	-1.0097	C	3.698284	0.291792	-0.941597
C	-3.704219	0.271605	0.894385	H	2.019848	1.364261	-1.73725
H	-1.961243	1.59885	1.924557	C	3.273835	-0.997357	1.040253
C	-3.255213	-1.147277	-0.995975	C	4.154282	-0.560137	0.056623
H	-1.252774	-1.108812	-1.762501	H	4.374309	0.634176	-1.713976

C	-4.147273	-0.654852	-0.048744	H	3.621394	-1.656291	1.82496
H	-4.375963	0.665132	1.646599	H	5.187216	-0.881378	0.068879
H	-3.594207	-1.861006	-1.734942	H	1.269352	-0.930448	1.793854
H	-5.177357	-0.986716	-0.041598	H	0.264749	-2.25271	-0.549508
H	-1.760979	2.114683	2.569835	H	0.887892	-2.789305	-0.780939
tsi8i10				**tsi9i11**			
C	2.699694	-2.145143	-0.201417	C	2.488954	2.305754	0.285994
C	3.169453	-0.851295	-0.285302	C	3.08668	1.068917	0.259232
C	2.301886	0.24955	-0.040479	C	2.314251	-0.107676	0.083082
C	0.955891	-0.019666	0.298484	C	0.910916	0.048287	-0.057792
C	0.525624	-1.368512	0.564406	C	0.343755	1.324955	-0.005378
C	1.403308	-2.417472	0.256868	C	1.081993	2.457112	0.133822
H	3.72223	1.829465	-0.429697	H	3.892801	-1.586866	0.146887
H	4.19596	-0.659191	-0.569205	H	3.096607	3.19135	0.425413
C	2.690104	1.600863	-0.196834	H	4.160066	0.983958	0.37162
C	-0.013862	1.007732	0.226151	C	2.826768	-1.427831	0.04329
H	1.11453	-3.438554	0.466452	C	0.046255	-1.06745	-0.226059
C	0.396542	2.319422	0.071617	H	0.640817	3.445588	0.147576
C	1.76057	2.611566	-0.095399	C	0.585206	-2.333996	-0.254582
H	-0.330277	3.117535	0.001276	C	1.981122	-2.500426	-0.123454
H	2.070202	3.640669	-0.22025	H	-0.047046	-3.201587	-0.39009
C	-2.669324	-1.544041	-0.315328	H	2.392678	-3.500681	-0.157114
C	-1.484298	-0.870681	-0.155093	C	-1.354082	-0.638419	-0.25196
C	-1.383209	0.491944	0.104967	C	-2.376136	-1.272975	0.43594
C	-2.576022	1.222479	0.159109	C	-1.562124	0.688673	-0.762809
C	-3.792872	0.581087	-0.043157	C	-3.591407	-0.626899	0.661831
C	-3.847191	-0.789199	-0.284984	H	-2.201707	-2.253605	0.859848
H	-2.703854	-2.612485	-0.48732	C	-2.800051	1.327812	-0.508978
H	-2.556132	2.284458	0.370307	C	-3.784906	0.683551	0.214261
H	-4.710045	1.153444	-0.00445	H	-4.373541	-1.130833	1.213029
H	-4.801436	-1.273142	-0.450717	H	-2.983066	2.311629	-0.92004
H	3.365465	-2.969749	-0.420885	H	-4.725746	1.182287	0.406674
H	-0.184403	-1.544254	1.362832	H	-1.035027	0.982425	-1.662448
tsi10p7				**tsi11p7**			
C	2.157908	-2.405857	-0.127171	C	2.166531	-2.417163	-0.05699
C	2.924582	-1.257255	-0.06137	C	2.932722	-1.271597	-0.072397
C	2.298423	0.016465	0.01317	C	2.309032	0.002511	-0.032378
C	0.90349	0.015373	0.074541	C	0.911033	0.003015	0.022344
C	0.106315	-1.165819	0.120844	C	0.122009	-1.165534	0.051293

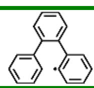
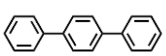
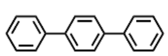
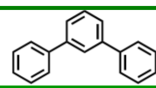
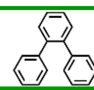
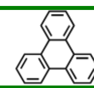
C	0.749204	-2.384877	-0.075469	C	0.750193	-2.385202	0.0087
H	3.999931	1.363775	-0.05782	H	4.013333	1.347482	-0.095205
H	4.003903	-1.325844	-0.104401	H	4.011888	-1.343093	-0.118595
C	2.920642	1.290298	-0.019994	C	2.934003	1.27631	-0.052687
C	0.105861	1.174836	0.039374	C	0.117456	1.173049	0.045304
H	0.195833	-3.312218	-0.137969	H	0.197322	-3.315157	0.032102
C	0.735903	2.399473	-0.003762	C	0.753407	2.394029	0.026349
C	2.1506	2.435591	-0.020289	C	2.168722	2.423505	-0.021089
H	0.179132	3.326811	-0.037888	H	0.202154	3.325127	0.044544
H	2.642602	3.398858	-0.051172	H	2.664404	3.385284	-0.036215
C	-2.49614	-1.397137	0.001694	C	-2.495303	-1.398618	-0.058645
C	-1.300598	-0.700261	0.041786	C	-1.288044	-0.707818	0.134969
C	-1.293169	0.718501	0.016179	C	-1.278159	0.728187	0.064183
C	-2.488558	1.419598	-0.040351	C	-2.470635	1.42637	-0.012792
C	-3.687406	0.710125	-0.079879	C	-3.669643	0.719278	-0.094827
C	-3.691338	-0.682128	-0.062646	C	-3.675893	-0.677573	-0.141422
H	-2.509874	-2.479022	0.024139	H	-2.508302	-2.479595	-0.096757
H	-2.496293	2.501679	-0.059051	H	-2.476929	2.508346	-0.039176
H	-4.625596	1.246657	-0.12674	H	-4.605036	1.258526	-0.158798
H	-4.632232	-1.214786	-0.09705	H	-4.615668	-1.201793	-0.251967
H	2.655527	-3.361402	-0.228261	H	2.659539	-3.379747	-0.091936
H	0.012759	-1.266063	1.976263	H	-1.2673	-0.841882	1.95253

Table S6. Harmonic Frequencies (cm^{-1}) of relevant reactants, intermediates, transition states and products.

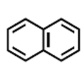
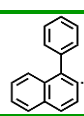
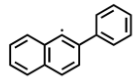
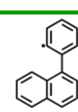
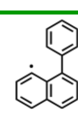
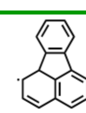
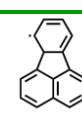
							
ν1	65.4	413.9	403.0	16.3	22.1	23.5	36.9
ν2	95.2	413.9	429.2	23.7	35.0	38.0	49.8
ν3	128.0	624.2	602.3	46.0	45.3	49.0	62.1
ν4	268.5	624.2	621.3	96.1	81.8	76.9	88.8
ν5	314.5	689.7	678.6	103.6	116.5	111.7	103.5
ν6	371.8	726.6	725.6	141.0	118.4	147.3	137.1
ν7	416.5	866.6	818.1	214.9	214.1	191.8	226.0
ν8	422.5	866.6	899.4	234.6	239.4	251.4	256.9
ν9	503.3	987.8	972.2	275.4	282.1	262.7	276.5
ν10	561.6	987.8	994.6	305.4	307.8	308.0	320.1
ν11	627.4	1015.4	1001.7	392.9	340.8	346.6	365.3
ν12	630.2	1021.1	1018.9	407.8	366.2	415.2	402.1
ν13	642.6	1030.7	1052.5	416.7	417.0	416.9	417.5
ν14	716.6	1062.3	1074.6	417.8	419.4	423.2	428.2
ν15	720.7	1062.3	1177.9	420.3	448.4	461.0	508.2
ν16	758.3	1176.8	1178.2	492.8	515.6	510.6	534.8
ν17	760.4	1200.6	1305.7	546.7	551.9	524.5	567.8
ν18	803.6	1200.6	1327.6	548.5	597.2	568.5	576.8
ν19	862.6	1335.0	1468.3	602.4	610.2	595.2	619.1
ν20	862.7	1390.2	1476.1	606.9	613.0	610.0	629.0
ν21	931.9	1518.9	1575.0	636.9	635.7	635.4	637.0
ν22	950.7	1518.9	1630.2	637.2	638.5	638.5	640.6
ν23	991.3	1637.5	3157.3	683.7	649.3	677.0	712.3
ν24	992.1	1637.5	3163.1	705.8	708.2	699.8	717.9
ν25	1008.3	3157.7	3176.1	717.9	718.0	706.9	724.3
ν26	1008.4	3167.4	3178.3	730.1	719.6	718.0	750.1
ν27	1014.9	3167.4	3189.5	751.0	754.5	750.2	767.9
ν28	1023.3	3183.1		752.6	773.6	775.3	785.9
ν29	1031.8	3183.1		784.6	783.4	784.0	787.7
ν30	1056.4	3193.2		793.4	801.0	791.9	799.3
ν31	1069.3			849.2	818.9	845.2	861.8
ν32	1104.8			857.2	861.4	850.5	862.6
ν33	1109.3			861.8	863.2	859.7	901.2
ν34	1184.6			915.3	864.1	923.4	939.6

ν35	1185.4	925.4	913.9	930.2	951.8
ν36	1206.3	934.4	934.4	939.7	977.3
ν37	1213.8	980.2	942.6	946.4	989.3
ν38	1298.8	982.9	978.5	978.5	991.2
ν39	1303.9	984.4	987.0	984.4	993.3
ν40	1326.5	987.3	991.5	986.4	1002.5
ν41	1363.3	987.8	1003.5	1000.7	1006.5
ν42	1365.0	1001.6	1007.6	1001.6	1018.0
ν43	1467.2	1006.3	1007.8	1005.6	1026.1
ν44	1495.5	1008.3	1016.6	1016.6	1031.4
ν45	1522.7	1022.2	1023.6	1021.8	1056.6
ν46	1543.2	1024.0	1026.0	1023.6	1060.9
ν47	1611.3	1044.3	1053.7	1036.0	1088.0
ν48	1626.2	1053.6	1058.0	1053.7	1104.9
ν49	1643.3	1056.5	1061.6	1057.7	1118.8
ν50	1646.5	1104.0	1103.5	1103.7	1143.9
ν51	3161.6	1108.7	1103.9	1111.5	1177.8
ν52	3162.5	1170.7	1128.3	1144.0	1184.2
ν53	3167.3	1183.6	1183.2	1183.0	1190.0
ν54	3170.0	1184.0	1184.3	1185.1	1207.4
ν55	3177.4	1194.6	1185.1	1187.2	1240.8
ν56	3181.2	1206.1	1199.5	1195.7	1276.6
ν57	3183.2	1208.4	1205.8	1205.8	1283.4
ν58	3186.4	1215.9	1207.8	1215.0	1302.6
ν59	3192.0	1238.1	1225.8	1227.7	1319.6
ν60	3193.4	1260.4	1272.1	1266.3	1322.4
ν61		1311.8	1290.5	1284.1	1328.0
ν62		1313.2	1298.2	1309.9	1360.5
ν63		1328.0	1334.9	1333.2	1440.0
ν64		1338.1	1339.6	1341.1	1469.4
ν65		1363.5	1345.6	1365.6	1480.7
ν66		1367.8	1365.2	1368.2	1488.8
ν67		1416.6	1367.1	1408.0	1516.3
ν68		1470.6	1441.9	1427.9	1536.6
ν69		1478.3	1482.6	1480.9	1569.7
ν70		1488.9	1488.3	1488.0	1604.1
ν71		1526.0	1528.0	1523.6	1619.6
ν72		1529.6	1529.7	1529.1	1634.2
ν73		1531.6	1560.7	1534.5	1638.0

ν74				1604.1	1589.2	1606.6	1644.6
ν75				1604.6	1619.7	1609.7	3157.8
ν76				1626.0	1627.1	1626.5	3161.0
ν77				1637.3	1642.8	1635.4	3164.0
ν78				1644.1	1644.3	1642.1	3165.3
ν79				2910.5	2887.6	2938.3	3168.2
ν80				3154.0	3153.8	3149.8	3174.3
ν81				3159.3	3155.7	3158.3	3175.8
ν82				3159.8	3161.5	3162.6	3177.8
ν83				3162.2	3162.6	3162.8	3183.8
ν84				3164.0	3167.7	3169.0	3184.3
ν85				3167.2	3171.3	3172.1	3187.9
ν86				3170.0	3172.0	3172.3	3191.8
ν87				3179.2	3177.9	3178.0	3192.9
ν88				3179.5	3178.9	3180.7	
ν89				3180.4	3179.9	3186.7	
ν90				3186.7	3184.3	3190.2	
ν91				3188.9	3190.1	3193.3	
ν92				3193.2	3192.1	3196.8	
ν93				3200.4	3198.5	3200.8	

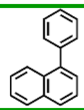
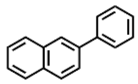
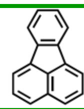
						
ν1	65.4	37.9	37.5	46.6	52.2	51.3
ν2	75.2	45.5	44.6	47.9	54.0	51.3
ν3	107.7	68.5	69.7	62.7	62.3	110.8
ν4	132.9	81.6	79.9	96.5	93.6	121.7
ν5	206.0	122.9	111.8	114.8	103.9	261.1
ν6	226.9	137.1	153.0	143.2	134.9	261.1
ν7	267.6	214.6	215.3	236.7	234.2	274.2
ν8	311.1	245.5	225.8	274.2	255.5	274.2
ν9	360.1	295.0	338.4	284.8	275.2	410.6
ν10	380.4	393.1	344.7	333.5	324.3	410.6
ν11	398.6	408.4	407.8	350.8	364.1	422.2
ν12	430.9	416.8	416.4	406.9	399.9	434.4
ν13	453.4	419.8	418.9	421.1	417.8	438.9
ν14	457.1	424.4	428.0	421.1	419.1	438.9
ν15	514.6	425.1	460.7	492.0	520.0	556.5
ν16	550.9	529.3	498.7	503.1	534.2	556.5
ν17	568.3	534.1	545.2	551.6	572.9	567.7

ν18	578.9	584.0	584.4	628.5	577.3	586.1
ν19	596.8	629.1	629.0	629.7	629.9	621.2
ν20	614.6	633.4	632.6	632.9	632.3	637.4
ν21	635.9	636.1	637.0	637.3	639.1	637.4
ν22	683.8	658.7	658.4	649.1	641.3	713.8
ν23	699.0	714.6	714.6	718.3	719.8	729.4
ν24	723.3	718.6	718.1	719.5	720.0	729.4
ν25	750.3	718.9	718.4	725.9	725.4	758.9
ν26	763.8	750.9	752.9	727.2	766.3	790.0
ν27	771.9	777.3	774.2	774.4	767.4	790.0
ν28	783.2	792.3	792.1	788.9	789.0	791.3
ν29	791.9	796.3	798.6	824.6	795.2	791.3
ν30	798.2	857.0	857.1	828.5	804.1	794.2
ν31	847.4	862.8	862.2	864.0	862.9	871.3
ν32	886.4	862.8	862.3	864.5	862.9	871.3
ν33	903.5	869.5	869.7	927.7	900.0	890.4
ν34	943.2	938.8	940.1	929.7	940.2	949.9
ν35	946.9	944.7	942.7	947.7	943.9	949.9
ν36	964.9	987.0	987.1	952.0	977.1	968.5
ν37	970.7	991.4	991.1	993.2	990.8	984.6
ν38	984.4	991.4	991.3	993.2	991.1	994.6
ν39	994.1	995.0	993.9	1000.5	1002.6	994.6
ν40	996.0	1007.7	1007.6	1009.3	1007.7	1022.2
ν41	1004.4	1007.9	1007.8	1009.3	1008.1	1022.2
ν42	1017.9	1016.1	1016.0	1013.5	1017.1	1028.7
ν43	1025.9	1020.1	1020.6	1021.3	1019.8	1079.5
ν44	1044.9	1028.3	1028.1	1022.5	1029.6	1079.5
ν45	1076.7	1030.5	1030.3	1034.0	1031.3	1089.5
ν46	1080.0	1050.0	1050.0	1052.4	1059.9	1137.1
ν47	1118.3	1061.9	1062.0	1065.5	1061.2	1137.1
ν48	1137.4	1071.9	1071.9	1087.1	1086.9	1172.9
ν49	1154.5	1106.4	1106.3	1106.1	1103.9	1195.3
ν50	1186.0	1106.9	1106.9	1106.6	1106.2	1195.3
ν51	1189.4	1144.7	1145.1	1122.4	1141.6	1208.3
ν52	1196.4	1184.7	1184.8	1184.9	1184.1	1247.1
ν53	1203.6	1184.8	1185.0	1184.9	1184.5	1273.2
ν54	1229.9	1207.2	1207.3	1200.0	1189.3	1273.2
ν55	1253.8	1209.3	1209.3	1208.8	1207.4	1321.3
ν56	1267.2	1220.5	1220.7	1209.3	1208.5	1321.3

ν57	1295.9	1287.1	1287.0	1265.0	1267.4	1325.4	
ν58	1304.9	1304.3	1304.1	1291.7	1277.7	1359.8	
ν59	1315.8	1307.6	1307.2	1308.7	1302.9	1368.3	
ν60	1331.4	1310.2	1309.7	1324.1	1311.1	1368.3	
ν61	1335.7	1323.7	1324.1	1331.8	1322.6	1472.5	
ν62	1344.4	1349.0	1349.1	1352.9	1327.4	1472.5	
ν63	1406.1	1360.7	1360.8	1358.6	1360.3	1480.4	
ν64	1435.7	1365.5	1365.5	1365.2	1361.2	1496.7	
ν65	1473.5	1436.2	1436.3	1437.3	1466.1	1537.0	
ν66	1486.1	1477.8	1477.8	1480.1	1478.8	1537.0	
ν67	1509.2	1489.5	1489.5	1492.5	1489.6	1589.7	
ν68	1522.4	1523.4	1523.5	1516.3	1512.5	1618.8	
ν69	1533.2	1533.1	1533.2	1534.8	1533.4	1618.8	
ν70	1594.3	1557.2	1557.0	1539.4	1539.1	1648.0	
ν71	1610.1	1588.5	1588.2	1610.4	1601.6	1648.0	
ν72	1619.1	1618.7	1618.8	1617.6	1618.0	1654.1	
ν73	1633.1	1623.0	1623.2	1626.2	1622.7	3167.3	
ν74	1642.0	1642.5	1642.3	1640.1	1638.0	3168.4	
ν75	2825.8	1644.5	1644.4	1645.2	1644.9	3168.4	
ν76	3159.0	1652.4	1652.3	1645.3	1645.0	3182.2	
ν77	3163.7	3162.1	3162.2	3162.0	3160.4	3182.2	
ν78	3165.9	3162.3	3162.4	3162.0	3160.5	3184.9	
ν79	3167.3	3167.1	3167.3	3165.9	3163.9	3199.0	
ν80	3176.5	3168.6	3168.9	3168.5	3167.8	3202.0	
ν81	3179.9	3169.0	3169.1	3168.7	3168.0	3202.0	
ν82	3182.9	3171.3	3171.6	3177.6	3172.6	3219.8	
ν83	3187.7	3179.1	3179.2	3178.2	3177.3	3219.8	
ν84	3192.6	3180.1	3180.3	3181.1	3177.5	3221.9	
ν85	3196.1	3183.1	3183.3	3182.3	3182.1		
ν86	3198.1	3185.4	3185.6	3185.2	3185.7		
ν87	3201.3	3187.1	3187.4	3185.8	3185.7		
ν88		3187.6	3188.0	3191.1	3191.8		
ν89		3192.8	3193.0	3192.6	3192.9		
ν90		3193.2	3193.4	3193.2	3193.0		
							
ν1	173.2	29.0	23.0	46.0	52.3	95.7	89.7
ν2	187.1	36.3	35.0	71.2	74.9	114.9	97.8

ν3	366.4	66.0	77.5	91.0	88.3	158.9	170.5
ν4	397.7	155.4	163.3	170.9	169.8	197.6	191.1
ν5	482.9	172.8	179.0	181.3	183.0	231.6	240.6
ν6	489.3	244.2	251.4	248.5	241.8	282.6	269.5
ν7	519.8	264.7	274.7	293.3	293.6	341.8	348.4
ν8	521.1	299.7	292.2	315.5	317.2	411.1	411.3
ν9	637.3	380.5	372.3	411.9	414.7	436.4	424.1
ν10	639.4	416.4	406.3	427.0	419.4	467.3	465.1
ν11	732.5	430.5	416.8	446.3	456.3	477.5	481.3
ν12	775.3	479.5	458.1	484.2	476.4	492.5	490.9
ν13	792.5	483.9	506.6	503.6	503.0	536.9	521.4
ν14	803.3	515.3	529.5	531.0	526.2	548.8	560.5
ν15	811.6	537.1	539.6	562.7	565.9	558.0	566.0
ν16	853.4	562.9	558.5	583.9	584.5	608.0	592.6
ν17	904.8	617.2	617.4	623.8	630.3	617.5	625.9
ν18	956.6	634.4	635.5	632.5	633.6	633.3	637.9
ν19	964.8	650.1	644.9	663.1	650.5	676.4	647.3
ν20	982.0	690.0	713.1	706.9	712.4	694.8	688.0
ν21	997.4	719.3	716.5	719.3	717.5	745.5	738.3
ν22	1003.4	728.8	723.2	749.1	752.6	760.6	762.3
ν23	1037.3	760.1	754.2	757.8	776.4	762.8	776.9
ν24	1047.8	774.9	766.2	800.3	786.2	781.9	791.9
ν25	1154.6	795.6	779.3	809.2	802.6	800.1	812.2
ν26	1170.9	799.6	798.8	822.0	834.2	822.5	817.7
ν27	1174.6	811.2	824.0	844.2	846.1	847.4	850.7
ν28	1187.4	845.7	854.1	863.1	860.6	879.3	879.8
ν29	1234.6	861.3	861.6	890.2	892.1	892.7	899.0
ν30	1275.4	891.1	874.7	933.8	929.4	899.8	916.3
ν31	1292.1	931.4	907.8	953.7	943.5	957.8	924.8
ν32	1393.1	939.8	933.4	976.6	965.0	962.9	970.3
ν33	1397.4	965.9	950.0	980.0	979.4	971.8	976.0
ν34	1424.9	971.4	956.2	992.1	990.5	978.7	980.3
ν35	1496.2	987.0	981.7	994.7	993.5	995.1	986.8
ν36	1496.9	991.9	987.4	996.6	1007.5	1026.3	991.4
ν37	1551.3	999.3	1001.4	1002.7	1020.5	1047.4	1026.0
ν38	1614.2	1007.8	1007.5	1046.1	1042.9	1070.2	1055.0
ν39	1642.7	1023.3	1023.3	1051.2	1054.8	1075.3	1066.1
ν40	1670.3	1053.6	1043.7	1086.2	1087.1	1108.2	1074.3
ν41	3156.7	1062.3	1053.5	1123.0	1107.2	1133.5	1130.2

ν42	3158.6	1097.1	1084.0	1143.3	1134.9	1159.1	1150.5
ν43	3160.8	1103.6	1103.5	1171.9	1168.2	1175.1	1164.5
ν44	3164.2	1142.0	1140.8	1178.2	1184.8	1182.2	1181.2
ν45	3175.0	1178.9	1165.3	1189.0	1191.8	1194.3	1195.8
ν46	3176.3	1182.3	1178.5	1211.2	1208.5	1198.9	1209.9
ν47	3187.9	1183.6	1183.7	1233.5	1212.5	1228.0	1236.5
ν48	3188.9	1194.7	1196.4	1252.4	1240.8	1234.3	1255.5
ν49		1205.5	1205.7	1275.3	1304.2	1286.3	1274.8
ν50		1207.3	1208.6	1308.3	1312.8	1293.8	1289.7
ν51		1234.0	1229.0	1324.3	1348.5	1320.0	1323.5
ν52		1237.8	1257.6	1363.5	1354.3	1324.8	1364.6
ν53		1275.1	1300.3	1386.3	1366.4	1360.6	1383.7
ν54		1306.0	1317.7	1429.6	1401.5	1380.9	1399.0
ν55		1338.3	1339.0	1440.8	1459.9	1426.7	1424.5
ν56		1340.8	1342.5	1476.6	1462.6	1469.8	1437.7
ν57		1369.0	1367.5	1479.9	1485.8	1473.8	1463.9
ν58		1391.6	1416.5	1499.6	1513.6	1496.4	1484.9
ν59		1441.6	1432.7	1548.5	1532.6	1508.0	1523.1
ν60		1472.2	1463.4	1568.3	1589.5	1530.4	1525.1
ν61		1488.6	1488.3	1614.0	1615.2	1610.3	1597.3
ν62		1518.3	1506.0	1629.6	1634.2	1617.5	1613.4
ν63		1529.9	1529.6	1637.3	1642.4	1620.4	1627.9
ν64		1555.3	1562.6	1661.5	1653.1	1647.5	1648.4
ν65		1596.7	1604.0	3158.8	3158.1	2841.5	2827.6
ν66		1626.3	1626.0	3159.2	3161.3	3155.9	3156.8
ν67		1628.4	1641.9	3162.4	3161.7	3160.5	3159.9
ν68		1642.8	1669.5	3165.5	3168.9	3161.7	3160.4
ν69		2943.0	2906.2	3170.7	3169.4	3167.0	3161.3
ν70		3153.1	3146.7	3174.7	3174.9	3174.1	3170.7
ν71		3154.7	3153.4	3176.0	3179.7	3177.8	3174.9
ν72		3157.2	3156.3	3185.2	3181.7	3178.7	3178.8
ν73		3162.0	3159.7	3187.7	3186.9	3185.9	3183.6
ν74		3162.4	3162.0	3188.9	3188.8	3187.1	3185.8
ν75		3171.2	3162.7	3199.6	3193.4	3190.1	3191.7
ν76		3174.5	3171.0				
ν77		3175.6	3171.1				
ν78		3179.2	3175.6				
ν79		3184.6	3179.1				
ν80		3189.1	3189.3				

ν81		3189.4	3190.1
			
ν1	44.2	52.8	103.0
ν2	75.4	62.8	122.9
ν3	84.8	94.2	166.8
ν4	169.4	172.8	207.6
ν5	183.7	188.5	257.2
ν6	245.2	262.9	299.3
ν7	293.6	278.3	357.1
ν8	316.5	339.6	440.1
ν9	411.7	404.6	441.7
ν10	418.4	419.7	471.0
ν11	446.7	437.2	478.5
ν12	483.9	490.1	494.6
ν13	505.5	516.7	571.8
ν14	531.9	529.0	572.8
ν15	571.8	560.6	579.9
ν16	587.4	571.2	629.0
ν17	633.9	634.3	637.9
ν18	635.5	644.5	656.9
ν19	670.7	674.0	686.8
ν20	712.3	711.9	755.8
ν21	722.0	718.0	762.0
ν22	752.5	758.9	779.2
ν23	783.9	780.5	796.7
ν24	801.9	787.3	803.1
ν25	809.8	796.5	820.0
ν26	825.7	841.2	850.6
ν27	845.3	862.4	891.2
ν28	865.8	872.4	909.3
ν29	891.8	882.1	922.4
ν30	931.9	925.0	931.0
ν31	945.5	944.9	957.4
ν32	978.5	962.6	982.9
ν33	983.4	973.4	991.1
ν34	992.0	990.0	992.1
ν35	993.6	992.2	995.1

ν36	1004.0	1000.1	1040.9
ν37	1009.8	1008.3	1045.9
ν38	1021.3	1020.2	1063.5
ν39	1046.8	1039.9	1109.6
ν40	1054.9	1046.4	1125.4
ν41	1083.7	1065.6	1164.2
ν42	1104.3	1107.0	1185.1
ν43	1142.8	1157.8	1187.2
ν44	1171.7	1175.5	1210.7
ν45	1184.3	1184.1	1237.3
ν46	1187.8	1185.5	1258.5
ν47	1207.0	1209.1	1294.9
ν48	1210.8	1221.2	1322.7
ν49	1237.5	1258.9	1342.3
ν50	1275.9	1294.2	1398.0
ν51	1309.5	1301.5	1405.4
ν52	1316.7	1316.5	1444.9
ν53	1354.9	1357.5	1458.0
ν54	1369.5	1384.0	1476.5
ν55	1386.9	1398.1	1490.1
ν56	1430.1	1405.8	1510.0
ν57	1468.8	1464.7	1525.7
ν58	1484.0	1488.5	1616.1
ν59	1497.6	1504.5	1641.7
ν60	1531.7	1534.2	1643.7
ν61	1548.9	1546.4	1646.2
ν62	1613.9	1605.7	1659.0
ν63	1618.5	1619.5	3161.7
ν64	1636.6	1643.7	3162.4
ν65	1643.7	1644.5	3162.4
ν66	1661.2	1668.6	3168.3
ν67	3158.7	3157.7	3172.1
ν68	3160.9	3160.4	3173.0
ν69	3161.4	3161.3	3178.6
ν70	3167.5	3163.1	3185.2
ν71	3170.2	3166.5	3186.0
ν72	3172.5	3169.4	3190.6
ν73	3177.3	3175.9	
ν74	3183.0	3178.1	

ν75	3185.2	3183.2
ν76	3186.7	3185.7
ν77	3191.2	3188.6
ν78	3202.6	3192.0

	tsi1	tsi1p1	tsi2	tsi2p2	tsi3	tsi3p3	tsp3i4 (H)
ν1	-317.1	-917.5	-332.0	-949.3	-320.7	-819.2	-898.2
ν2	15.0	37.4	14.5	42.8	25.8	47.9	44.9
ν3	26.0	46.1	27.3	46.1	37.0	54.1	49.1
ν4	43.5	66.4	46.1	59.1	49.1	60.3	58.7
ν5	76.0	83.7	80.3	97.4	78.0	102.3	90.4
ν6	93.0	126.5	94.3	113.2	96.8	107.5	101.5
ν7	116.8	137.0	108.5	143.8	122.6	138.6	128.0
ν8	138.5	213.6	144.2	233.3	139.9	225.8	182.3
ν9	164.3	240.2	171.6	268.9	165.6	255.7	233.2
ν10	262.3	294.0	271.3	269.5	243.4	281.9	246.2
ν11	320.6	383.2	314.6	328.0	322.3	314.3	260.0
ν12	368.5	403.2	358.1	350.6	361.3	358.6	290.6
ν13	400.8	406.0	390.2	404.3	394.4	406.7	322.6
ν14	417.0	418.9	399.9	419.2	400.4	418.5	362.2
ν15	422.6	419.5	421.0	419.2	421.5	419.4	400.2
ν16	443.2	421.6	445.8	439.7	447.9	453.7	418.5
ν17	467.5	447.3	499.5	488.3	498.9	508.0	424.4
ν18	534.1	522.0	545.0	505.1	562.1	534.3	520.2
ν19	582.8	527.5	590.9	552.5	577.6	558.7	531.1
ν20	614.9	557.5	615.4	564.6	614.9	570.9	573.6
ν21	623.1	585.6	624.3	628.2	623.0	577.8	576.4
ν22	625.7	631.5	626.0	631.6	624.1	628.7	620.2
ν23	640.3	633.6	638.7	637.4	639.7	632.5	624.3
ν24	696.0	636.6	691.3	639.8	696.0	638.3	634.5
ν25	715.9	653.9	696.6	648.5	715.7	640.8	638.8
ν26	718.1	711.8	719.1	704.9	718.6	713.8	714.9
ν27	730.8	716.8	731.4	718.1	732.5	718.5	720.2
ν28	753.2	718.5	756.9	718.5	750.4	719.5	725.8
ν29	772.7	745.3	767.9	727.3	754.5	759.6	759.5
ν30	813.4	776.9	802.0	773.0	796.4	772.2	767.3
ν31	839.3	786.1	839.6	787.4	839.9	786.7	787.1
ν32	842.1	798.5	863.8	818.5	861.4	792.9	788.1
ν33	860.8	843.6	866.0	829.4	864.3	805.9	801.3

ν34	885.3	860.5	905.4	861.0	894.2	860.5	863.8
ν35	907.4	861.1	906.1	863.4	907.9	863.0	869.9
ν36	937.9	867.2	907.0	911.6	939.3	896.1	900.5
ν37	972.2	938.5	945.1	925.0	966.4	939.4	927.9
ν38	975.2	943.0	971.7	943.9	972.9	943.9	942.2
ν39	988.9	987.6	989.3	946.5	991.2	974.5	959.9
ν40	991.3	990.0	992.0	990.4	992.8	989.5	972.1
ν41	997.6	991.7	997.3	992.4	999.1	992.0	978.7
ν42	999.8	993.3	1000.0	997.0	1000.5	999.7	991.7
ν43	1007.0	1007.9	1008.4	1004.9	1007.8	1007.5	998.8
ν44	1012.1	1008.3	1010.1	1008.5	1009.8	1008.6	1004.1
ν45	1020.6	1012.4	1020.3	1009.3	1020.7	1014.0	1008.6
ν46	1022.8	1020.3	1024.3	1020.7	1024.8	1020.1	1018.1
ν47	1031.4	1023.1	1038.5	1021.9	1036.2	1025.6	1023.6
ν48	1043.6	1027.5	1050.0	1032.8	1054.2	1029.7	1028.9
ν49	1058.6	1043.4	1062.4	1051.2	1058.2	1058.7	1031.4
ν50	1064.6	1060.9	1065.3	1064.8	1064.7	1060.7	1059.9
ν51	1081.8	1067.3	1082.7	1077.9	1082.3	1081.0	1063.8
ν52	1093.4	1106.1	1089.1	1105.7	1088.6	1103.7	1087.1
ν53	1107.3	1107.6	1106.8	1106.6	1110.4	1106.5	1103.9
ν54	1178.6	1144.7	1178.4	1120.4	1179.0	1140.7	1130.9
ν55	1178.7	1184.9	1178.8	1184.7	1182.4	1184.0	1143.3
ν56	1184.9	1185.4	1184.6	1185.0	1185.7	1184.8	1182.0
ν57	1185.8	1207.3	1186.3	1197.0	1185.9	1188.1	1184.4
ν58	1205.3	1209.6	1193.9	1208.8	1200.0	1207.9	1189.8
ν59	1212.1	1216.3	1209.2	1209.3	1215.1	1209.8	1208.3
ν60	1287.5	1274.6	1294.1	1256.2	1291.4	1259.2	1252.2
ν61	1305.3	1290.7	1296.9	1282.5	1292.3	1267.8	1267.2
ν62	1321.2	1305.6	1321.7	1308.8	1320.8	1296.5	1286.4
ν63	1322.9	1307.7	1322.6	1321.7	1322.5	1305.3	1307.8
ν64	1329.2	1322.5	1329.8	1322.3	1328.8	1321.4	1316.9
ν65	1362.3	1344.2	1355.6	1348.9	1359.0	1328.2	1322.4
ν66	1365.0	1361.1	1362.3	1358.1	1367.1	1360.1	1327.0
ν67	1468.0	1365.0	1451.1	1363.5	1449.7	1363.3	1361.8
ν68	1469.7	1441.9	1469.8	1420.0	1469.6	1459.7	1446.6
ν69	1484.5	1476.3	1484.7	1479.5	1484.5	1475.1	1469.3
ν70	1494.2	1489.4	1489.0	1489.1	1490.0	1487.2	1485.0
ν71	1506.4	1516.1	1511.6	1506.8	1516.4	1499.8	1486.3
ν72	1536.1	1532.8	1535.6	1533.3	1538.3	1531.4	1517.9

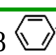
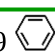
ν73	1563.8	1543.8	1580.0	1535.4	1575.8	1533.7	1536.5
ν74	1583.1	1557.6	1586.4	1592.7	1583.9	1579.3	1580.0
ν75	1611.8	1618.2	1602.8	1611.6	1610.0	1615.1	1603.6
ν76	1616.9	1621.3	1620.7	1621.8	1618.1	1619.6	1619.6
ν77	1627.7	1629.3	1627.7	1624.4	1626.9	1624.6	1628.8
ν78	1642.5	1643.9	1644.6	1644.2	1642.2	1642.6	1639.0
ν79	3144.2	1645.0	3143.8	1645.0	3144.0	1643.2	1644.1
ν80	3153.8	3161.8	3154.7	3161.7	3155.0	3160.7	2315.3
ν81	3162.1	3162.1	3161.4	3161.8	3162.4	3161.0	3159.7
ν82	3162.8	3167.8	3162.3	3167.0	3164.0	3166.3	3160.5
ν83	3165.6	3169.0	3163.7	3168.3	3165.5	3168.6	3164.7
ν84	3167.8	3171.3	3166.6	3168.9	3170.0	3168.6	3168.0
ν85	3169.5	3173.3	3168.9	3177.6	3171.4	3175.7	3169.8
ν86	3171.5	3178.4	3171.2	3177.8	3172.7	3177.7	3174.5
ν87	3177.0	3180.0	3178.0	3182.8	3178.0	3178.3	3177.5
ν88	3181.5	3184.0	3182.5	3183.5	3183.5	3185.7	3178.0
ν89	3184.5	3185.2	3183.7	3186.5	3185.8	3186.3	3183.9
ν90	3185.0	3189.5	3185.0	3187.6	3186.7	3186.7	3185.7
ν91	3187.8	3190.7	3186.3	3191.7	3191.6	3193.0	3189.6
ν92	3191.9	3192.4	3191.7	3192.1	3194.9	3193.4	3192.6
ν93	3193.6	3193.4	3193.1	3194.3	3200.8	3194.2	3193.0

	tsp3i4 	tsi4i5	tsi5p4
ν1	-1623.1	-249.3	-959.6
ν2	12.5	56.2	52.1
ν3	15.4	76.0	62.6
ν4	25.9	98.6	113.7
ν5	48.3	106.7	122.2
ν6	51.3	164.4	247.9
ν7	60.9	222.2	250.1
ν8	87.5	238.4	272.7
ν9	98.0	271.0	286.3
ν10	112.2	335.1	386.2
ν11	142.2	372.5	407.0
ν12	154.7	399.5	408.2
ν13	177.2	411.7	426.8
ν14	240.8	442.1	437.0
ν15	262.1	471.3	442.8
ν16	288.3	546.5	487.8

ν17	326.9	563.1	502.0
ν18	366.5	581.7	560.0
ν19	400.6	589.6	562.5
ν20	404.9	620.4	575.3
ν21	418.5	627.4	584.3
ν22	430.3	632.7	623.2
ν23	442.0	712.3	634.9
ν24	522.7	721.4	638.3
ν25	535.9	734.3	708.0
ν26	574.7	749.1	730.2
ν27	577.9	756.0	738.8
ν28	619.6	782.6	757.8
ν29	620.8	787.3	784.9
ν30	627.2	797.6	790.1
ν31	634.2	851.5	791.6
ν32	639.6	869.6	796.1
ν33	680.1	891.0	802.8
ν34	702.3	898.5	876.4
ν35	719.4	951.1	877.6
ν36	727.1	959.5	898.9
ν37	729.3	974.1	959.0
ν38	737.3	990.7	961.5
ν39	763.8	991.9	969.3
ν40	766.8	999.0	989.0
ν41	789.8	1001.4	995.5
ν42	790.4	1014.7	996.6
ν43	802.1	1025.4	1015.0
ν44	849.3	1034.8	1022.8
ν45	863.1	1055.0	1027.9
ν46	881.0	1061.3	1072.2
ν47	900.4	1082.5	1079.8
ν48	914.4	1089.1	1086.5
ν49	941.2	1122.7	1133.8
ν50	963.2	1144.4	1134.8
ν51	977.9	1181.4	1171.7
ν52	979.2	1181.7	1193.0
ν53	990.5	1190.3	1194.4
ν54	993.0	1195.2	1205.5
ν55	1000.4	1248.2	1247.1

ν56	1003.7	1273.9	1265.9
ν57	1004.8	1287.7	1270.0
ν58	1007.5	1305.9	1310.5
ν59	1018.1	1319.5	1317.1
ν60	1019.1	1323.0	1324.9
ν61	1026.1	1334.0	1348.1
ν62	1030.7	1348.5	1361.2
ν63	1044.0	1442.2	1364.3
ν64	1060.0	1457.7	1465.2
ν65	1060.7	1477.6	1470.2
ν66	1078.6	1492.8	1477.0
ν67	1080.5	1510.1	1494.1
ν68	1093.8	1528.7	1527.3
ν69	1103.9	1576.0	1535.0
ν70	1121.6	1591.3	1578.3
ν71	1141.0	1602.9	1603.1
ν72	1167.9	1610.5	1619.2
ν73	1181.2	1631.8	1636.4
ν74	1184.0	1638.9	1645.4
ν75	1184.5	3151.0	1650.6
ν76	1189.8	3161.4	3168.1
ν77	1190.3	3162.2	3169.0
ν78	1208.2	3164.4	3170.0
ν79	1243.1	3167.8	3182.3
ν80	1266.6	3170.2	3183.2
ν81	1280.2	3173.6	3185.8
ν82	1292.6	3174.6	3197.8
ν83	1307.7	3182.6	3200.3
ν84	1317.5	3184.2	3203.4
ν85	1323.1	3187.1	3215.7
ν86	1327.0	3191.1	3217.2
ν87	1331.1	3194.3	3223.0
ν88	1361.4		
ν89	1377.0		
ν90	1459.8		
ν91	1471.6		
ν92	1480.3		
ν93	1486.6		
ν94	1499.4		

ν95	1505.1
ν96	1519.5
ν97	1536.5
ν98	1590.4
ν99	1602.7
ν100	1605.1
ν101	1619.8
ν102	1625.7
ν103	1630.7
ν104	1638.7
ν105	1644.0
ν106	3154.2
ν107	3157.2
ν108	3160.0
ν109	3160.3
ν110	3164.3
ν111	3167.3
ν112	3167.9
ν113	3169.5
ν114	3174.7
ν115	3175.2
ν116	3176.8
ν117	3177.5
ν118	3184.2
ν119	3185.8
ν120	3186.4
ν121	3188.3
ν122	3192.9
ν123	3193.3

	tsi6	tsi6p5	tsi7	tsi7p6	tsp5i8 	tsp5i9 
ν1	-294.5	-807.7	-311.0	-917.2	-1610.9	-1679.5
ν2	11.9	43.4	12.9	50.1	15.4	16.6
ν3	34.1	75.0	32.9	60.3	20.8	24.9
ν4	53.9	85.3	55.8	91.1	28.3	34.2
ν5	112.3	167.4	115.1	174.4	52.4	51.0
ν6	123.8	188.5	129.6	185.1	72.4	68.1
ν7	176.5	245.7	186.7	265.4	80.7	83.1
ν8	197.2	286.7	204.2	271.7	125.7	123.7

ν9	363.0	309.1	367.3	333.5	140.5	135.6
ν10	369.0	407.3	384.1	383.7	166.7	168.0
ν11	399.5	417.9	399.8	419.4	177.9	179.8
ν12	440.1	422.3	441.4	430.1	200.5	208.6
ν13	475.2	444.2	449.2	438.1	256.4	245.0
ν14	498.3	486.7	490.3	487.1	299.0	299.9
ν15	516.2	502.5	516.2	517.5	329.1	322.2
ν16	519.5	526.4	523.5	526.0	405.8	405.5
ν17	570.7	538.7	568.2	544.9	409.1	415.7
ν18	613.9	576.0	614.6	565.3	433.3	425.6
ν19	625.3	580.4	629.7	583.8	441.3	445.1
ν20	640.0	635.7	635.2	635.1	447.7	465.7
ν21	693.9	637.7	695.0	643.1	484.5	485.8
ν22	729.1	666.0	730.6	672.3	508.2	509.5
ν23	736.7	713.2	748.2	712.3	532.2	530.7
ν24	767.9	721.7	770.1	718.3	574.5	573.5
ν25	789.5	748.2	776.1	760.2	588.0	590.9
ν26	801.4	784.4	807.7	777.0	620.6	619.4
ν27	809.6	794.6	819.7	783.7	622.4	623.1
ν28	836.5	807.7	838.4	791.0	631.6	633.3
ν29	855.9	824.1	843.6	834.6	669.6	656.0
ν30	887.8	845.0	895.2	860.3	680.9	667.2
ν31	904.7	864.1	903.7	869.9	702.4	700.6
ν32	914.6	890.9	906.0	881.8	716.8	719.3
ν33	958.7	921.6	953.3	915.2	732.0	730.0
ν34	970.2	944.6	966.8	943.0	738.5	739.8
ν35	971.3	978.1	971.1	957.9	752.5	766.8
ν36	984.7	982.7	988.6	971.9	774.4	783.4
ν37	997.6	989.4	995.9	990.5	801.3	794.2
ν38	998.7	992.9	999.6	991.6	810.0	806.9
ν39	1003.9	1003.3	1003.7	999.7	824.0	843.0
ν40	1024.9	1009.6	1018.5	1008.4	846.3	846.4
ν41	1037.6	1021.8	1032.0	1020.6	849.0	861.2
ν42	1050.2	1048.2	1045.0	1033.0	885.8	864.3
ν43	1056.4	1055.2	1057.8	1044.9	890.8	911.4
ν44	1081.3	1087.8	1081.9	1061.2	914.5	916.8
ν45	1143.1	1105.3	1140.4	1106.4	936.4	933.9
ν46	1165.4	1138.0	1163.3	1156.2	965.7	943.7
ν47	1170.7	1169.9	1173.6	1175.3	977.7	972.9

ν48	1178.5	1184.1	1178.6	1183.4	979.4	978.2
ν49	1184.6	1186.3	1183.8	1185.0	984.3	985.1
ν50	1185.2	1203.8	1185.4	1209.1	993.0	991.5
ν51	1222.0	1207.5	1227.3	1218.4	994.1	994.1
ν52	1265.0	1237.6	1271.3	1251.9	1001.0	1002.2
ν53	1288.4	1270.1	1292.7	1288.4	1003.8	1008.6
ν54	1319.9	1308.8	1321.0	1297.4	1004.6	1017.2
ν55	1328.4	1309.9	1328.8	1316.0	1019.2	1021.6
ν56	1372.0	1346.0	1381.3	1353.5	1044.4	1032.6
ν57	1381.9	1362.0	1395.5	1374.7	1046.3	1051.7
ν58	1419.5	1378.3	1421.3	1388.9	1054.2	1057.0
ν59	1469.0	1423.7	1469.5	1409.9	1079.1	1066.4
ν60	1479.8	1467.5	1479.3	1461.6	1083.1	1078.2
ν61	1487.6	1482.8	1486.6	1486.9	1086.1	1091.8
ν62	1492.5	1489.7	1490.2	1493.9	1123.0	1104.9
ν63	1540.0	1530.3	1536.1	1532.4	1144.0	1140.8
ν64	1581.1	1545.1	1580.9	1534.6	1172.0	1169.5
ν65	1590.0	1594.5	1587.0	1590.3	1175.9	1177.9
ν66	1608.1	1614.9	1626.2	1620.4	1181.2	1184.5
ν67	1627.4	1619.5	1627.8	1634.5	1186.7	1189.5
ν68	1654.4	1642.6	1645.4	1643.8	1188.4	1193.6
ν69	3143.8	1655.2	3143.4	1653.6	1190.3	1204.0
ν70	3153.3	3160.7	3153.1	3160.1	1211.0	1206.4
ν71	3158.2	3162.6	3156.8	3162.6	1236.8	1215.7
ν72	3161.0	3164.4	3159.1	3163.1	1241.8	1237.1
ν73	3162.5	3169.9	3162.1	3165.6	1275.4	1296.3
ν74	3163.8	3172.5	3162.4	3169.3	1287.8	1310.9
ν75	3169.6	3177.6	3166.4	3173.5	1313.7	1317.6
ν76	3170.2	3179.5	3169.0	3178.1	1325.6	1327.3
ν77	3176.1	3185.4	3175.7	3179.8	1331.0	1352.3
ν78	3178.0	3186.7	3178.1	3185.8	1365.7	1359.2
ν79	3184.2	3190.7	3184.4	3190.5	1368.0	1364.8
ν80	3188.9	3192.6	3188.6	3191.1	1387.7	1368.2
ν81	3190.7	3201.8	3189.5	3193.3	1428.8	1414.0
ν82					1461.0	1463.9
ν83					1475.3	1477.7
ν84					1482.5	1484.2
ν85					1495.3	1485.1
ν86					1504.0	1504.8

ν87					1507.5	1528.0
ν88					1548.6	1533.4
ν89					1590.3	1597.8
ν90					1605.0	1603.8
ν91					1617.0	1617.1
ν92					1626.7	1627.5
ν93					1630.3	1635.4
ν94					1637.6	1644.3
ν95					1661.3	1650.6
ν96					3154.6	3153.7
ν97					3157.9	3157.5
ν98					3159.3	3160.3
ν99					3160.6	3160.4
ν100					3162.4	3160.6
ν101					3165.2	3166.8
ν102					3170.0	3167.2
ν103					3170.8	3170.1
ν104					3174.9	3172.9
ν105					3175.9	3176.2
ν106					3176.6	3176.8
ν107					3185.4	3181.9
ν108					3186.5	3182.6
ν109					3187.3	3186.0
ν110					3190.1	3187.4
ν111					3200.3	3191.6

	tsp5i9 (H)	tsp5i8 (H)	tsi8i10	tsi9i11	tsi10p7	tsi11p7
ν1	-959.1	-890.5	-444.5	-423.2	-870.9	-899.9
ν2	37.3	42.6	84.7	80.5	104.3	106.1
ν3	70.7	75.6	101.3	101.5	123.3	118.0
ν4	82.9	81.7	160.2	169.9	170.7	167.4
ν5	155.2	167.4	191.1	184.3	205.0	204.8
ν6	167.9	177.6	254.8	231.3	252.2	252.5
ν7	210.7	180.8	262.3	288.5	286.1	291.8
ν8	242.0	241.1	352.0	352.4	347.5	353.3
ν9	292.8	261.1	407.1	399.2	374.7	387.3
ν10	316.0	298.7	420.7	425.9	436.6	431.9
ν11	347.9	315.6	442.4	444.1	445.4	456.3
ν12	416.6	408.7	478.1	474.5	461.0	466.0

ν13	419.4	427.3	509.8	508.2	475.6	472.8
ν14	457.8	444.4	520.4	533.6	487.6	492.4
ν15	483.5	483.7	547.8	557.7	495.3	501.6
ν16	503.9	507.3	568.3	582.0	570.9	571.6
ν17	528.3	531.5	599.7	610.3	574.4	572.7
ν18	572.6	569.4	616.7	612.4	577.3	576.7
ν19	585.6	585.5	647.8	648.5	629.7	629.8
ν20	624.8	620.7	688.4	683.4	633.2	638.0
ν21	632.6	628.5	715.6	728.8	657.3	654.1
ν22	660.7	667.8	751.9	750.2	687.4	682.0
ν23	702.0	706.4	769.6	760.5	753.0	752.3
ν24	719.7	726.4	775.3	788.4	762.6	759.6
ν25	762.3	751.6	793.4	804.3	777.2	776.7
ν26	781.7	768.8	804.7	814.9	790.3	795.9
ν27	790.4	800.1	825.6	838.4	800.7	800.8
ν28	805.8	809.6	864.0	859.3	819.0	819.7
ν29	835.4	823.8	870.7	880.8	851.3	852.4
ν30	836.8	844.7	879.8	898.1	890.9	884.6
ν31	863.8	873.5	909.7	920.2	908.7	905.4
ν32	898.6	890.8	948.8	952.8	914.0	920.9
ν33	929.2	920.3	972.0	970.2	925.7	929.9
ν34	934.9	936.0	977.0	978.8	958.8	956.5
ν35	944.0	962.5	984.8	986.8	984.4	984.0
ν36	964.4	973.3	990.8	989.1	990.7	990.8
ν37	983.2	978.1	1004.9	1018.7	993.8	991.7
ν38	991.1	984.4	1041.5	1035.7	994.1	993.8
ν39	994.3	993.0	1055.3	1042.2	1045.7	1041.9
ν40	1009.0	1000.0	1080.2	1068.9	1046.5	1042.1
ν41	1021.4	1003.4	1117.7	1090.8	1068.7	1064.5
ν42	1030.0	1018.1	1141.4	1138.1	1109.4	1109.4
ν43	1053.5	1046.8	1156.4	1166.8	1124.4	1115.8
ν44	1071.6	1055.6	1177.3	1177.5	1161.0	1164.7
ν45	1098.9	1085.5	1181.6	1191.0	1184.8	1182.1
ν46	1106.3	1129.7	1202.4	1201.8	1185.5	1187.5
ν47	1134.2	1144.9	1227.0	1210.9	1209.1	1208.9
ν48	1168.3	1172.0	1250.4	1243.6	1234.9	1237.6
ν49	1184.5	1181.6	1266.6	1285.3	1254.0	1258.3
ν50	1198.5	1188.1	1316.3	1318.9	1294.1	1294.5
ν51	1207.1	1211.2	1323.6	1336.1	1322.1	1318.5

v52	1213.5	1237.1	1360.9	1361.0	1340.7	1333.6
v53	1240.7	1257.1	1373.2	1382.6	1386.4	1395.7
v54	1307.5	1277.5	1406.7	1419.0	1399.9	1398.2
v55	1311.5	1313.1	1441.5	1449.8	1428.0	1439.9
v56	1351.0	1323.1	1462.8	1458.1	1458.2	1455.8
v57	1360.5	1365.9	1474.8	1467.4	1468.4	1472.3
v58	1364.4	1387.2	1489.1	1506.7	1490.6	1481.5
v59	1397.1	1428.3	1523.9	1516.2	1505.7	1508.5
v60	1461.7	1447.8	1569.6	1566.2	1523.6	1526.3
v61	1471.6	1475.4	1585.5	1584.8	1609.0	1589.1
v62	1483.3	1486.4	1600.0	1600.2	1618.8	1626.9
v63	1519.6	1500.7	1620.2	1628.6	1633.8	1639.3
v64	1532.9	1548.8	1635.1	1648.7	1645.5	1640.0
v65	1594.1	1579.5	3129.6	3130.4	1648.6	1658.3
v66	1617.1	1616.1	3153.5	3153.7	3163.2	3162.8
v67	1634.9	1629.5	3159.4	3160.1	3163.7	3163.4
v68	1644.5	1637.0	3161.4	3163.0	3164.6	3165.0
v69	1651.5	1661.4	3162.7	3166.3	3170.1	3171.6
v70	2267.1	2335.5	3169.5	3169.0	3174.3	3173.5
v71	3159.5	3159.7	3173.9	3172.4	3177.1	3174.5
v72	3161.8	3160.2	3175.6	3177.9	3180.0	3182.4
v73	3162.3	3163.2	3185.1	3181.1	3186.7	3186.1
v74	3168.6	3166.7	3186.0	3185.7	3188.2	3186.9
v75	3168.7	3171.5	3187.5	3191.6	3191.4	3192.8
v76	3175.0	3176.0				
v77	3177.8	3176.5				
v78	3183.3	3186.4				
v79	3184.2	3188.3				
v80	3189.0	3189.8				
v81	3192.2	3201.7				

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