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Gas-Phase Synthesis of Corannulene – A Molecular Building Block of Fullerenes

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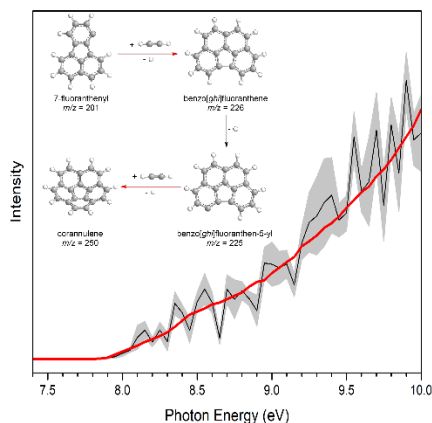
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Abstract: Fullerenes (C_{60} , C_{70}) detected in planetary nebulae and carbonaceous chondrites have been implicated to play a key role in the astrochemical evolution of the interstellar medium. However, the formation mechanism of even their simplest molecular building block — the corannulene molecule ($C_{20}H_{10}$) — has remained elusive. Here we demonstrate via a combined molecular beams and *ab initio* investigation that corannulene can be synthesized in the gas phase through the reactions of 7-fluoranthenyl ($C_{16}H_9^{\bullet}$) and benzo[ghi]fluoranthen-5-yl ($C_{18}H_9^{\bullet}$) radicals with acetylene (C_2H_2) mimicking conditions in carbon-rich circumstellar envelopes. This reaction sequence reveals a reaction class in which a polycyclic aromatic hydrocarbon (PAH) radical undergoes ring expansion while simultaneously forming an out-of-plane carbon backbone central to 3D nanostructures such as buckybowls and buckyballs. These fundamental reaction mechanisms are critical in facilitating an intimate understanding of the origin and evolution of the molecular universe and, in particular, of carbon in our galaxy.



Corannulene can be formed through molecular mass growth processes in circumstellar envelopes.

1. INTRODUCTION

For more than half a century, carbon-rich Asymptotic Giant Branch (AGB) stars such as IRC +10216 (CW Leonis)¹ and their descendants, planetary nebulae (PNe) like NGC 7293 (Helix Nebula),² have emerged as natural laboratories for developing our fundamental understanding of the chemical evolution of carbon-rich circumstellar envelopes (CSE).^{3,4} The ejection of carbonaceous matter at a level of some 10^{-5} solar masses per year causes the formation of extended envelopes at temperatures of a few 1,000 K close to the central star⁵ and drive the (photochemical) synthesis of hydrogen-deficient molecules like fullerenes (C_{60} , C_{70}).⁶ A fullerene is an allotrope of carbon whose carbon atoms are arranged via fused rings of five and six atoms to form a hollow, soccer-ball (C_{60}) or ellipsoid, rugby-ball type sphere (C_{70}) (Scheme 1).⁷ These circumstellar molecules act as the molecular feedstock for carbonaceous nanoparticles (interstellar grains),⁸ which in turn have been suggested to be linked to the formation of astrobiologically relevant organics (amino acids, sugars) on their ice coated surfaces through processing by ionizing radiation.⁹ Carbonaceous organics also contribute critically to the galactic carbon budget with up to 80% of the ejected material infused into the interstellar medium.^{6,10} However, with nearly 100 molecules detected in carbon-rich circumstellar environments, the fundamental processes involved in synthesizing the chemically most intriguing class of carbonaceous molecules - fullerenes¹¹⁻¹⁴ remain poorly explored. These pathways are critical to an understanding at the molecular level on how circumstellar envelopes — among them TC 1 as the planetary nebula toward which Buckminsterfullerene (C_{60}) was first observed via the 7.0, 8.5, 17.4, and 19.0 μm emissions¹¹ — evolve thus constraining the chemistry and the distribution of carbon in our galaxy.^{7,12,15-19}

In circumstellar envelopes, sophisticated *bottom-up* and *top-down* strategies have been advocated to synthesize fullerenes. Generic molecular mass growth processes incorporating often unsubstantiated gas-phase chemistries are implicated in the *bottom-up* synthesis from simple molecular building blocks involving a self-assembly of atomic carbon and dicarbon²⁰⁻²² and photochemical processing along with dehydrogenation of polycyclic aromatic hydrocarbons (PAHs) such as naphthalene in conjunction with nucleation of the C_{10} fragments.^{23,24} The *top-down* strategy favors an ultraviolet photo processing of complex PAHs such as $C_{66}H_{20}$ ²⁴⁻²⁷ or hydrogenated amorphous carbon particles near the central star.²⁸ These pathways likely involve graphene sheets, which have been suggested to be converted to fullerenes through atomic carbon

loss accompanied by formation of five-membered rings as a prerequisite to out-of-plane bent carbon sheets. In the laboratory, solid state routes revealed the conversion of graphene to buckminsterfullerene (C_{60}) by energetic electrons²⁹ and heating of proxies of circumstellar silicon carbide nanoparticles to 1,300 K while exposing the samples to 150 keV xenon ions.³⁰ These pathways complement synthetic routes involving targeted organic precursors with predominantly existing carbon connections via flash pyrolysis of, e.g., $C_{60}H_{27}Cl_3$,³¹⁻³⁵ laser-assisted cyclodehydrogenation of $C_{60}H_{30}$,³⁵ and platinum-catalyzed cyclodehydrogenation of precursors with prevailing fullerene-type carbon skeletons such as $C_{57}H_{33}N_3$ and $C_{60}H_{30}$.^{26, 36}

It is remarkable that both the bottom-up and top-down strategies to fullerenes have faced limited efficiencies under conditions prevailing in circumstellar envelopes²⁵ with observed abundances challenging high-temperature circumstellar reaction networks derived from the chemistry of sooty environments in hydrocarbon flames.³⁷ The impending involvement of PAHs within the framework of a bottom-up^{38, 39} and top-down²⁷ synthesis of circumstellar fullerenes advocates a promising link between PAHs and fullerenes considering that these are known to coexist towards, e.g., TC 1.¹¹ However, despite this possible connection between fullerenes and PAHs, even the synthetic routes to ‘bent’ PAHs such as corannulene ($C_{20}H_{10}$) in carbon rich circumstellar envelopes are still unknown. The carbon skeleton of corannulene — the simplest representative of a circulene in which a central polygon is surrounded by and fused with benzene rings — represents the fundamental molecular building block of fullerenes and hence may signify an essential reaction intermediate in the molecular mass growth processes leading ultimately to fullerenes. This hypothesis requires the untangling of the elusive synthetic pathways to viable PAH precursors carrying an out-of-plane carbon backbone as a critical prerequisite of yielding fullerenes: corannulene ($C_{20}H_{10}$) (Scheme 1).

Here, we present a combined molecular beam and high-level *ab initio* investigation on the facile gas phase synthesis of corannulene ($C_{20}H_{10}$) in high temperature environments mimicking the conditions in carbon-rich circumstellar envelopes. The Hydrogen-Abstraction/aCetylene-Addition (HACA) and Hydrogen-Abstraction/Vinylacetylene-Addition (HAVA) mechanisms have been instrumental in elucidating the synthetic routes to the formation of planar PAHs carrying up to four fused benzene rings like triphenylene ($C_{18}H_{12}$),⁴⁰ but their validity to synthesize out-of-plane PAHs carrying a five-membered ring as present in corannulene ($C_{20}H_{10}$) has not been explored yet. Here, the gas phase synthesis of corannulene ($C_{20}H_{10}$) reveals

previously elusive chemistries of the 7-fluoranthenyl ($C_{16}H_9^{\bullet}$) and benzo[*ghi*]fluoranthen-5-yl ($C_{18}H_9^{\bullet}$) radicals with acetylene (C_2H_2) involving the HACA mechanism⁴¹ via benzo[*ghi*]fluoranthene ($C_{18}H_{10}$) intermediates through sequential bay closures accompanied by aromatization and out-of-plane bending of the carbon skeleton (Scheme 2). Corannulene represents a viable prototype intermediate and critical building block in bottom-up molecular mass growth processes from PAHs to Buckminsterfullerene (C_{60}) thus bringing us closer to an understanding of the carbon budget in our galaxy and the fundamental molecular processes of synthesizing fullerenes in circumstellar environments. Detailed experimental method and synthesis processes are provided in Supplementary Information (Supplementary Notes 1 and 2, Supplementary Schemes 1 and 2; Supplementary Figures 1–7). Briefly, a high temperature chemical reactor was used to investigate the reactions of the 7-fluoranthenyl ($C_{16}H_9^{\bullet}$) radical — generated *in situ* from 1-(2,6-dibromophenyl)naphthalene ($C_{16}H_{10}Br_2$) — with acetylene to benzo[*ghi*]fluoranthene ($C_{18}H_{10}$) and of the benzo[*ghi*]fluoranthen-5-yl radical ($C_{18}H_9^{\bullet}$) — formed *in situ* from benzo[*ghi*]fluoranthene ($C_{18}H_{10}$) — with a second acetylene molecule to corannulene ($C_{20}H_{10}$) at 1450 ± 10 K (Scheme 2). This reactor consists of a heated silicon carbide (SiC) tube and is incorporated within the source chamber of a molecular beam machine equipped with a Wiley–McLaren reflectron time-of-flight mass spectrometer (Re-TOF-MS). The reaction intermediates and products were probed isomer specifically through fragment-free photoionization in a molecular beam by tunable vacuum ultraviolet (VUV) light in tandem with the identification of the ionized molecules in a reflectron time-of-flight mass spectrometer. Mass spectra were collected by recording the arrival time of the ions as a function of mass-to-charge (m/z) ratios.

2. EXPERIMENTAL

The experiments were carried out at the Advanced Light Source (ALS) at the Chemical Dynamics Beamline (9.0.2.) utilizing a chemical reactor.⁴²⁻⁵¹ Briefly, the high temperature chemical reactor consisted of a resistively heated silicon carbide (SiC) tube of 20 mm in length and 1 mm inner diameter. In the experiment, the 7-fluoranthenyl radicals ($C_{16}H_9^{\bullet}$) were produced *in situ* at concentrations of less than 0.1 % via pyrolysis of the 1-(2,6-dibromophenyl)naphthalene ($C_{16}H_{10}Br_2$) seeded in acetylene (99.9 %; Matheson Gas) carrier gas at a pressure of 100 Torr (Supplementary Figure 4). Acetone traces in acetylene were removed by passing the acetylene gas in a cooling coil cooled through dry ice. The acetylene–1-(2,6-

dibromophenyl)naphthalene gas mixture was introduced into the silicon carbide tube (“pyrolytic reactor”) at the temperature of 1450 ± 10 K as monitored by a Type-C thermocouple. After exiting the reactor, the molecular beam, which contained the reaction products, passed through a skimmer and entered into a detection chamber, which housed the Wiley-McLaren Reflectron Time-of-Flight Mass Spectrometer (ReTOF-MS). The products were photoionized in the extraction region of the spectrometer and detected with a microchannel plate (MCP) detector. Vacuum ultraviolet (VUV) single photon ionization represents essentially a fragment-free ionization technique.⁵² Here, mass spectra were taken in 0.05 eV intervals from 7.40 eV to 10.00 eV. The photoionization efficiency (PIE) curves, which report the intensity of a specific mass-to-charge ratio (m/z) versus the photon energy, were extracted by integrating the signal collected at a well-defined m/z selected for the species of interest over the range of photon energies and normalized to the incident photon flux. The residence times of the reactants in the reactor tube (20 mm) under our experimental condition are tens of μs .⁵³⁻⁵⁵ A control experiment was also conducted by expanding neat helium carrier gas with the 1-(2,6-dibromophenyl)naphthalene ($\text{C}_{16}\text{H}_{10}\text{Br}_2$) precursor into the resistively-heated silicon carbide tube. No signal at $m/z = 226$, 227 or 250 was observed in the control experiment. 1-(2,6-Dibromophenyl)naphthalene ($\text{C}_{16}\text{H}_{10}\text{Br}_2$) was synthesized in house (Supplementary Scheme 1).

3. COMPUTATIONAL

The calculations of the energies and molecular parameters including geometries, rotational constants, and vibrational frequencies of the reactants, possible products, various intermediates and transition states for the reactions of 7-fluoranthenyl and benzo[*ghi*]fluoranthen-5-yl radicals with acetylene proceeding on the $\text{C}_{18}\text{H}_{11}$ and $\text{C}_{20}\text{H}_{11}$ potential energy surfaces (PESs), respectively, were carried out at the G3(MP2,CC)//B3LYP/6-311G(d,p) level of theory. Within this theoretical approach, geometries were optimized and vibrational frequencies were calculated using the density functional B3LYP method^{17,18} with the 6-311G(d,p) basis set. Using the optimized geometries, single-point energies were refined using a series of coupled clusters CCSD(T) and second-order Møller-Plesset perturbation theory MP2 calculations, with the final energy being computed as

$$\begin{aligned} E[\text{G3}(\text{MP2},\text{CC})] &= E[\text{CCSD}(\text{T})/6-311\text{G}(\text{d},\text{p})] + E[\text{MP2}/\text{G3Large}] - E[\text{MP2}/6-311\text{G}(\text{d},\text{p})] \\ &+ \text{ZPE} [\text{B3LYP}/6-311\text{G}(\text{d},\text{p})]^{19-21} \end{aligned}$$

The G3(MP2,CC) model chemistry approach normally provides chemical accuracy of 0.01–0.02 Å for bond lengths, 1–2° for bond angles, and 3–6 kJ mol⁻¹ for relative energies of hydrocarbons, their radicals, reaction energies, and barrier heights in terms of average absolute deviations.²⁰ The adiabatic ionization energies were calculated using the same G3(MP2,CC)//B3LYP/6-311G(d,p) method with the expected accuracy of ±0.1 eV. The GAUSSIAN 09²² and MOLPRO 2010²³ program packages were employed for the ab initio calculations.

Pressure- and temperature-dependent rate constants and product branching ratios for the 7-fluoranthenyl + C₂H₂ and benzo[ghi]fluoranthen-5-yl + C₂H₂ were evaluated using the Rice-Ramsperger-Kassel-Marcus Master Equation (RRKM-ME) theoretical approach utilizing the MESS software package.^{24,25} Densities of states and partition functions for local minima and numbers of states for transition states were computed within the Rigid-Rotor, Harmonic-Oscillator (RRHO) model. Tunneling corrections using asymmetric Eckart potentials were included in rate constant calculations. We used collision parameters for RRKM-ME calculations derived in the literature for systems of similar size; the Lennard-Jones parameters ϵ and σ for hydrocarbons were taken from Wang and Frenklach²⁶ and those for N₂ bath gas from Vishnyakov et al.^{27,28} The temperature dependence of the range parameter α for the deactivating wing of the energy transfer function was expressed as $\alpha(T) = \alpha_{300}(T/300 \text{ K})^n$, with $n = 0.62$ and $\alpha_{300} = 424 \text{ cm}^{-1}$ derived by Jasper from classical trajectory calculations²⁹ and used earlier by us in the studies of the reactions of C₂H₂ addition to various PAH radicals.³⁰⁻³² The main results of the RRKM-ME calculations of the rate constants and product branching ratios are described in Supplementary Note 2. The input files for the MESS calculations which including optimized Cartesian coordinates, vibrational frequencies, and relative energies of all species involved is provided as Supplementary Note 3.

4. RESULTS & DISCUSSION

Figure 1 displays characteristic mass spectra collected at a photoionization energy of 9.50 eV for the 1-(2,6-dibromophenyl)naphthalene (C₁₆H₁₀Br₂) precursor seeded in helium (Figure 1a) and in acetylene (Figure 1b) at a reactor temperature of 1450 ± 10 K. The 1-(2,6-dibromophenyl)naphthalene — helium system serves as a reference when compared to the 1-(2,6-dibromophenyl)naphthalene — acetylene system to unambiguously identify the m/z value(s) associated with the reaction of the radical intermediates with acetylene (Scheme 2). In the 1-(2,6-

dibromophenyl)naphthalene — helium system, signal can be observed at $m/z = 360, 362,$ and 364 . These ions can be linked to non-pyrolyzed precursor molecules: $C_{16}H_{10}^{79}Br_2$ (360 amu), $C_{16}H_{10}^{79}Br^{81}Br$ (362 amu), and $C_{16}H_{10}^{81}Br_2$ (364 amu). These precursors undergo a single carbon-bromine bond rupture yielding the 1-(1-naphthyl)-2-bromophenyl radical ($C_{16}H_{10}^{79}Br^{\bullet}$, 281 amu; $C_{16}H_{10}^{81}Br^{\bullet}$, 283 amu). Note that according to our B3LYP/6-311G** calculations, the hydrogen bromide (HBr) elimination from 1-(2,6-dibromophenyl)naphthalene is endothermic by 307 kJ mol^{-1} compared to 312 kJ mol^{-1} for the bromine atom loss, but features a barrier of 336 kJ mol^{-1} , while the atomic bromine loss occurs without an exit barrier. Thus, the atomic bromine elimination is favorable over the molecular hydrogen bromide loss both in terms of enthalpy and entropy and hence represents the dominant decomposition channel of the precursor. The 1-(1-naphthyl)-2-bromophenyl radical then undergoes a cycloaddition accompanied by atomic hydrogen loss and aromatization to 7-bromofluoranthene ($C_{16}H_9^{79}Br$, 280 amu; $C_{16}H_9^{81}Br$, 282 amu) (Supplementary Figure 8). The signal at $m/z = 280$ and 282 is clearly observable in the 1-(2,6-dibromophenyl)naphthalene–helium reference system and hence can be associated with 7-bromofluoranthene; smaller signals at a level of about $15 \pm 2\%$ are associated to $^{13}CC_{15}H_9^{79}Br$ (281 amu) and $^{13}CC_{15}H_9^{81}Br$ (283 amu). The *in situ* formed 7-bromofluoranthene can also undergo a carbon–bromine bond rupture yielding the 7-fluoranthenyl radical ($C_{16}H_9^{\bullet}$, 201 amu) which may recombine with a hydrogen atom in the reactor to fluoranthene ($C_{16}H_{10}$; 202 amu). Ion counts at $m/z = 202$ and 203 can be linked to molecules of the formulae $C_{16}H_{10}$ ($m/z = 202$) and $^{13}CC_{15}H_{10}$ ($m/z = 203$). The aforementioned ion counts are also observable in the 1-(2,6-dibromophenyl)naphthalene–acetylene system (Figure 1b) with signal at $m/z = 202$ and 203 reduced compared to the 1-(2,6-dibromophenyl)naphthalene–helium system under same counting conditions. Instead, ion counts at $m/z = 226$ and 227 dominate the mass spectrum in the 1-(2,6-dibromophenyl) naphthalene–acetylene system. Considering the mass difference of 24 amu to the reduced ion counts at $m/z = 202$ and 203 , signal at $m/z = 226$ and 227 can be connected to the product of the reaction of the 7-fluoranthenyl radical ($C_{16}H_9^{\bullet}$, 201 amu) with acetylene (C_2H_2 , 26 amu) leading to the molecules of the formulae $C_{18}H_{10}$ (226 amu) and $^{13}CC_{17}H_{10}$ (227 amu). Further molecular mass growth processes are evident from the detection of signal at $m/z = 250$ ($C_{20}H_{10}$): the $C_{18}H_{10}$ (226 amu) hydrocarbon could lose a hydrogen atom via abstraction by atomic hydrogen and/or bromine in the reactor leading to the $C_{18}H_9^{\bullet}$ radical (225 amu), which reacts with acetylene (C_2H_2 , 26 amu) to a $C_{20}H_{11}^{\bullet}$ radical intermediate (251 amu)

which is then stabilized by hydrogen atom elimination yielding a hydrocarbon with the molecular formula $C_{20}H_{10}$ (250 amu). Signal at $m/z = 304$ and 306 is observable in the 1-(2,6-dibromophenyl)-naphthalene–acetylene system, but absent in the control experiment. Considering the nearly equal intensities of both peaks and the molecular weights, these ion counts can be associated with $C_{18}H_9^{79}Br$ (304 amu) and $C_{18}H_9^{81}Br$ (306 amu) produced via the recombination of atomic bromine and the $C_{18}H_9^{\bullet}$ radical. To identify the nature of the isomers generated 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; the PIE calibration curves recorded in the present setup (Supplementary Figure 9).

In both the 1-(2,6-dibromophenyl)naphthalene–helium and 1-(2,6-dibromophenyl)naphthalene–acetylene systems, the PIE curves of $m/z = 360$, 362 , and 364 are superimposable after scaling and reveal an onset of the ion counts at 7.90 ± 0.05 eV. This onset correlates nicely with the computed adiabatic ionization energy of 7.85 ± 0.1 eV for the 1-(2,6-dibromophenyl)naphthalene precursor (Supplementary Figure 10). Likewise, the PIEs of $m/z = 280$ to 283 are identical within our error limits for both systems. The experimentally determined onsets of the ion counts at 7.90 ± 0.05 eV is in excellent agreement with the adiabatic ionization energy of the 7-bromofluoranthene molecule ($C_{16}H_9^{79}Br$, $C_{16}H_9^{81}Br$) of 7.88 ± 0.1 eV. Finally, the extracted PIE curves of $m/z = 202$ and 203 overlap for both systems after scaling. These graphs can be fit with the reference curve of fluoranthene ($C_{16}H_{10}$; 202 amu) along with its ^{13}C counterpart (Figure 2). At both m/z ion counts rise at 7.85 ± 0.05 eV, which correlates with the adiabatic ionization energy of fluoranthene from the reference PIE curve (7.85 ± 0.05 eV) and from literature data (7.9 ± 0.1 eV).⁵⁶ The ion counts at $m/z = 226$ ($C_{18}H_{10}$), 227 ($^{13}CC_{17}H_{10}$), and 250 ($C_{20}H_{10}$) are unique to the 1-(2,6-dibromophenyl)naphthalene–acetylene systems and hence are reaction products of the radical intermediates with acetylene. The analysis of the PIE curves underlines these findings. The PIE curves at $m/z = 226$ and 227 are superimposable after scaling and can be reproduced with a linear combination of reference PIE curves of the 7-ethynylfluoranthene and benzo[ghi]fluoranthene molecules; as revealed from the fitting procedure and visualized in Figure 2, ion counts from benzo[ghi]fluoranthene clearly dominate at a level of 96.9 ± 1.0 % at

10.0 eV. The onsets of the ion counts at 7.85 ± 0.05 eV agree well with the adiabatic ionization energy of benzo[*ghi*]fluoranthene of 7.85 ± 0.05 eV measured in this work (Supplementary Figure 9). Having established the predominant contribution of benzo[*ghi*]fluoranthene as a contributor of ion signal at $m/z = 226$ and 227 , we are analyzing the ion counts at $m/z = 250$. The corannulene reference PIE curve correlates well with the experimentally recorded PIE curve of $m/z = 250$ in the 1-(2,6-dibromophenyl)naphthalene–acetylene system. The onsets of the ion counts at 7.85 ± 0.05 eV (reference curve) and 7.85 ± 0.05 eV (experimental PIE curve) replicate well the adiabatic ionization energy of corannulene of 7.83 ± 0.02 eV,⁵⁷ respectively. Altogether, the experiments propose that in the 1-(2,6-dibromophenyl)naphthalene–acetylene system, benzo[*ghi*]fluoranthene (C₁₈H₁₀) and corannulene (C₂₀H₁₀) represent distinct reaction products, which are absent in the control experiment when acetylene is absent. On the other hand, fluoranthene (C₁₆H₁₀) is formed in both systems suggesting that it is the hydrogen recombination product of the reaction of 7-fluoranthenyl radical (C₁₆H₉[•]) with atomic hydrogen in both systems.

Our experimental investigations reveal that corannulene (C₂₀H₁₀, 250 amu) — a prototype non-planar PAH and molecular building block of fullerenes — is synthesized via molecular mass growth processes involving reactions of the 7-fluoranthenyl radical (C₁₆H₉[•], 201 amu) and of the benzo[*ghi*]fluoranthene-5-yl radical (C₁₈H₉[•], 225 amu) with acetylene (C₂H₂, 26 amu). To unravel the underlying reaction mechanisms, we combined these experimental findings with electronic structure calculations (Figure 3). Our computations reveal that molecular mass growth processes can account for the formation of benzo[*ghi*]fluoranthene (C₁₈H₁₀) (Figure 3a) and corannulene (C₂₀H₁₀) (Figure 3b, Supplementary Figure 11). The 7-fluoranthenyl radical (C₁₆H₉[•]) can add with its radical center to one of the carbon atoms of the acetylene molecule via an entrance barrier of 10 kJmol⁻¹ yielding a doublet radical intermediate **i1**. The latter can ring-close to **i4** by overcoming a barrier to isomerization of only 66 kJmol⁻¹. This intermediate can eliminate a hydrogen atom from the C1 position of the fluoranthene moiety yielding benzo[*ghi*]fluoranthene (C₁₈H₁₀) (**p1**) via a tight exit transition state in an overall exoergic reaction (−195 kJmol⁻¹). Alternatively, in a more energetically favorable pathway, a hydrogen shift from C1 of the fluoranthene unit to the terminal carbon atom of the acetylenic side chain can form intermediate **i2** which subsequently undergoes ring closure to **i3**. The latter loses atomic hydrogen accompanied by aromatization to form the planar, C_{2v} symmetric benzo [*ghi*]fluoranthene (C₁₈H₁₀). Our computations also propose that 7-ethynylfluoranthene (**p2**) is formed via hydrogen

loss from intermediate **i1**. According to RRKM-Master Equation (RRKM-ME) calculations at the conditions inside the chemical reactor, relative yields of **p1** and **p2** constitute 93% and 7%, respectively (Supplemental Note 2, Supplementary Figure 12).

The mechanism of the transformation from benzo[*ghi*]fluoranthene ($C_{18}H_{10}$) to corannulene ($C_{20}H_{10}$) mirrors the conversion from fluoranthene ($C_{16}H_{10}$) to benzo[*ghi*]fluoranthene ($C_{18}H_{10}$). This sequence is initiated by a carbon-hydrogen bond cleavage and hydrogen atom loss from benzo[*ghi*]fluoranthene ($C_{18}H_{10}$) to the benzo[*ghi*]fluoranthen-5-yl radical ($C_{18}H_9^{\bullet}$). In the chemical reactor, this might be induced by hydrogen abstraction, whereas in the circumstellar envelope, photolysis may lead to atomic hydrogen elimination. The benzo[*ghi*]fluoranthen-5-yl radical ($C_{18}H_9^{\bullet}$) adds then with its radical center to the acetylenic bond of acetylene passing an entrance barrier of 18 kJmol^{-1} to access a planar, C_s symmetric doublet radical intermediate **i5**. This radical may undergo ring closure and out-of-plane bending to **i6** via a barrier of 88 kJmol^{-1} followed by hydrogen ejection from the C10 carbon atom through a tight, C_1 symmetric transition state forming the C_{5v} symmetric corannulene ($C_{20}H_{10}$, **p3**) in an overall exoergic reaction (-144 kJmol^{-1}). A second, more preferable pathway to corannulene ($C_{20}H_{10}$) involves a hydrogen migration from the C6 atom of the benzo[*ghi*]fluoranthene moiety to the terminal carbon atom of the acetylenic side chain yielding intermediate **i7**. The latter subsequently can isomerize via ring closure and out-of-plane bending to **i8**, which ejects a hydrogen atom accompanied by bay closure and aromatization, yielding eventually corannulene ($C_{20}H_{10}$, **p3**). Alternatively, **i6** can also isomerize to **i8** via hydrogen migration from C10 to C1 eventually yielding corannulene through atomic hydrogen loss. The computations suggest that 5-ethynylbenzo[*ghi*]fluoranthene ($C_{20}H_{10}$, **p4**), might be also formed from **i5**. RRKM-ME calculated relative yields of **p3** and **p4** are 73% and 27%, respectively (Supplementary Notes 4 and 5; Supplementary Figure 13). It should be highlighted that our experiments reveal branching ratios of ion counts; due to the lack of available photoionization cross sections, branching ratios of the products cannot be estimated. Nevertheless, both the experiments and computations reveal the formation of corannulene; our computations predict that the 5-ethynylbenzo[*ghi*]fluoranthene isomer could also be a contributor, but at lower fractions than corannulene. We would like to recall that the PIE curve at $m/z = 250$ could be replicated by calibration curve of corannulene recorded within the same experimental setup.

5. CONCLUSIONS

The high-temperature formation of corannulene ($C_{20}H_{10}$) defines a benchmark of sequential HACA-type bay closures on armchair edges of PAH molecules involving molecular mass growth processes from *planar* PAHs (fluoranthene ($C_{16}H_{10}$), benzo[*ghi*]fluoranthene ($C_{18}H_{10}$)) to a *non-planar* PAH (corannulene ($C_{20}H_{10}$)) via 7-fluoranthenyl ($C_{16}H_9^{\bullet}$) and benzo[*ghi*]fluoranthen-5-yl radicals ($C_{18}H_9^{\bullet}$) (Scheme 2). In carbon rich circumstellar envelopes of Asymptotic Giant Branch stars and of planetary nebulae, the 7-fluoranthenyl ($C_{16}H_9^{\bullet}$)–acetylene (C_2H_2) and benzo[*ghi*]fluoranthen-5-yl ($C_{18}H_9^{\bullet}$)–acetylene (C_2H_2) reactions can be initiated through abstraction of a hydrogen atom from the 7- and 5-position of fluoranthene ($C_{16}H_{10}$) and benzo[*ghi*]fluoranthene ($C_{18}H_{10}$), respectively. The barriers for the hydrogen abstraction can be easily overcome in high temperature circumstellar environments at temperatures of a few 1,000 K.⁶ Alternatively, the strong photon field of the central star might lead to homolytic carbon-hydrogen bond rupture processes leading to 7-fluoranthenyl ($C_{16}H_9^{\bullet}$) and benzo[*ghi*]fluoranthen-5-yl ($C_{18}H_9^{\bullet}$) from fluoranthene ($C_{16}H_{10}$) and benzo[*ghi*]fluoranthene ($C_{18}H_{10}$), respectively. In these high temperature environments, the fluoranthene molecule ($C_{16}H_{10}$) can be easily synthesized through the Phenyl-Addition-Cyclization (PAC) mechanism⁵⁸ from 1-phenylnaphthalene ($C_{16}H_{12}$), which in turn can be formed via the elementary reaction of the phenyl radical ($C_6H_5^{\bullet}$) with naphthalene ($C_{10}H_8$) (Scheme 2).⁵⁸ Note that naphthalene ($C_{10}H_8$) is accessible from the phenyl radical ($C_6H_5^{\bullet}$) either via the HACA⁵¹ or HAVA pathway.⁵⁵ In carbon rich circumstellar envelopes, this bottom-up synthesis eventually leads from a single ring aromatic (phenyl ($C_6H_5^{\bullet}$)) through successive molecular mass growth processes (of the reaction intermediates) involving vinylacetylene (C_4H_4), acetylene (C_2H_2) to a prototype of a non-planar PAH — corannulene ($C_{20}H_{10}$) — through highly complementary reaction mechanisms (HACA, HAVA, PAC).

The complementary nature of the PAC, HAVA, and HACA mechanisms along with their critical role in the bottom-up synthesis of non-planar PAHs (corannulene ($C_{20}H_{10}$)) is highlighted in Schemes 1 and 2. The aromatic corannulene molecule consists of a five-membered ring fused with five benzene rings and is classified as a [5]circulene. This bowl-shaped geodesic polyarene represents *the* most fundamental, buckybowl-type molecular building blocks of fullerenes and also of carbon nanotubes. The aromaticity of corannulene can be best understood in terms of the

annulene-within-an-annulene model⁵⁹ defining corannulene via a central 6π cyclopentadienyl anion surrounded by an aromatic 14 π annulenyl cation.⁶⁰ Whereas the next higher member of the circulenes — [6]circulene or coronene ($C_{24}H_{12}$) — consists of a central hexagon fused with six benzene rings and represents a central PAH intermediate to 2-dimensional carbonaceous nanostructures detected as 80 nm graphitized carbon grains in carbonaceous meteorites like Murchison and Allende,⁶¹ the [5]circulene — corannulene — defines a central molecular fragment of fullerenes (C_{60} , C_{70}) along with 3-dimensional carbonaceous nanostructures (carbon nanotubes) proposed to exist in chondrites (Scheme 1).

Previous high-temperature circumstellar reaction networks borrowed from sooty hydrocarbon flames have revealed limited efficiencies under conditions prevailing in circumstellar envelopes to synthesize fullerenes predominantly due to the lack of constrained and validated mechanisms leading to PAHs and fullerenes.^{58, 62} These high temperature reaction mechanisms in carbon rich circumstellar envelopes are similar — albeit under the exclusion of oxygen — to the bottom-up formation of PAHs probed in sooting combustion flames of, e.g., methane,⁶³ acetylene,⁶⁴ and benzene⁶⁵ revealing the ubiquitous presence of aromatics like fluoranthene, benzo[*ghi*]fluoranthene, and corannulene along with fullerenes (C_{60} , C_{70}). The reaction pathways to corannulene revealed in the present study and the potential role of corannulene in the formation of fullerenes gain strong support from sophisticated examinations of carbonaceous chondrites. Along with $^{13}C/^{12}C$ isotopic analysis, fluoranthene ($C_{16}H_{10}$),⁶⁶ benzo[*ghi*]fluoranthene ($C_{18}H_{10}$),^{66, 67} corannulene ($C_{20}H_{10}$),⁶⁷ buckminsterfullerene (C_{60}),⁶⁷⁻⁷² and rugbyballene (C_{70})^{67, 68, 71, 72} have been detected in, e.g., Murchison, Allende, Orgueil, and Tagish Lake thus corroborating impending molecular mass growth processes from fluoranthene via benzo[*ghi*]fluoranthene to corannulene and conceivably to fullerenes. It is important to point out that once PAHs form in circumstellar envelopes of carbon rich stars and are injected into the interstellar medium, they can be destroyed by photons, shocks and galactic cosmic rays envisaging lifetimes of only about 10^8 years.⁷³ However, the PAH abundance injected into the interstellar medium is in the order of 10% of the elemental carbon,⁷⁴ whereas the concentrations of PAHs in meteorites are measured only in parts per million (ppm). These considerations reveal that the absolute amount of PAHs synthesized in circumstellar envelopes and incorporated in carbonaceous chondrites is small, but nevertheless measurable. Overall, our findings establish a rigorous framework of a bottom-up synthesis of corannulene ($C_{20}H_{10}$) and provide a molecular

tracer to allow astrochemists to establish a mechanistic understanding, verified both by experiment and theory and able to explain the presence of PAHs and potentially fullerenes in deep space. These findings eventually transform the way how we think about the origin and evolution of carbonaceous matter in our galaxy.

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Author contributions

R.I.K. directed the overall project. R.K.M. synthesized the molecular precursor; L.Z., W.L. and O.K. carried out the experimental measurements; L.Z. performed the data analysis; L.B.T., A.N.M., V.N.A. and A.M.M. carried out the theoretical analysis; R.I.K., A.M.M., and M.A. discussed the data and supervised the project. F.R.F. supervised the synthesis of the molecular precursor. A.H.H. synthesized 7-ethynylfluoranthene and S.F.W. supervised the synthesis.

Competing financial interests

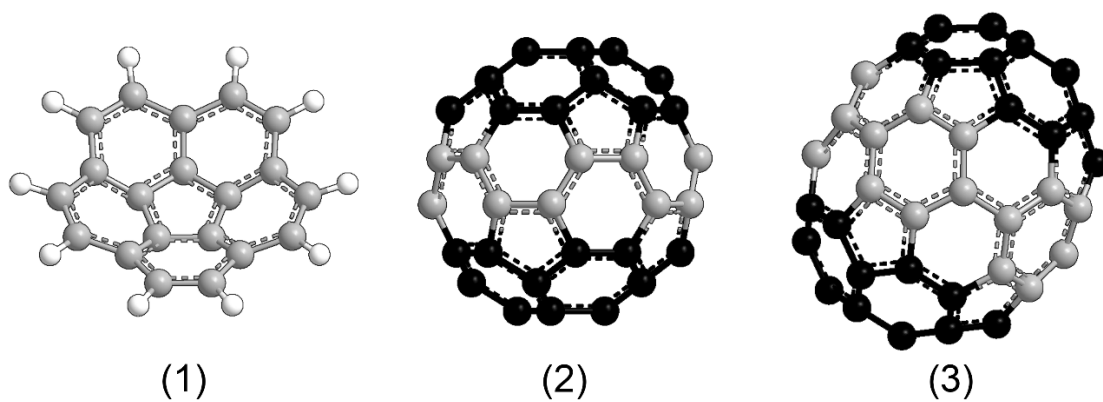
The authors declare no competing financial interests.

References

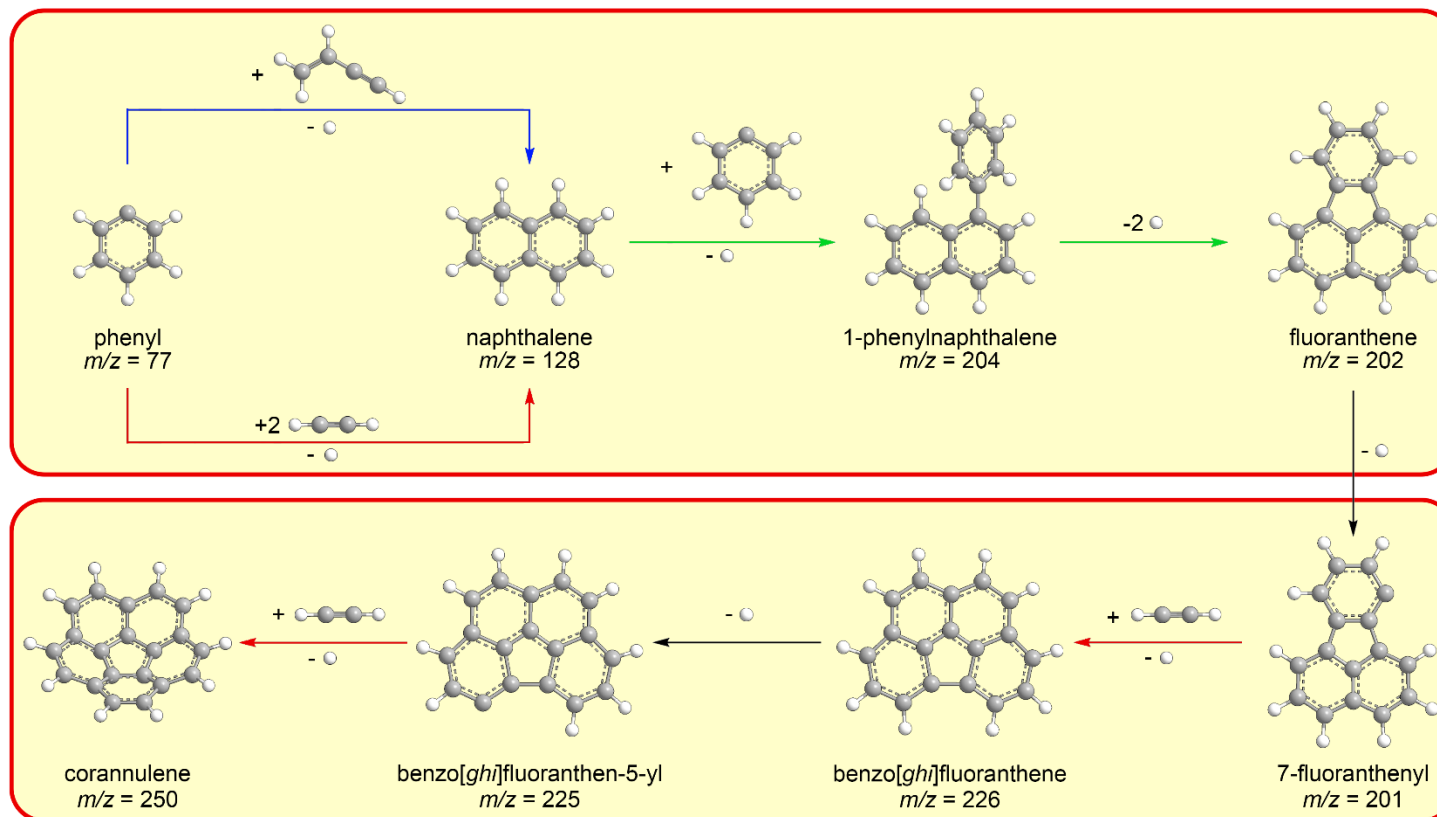
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Scheme 1. Corannulene ($C_{20}H_{10}$, **1**) as fundamental molecular building blocks of buckminsterfullerene (C_{60} ; **2**) and rugbyballene (C_{70} ; **3**) fullerenes; the corannulene moiety is highlighted in black.



Scheme 2. Schematic representation of the formation of corannulene from the phenyl radical. Upper sequence: the bottom-up formation of fluoranthene from the phenyl radical involving three key molecular mass processes via Hydrogen-Abstraction-acetylene-Addition (HACA) (red), Hydrogen-Abstraction-Vinylacetylene-Addition (HAVA) (blue), and Phenyl-Addition-Cyclization (PAC) (green) mechanisms. Lower sequence: the formation of benzo[ghi]fluoranthene and corannulene through the reaction of the 7-fluoranthenyl radical ($C_{16}H_9^{\bullet}$) with acetylene (C_2H_2) via HACA mechanism.

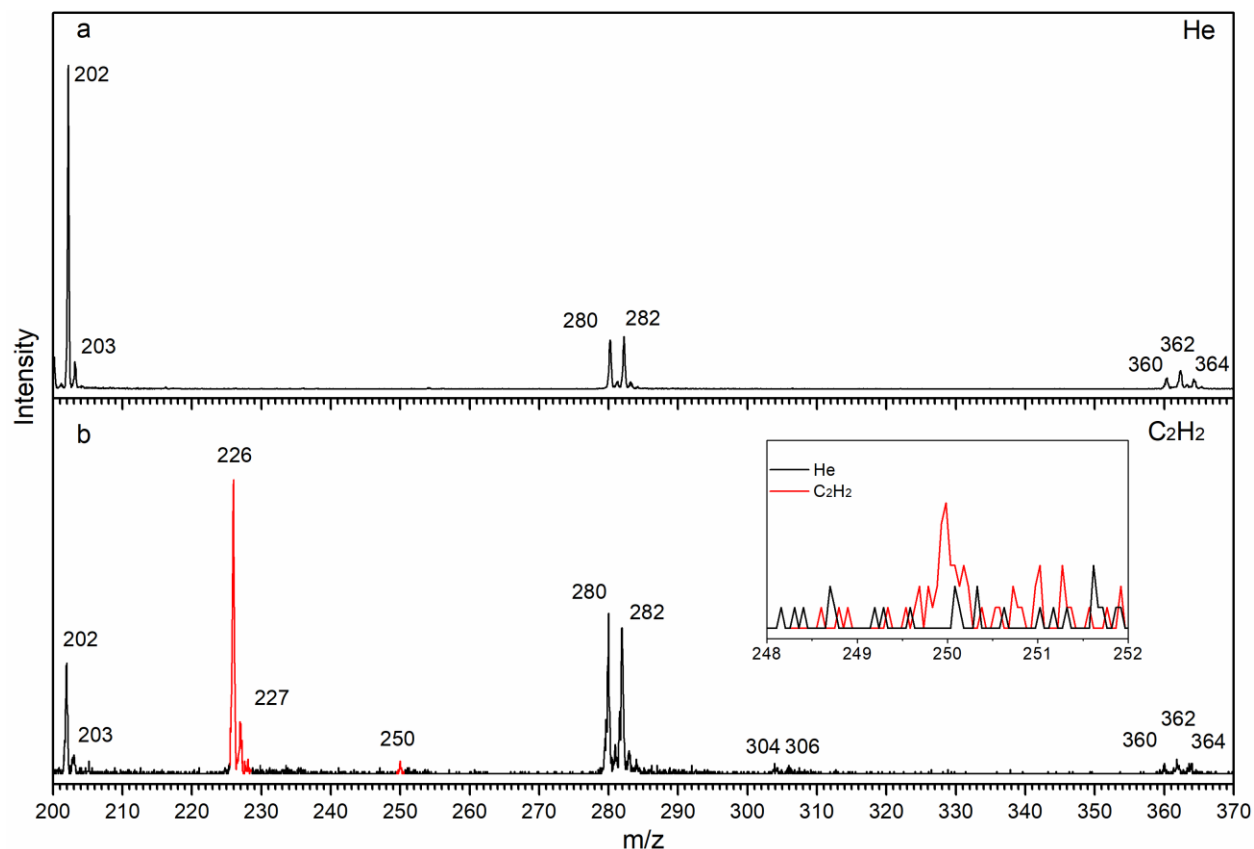


Figure 1. Photoionization mass spectra recorded at a photoionization energy of 9.5 eV at a reactor temperature of 1450 ± 10 K. (a) 1-(2,6-dibromophenyl)naphthalene ($C_{16}H_{10}Br_2$)–helium (He) system; (b) 1-(2,6-dibromophenyl)naphthalene ($C_{16}H_{10}Br_2$)–acetylene (C_2H_2) system. The mass peaks of the newly formed species at $m/z = 226$, 227 and 250 are highlighted in red. The inset shows the expanded region around $m/z = 250$.

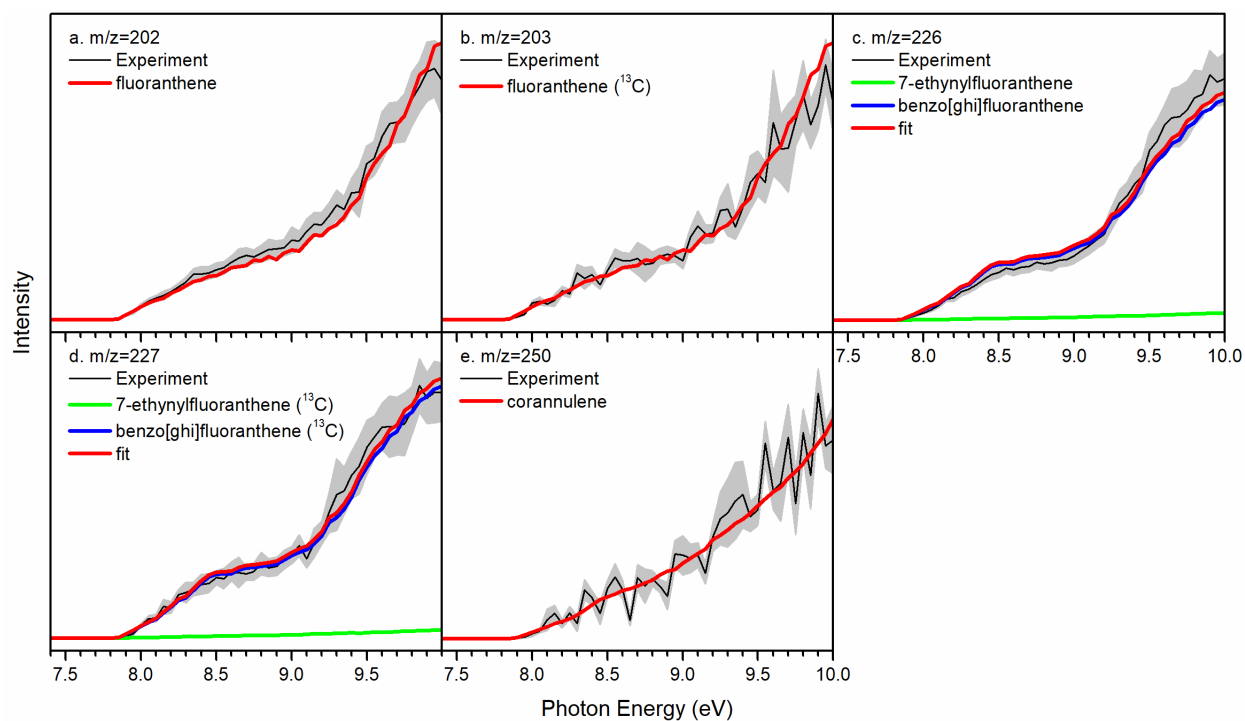


Figure 2. Photoionization efficiency (PIE) curves for $m/z = 202$, 203 , 226 , 227 and 250 . Black: experimentally derived PIE curves with the error area presented in gray; red: reference PIE curve. The overall error bars consist of two parts: $\pm 10\%$ based on the accuracy of the photodiode and a 1σ error of the PIE curve averaged over the individual scans.

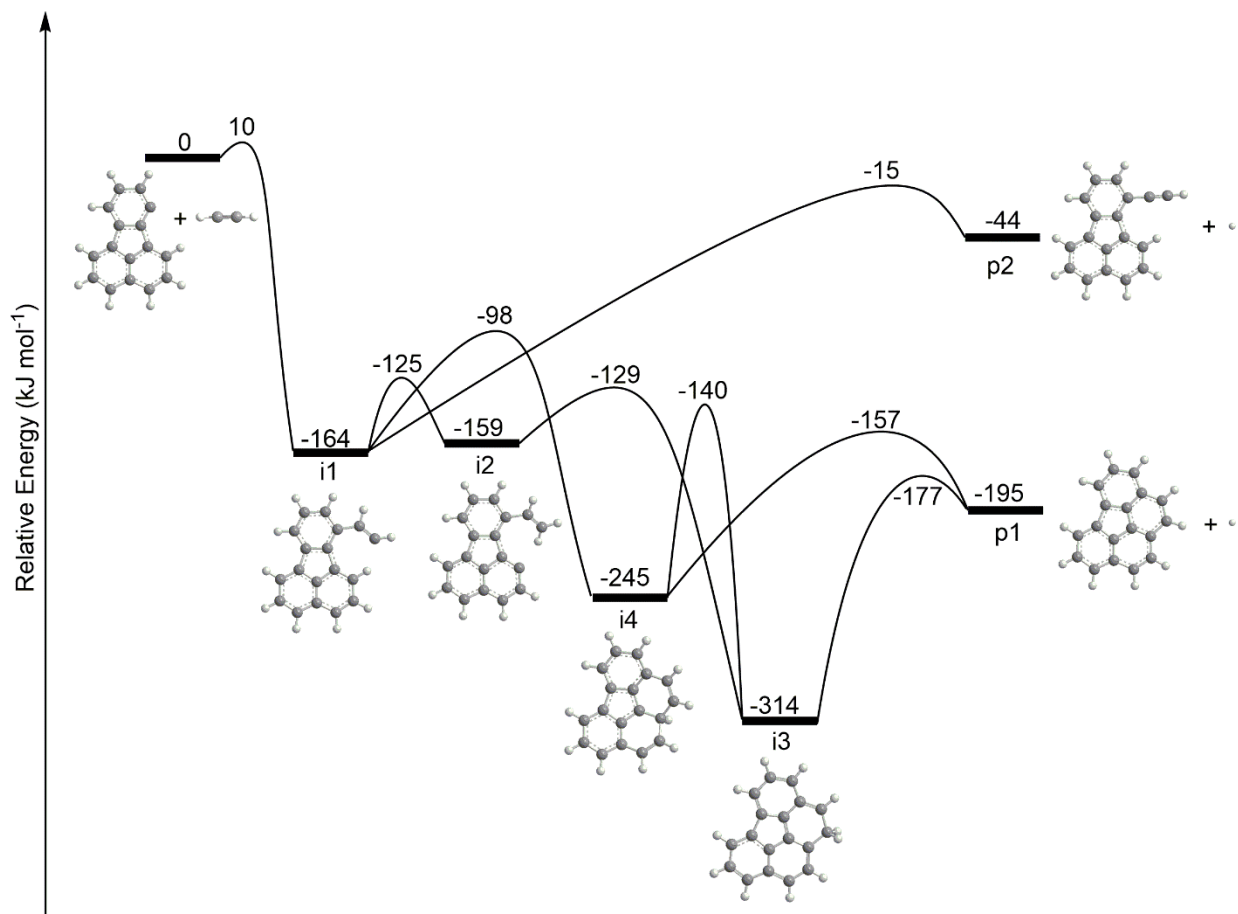


Figure 3a. Potential energy surface (PES) for the reaction of the 7-fluoranthenyl radical ($\text{C}_{16}\text{H}_9^{\bullet}$) with acetylene (C_2H_2) calculated at the G3(MP2,CC)//B3LYP/6-311G(d,p) level of theory. The relative energies are given in kJ mol^{-1} . Cartesian coordinates of reactants, intermediates, products, and transition states are provided in the Supplementary Note 3.

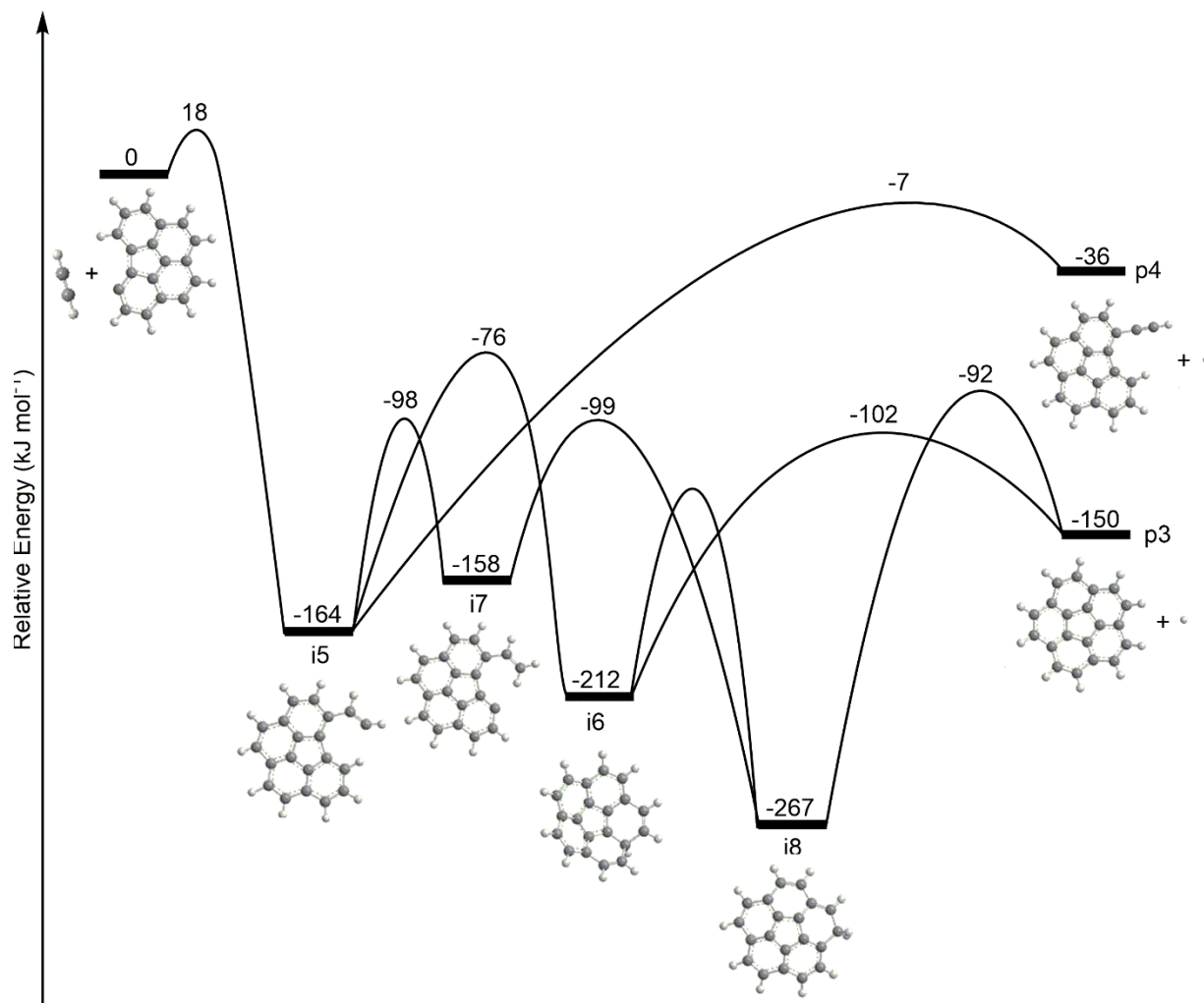


Figure 3b. Potential energy surface (PES) for the reaction of the benzofluoranthren-5-yl (C₁₈H₉) with acetylene (C₂H₂) calculated at the G3(MP2,CC)//B3LYP/6-311G(d,p) level of theory. The relative energies are given in kJmol⁻¹. Cartesian coordinates of reactants, intermediates, products, and transition states are provided in the Supplementary Note 3.

Supplementary Information

Gas-Phase Synthesis of Corannulene – A Molecular Building Block of Fullerenes

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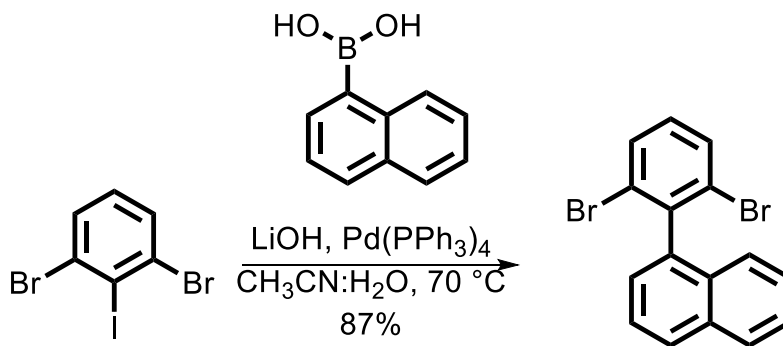
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Supplementary Note 1. Materials and Synthetic Methods.

Unless otherwise stated, all manipulations of air and/or moisture sensitive compounds were carried out in oven-dried glassware, under an atmosphere of N₂. 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 N₂ or Ar 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 ¹H and ¹³C NMR spectra were recorded on Bruker AVB-400 and AVQ-400 MHz spectrometers, and are referenced to residual solvent peaks (CDCl₃ ¹H NMR = 7.26 ppm, ¹³C NMR = 77.16 ppm). ESI mass spectrometry was performed on a Finnigan LTQFT (Thermo) spectrometer in positive ionization mode.

Synthetic Procedure for 1-(2,6-dibromophenyl)naphthalene



Supplementary Scheme 1. Synthetic pathway for 1-(2,6-dibromophenyl)naphthalene.

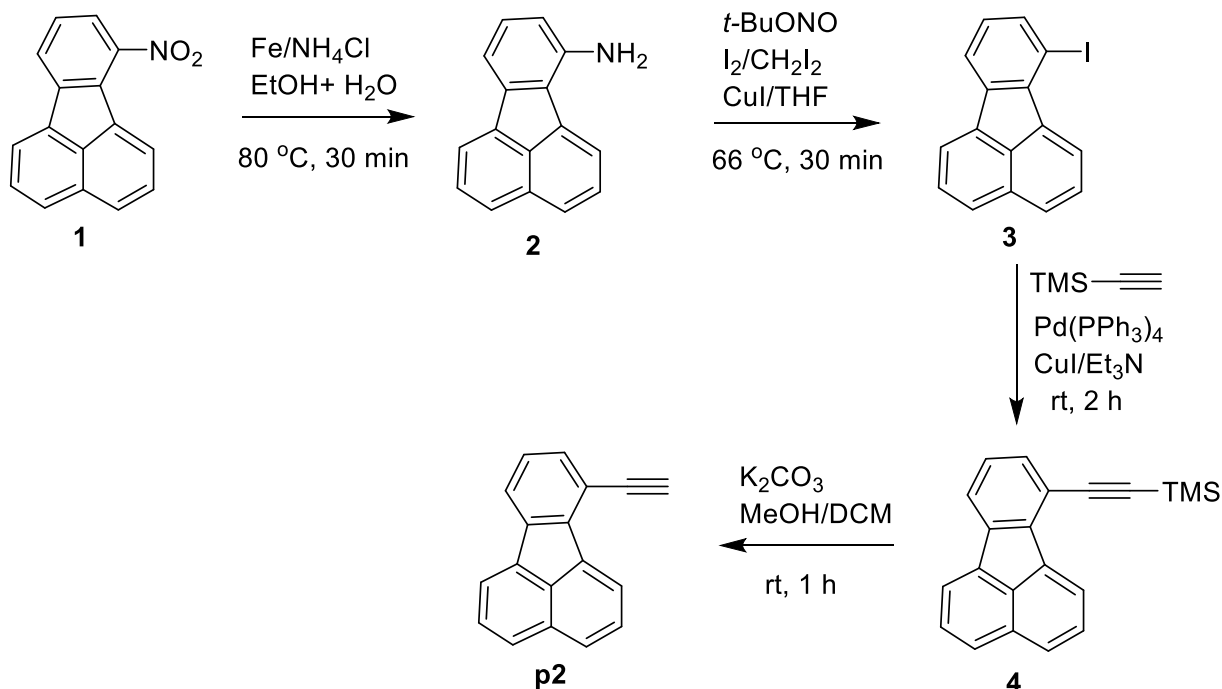
1-(2,6-dibromophenyl)naphthalene

1.2 g (3.36 mmol) of 1,3-Dibromo-2-iodobenzene, 0.58 g (3.36 mmol) of naphthalen-1-ylboronic acid, 0.55 g (13.2 mmol) LiOH, 0.4 g (0.336 mmol) of Pd(PPh₃)₄ in 3:1 N₂ degassed mixture of CH₃CN:H₂O were stirred at 70 °C overnight. After cooling to 24 °C, the product was extracted with ethyl acetate and the organic layer was dried with sodium sulfate. After the solvent was removed, the residue was purified by silica gel column chromatography (hexane), thus yielding 1.04 g (87% yield) of 1-(2,6-dibromophenyl)naphthalene as a colorless solid.

^1H NMR (400 MHz, in CDCl_3): δ = 7.95 (t, J = 7.4 Hz, 2H), 7.72 (d, J = 8.0 Hz, 2H), 7.59 (t, J = 7.6 Hz, 1H); 7.52 (t, J = 7.4 Hz, 1H), 7.44 (t, J = 7.5 Hz, 1H), 7.34 (t, J = 6.7 Hz, 2H), 7.18 (t, J = 8.0 Hz, 1H) ppm; ^{13}C NMR (101 MHz, in CDCl_3): δ = 141.7, 139.1, 133.6, 132.0, 131.0, 130.3, 128.8, 128.6, 127.1, 126.6, 126.2, 125.7, 125.5, 125.0 ppm; HRMS (EI-TOF): Calcd for $\text{C}_{16}\text{H}_{10}\text{Br}_2$, 359.9149; found 359.9152

Synthesis of 7-Ethynylfluoranthene **p2**

The 7-ethynylfluoranthene **p2** has been synthesized from 7-nitrofluoranthene **1** which has been prepared by reported protocol.¹⁵ Thus, reduction of **1** with Fe powder/ NH_4Cl gave 7-aminofluoranthene **2** (Supplementary Scheme 2). Subsequent, diazotization-iodination of **2** with *t*-BuONO/ $\text{CH}_2\text{I}_2/\text{I}_2/\text{CuI}$ afforded 7-iodofluoranthene **3**. Sonogashira coupling of **3** with TMS-acetylene in presence of $\text{Pd}(\text{PPh}_3)_4/\text{CuI}$ in Et_3N gave TMS protected 7-ethynylfluoranthene **4** which on desilylation with K_2CO_3 provided 7-ethynylfluoranthene **p2**.



Supplementary Scheme 2. Synthesis of 7-Ethynylfluoranthene **p2**

7-Aminofluoranthene **2**

Iron powder (1.10 g, 19.7 mmol) was added to the solution of NH₄Cl (1.05 g, 19.7 mmol) in H₂O/EtOH (30 mL, 1:1) in 100 mL flask equipped with a stir bar. The mixture was stirred at 60 °C for 30 min to activate the iron powder. Then 7-nitrofluoranthene **1**¹⁵ (742 mg, 3.0 mmol) was added and the temperature of reaction mixture was raised to 80 °C and stirring was continued for another 30 min. The mixture was cooled with ice-bath, basified with dilute aqueous NaOH to pH ~12 and was filtered to remove solid residue. The filtrate was concentrated under reduced pressure and extracted with EtOAc. The organic phase was separated, dried over anhydrous Na₂SO₄, filtered, and evaporated. The residue was purified by column chromatography (20 → 30% EtOAc/hexane) to give **2** (534 mg, 82%) as a yellow solid. ¹H NMR (400 MHz, CDCl₃) δ = 7.93 (d, *J* = 6.8 Hz 1H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.81–7.75 (m, 2H), 7.66–7.59 (m, 2H), 7.45 (dd, *J* = 7.4, 0.8 Hz, 1H), 7.23 (t, *J* = 7.6 Hz, 1H), 6.76 (dd, *J* = 8.0, 0.8 Hz, 1H), 4.22 (s, 2H) ppm; ¹³C NMR (101 MHz, CDCl₃) δ = 143.2, 140.8, 137.4, 137.0, 132.3, 130.1, 128.83, 128.1, 128.0, 126.7, 125.6, 123.7, 121.0, 120.3, 116.6, 113.0 ppm.

7-Iodofluoranthene **3**

Iodine (467 mg, 1.84 mmol), CuI (420 g, 2.20 mmol), CH₂I₂ (445 μL, 5.52 mmol), and tert-butyl nitrite (660 μL, 5.55 mmol) were added to a solution of **2** (400 mg, 1.84 mmol) in dry THF (15 mL). The reaction mixture was stirred at 66 °C for 30 min, cooled to 24 °C, and filtered. The filtrate was concentrated under reduced pressure and extracted with EtOAc. The organic phase was separated, dried over anhydrous Na₂SO₄, filtered, and evaporated. The residue was purified by column chromatography (5 → 10% EtOAc/hexane) to give **3** (428 mg, 71%) as an off-white solid. ¹H NMR (400 MHz, CDCl₃) δ = 8.84 (d, *J* = 7.2 Hz, 1H), 7.97 (d, *J* = 6.8 Hz, 1H), 7.95–7.89 (m, 3H), 7.82 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.74 (dd, *J* = 8.0, 6.8 Hz, 1H), 7.67 (dd, *J* = 8.0, 6.8 Hz, 1H), 7.09 (t, *J* = 7.6 Hz, 1H) ppm; ¹³C NMR (101 MHz, CDCl₃) δ = 142.0, 141.2, 138.7, 137.4, 135.4, 132.5, 130.0, 128.5, 128.0, 127.8, 127.6, 127.5, 123.1, 121.1, 120.2, 90.0 ppm.

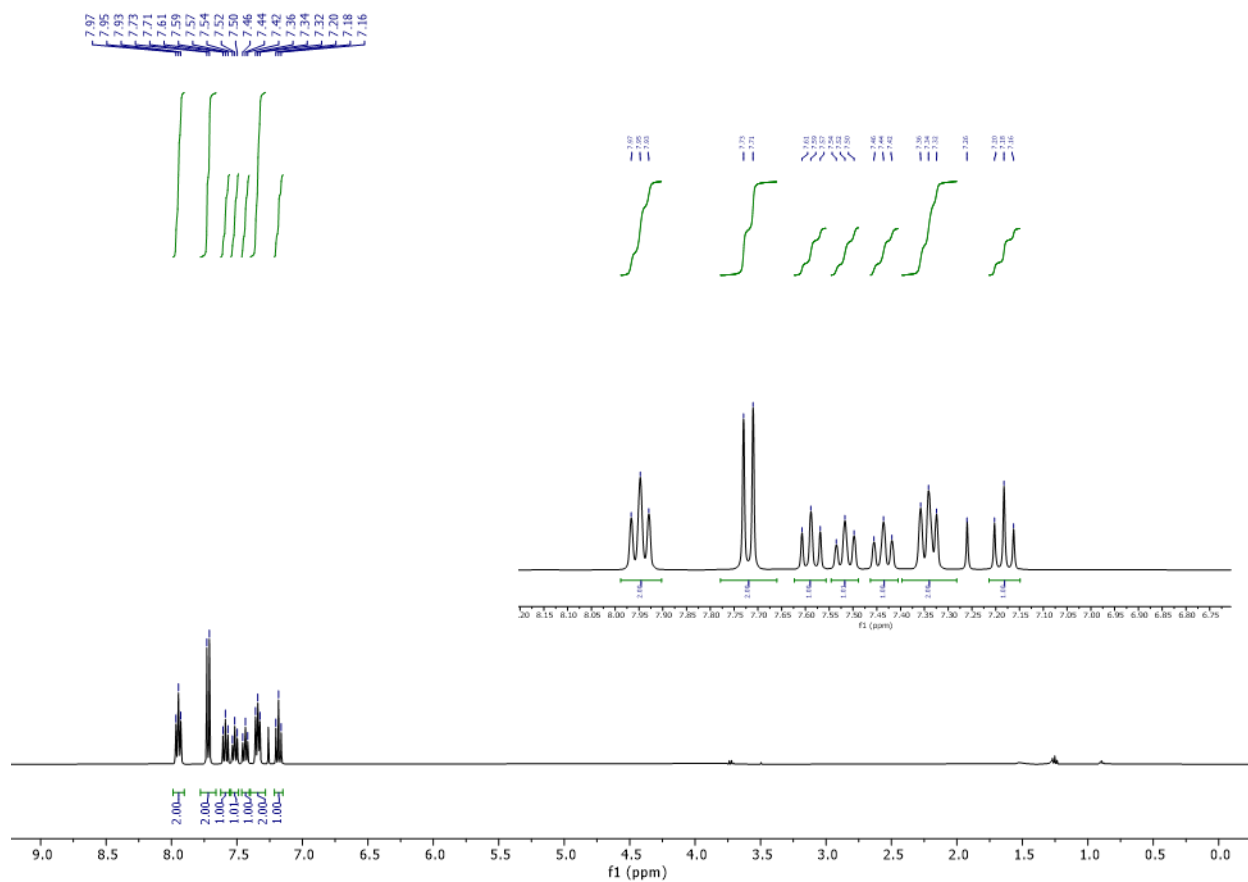
7-[2-(Trimethylsilyl)ethynyl]fluoranthene **4**

Pd(PPh₃)₄ (28.2 mg, 0.024 mmol) and Cu(I)I (9.1 mg, 0.048 mmol) were added to dry Et₃N (10 mL) in a flame-dried flask equipped with a stirring bar under N₂ at 24 °C. Then **3** (400 mg, 1.22 mmol) was added followed by TMS-acetylene (347 μL, 2.44 mmol). The resulting mixture was stirred for 2 h at 24 °C [progress of the reaction was monitored by TLC (n-hexane)]. Volatiles

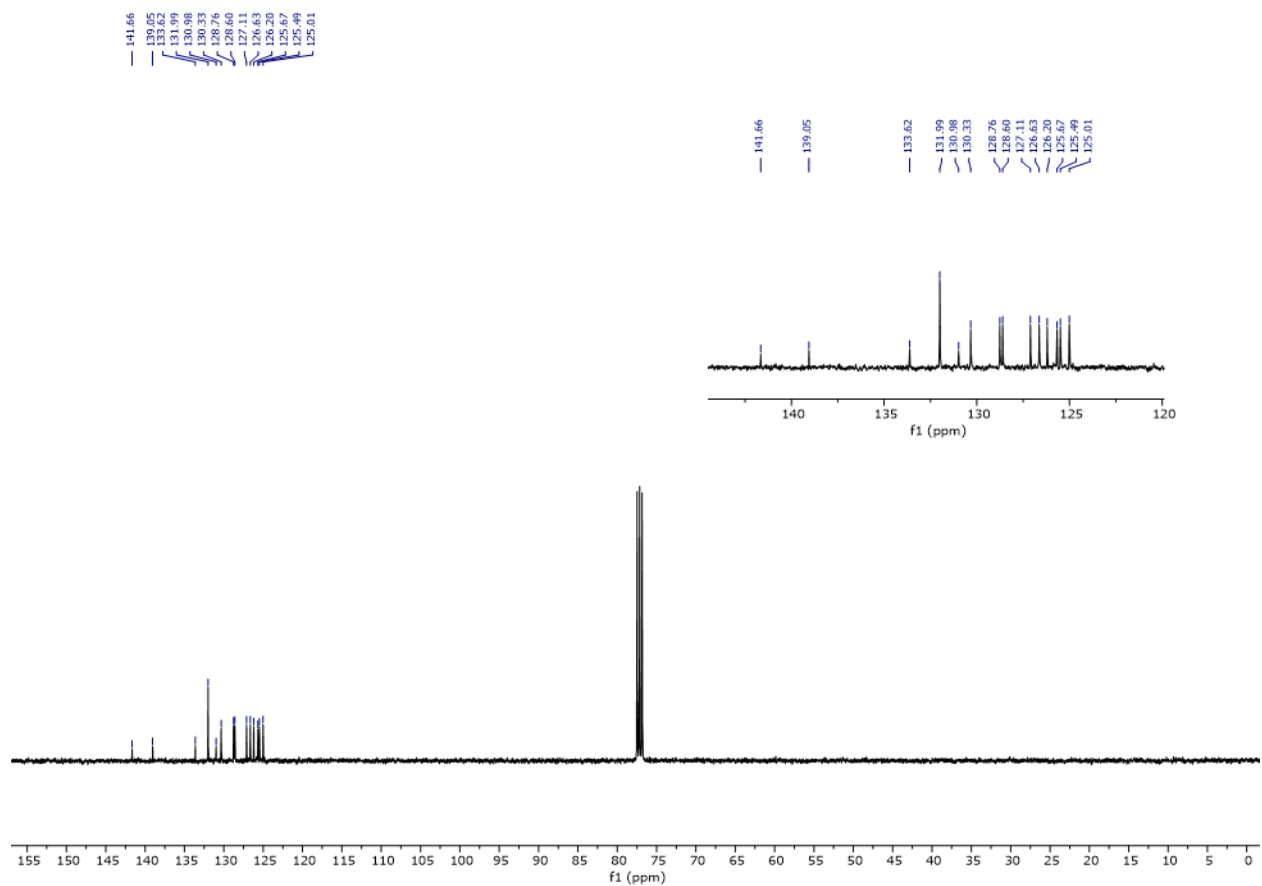
were evaporated and the residue was purified by column chromatography (0 → 5% EtOAc/hexane) to give **4** as light yellow solid (331 mg, 91%). ¹H NMR (400 MHz, CDCl₃) δ = 8.57 (d, *J* = 6.8 Hz, 1H), 7.95 (d, *J* = 7.2 Hz, 1H), 7.92–7.86 (m, 3H), 7.72–7.63 (m, 2H), 7.49 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.34 (t, *J* = 7.6 Hz, 1H), 0.42 (s, 9H) ppm; ¹³C NMR (101 MHz, CDCl₃) δ = 139.7, 139.7, 136.5, 135.8, 132.6, 131.8, 129.9, 128.2, 127.9, 127.3, 127.18, 127.1, 123.5, 121.9, 120.3, 117.7, 104.0, 99.2, 0.2 ppm.

7-Ethynylfluoranthene p2

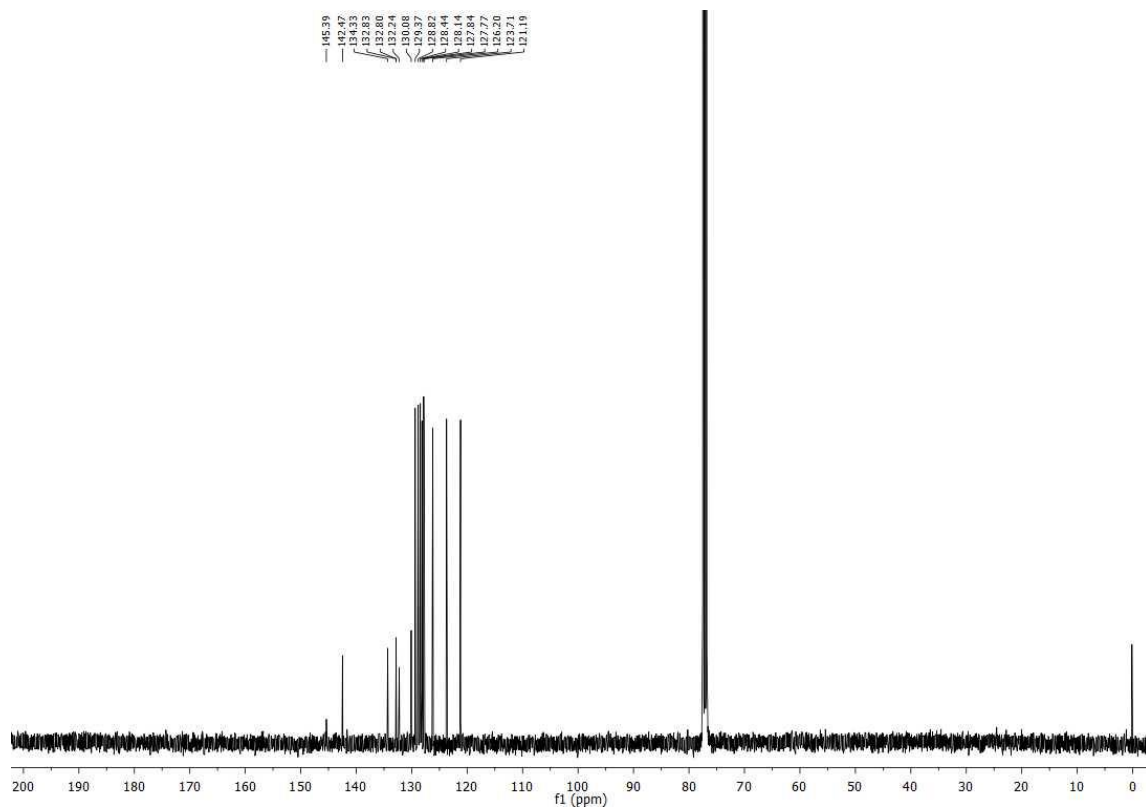
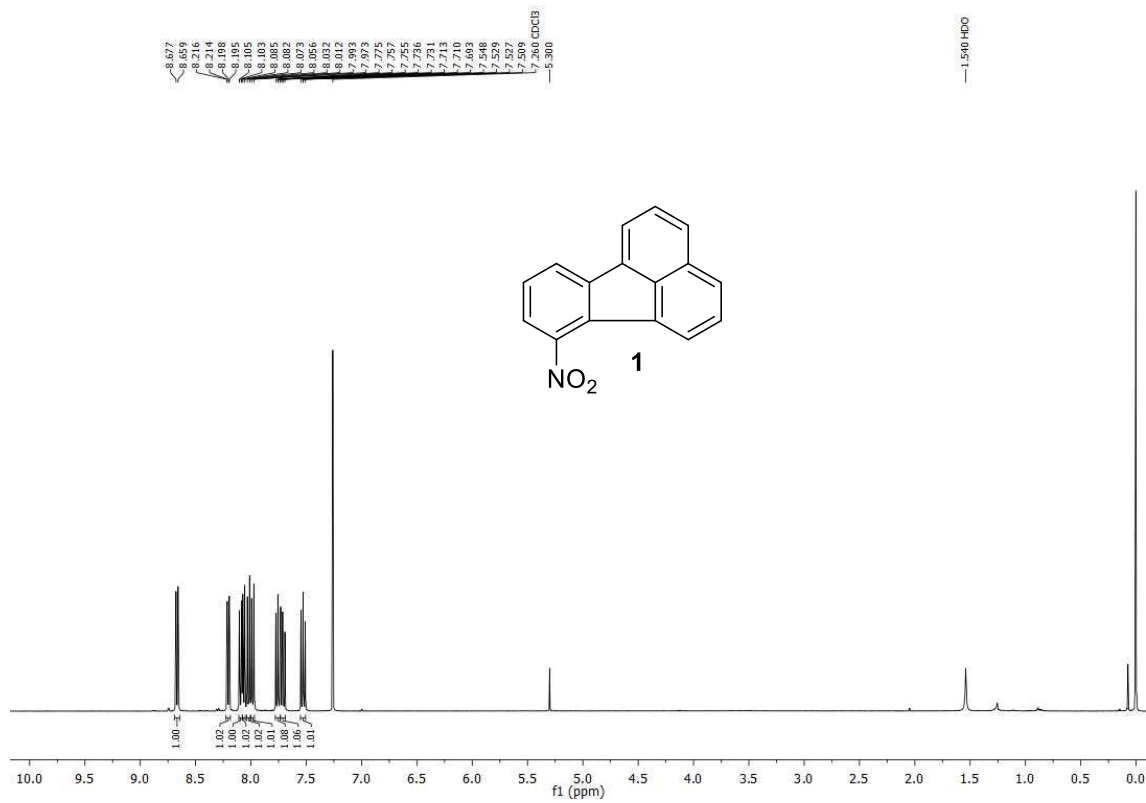
Anhydrous K₂CO₃ (370 mg, 2.68 mmol) was added to a stirred solution of mixture of **4** (200 mg, 0.67 mmol) in dry MeOH/DCM (10 mL, 1:1) at 24 °C. After 2 h, volatiles were evaporated and the residue was column chromatographed (0 → 5% EtOAc/hexane) to give **p2** as an off-white solid (140 mg, 92%). ¹H NMR (400 MHz, CDCl₃) δ = 8.58 (d, *J* = 7.2 Hz, 1H), 7.96 (d, *J* = 6.8 Hz, 1H), 7.93 (dd, *J* = 7.4, 1.0 Hz, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.7–7.63 (m, 2H), 7.52 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.36 (t, *J* = 7.8 Hz, 1H), 3.57 (s, 1H) ppm; ¹³C NMR (101 MHz, CDCl₃) δ = 140.0, 139.8, 136.2, 135.7, 132.5, 132.2, 130.0, 128.3, 127.93, 127.4, 127.3, 127.2, 123.5, 122.1, 120.4, 116.7, 82.6, 81.8 ppm.



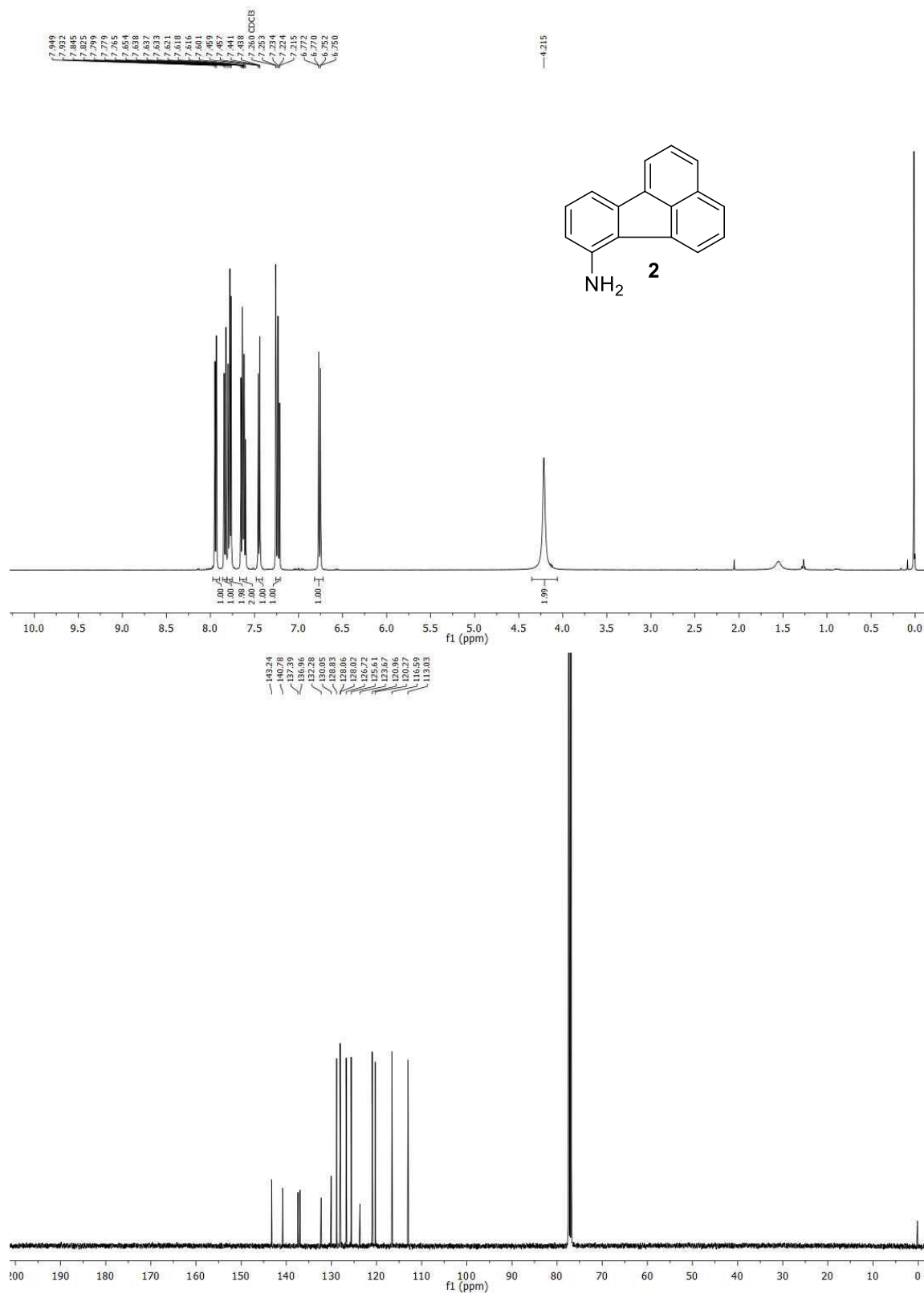
Supplementary Figure 1. ^1H NMR spectrum of 1-(2,6-dibromophenyl)naphthalene.



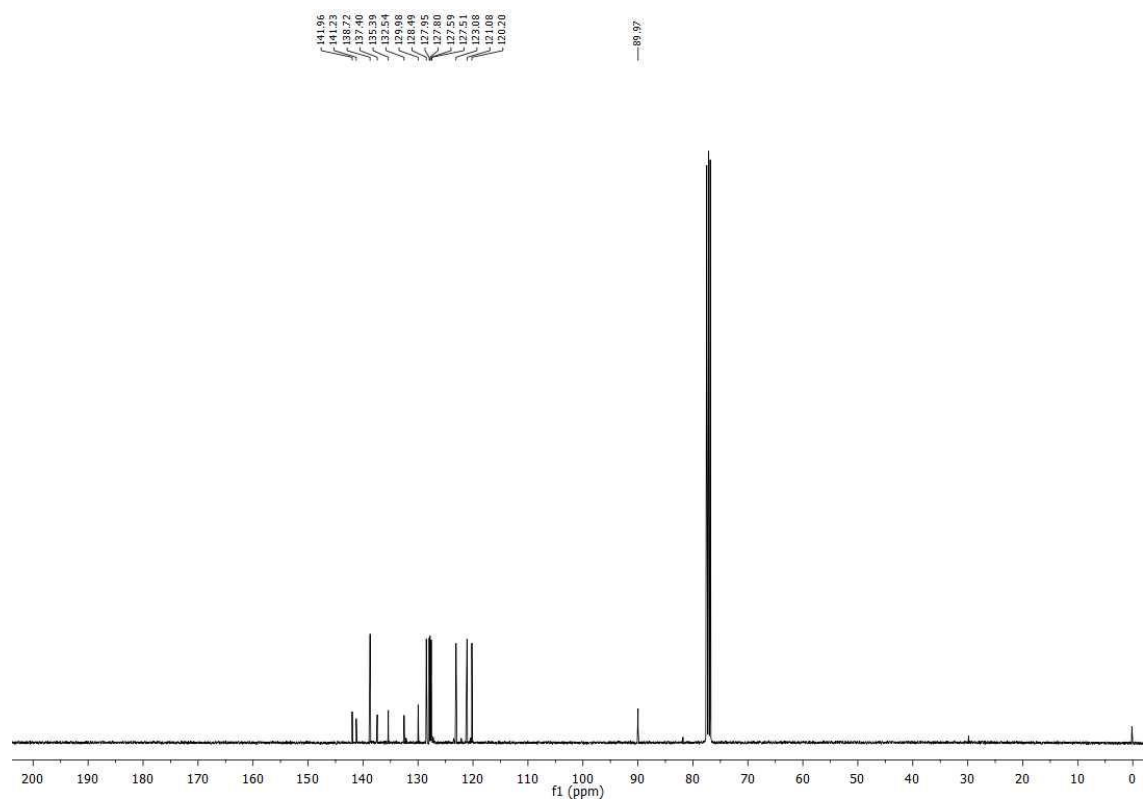
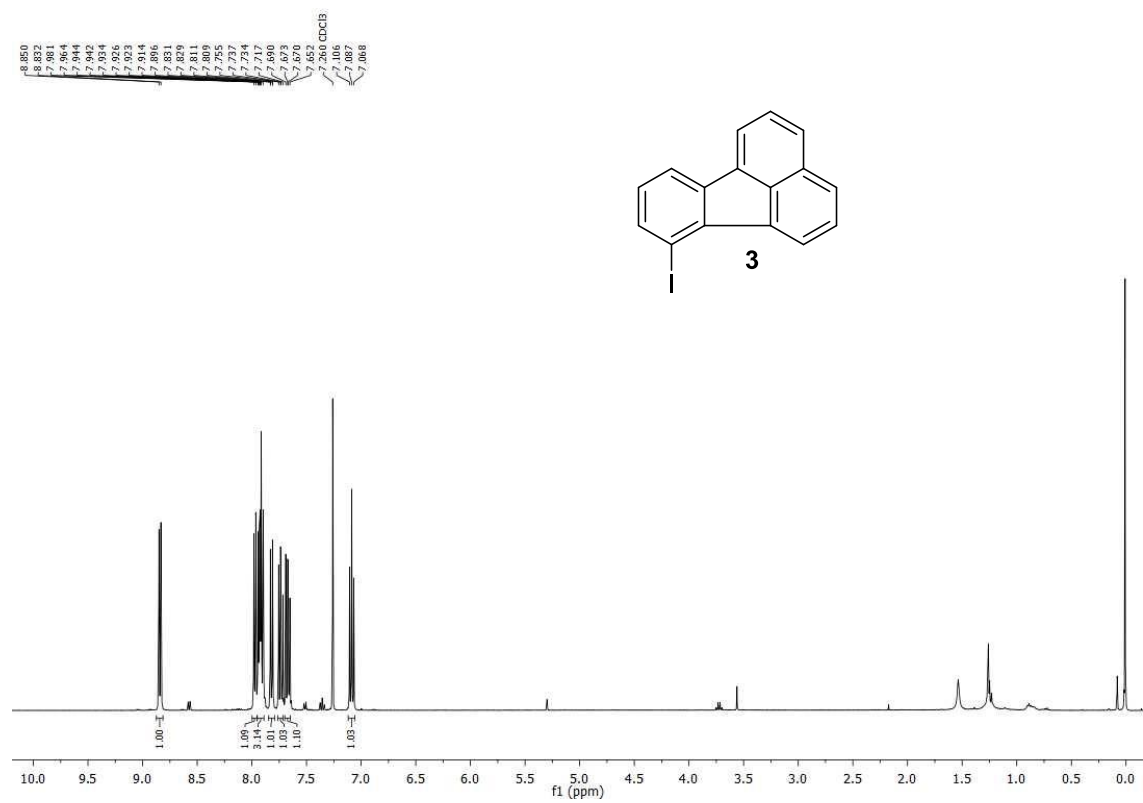
Supplementary Figure 2. ^{13}C NMR spectrum of 1-(2,6-dibromophenyl)naphthalene.



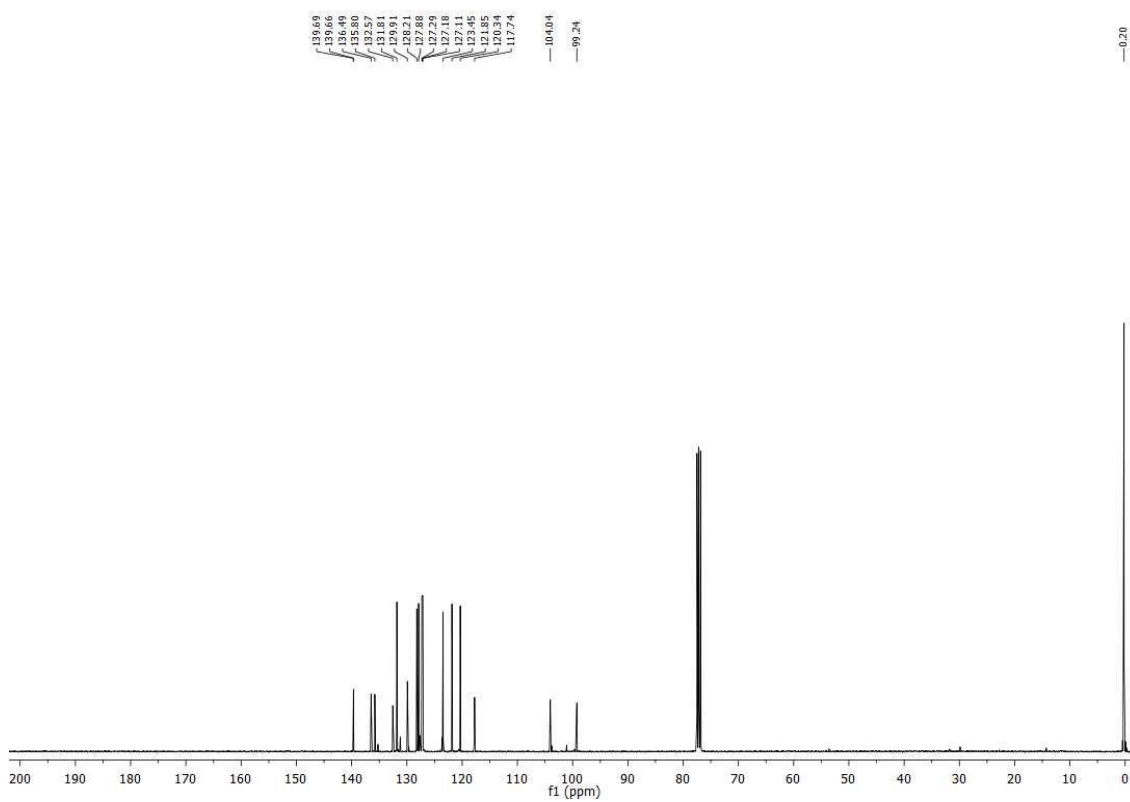
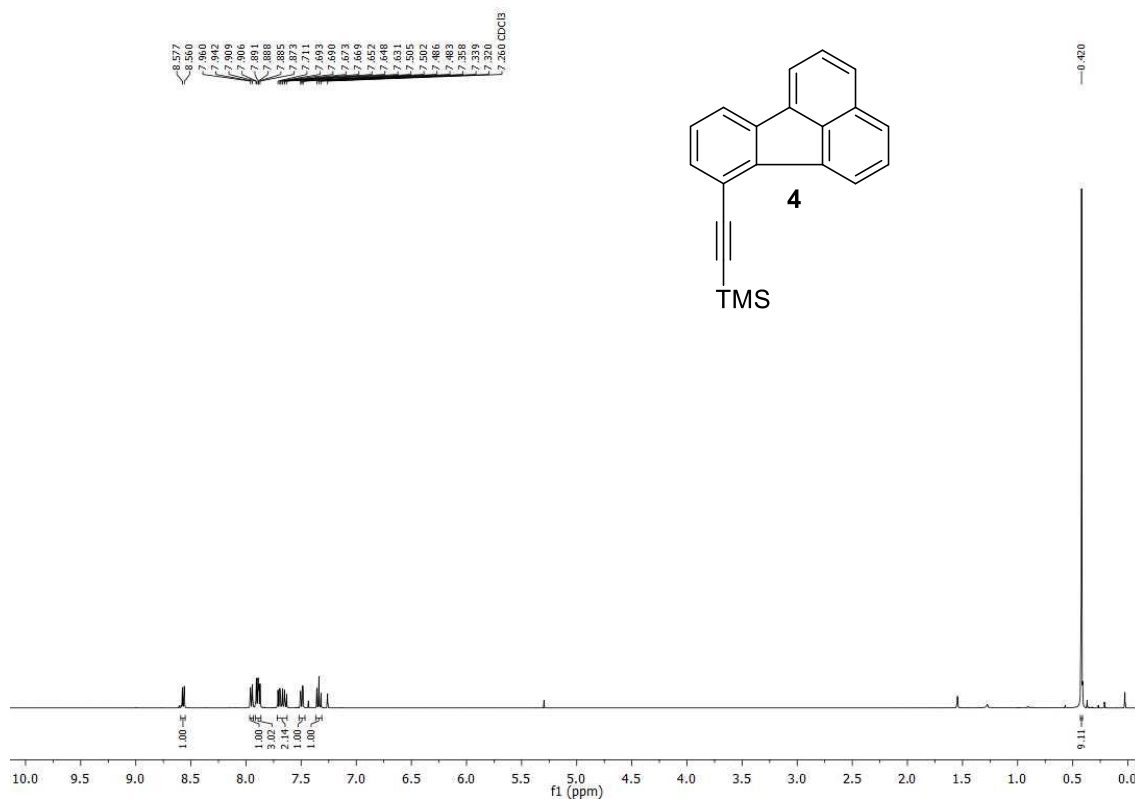
Supplementary Figure 3. ¹H NMR and ¹³C NMR spectra of compound **1** in CDCl₃.



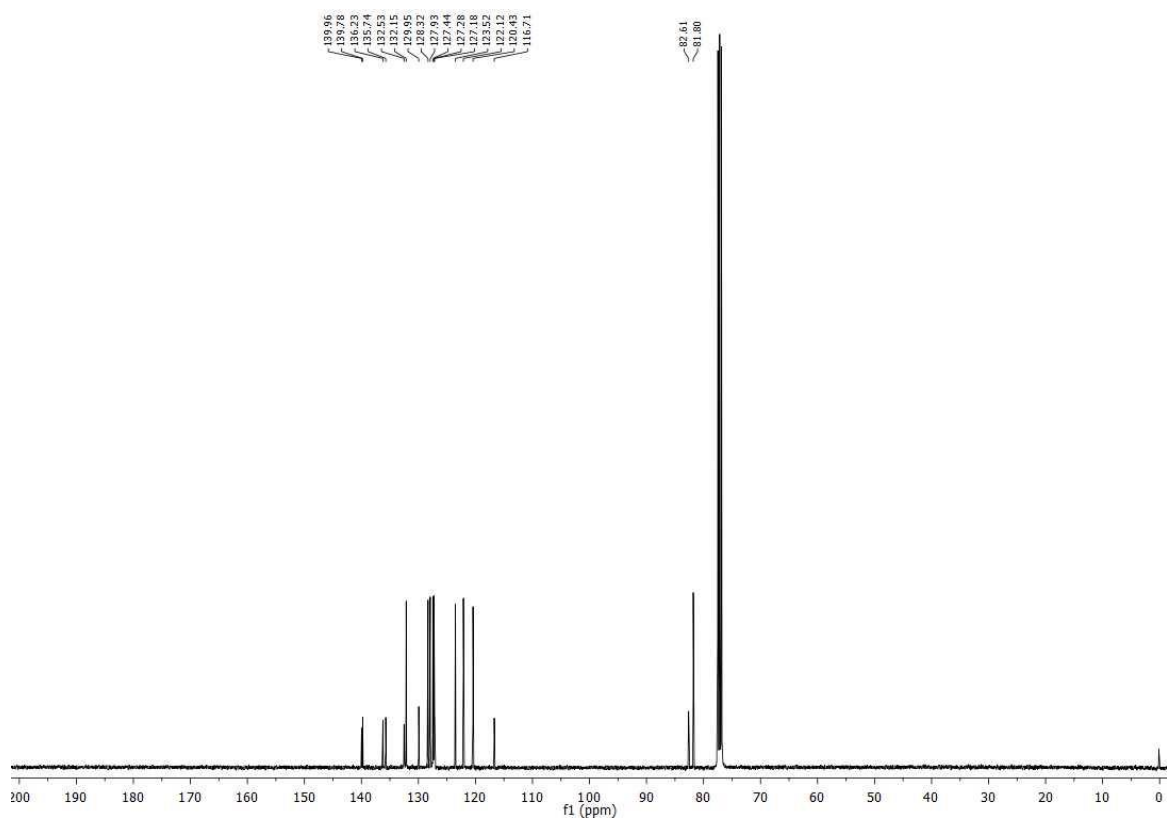
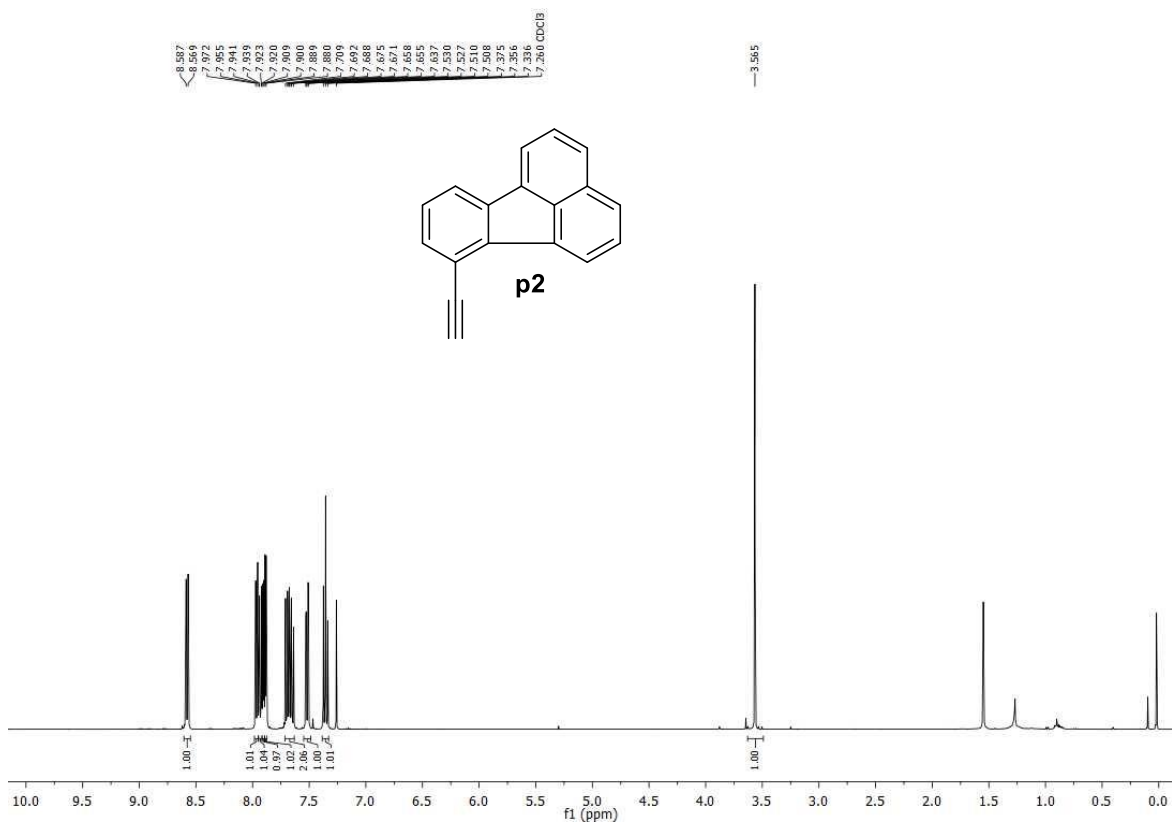
Supplementary Figure 4. ¹H NMR and ¹³C NMR spectra of compound 2 in CDCl₃.



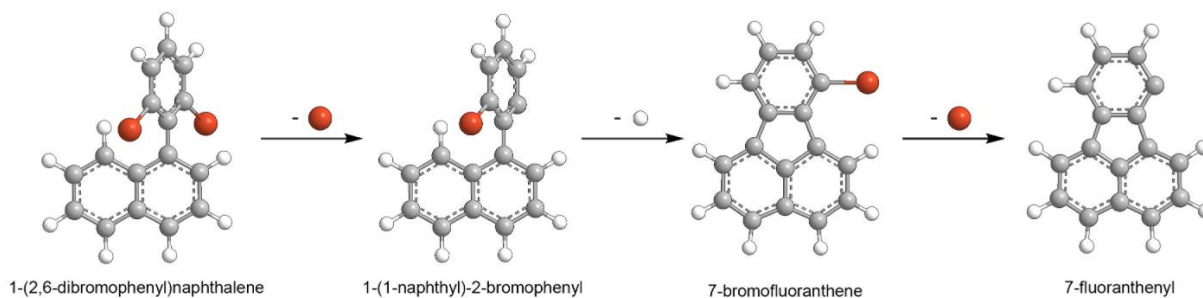
Supplementary Figure 5. ¹H NMR and ¹³C NMR spectra of compound **3** in CDCl₃.



Supplementary Figure 6. ¹H NMR and ¹³C NMR spectra of compound **4** in CDCl₃.

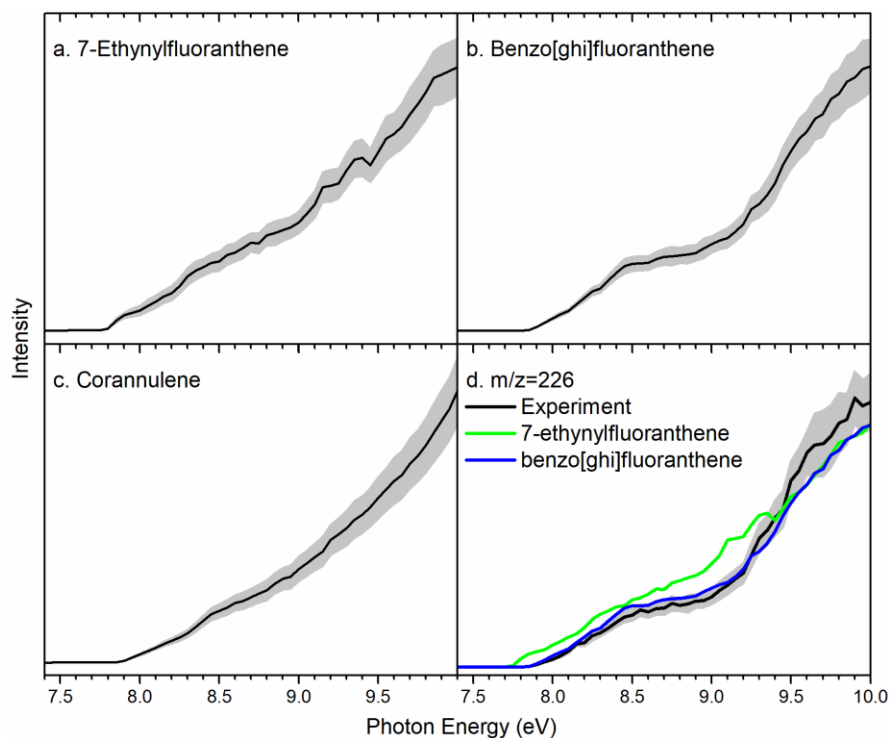


Supplementary Figure 7. ¹H NMR and ¹³C NMR spectra of compound **p2** in CDCl₃.



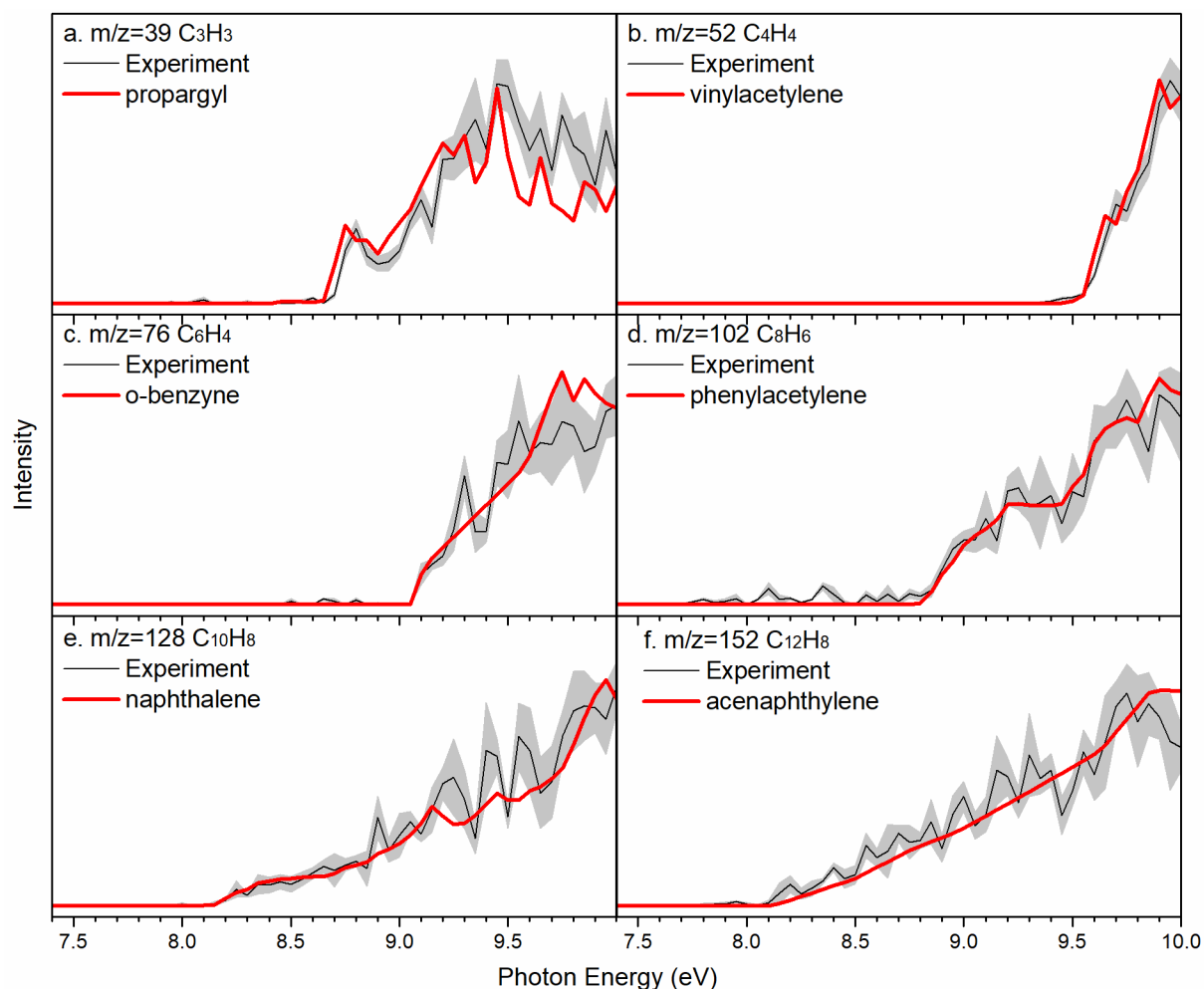
Supplementary Figure 8. Reaction scheme for the pyrolysis of the precursor 1-(2,6-dibromophenyl)naphthalene ($C_{16}H_{10}Br_2$) forming the 7-fluoranthenyl ($C_{16}H_9^{\bullet}$) radical via the 1-(1-naphthyl)-2-bromophenyl radical ($C_{16}H_{10}Br^{\bullet}$) and 7-bromofluoranthene ($C_{16}H_9Br$).

Since both carbon-bromine bonds are equivalent, the cleavage of either bond leads to the formation of the 1-(1-naphthyl)-2-bromophenyl radical. This radical undergoes ring closure followed by hydrogen atom loss from the C8 position of the naphthyl moiety leading to 7-bromofluoranthene. This reaction sequence is in analogy to the phenyl-addition-dehydrocyclization (PAC) mechanism extracted for the formation of fluoranthene from the reaction of phenyl with naphthalene.¹ The carbon-bromine bond in 7-bromofluoranthene can be cleaved by pyrolysis forming the 7-fluoranthenyl radical reactant *in situ*.



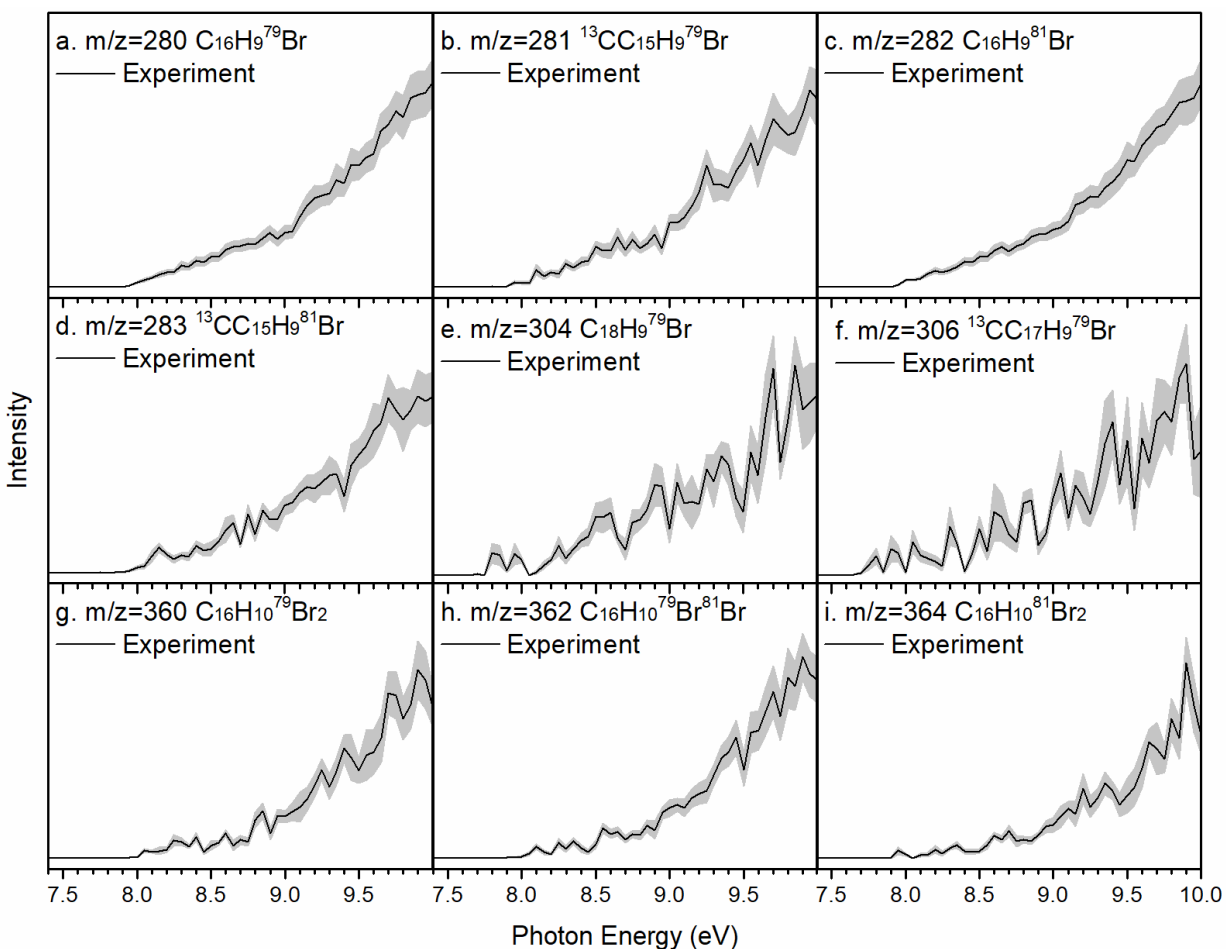
Supplementary Figure 9. PIE calibration curves for 7-ethynylfluoranthene, benzo[*ghi*]-fluoranthene and corannulene, along with the comparison between the calibration curves and experimental measurement at $m/z = 226$.

These PIE calibration curves were newly recorded in this work and are shown as black along with the error limits (grey area). The adiabatic ionization energies of these isomers are 7.80 ± 0.05 , 7.85 ± 0.05 and 7.85 ± 0.05 eV, respectively. The scaled PIE curve at $m/z = 226$ presents a discrepancy between the 7-ethynylfluoranthene calibration curve alone and experiment data. Combined with Fig. 2 in the manuscript, it is concluded that 7-ethynylfluoranthene is just a minor contributor while benzo[*ghi*]fluoranthene the major. The overall error bars consist of two parts: $\pm 10\%$ based on the accuracy of the photodiode and a 1σ error of the PIE curve averaged over the individual scans.



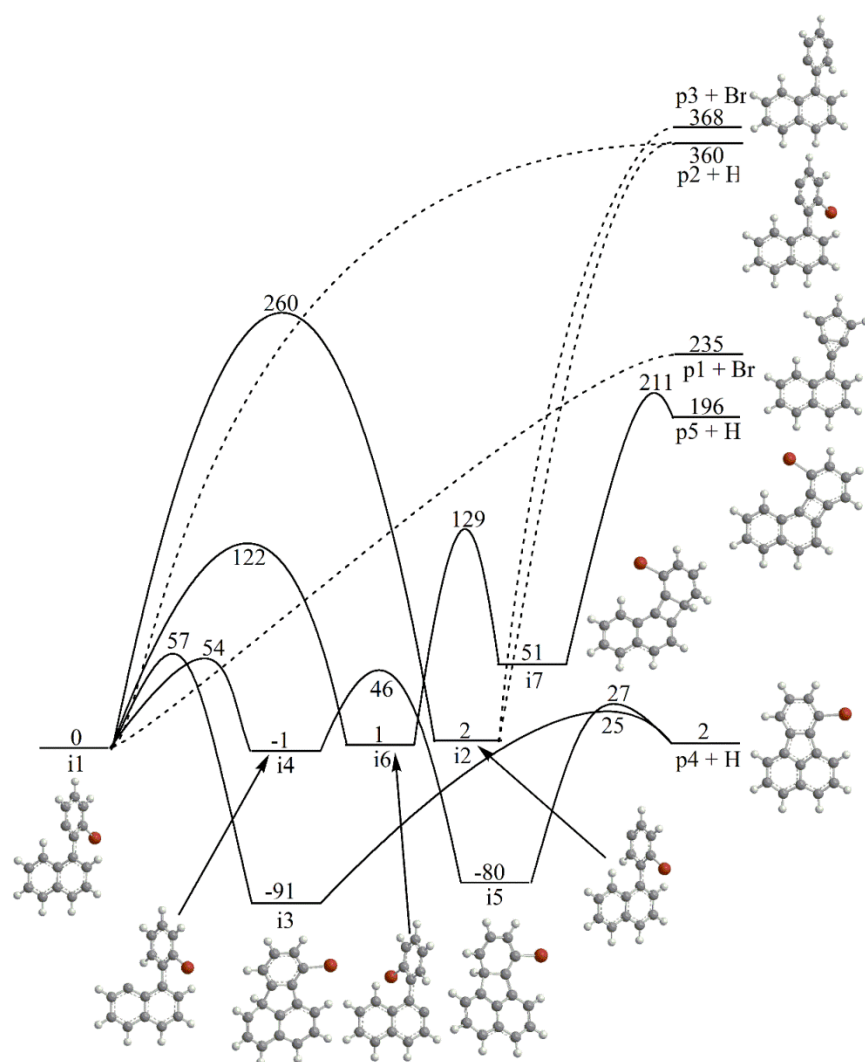
Supplementary Figure 10a. Photoionization efficiency (PIE) curves of distinct ions detected in 1-(2,6-dibromophenyl)naphthalene ($C_{16}H_{10}Br_2$)–acetylene (C_2H_2) system. The black lines shows the experimental measurements along with the error areas labelled in grey. The red lines present the calibration PIE curves of each species. The overall error bars consist of two parts: $\pm 10\%$ based on the accuracy of the photodiode and a 1σ error of the PIE curve averaged over the individual scans.

These species are decomposition products in the pyrolysis of 1-(2,6-dibromophenyl)naphthalene. Due to the short residence time leading to quite limited secondary reactions, the intensities of these species are very low compared with those at $m/z > 200$. Thus, accounting for their m/z ratios and low concentrations, these smaller products cannot yield corannulene via recombination processes, to interfere the conclusion of the present study. This was also validated in our previous studies.¹⁻⁸



Supplementary Figure 10b. Photoionization efficiency (PIE) curves of distinct ions detected in 1-(2,6-dibromophenyl)naphthalene ($C_{16}H_{10}Br_2$)–acetylene (C_2H_2) system. The overall error bars consist of two parts: $\pm 10\%$ based on the accuracy of the photodiode and a 1σ error of the PIE curve averaged over the individual scans.

Signal at $m/z = 360$, 362 and 364 refers to the precursor 1-(2,6-dibromophenyl)naphthalene ($C_{16}H_{10}^{79}Br_2$, $C_{16}H_{10}^{79}Br^{81}Br$ and $C_{16}H_{10}^{81}Br_2$). The C–Br cleavage of the precursor leads to the formation 1-(1-naphthyl)-2-bromophenyl radical ($C_{16}H_{10}^{79}Br$, $m/z = 281$; $C_{16}H_9^{81}Br$, $m/z = 282$). This radical can rapidly undergo ring closure followed by hydrogen atom loss to 7-bromofluoranthene ($C_{16}H_9^{79}Br$, $m/z = 280$; $^{13}CC_{15}H_9^{79}Br$, $m/z = 281$; $C_{16}H_9^{81}Br$, $m/z = 282$; $^{13}CC_{15}H_9^{81}Br$, $m/z = 283$). Based on Supplementary Figures 5a–5d, these PIE curves are superimposable suggesting that they are connected to 7-bromofluoranthene and its $^{13}C/^{81}Br$ counterparts; no 1-(1-naphthyl)-2-bromophenyl radical was detected. Signal at $m/z = 304$ and 306 — based on the nearly equal intensities of the two peaks in the mass spectra (Figure 1) — can be linked to $C_{18}H_9^{79}Br$ (304 amu) and $C_{18}H_9^{81}Br$ (306 amu) produced via the recombination of atomic bromine and the $C_{18}H_9^{\bullet}$ radical.

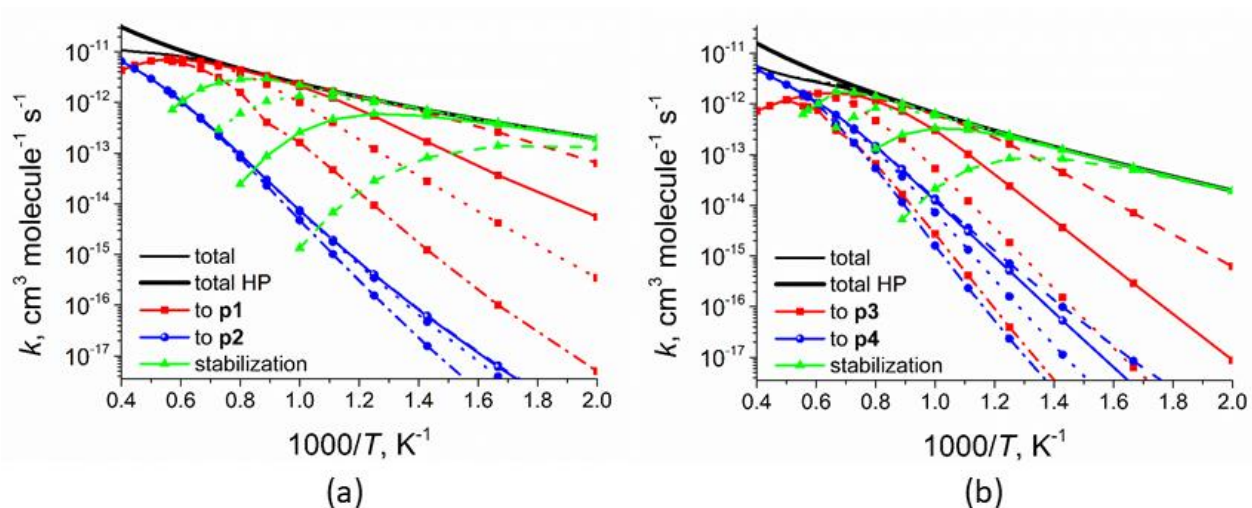


Supplementary Figure 11. B3LYP/6-311G** calculated potential energy diagram for various isomerization and dissociation pathways of the 1-(1-naphthyl)-2-bromophenyl radical produced via a C-Br bond cleavage in the 1-(2,6-dibromophenyl)naphthalene precursor. The energies are given in kJmol^{-1} with respect to the separated reactants.

The results of these computations demonstrate that the pathways leading to 7-bromofluoranthene are significantly more favorable than immediate H and Br atom losses and H migrations (except the 1,5-H shift which eventually results in the same 7-bromofluoranthene product). In fact, relative product yields at the experimental temperature of 1,450 K based on the barriers required are 1 (p4 + H) / $2.2\text{E}-6$ (p5 + H) / $3.0\text{E}-7$ (p1 + Br) / $9.5\text{E}-12$ (p2 + H) / $4.9\text{E}-12$ (p3 + Br). This reveals that 7-bromofluoranthene (p4) is the nearly exclusive product. Next, the weakest C-Br bond in 7-bromofluoranthene radical is cleaved in the reactor producing the fluoranthene-7-yl radical; this and only this isomer of fluoranthenyl can be formed due to the targeted and specific design of the initial precursor in the present study as demonstrated previously.^{1-3, 5, 6}

Supplementary Note 2. Rate constants and product branching ratios for C₂H₂ addition reactions

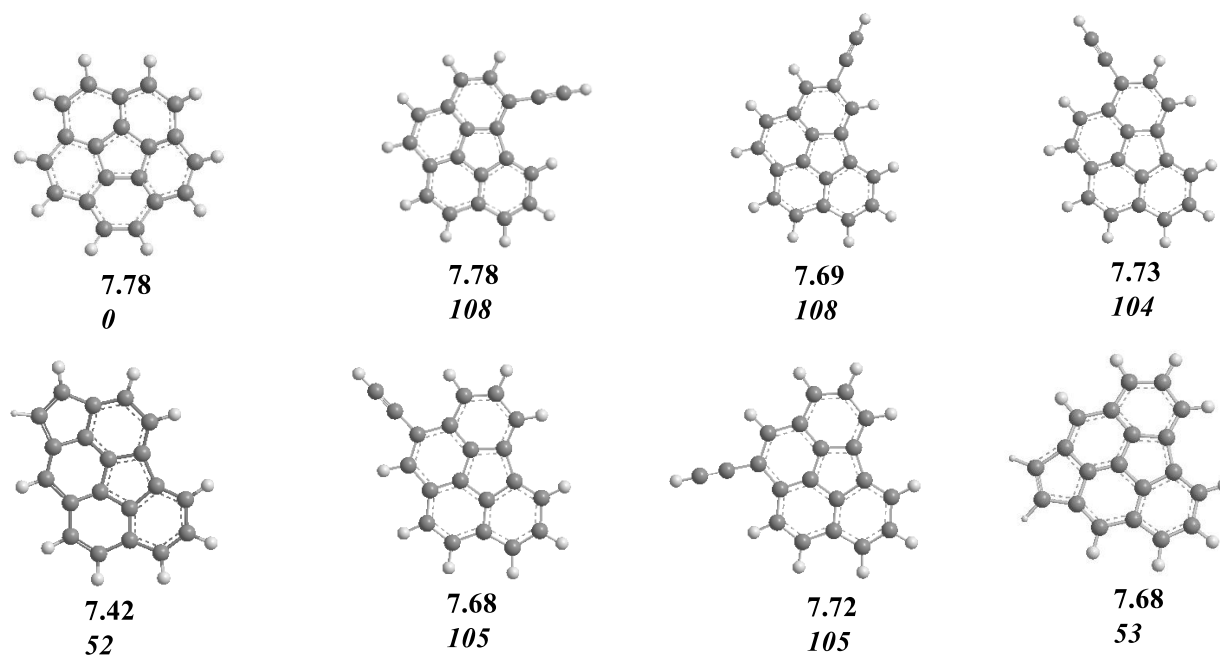
Computed rate constants for the 7-fluoranthenyl + C₂H₂ and benzo[*ghi*]fluoranthen-5-yl + C₂H₂ reactions are illustrated in Supplementary Figure 12, whereas the rate constants for all possible reaction channels in the temperature range of 500-2500 K and at pressures of 0.04, 1, 10, and 100 atm are given in Supplementary Note 5 in the form of output files of MESS calculations.



Supplementary Figure 12. Calculated total and individual channel rate constants for the 7-fluoranthenyl + C₂H₂ (a) and benzo[*ghi*]fluoranthen-5-yl + C₂H₂ (b) reactions. Individual channels include the formation of bimolecular products **p1** and **p2** (a), **p3** and **p4** (b), and overall collisional stabilization of various intermediates. Dashed, solid, dotted, and dash-dotted lines show rate constants computed at the pressures of 0.04, 1, 10, and 100 atm, respectively. Bold lines show the total rate constants at the high-pressure limit (HP).

Both reactions are predicted to be fast with the total HP limit rate constants varying from 1.9×10^{-13} to 3.1×10^{-11} and from 2.0×10^{-14} to 1.6×10^{-11} cm³ molecule⁻¹ s⁻¹ in the 500–2500 K temperature range for 7-fluoranthenyl + C₂H₂ and benzo[*ghi*]fluoranthen-5-yl + C₂H₂, respectively. The former reaction is faster than the latter due to a low entrance barrier, 10 vs. 18 kJmol⁻¹. At low temperatures, collisional stabilization of intermediates prevails, especially at

high pressures, but at 0.04 and 1 atm and above 1000 K both reactions mostly form bimolecular products. For the reactor conditions around 0.04 atm, the branching ratio for the extra six-membered formation (**p1**) varies from 99.6% at 1000 K and 92.7% at 1500 K to 39.9% at 2500 K and, except for the highest temperatures, exceeds the branching ratio for ethynyl-substituted fluoranthene (**p1**) produced by the immediate H loss from the initial complex, 0.3-60.1% in the same 1000-2500 K range. Due to the lower energy difference between corannulene (**p3**) and 5-ethynylbenzo[*ghi*]fluoranthene (**p4**), 108 kJmol⁻¹ vs. a 151 kJmol⁻¹ difference between **p1** and **p2**, the preference for the formation of **p3** over **p4** is less pronounced. For instance, the calculated **p3/p4** branching ratios vary from 94.3/5.1 at 1000 K, to 72.7/27.3 at 1500 K, 33.2/66.8 at 2000 K, and to 13.1/86.9 at 2500 K. Nevertheless, at the typical conditions of hydrocarbon flame combustion on Earth (1500 K and 1 atm) and in low-pressure circumstellar environments at temperatures of 1000–1500 K both reactions favor the growth of an extra six-membered ring thus leading to the formation of corannulene.



Supplementary Figure 13. Calculated structures, adiabatic ionization energies (eV), and relative energies (kJ mol^{-1} , in italics) of various $\text{C}_{20}\text{H}_{10}$ isomers calculated at the G3(MP2,CC)//B3LYP level of theory. Distinct $\text{C}_{20}\text{H}_{10}$ isomers are distinguishable, with the exception of ethynyl-benzo[ghi]fluoranthene (p4). The other isomers, especially those containing two five-member rings have noticeably lower adiabatic ionization energies, which contradicts our experimental onset of the PIE curves. Recall that p4 was predicted computationally to be a less important isomer formed.

Supplementary Note 3. Input files for RRRKM-ME calculations using the MESS package containing optimized Cartesian coordinates, vibrational frequencies, and relative energies of all species and output files including all computed rate constants

3.1. Input file for RRKM-ME calculations for the 7-fluoranthenyl + C₂H₂ reaction using MESS package

```

Temperature List[K]          300. 400. 500. 600. 700. 800. 900.
1000. 1125. 1250. 1375. 1500. 1650. 1750. 1800. 2000. 2250. 2500.
PressureList[atm]           0.03947368 1. 10. 100.
EnergyStepOverTemperature   0.2          #Ratio of
discretization energy step to T
ExcessEnergyOverTemperature 100
ModelEnergyLimit[kcal/mol]  900
WellCutoff                  10
ChemicalEigenvalueMax      0.2
ChemicalEigenvalueMin      1.e-6          #only for direct
diagonalization method
CalculationMethod          direct
EigenvalueOutput           eigenvalue.out

Reactant  p0      #ground energy of bimolecular species will be used as a
reference.
Model
EnergyRelaxation
Exponential
Factor[1/cm]              424      ! Jasper calc N2
Power                     0.62
ExponentCutoff            15
End
CollisionFrequency
  LennardJones
    Epsilons[1/cm]        101.5  866.4   ! N2 Frenklach correlation
with molecular weight
    Sigmas[angstrom]     3.6154  7.56   ! N2 Frenklach correlation
with molecular weight
Masses[amu]               28.   227.08608
End
OutputTemperatureStep[K]  100
OutputTemperatureSize    20
OutputReferenceEnergy[kcal/mol]  0.
!-----
-----
!-----fl_i1-----
Well      i1
Species
RRHO
Geometry[angstrom]      29
C  -1.3144481226   -1.2356813834   -0.0011007583
C  -1.3187469508   -2.6374728291   -1.208466E-4

```

C	-0.0458075819	-3.2713260426	-0.007364328
C	1.1005508475	-2.5038777916	-0.0147926632
C	1.0711310893	-1.0827757707	-0.0155551733
C	-0.1450795715	-0.4291444152	-0.008668726
C	-2.4855960422	-0.4485884254	0.0053078178
C	-3.7107923156	-1.0804667322	0.0130972592
C	-3.7455957638	-2.4993930082	0.014300557
C	-2.5947640719	-3.2645134485	0.0079467913
C	-0.6082649638	0.9786429642	-0.0069293962
C	-2.0385287767	0.9522668226	0.0015532757
C	-2.7920917747	2.1166951428	0.0048137832
C	-2.1294660073	3.3438440196	-3.705793E-4
C	-0.7423834949	3.3849936569	-0.0085293872
C	0.0564702305	2.221275258	-0.0119607719
C	1.5110925075	2.4464596563	-0.0203143762
C	2.523888061	1.6080488941	-0.0255250942
H	0.0209702472	-4.3541719728	-0.0070459897
H	2.0667251271	-2.9964011274	-0.0202958613
H	2.0044559953	-0.5319721894	-0.0215313461
H	-4.6418001222	-0.5240318932	0.0182842471
H	-4.7099233028	-2.9952937709	0.0204102404
H	-2.6628068575	-4.3472726837	0.0090845889
H	-3.8755928118	2.0748337462	0.0113080998
H	-2.694601406	4.2688231034	0.0019411038
H	-0.2438163065	4.3483800993	-0.0124146121
H	1.7778518612	3.5110323248	-0.0227027753
H	3.6002272778	1.695329796	-0.0315550791

Core RigidRotor

SymmetryFactor 1.0

End

Frequencies[1/cm] 81

47.9990	91.5179	118.7530
163.1597	177.3328	215.4045
237.1318	264.9680	309.8782
343.3988	438.3173	452.8191
460.5807	464.9915	504.3784
521.0929	536.5225	572.0162
579.1186	612.9753	628.7553
635.7394	642.1052	679.6962
750.4643	772.1157	772.6487
789.0795	800.8630	810.1245
817.6426	842.5528	852.5788
888.0668	915.3485	916.6415
926.3043	970.3916	973.3170
977.6368	987.6560	1020.9226
1057.0036	1063.8220	1090.5575
1134.1952	1165.9140	1184.6322
1202.3248	1206.4009	1227.3860
1247.5428	1259.3420	1297.0534
1309.1777	1341.5506	1396.6118
1402.9048	1420.6844	1453.6177
1466.0865	1477.3890	1507.6610
1525.0254	1598.8263	1628.0919

1639.8542	1641.9582	1657.0986
1659.8209	3004.0267	3148.1562
3160.5631	3161.4280	3163.9225
3170.3034	3172.1501	3181.2894
3184.5916	3187.7386	3237.4644

ZeroEnergy[kcal/mol] -39.2
 ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----fl_i2-----

Well i2

Species

RRHO

Geometry[angstrom] 29

C	-0.6782458462	-1.2737605139	0.0202956166
C	-0.6972104237	-2.6762027154	0.027658191
C	0.5629241861	-3.3386382632	0.0391124672
C	1.7321639571	-2.5939993267	0.0403561542
C	1.6584386425	-1.1948831002	0.0285786205
C	0.5051917784	-0.4719890415	0.0171237158
C	-1.8350869873	-0.4637751	0.0152309873
C	-3.0679963152	-1.0816905229	0.0142209443
C	-3.1226975514	-2.4998822084	0.0178714636
C	-1.9838005473	-3.2826855524	0.0251438437
C	0.0617727098	0.9378900036	0.0162808466
C	-1.3667928211	0.9310546945	0.0240532516
C	-2.0934553549	2.1124792171	0.0701813761
C	-1.4002503015	3.3217846879	0.1289908778
C	-0.010985177	3.3348883939	0.1350546856
C	0.7615821206	2.1572585287	0.0597841377
C	2.2232391885	2.3234446473	0.0442120453
C	3.1533493501	1.4999736506	-0.4460837061
H	0.6091241711	-4.4227973121	0.0479236361
H	2.6953271302	-3.0925790401	0.0508346893
H	-3.9913500424	-0.5125518986	0.0114861697
H	-4.0940881793	-2.9815741709	0.0162372879
H	-2.0689269706	-4.3640778702	0.0298633774
H	-3.1775927842	2.0975074543	0.0767733801
H	-1.9452666213	4.2576266226	0.1774016666
H	0.5084000481	4.285940415	0.1864924667
H	2.5585371377	3.2737422163	0.4550515475
H	2.9145022518	0.5530863556	-0.9129911014
H	4.2022752515	1.7700907491	-0.4023486387

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 81

46.2792	87.5061	107.6800
158.5739	171.0001	203.6578
242.2442	265.8166	297.8059
344.5362	432.7634	445.0316

454.2476	467.8911	487.2611
523.2452	539.7542	563.8073
578.4938	616.5200	627.2056
632.5180	636.4826	708.1789
753.0109	767.4992	772.5228
785.0953	803.4974	823.0663
825.8912	836.6068	913.8482
919.7216	937.9979	948.0368
954.7686	975.2611	982.1957
992.1317	1025.9045	1049.1073
1067.5129	1097.9764	1099.5354
1138.7678	1161.1768	1186.6242
1205.2709	1225.5607	1237.5251
1250.1765	1294.1243	1308.5732
1346.5559	1355.6352	1391.6886
1416.4052	1435.3891	1446.5843
1460.8962	1479.1282	1493.7553
1514.6981	1598.4076	1605.4641
1628.0816	1637.5202	1649.4571
1687.6223	3123.7963	3141.4836
3159.9553	3161.0323	3162.2839
3171.0189	3172.4768	3176.3612
3185.6783	3187.3031	3224.4390

ZeroEnergy[kcal/mol] -38.1
 ElectronicLevels[1/cm] 1

0 2
 End

End
 !-----

!-----fl_i3-----
 Well i3

Species
 RRHO

Geometry[angstrom] 29

C	-0.7012180971	-1.2072199836	0.229018029
C	-0.7222528205	-2.5994526068	0.2036670863
C	0.571939824	-3.2213745895	0.2021147921
C	1.7489723987	-2.4788919938	0.2243979762
C	1.7374502117	-1.0502065706	0.2502024937
C	0.4944521394	-0.4912048306	0.2510057337
C	-1.8112640032	-0.3163614075	0.2367594655
C	-3.0561710281	-0.9095123901	0.2166595576
C	-3.1346459645	-2.3349248759	0.1902994512
C	-2.0273154964	-3.1686310486	0.1835657498
C	0.1699281745	0.891689623	0.2736251348
C	-1.2246206473	1.0664584096	0.2662453436
C	-1.6848379721	2.3834440065	0.2866413785
C	-0.7249734425	3.4260258857	0.3129409158
C	0.6504711022	3.2131139251	0.319585794
C	1.1628845799	1.8804294473	0.2991938197
C	2.4981367901	1.4128930878	0.3009244957
C	2.8976296121	-0.063534053	0.2764166338
H	0.6391452519	-4.3043082802	0.1830329729

```

H  2.6952707616   -3.0112688594   0.2218773203
H  -3.9746444443   -0.3325244829   0.2201508801
H  -4.1209960563   -2.7859550418   0.1747003728
H  -2.164295318    -4.2446957289   0.1631128519
H  -2.7406431921    2.6289017971   0.2831531808
H  -1.0857572959    4.4490202353   0.3287969269
H  1.3249047093    4.0625379096   0.3401749017
H  3.3175501587    2.1240974332   0.3204071361
H  3.5425524132    -0.2705973181   1.1450997222
H  3.5539396497    -0.2385086987  -0.5908591162

```

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Core RigidRotor
SymmetryFactor 1.0
End

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```

Frequencies[1/cm]  81
71.4867           112.0640           152.5461
216.7730          254.8555           271.4370
291.8218          309.6623           414.7604
429.0355          436.0349           458.8412
495.3527          522.1728           538.1348
566.9434          573.3464           578.5430
627.8705          630.9999           638.7780
652.9769          687.3054           741.4202
746.8059          768.2386           776.6932
795.3987          806.5929           839.1180
864.8787          880.3855           916.0119
916.1682          923.7736           960.9499
965.2378          967.9371           982.0430
1000.2026         1041.2206          1051.2614
1055.6133         1148.0192          1158.1762
1172.6751         1185.3510          1187.4965
1201.1069         1223.7010          1246.8119
1263.5511         1285.8592          1323.1319
1334.0110         1384.1091          1396.7254
1411.7497         1432.8088          1446.5627
1451.1134         1458.8330          1474.4142
1504.9794         1519.4675          1575.5732
1607.9449         1634.9051          1654.8210
1710.1562         2958.7685          2960.3987
3153.4707         3157.9790          3159.0948
3163.1520         3170.4828          3172.2714
3172.7977         3182.5375          3184.4594

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ZeroEnergy[kcal/mol] -75.0
ElectronicLevels[1/cm] 1
0 2

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End
End

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!-----
!-----fl_i4-----
Well      i4

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Species
RRHO
Geometry[angstrom]  29
C  -0.7554633883   -1.233079212   0.0526156337

```

C	-0.7745900476	-2.628456502	0.0052143609
C	0.5526800984	-3.2612495195	-0.0127570871
C	1.7147015817	-2.5649469064	-0.0223656597
C	1.772734743	-1.0483925424	-0.2042505235
C	0.4311672142	-0.4988221953	0.0309066449
C	-1.8502949924	-0.3919589624	0.4082924898
C	-3.0835194453	-1.0132665573	0.5477135062
C	-3.1593390396	-2.4159902758	0.3891600111
C	-2.0360980494	-3.2230489482	0.1580225622
C	0.1493912091	0.7886311619	0.4899965869
C	-1.2526819871	0.943277634	0.6971732081
C	-1.6654316848	2.1551410659	1.2332037918
C	-0.6854507018	3.1113873337	1.5849879775
C	0.6921188649	2.8725798088	1.4767700448
C	1.1453204857	1.6611841061	0.9332425623
C	2.5031941401	1.0967684517	0.9300564274
C	2.7936295649	-0.1543073191	0.4991503621
H	0.5974008055	-4.3450965284	0.042483755
H	2.6569542278	-3.1040955187	-0.0019999846
H	2.0199792202	-0.9252315559	-1.2850457704
H	-3.9793781562	-0.4601659399	0.8086838361
H	-4.1258381806	-2.8944961902	0.502475473
H	-2.149206452	-4.301932581	0.135357388
H	-2.7110160682	2.3737090985	1.4218038448
H	-1.0156049716	4.0546587072	2.0058991389
H	1.393249525	3.6129421439	1.8476830712
H	3.3029159842	1.6998140483	1.3502429748
H	3.8170035003	-0.5122073056	0.5587273738

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 81

90.3363	105.8798	184.2787
208.1437	254.9383	275.5309
296.4094	394.1259	404.7777
424.3205	442.9973	456.0702
479.4879	538.7268	539.4914
567.3763	569.4683	589.0460
621.3818	629.5629	632.6195
677.3564	732.6130	751.5327
753.8141	766.1517	769.8767
809.4824	822.2544	839.6533
861.6368	905.1072	910.4654
913.6768	959.0088	961.9533
963.3979	981.6585	987.0756
1018.3440	1032.8386	1046.7619
1050.5167	1111.0438	1134.3293
1157.6795	1172.7368	1178.1546
1207.1437	1211.9609	1223.8541
1244.6461	1271.5675	1285.6522
1322.7767	1366.3093	1381.2019
1390.0443	1416.7142	1419.6335
1429.6340	1496.7316	1505.6988

1535.2498	1552.6935	1582.6891
1596.9374	1605.0714	1637.3244
1649.5440	2783.5580	3145.6366
3146.4432	3158.7719	3159.2070
3165.5353	3167.0285	3168.2828
3169.3757	3182.5791	3183.3999

ZeroEnergy[kcal/mol] -58.6
 ElectronicLevels[1/cm] 1
 0 2

End
 End

!-----
 !-----c2h2_c16h9_fl_p0-----

Bimolecular fl_p0
 Fragment c16h9

RRHO

Geometry[angstrom] 25

C	0.002979243	-1.2242687746	0.0
C	0.002927131	-2.625290378	0.0
C	1.2804201651	-3.2521834629	0.0
C	2.4295235094	-2.484850224	0.0
C	2.399259978	-1.0638171069	0.0
C	1.1759217869	-0.4314156414	0.0
C	-1.1677046206	-0.4272702325	0.0
C	-2.3911245603	-1.0618962694	0.0
C	-2.4231727914	-2.4826265394	0.0
C	-1.2746488757	-3.2510339572	0.0
C	0.7204653547	0.9691772575	0.0
C	-0.7151126344	0.9773328182	0.0
C	-1.4103313867	2.1813107224	0.0
C	-0.705828709	3.389270637	0.0
C	0.697670027	3.404386394	0.0
C	1.344822846	2.1880747675	0.0
H	1.3510489887	-4.3347117916	0.0
H	3.3938638383	-2.9808574969	0.0
H	3.3282232827	-0.5050325848	0.0
H	-3.3235319598	-0.5079706134	0.0
H	-3.388090729	-2.977467472	0.0
H	-1.3464584441	-4.3334961311	0.0
H	-2.4946223621	2.1906915881	0.0
H	-1.2467582987	4.3295520947	0.0
H	1.2395052211	4.3435473967	0.0

Core RigidRotor
 SymmetryFactor 1
 End

Frequencies[1/cm] 69

99.7431	125.9431	167.1969
207.6710	256.0968	293.5303
358.2715	431.9756	459.4859
470.2009	478.8379	495.1143
558.6415	569.5332	573.3931
618.4091	632.4881	642.3197
681.8167	729.6749	754.2886

```

769.6279          787.6522          789.8306
816.7372          839.8720          892.2529
909.7508          917.8925          927.8944
964.1723          977.8681          978.4598
988.2375          1033.4262         1060.4533
1061.6062         1096.2567         1122.1222
1164.6247         1174.5731         1203.8534
1212.3951         1247.4732         1261.3191
1283.9902         1325.9551         1393.2838
1394.7080         1421.8962         1448.4648
1454.8476         1468.3252         1496.4499
1520.2721         1558.3796         1638.7613
1640.5995         1642.1708         1658.8976
3160.1197         3161.6410         3162.6669
3172.0359         3173.0338         3176.2281
3183.5429         3185.2571         3187.7365
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0 2
End
Fragment      c2h2
RRHO
Geometry[angstrom]      4
C 0.0  0.0  0.5990703976
C 0.0  0.0 -0.5990703976
H 0.0  0.0  1.6619081422
H 0.0  0.0 -1.6619081422
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm]      7
642.0679          642.0679          772.6955
772.6955          2069.5209         3420.9273
3523.7963
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0 1
End
GroundEnergy[kcal/mol] 0.0
End
!-----h_c18h10_fl_p1-----
Bimolecular  fl_p1
Fragment      c18h10
RRHO
Geometry[angstrom]      28
C -0.5502694157  -0.9565243136   0.0
C -0.5595199471  -2.3454509872   0.0
C  0.7506026828  -2.9596611191   0.0
C  1.9233333496  -2.224556092    0.0
C  1.9117329772  -0.7803577102   0.0
C  0.6459608764  -0.2373527522   0.0
C -1.6594257039  -0.0674997223   0.0
C -2.9036393746  -0.6674139362   0.0

```

C	-2.9732392899	-2.091689745	0.0
C	-1.8589317508	-2.921279756	0.0
C	0.3427181547	1.1250780135	0.0
C	-1.0658596201	1.3161364158	0.0
C	-1.4885848833	2.6311533729	0.0
C	-0.5044808179	3.6631148795	0.0
C	0.8645780423	3.4273658447	0.0
C	1.3427954813	2.0889498588	0.0
C	2.6907289958	1.5628780201	0.0
C	2.9662304887	0.2064945353	0.0
H	0.8187109574	-4.0428029772	0.0
H	2.870157015	-2.7547367768	0.0
H	-3.8254867632	-0.0960500739	0.0
H	-3.9567636451	-2.5487367549	0.0
H	-1.9917758684	-3.9980492222	0.0
H	-2.5378925711	2.9054018711	0.0
H	-0.8510848808	4.6907716725	0.0
H	1.5532853502	4.2656746832	0.0
H	3.5225391939	2.2599623914	0.0
H	4.0029099664	-0.1142276199	0.0

Core RigidRotor

SymmetryFactor 1

End

Frequencies[1/cm] 78

71.0088	119.9158	185.3537
246.9106	276.2699	297.5283
299.8689	424.9032	437.0839
444.9036	448.1960	461.7271
515.9473	548.9595	567.3113
577.2208	578.9884	609.2500
639.9126	652.0372	670.6766
679.1012	759.5321	760.2025
776.3306	781.8340	783.3880
840.3041	841.8788	844.1167
878.0951	921.3342	925.9549
946.6698	964.2032	970.6723
979.8556	981.5520	982.1366
1041.0663	1041.9694	1070.3056
1148.1826	1156.9303	1159.5132
1185.9383	1211.3844	1215.7561
1234.7759	1251.6646	1261.8950
1306.6321	1350.1155	1396.7422
1402.0487	1425.0006	1436.5617
1451.4117	1456.0421	1484.2730
1494.1579	1514.3522	1539.4460
1626.7215	1627.1398	1652.5787
1677.7917	1701.6136	3157.0823
3157.5538	3160.0434	3160.3549
3170.9804	3171.8897	3174.2216
3175.2973	3183.4493	3184.2686

ZeroEnergy[kcal/mol] 0.0

ElectronicLevels[1/cm] 1

0 1

```

End
Fragment          H
Atom
Mass[amu]         1
ElectronicLevels[1/cm]      1
0  2
End
GroundEnergy[kcal/mol] -46.7
End
!-----h_c18h10_fl_p2-----
Bimolecular      fl_p2
Fragment          c18h10
RRHO
Geometry[angstrom]  28
C  -0.3149270684   -1.005221708    0.0
C  -0.3192307352   -2.4064367895   0.0
C   0.9559272621   -3.0366177098   0.0
C   2.105408558    -2.2704395833   0.0
C   2.0799506513   -0.8494847127   0.0
C   0.8578045424   -0.2090662882   0.0
C  -1.4836943422   -0.2090543869   0.0
C  -2.7090300757   -0.8395672926   0.0
C  -2.7452106046   -2.2598054868   0.0
C  -1.5976537982   -3.029868379    0.0
C   0.3999691201    1.1925806348    0.0
C  -1.026229576    1.1919916936    0.0
C  -1.7375490502    2.3832888326    0.0
C  -1.0345940358    3.5920721461    0.0
C   0.3543514924    3.6065389449    0.0
C   1.098912587     2.4080135462    0.0
C   2.5244376473    2.4679218451    0.0
C   3.7264354705    2.5487181111    0.0
H   1.0242440013   -4.1193608935    0.0
H   3.0692566879   -2.7675280337    0.0
H   3.0094274278   -0.2952687343    0.0
H  -3.6399231253   -0.2829896406    0.0
H  -3.7111104038   -2.7527507284    0.0
H  -1.6708332061   -4.1122764285    0.0
H  -2.8219109106    2.382764255     0.0
H  -1.5766339932    4.5307453998     0.0
H   0.8893533337    4.5482707482     0.0
H   4.7863221438    2.6202616381     0.0
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]  78
63.2892             102.1840             119.0055
164.7422            167.2881             225.4728
256.4859            292.5088             349.7901
391.1302            402.0298             436.9020
467.6160            476.1145             520.0298
549.1964            550.4628             588.5571
597.3385            607.0681             628.6545

```

639.2620	642.3045	660.8276
690.3794	749.8436	773.8291
775.6188	790.6023	815.7083
818.0269	825.4524	842.7638
917.6979	920.7253	929.7015
955.3913	977.4887	979.8083
989.8285	1009.1158	1051.8150
1062.7029	1081.0408	1137.3272
1165.0680	1185.1350	1205.7455
1208.6088	1240.8904	1255.9780
1265.4143	1295.2797	1342.8920
1397.5584	1401.4911	1418.1761
1453.6496	1466.6704	1477.2723
1507.4634	1524.4409	1609.7720
1628.6461	1640.9011	1641.8431
1659.2335	2201.9449	3160.9473
3162.6446	3167.6198	3171.5866
3179.5595	3181.6465	3184.6338
3195.8323	3206.0382	3476.1748

ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
Fragment H
Atom
Mass[amu] 1
ElectronicLevels[1/cm] 1
0 2
End
GroundEnergy[kcal/mol] -10.4
End
!-----fl_ts1-----
Barrier ts1 fl_p0 i1
RRHO
Geometry[angstrom] 29
C 1.273246293 0.1674414348 8.511321E-4
C 2.5172312368 0.8113732292 -0.0358493355
C 2.4883083229 2.233654419 -0.005466473
C 1.2796839351 2.9002006121 0.0527304518
C 0.0315996931 2.2203322565 0.0870457071
C 0.0296458105 0.8424661431 0.0649607566
C 1.1039157847 -1.2382067567 -0.0276084806
C 2.2288947286 -2.0318985097 -0.0925594632
C 3.5047487069 -1.4072157885 -0.1280577569
C 3.6592593445 -0.0343216845 -0.1014651831
C -1.0063565754 -0.2081430936 0.0841933327
C -0.3496286861 -1.4822166983 0.0237184062
C -1.0919310818 -2.6572830709 0.0208372643
C -2.4872052682 -2.5908592872 0.078124216
C -3.1436831234 -1.3542496767 0.1412359026
C -2.3795854788 -0.2023492539 0.1503505677
C -3.60182625 1.7721488085 0.4437738527
C -4.0378348169 2.1978658344 -0.6068391021


```

H 3.4170925307 2.7937762322 -0.0307303873
H 1.2768207562 3.9845940268 0.0713489072
H -0.8905501328 2.7879960368 0.1229776832
H 2.1650005011 -3.1143145142 -0.1174792743
H 4.3869050184 -2.035980645 -0.1787565947
H 4.6527723817 0.4004743957 -0.1315429542
H -0.597782012 -3.6215065428 -0.0269414637
H -3.071094222 -3.5052644114 0.07331885
H -4.2266102687 -1.3101923107 0.182788621
H -3.4067389919 1.6936427473 1.4882368215
H -4.3327241364 2.4297630678 -1.6021160041
Core RigidRotor
SymmetryFactor 0.5
End
      Rotor      Hindered      ! C2H2      26.2281
      Group      18 28 29
      Axis      16 17
      Symmetry      1
      Potential[kcal/mol] 12
0      0.169427589 0.771836796 1.738201564 0.363955562 0.031375479 0.062750959
      0.451806905 1.229918796 2.321785483 0.721636029 0.175702685
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 316.0056
WellDepth[kcal/mol] 2.3
WellDepth[kcal/mol] 41.5
End
Frequencies[1/cm] 79
43.1170
88.9245      101.3543      126.1783
167.2305      209.5624      216.4630
257.2134      299.2307      358.0450
432.2661      458.9077      466.7431
475.1261      493.5155      533.1059
564.3705      572.0052      577.0669
622.6346      633.1834      644.8694
652.4241      657.5877      738.1090
759.7827      765.1078      770.4947
777.3325      788.8213      795.0717
816.5373      840.6810      898.0055
909.8489      917.8341      930.2529
965.8007      974.7732      977.9210
988.3022      1032.6167      1060.9911
1064.4072      1092.3202      1123.2755
1164.1999      1175.9712      1204.3247
1214.1278      1247.5377      1262.2195
1284.4317      1328.2514      1393.5961
1395.8177      1419.3309      1449.7202
1455.0003      1467.1619      1495.8180
1520.1009      1561.6418      1634.9726
1639.9667      1641.0143      1657.9895
1941.9756      3156.4206      3160.0994
3161.3400      3168.9983      3171.4119

```

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3177.3014          3180.4155          3183.8990
3191.6983          3395.3631          3482.5325
ZeroEnergy[kcal/mol]  2.3
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----fl_ts2-----
Barrier      ts2  i1  fl_p2
RRHO
Geometry[angstrom]  29
C  -1.3318726625  -1.2046444567  -0.0344227307
C  -1.328220557   -2.6038812614  -0.1072766268
C  -0.0493919927  -3.2258386367  -0.1399733301
C  1.0957618565   -2.4544879413  -0.0987402558
C  1.0620354836   -1.0356293795  -0.0242565812
C  -0.1637011249  -0.4028417058  0.0064924119
C  -2.5051934128  -0.416304021   0.0088757066
C  -3.7269599128  -1.0528857475  -0.0227829939
C  -3.7551068347  -2.4712597614  -0.0977284947
C  -2.6031552239  -3.2336011645  -0.1390822364
C  -0.6295483703  0.9937718429   0.0787754181
C  -2.0556946673  0.9852492446   0.0815453648
C  -2.773369004   2.1712199269   0.1440198045
C  -2.0768784866  3.3815556745   0.2067757237
C  -0.6872138765  3.4032437098   0.2052381395
C  0.0595935823   2.2105395489   0.1427817246
C  1.4974526059   2.2857451003   0.15968539
C  2.6432471447   2.5013309884   0.5113940904
H  0.0251224378  -4.3066605579  -0.1968106446
H  2.0624197853  -2.9452537379  -0.1240027467
H  1.9894693679  -0.4789257566  0.0067581903
H  -4.6609320116  -0.5023281783  0.0075910828
H  -4.7181009109  -2.9691178333  -0.1230339791
H  -2.6702512759  -4.3148882327  -0.1958429353
H  -3.8576932154  2.1647374043   0.1437166854
H  -2.6230277379  4.3164650646   0.2566005558
H  -0.1568895571  4.3462727129   0.2521517979
H  1.7473095114   1.7136717391   -1.6220838591
H  3.6888770594   2.636470415    0.6493183282
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  790.0351
WellDepth[kcal/mol]  35.5
WellDepth[kcal/mol]  6.7
End
Frequencies[1/cm]  80
62.5990          91.9360
102.0263         161.2280         171.6647
173.1978         239.1787         258.0035
294.4064         351.8310         388.4941

```

415.5305	436.7948	465.7811
468.5801	481.6739	520.0629
550.8899	552.7460	586.9453
600.8773	607.1880	633.5685
640.3058	646.3144	662.9600
692.5351	751.1348	774.5555
775.7447	790.8321	815.7269
822.7636	825.6002	843.2900
918.6186	921.7191	931.2693
955.2090	978.0642	980.2987
990.3295	1008.0876	1051.2904
1063.1073	1081.3356	1137.7485
1164.9455	1185.3030	1201.7450
1208.3207	1237.6451	1254.5704
1266.0949	1295.4806	1342.8345
1397.9567	1401.8090	1419.0808
1453.7784	1467.3706	1476.4439
1507.1755	1524.2862	1610.7458
1628.7651	1640.9313	1641.9151
1659.1698	2097.7229	3161.4061
3163.2097	3168.1997	3171.7568
3180.1185	3182.4192	3185.1663
3197.1588	3206.1581	3459.9939

ZeroEnergy[kcal/mol] -3.7

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----fl_ts3-----

Barrier ts3 i1 i2

RRHO

Geometry[angstrom] 29

C	-1.3472323463	-1.1941113717	-0.0060284311
C	-1.2792031996	-2.591015176	-0.007055374
C	0.031637137	-3.1579852619	-0.0161569339
C	1.1560778993	-2.3462356334	-0.0234437676
C	1.0285467189	-0.9368798683	-0.0220125089
C	-0.2081846989	-0.3569941332	-0.0133956019
C	-2.5372853615	-0.4292430154	0.002328135
C	-3.7350319786	-1.1129669931	0.0101431697
C	-3.7086471633	-2.534807288	0.0093876721
C	-2.5325639571	-3.2639386967	0.0011440443
C	-0.687713791	1.019767004	-0.0095905179
C	-2.1124932803	0.9894748768	3.59419E-5
C	-2.8284436775	2.1782239988	0.0053750718
C	-2.1219002107	3.3878052463	0.0010990366
C	-0.7310214057	3.4098097942	-0.0083055677
C	0.0285949235	2.2221757353	-0.0139381299
C	1.4953609466	2.2901628162	-0.0238538809
C	2.3750928013	1.288814767	-0.0302092371
H	0.1505534939	-4.2368636295	-0.0174022216
H	2.1401448541	-2.8020741838	-0.0303116719
H	1.942325037	0.0231782399	-0.027801424

```

H -4.6906208122 -0.5997845035 0.0168091412
H -4.6539739427 -3.0661658053 0.0155613626
H -2.5687513212 -4.3481859602 9.507312E-4
H -3.9128027126 2.1802164022 0.0127162068
H -2.6675852135 4.3245883727 0.0051834589
H -0.2133835832 4.3634525994 -0.0114172566
H 1.896513202 3.3063991101 -0.0261836729
H 3.4550956423 1.3869485571 -0.0374657742
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1634.4125
WellDepth[kcal/mol] 9.4
WellDepth[kcal/mol] 8.3
End
Frequencies[1/cm] 80
88.3143 99.7836
162.1905 200.6370 244.7092
247.7592 298.1202 332.3279
358.3172 370.8837 434.2963
455.0332 475.0256 508.3952
514.0240 535.0056 553.0121
571.5072 579.7334 629.0993
634.3831 640.8409 669.3041
702.9321 755.9936 774.1490
777.8615 794.9867 825.7331
831.7391 835.2151 841.3274
909.7418 921.4453 928.7775
956.2527 961.2062 975.1997
982.8021 993.9241 1029.2065
1044.7927 1070.5127 1086.3347
1112.0907 1143.1580 1162.1026
1188.7950 1207.9950 1229.1216
1243.6260 1256.9336 1286.0000
1302.6979 1334.1970 1374.5162
1401.1278 1421.6657 1438.6266
1447.5357 1466.1047 1497.6175
1510.9840 1520.7258 1608.9598
1627.3634 1632.7210 1643.0245
1650.9256 1663.2211 3071.1425
3158.3210 3160.5248 3160.9863
3170.3251 3171.6270 3176.2868
3178.9934 3184.2637 3186.3449
ZeroEnergy[kcal/mol] -29.8
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----fl_ts4-----
Barrier ts4 i2 i3
RRHO
Geometry[angstrom] 29

```

```

C -0.8375884419 -1.2044156539 0.4815857741
C -0.8829137082 -2.5995822305 0.5702644892
C 0.378561246 -3.2631266267 0.6604671755
C 1.5711004607 -2.5443778561 0.6454693668
C 1.5524555058 -1.1368583458 0.5485048116
C 0.3687802352 -0.4721214202 0.4632078183
C -1.9578113476 -0.3401748306 0.3718875833
C -3.2059293594 -0.9258686204 0.3580011544
C -3.2971734041 -2.3435538557 0.4507474697
C -2.188823565 -3.165774173 0.5537324213
C 0.0060082219 0.9307951292 0.3595570722
C -1.408400395 1.0391883594 0.3188652281
C -1.9778113838 2.3070235189 0.3254050194
C -1.1325386423 3.425818658 0.4124339227
C 0.2525645281 3.2996662409 0.5028615334
C 0.8619056763 2.0298114719 0.4584526396
C 2.28472969 1.7480834273 0.6379271128
C 2.9071897257 0.6673344332 0.0599459259
H 0.4119619891 -4.3454084287 0.7398226595
H 2.5113846176 -3.0813479875 0.7132492301
H -4.1157737291 -0.3406709549 0.2776983655
H -4.2831685557 -2.7949640233 0.438803028
H -2.3188577319 -4.2407634078 0.6212000487
H -3.0531335343 2.4438896549 0.2949159351
H -1.5724774429 4.4167452848 0.4296205498
H 0.8676621768 4.188456736 0.5954704313
H 2.8227801442 2.3392399381 1.3749677084
H 3.9321810667 0.4312202523 0.3202688461
H 2.5684929572 0.2917293102 -0.8966563208
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 417.5671
WellDepth[kcal/mol] 7.3
WellDepth[kcal/mol] 44.2
End
Frequencies[1/cm] 80
86.6492 99.0673
168.5217 203.7632 242.3427
268.4871 283.8184 329.2334
358.2321 418.6858 431.4526
458.7025 474.7491 492.3428
534.9351 541.1801 576.0056
579.8911 616.0712 634.0536
638.0884 654.2695 711.9695
747.8215 756.3414 770.7455
779.8186 791.9421 819.1374
836.8946 838.8590 888.0781
910.8769 921.3325 939.3021
954.9324 956.9935 974.2581
981.3105 987.8392 1041.1174
1063.1682 1078.1159 1097.9193

```

1140.6690	1159.8029	1185.9991
1213.5369	1230.3179	1240.8913
1251.1126	1267.3097	1282.7259
1327.0109	1363.7808	1392.8791
1407.3380	1431.9140	1434.2209
1447.7442	1476.8342	1494.8895
1507.7204	1542.0874	1607.5026
1618.1753	1623.3205	1637.6715
1645.2715	3136.0253	3144.1219
3153.6301	3159.9040	3161.0257
3169.6953	3170.7088	3171.5903
3183.4390	3185.0481	3226.8231

ZeroEnergy[kcal/mol] -30.8

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----fl_ts5-----

Barrier ts5 i3 fl_p1

RRHO

Geometry[angstrom] 29

C	-0.7066088264	-1.2012227186	0.2336914036
C	-0.7117477756	-2.5905496394	0.2371788397
C	0.5974520665	-3.2003991634	0.3024978387
C	1.7667729279	-2.4608260255	0.3584618277
C	1.7481084857	-1.0199096457	0.3560751413
C	0.4863158935	-0.4785399212	0.2896514584
C	-1.8178083919	-0.3164209067	0.1888606644
C	-3.0589369358	-0.9198388894	0.1358494273
C	-3.1239367581	-2.3442182507	0.1315257501
C	-2.0083805987	-3.170258104	0.1806223074
C	0.1757888826	0.8848778318	0.2867566119
C	-1.2308394209	1.0692540432	0.2272322084
C	-1.6624355251	2.3824042211	0.2381311051
C	-0.6873766226	3.4195798236	0.3105796951
C	0.6811363804	3.1916908583	0.3762197824
C	1.1684520316	1.8556195973	0.3669100388
C	2.512121919	1.3421031985	0.4486713301
C	2.8074147651	-0.0241270206	0.3981539567
H	0.6692455913	-4.2832768622	0.3082131773
H	2.7147314328	-2.9868393978	0.4020268238
H	-3.9815445176	-0.3508625776	0.0988792249
H	-4.1049796132	-2.8046476603	0.0889398657
H	-2.1380740929	-4.2473819598	0.1766012623
H	-2.7128409532	2.6493656952	0.1981849046
H	-1.0403062218	4.445036344	0.3177766746
H	1.3633877523	4.0331170393	0.4344865773
H	3.3378987133	2.0411382792	0.5292640849
H	3.8301476339	-0.3368490367	0.5741851625
H	3.4091207781	-0.1824291521	-1.4988501449

Core RigidRotor

SymmetryFactor 0.5

End

```

Tunneling      Eckart
ImaginaryFrequency[1/cm]  619.7609
WellDepth[kcal/mol]  32.6
WellDepth[kcal/mol]  4.3
End
Frequencies[1/cm]  80
71.6798          118.2113
176.8442         232.8532          275.5792
279.9193         287.1989          307.0053
344.4191         425.5817          438.9539
444.0830         459.0054          468.5905
523.3798         549.9178          567.7933
577.1983         581.0395          608.2714
639.0929         649.0972          669.0057
688.3326         759.1926          760.1861
776.0859         782.8596          794.0788
838.6498         841.9194          852.5220
877.7587         921.0254          926.1863
945.8565         968.2123          977.5338
980.7908         981.8485          987.3261
1041.5287        1042.6961         1068.5506
1141.3971        1151.9769         1159.6140
1185.6434        1202.9587         1217.6340
1233.9252        1250.1957         1261.6837
1304.4369        1349.0793         1394.5745
1397.9804        1422.0068         1437.2090
1442.0661        1453.4924         1471.6488
1493.0682        1511.3460         1536.7777
1622.7717        1627.6737         1648.4620
1671.0226        1697.2413         3158.8708
3160.5660        3161.1927         3164.8116
3171.5518        3172.6510         3176.2002
3181.0559        3183.7738         3184.7121
ZeroEnergy[kcal/mol]  -42.4
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----fl_ts6-----
Barrier      ts6  i1  i4
RRHO
Geometry[angstrom]  29
C  -0.8387351534   -1.2494858835   -0.1466569779
C  -0.7725904623   -2.6317131876    0.0526635962
C   0.5541529204   -3.1865002588    0.0714125938
C   1.6582890808   -2.410186767    -0.1863881908
C   1.570591159    -0.9916930702   -0.4772565943
C   0.2873447579   -0.4344306089   -0.3579202521
C  -2.0306235265   -0.475474136    -0.1507927785
C  -3.2244759258   -1.1511953943    0.0076339039
C  -3.194122617    -2.5582725535    0.1958455399
C  -2.0132288449   -3.2890219893    0.2312618431
C  -0.1734978498    0.9254332518   -0.3214175477

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C -1.5960764178 0.9378587805 -0.2615546625
C -2.2477909604 2.15991258 -0.1655120632
C -1.4756823597 3.3297285145 -0.0640574768
C -0.0846296707 3.2823082721 0.0335254985
C 0.59933244 2.0566709936 -0.0537892014
C 2.0037096796 1.8790734147 0.3506232627
C 2.6392029184 0.7181030796 0.4699152873
H 0.6821201234 -4.2493219031 0.2510895916
H 2.6320481323 -2.8849943235 -0.2380178363
H 2.2953004033 -0.5915886334 -1.1767478916
H -4.1796358438 -0.6371916239 0.0029898472
H -4.1356665067 -3.079818908 0.3277392835
H -2.0465603249 -4.3602552065 0.3998418545
H -3.3298253346 2.222556472 -0.1277955722
H -1.9770873701 4.2884678095 0.0063910593
H 0.4706881597 4.1949475341 0.2245291328
H 2.5163941115 2.7875963381 0.6809306165
H 3.6520662822 0.5035624072 0.7836561346
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 525.3918
WellDepth[kcal/mol] 15.8
WellDepth[kcal/mol] 35.2
End
Frequencies[1/cm] 80
94.2555 107.2735
172.8754 201.6823 255.3612
267.5091 290.7340 333.1747
359.3872 430.1677 448.8206
461.0211 476.1005 508.8794
540.6174 549.5305 574.3795
576.8436 618.3174 624.9231
642.9289 653.6794 699.8204
739.0386 753.0067 770.8759
771.7961 791.6826 813.2984
824.6169 835.0124 847.3574
887.0179 909.9356 917.6605
921.0617 966.7072 967.0581
974.1858 976.3893 1025.7214
1050.1249 1060.2854 1069.5407
1135.3930 1156.7471 1179.6635
1189.9074 1202.8711 1213.3542
1241.0022 1259.8907 1281.5344
1290.3300 1335.3889 1388.1486
1402.5144 1417.6671 1436.7212
1455.2437 1478.5186 1499.3604
1510.5110 1563.0027 1598.2813
1616.3143 1631.5285 1633.0345
1639.5392 3048.7484 3144.2053
3157.8489 3158.2929 3160.1359
3168.7528 3170.5836 3177.7743

```



```

3183.4475          3184.4494          3210.2102
ZeroEnergy[kcal/mol] -23.4
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----fl_ts7-----
Barrier      ts7  i4  fl_p1
RRHO
Geometry[angstrom]  29
C  -0.7423140114   -1.2871209556    0.2582687696
C  -0.7611435381   -2.6618143415    0.0512185608
C   0.548534867    -3.2752767678   -0.0754003892
C   1.7211696618   -2.5600035006   -0.0072099885
C   1.7284343499   -1.1028890025    0.1392813171
C   0.45473303     -0.5731138367    0.3255382235
C  -1.8408496534   -0.4340958544    0.5543930409
C  -3.0832424542   -1.0406665375    0.5714532597
C  -3.162464784    -2.4380967846    0.3142691202
C  -2.0534619219   -3.2432410041    0.0720158955
C   0.165170792    0.7404613862    0.6969226645
C  -1.2387144986    0.9112470809    0.8454493209
C  -1.6492639934    2.163253482     1.264600739
C  -0.6600750834    3.1529616453    1.5238578468
C   0.7081824521    2.9270674021    1.4069202826
C   1.1712467864    1.6557021078    0.9852831096
C   2.5201747799    1.1299349759    0.8776335261
C   2.7921155057   -0.1672017576    0.5104517188
H   0.6073184888   -4.3511051603   -0.2062723722
H   2.6656608736   -3.0854320276   -0.0988109322
H   1.9996495343   -0.8503281702   -1.5892323155
H  -3.9937139158   -0.4923556759    0.7876695225
H  -4.1429616845   -2.9012731741    0.3290231587
H  -2.188289366    -4.3081917714   -0.0851831523
H  -2.6943794263    2.4107307582    1.4157340752
H  -0.9954278175    4.1312230138    1.8504576735
H   1.4054616308    3.7212827286    1.6519383737
H   3.3525872011    1.7826162291    1.1207106764
H   3.8245471952   -0.4961454874    0.461356274
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  975.1678
WellDepth[kcal/mol]  21.0
WellDepth[kcal/mol]  9.1
End
Frequencies[1/cm]  80
78.7308          117.2933
182.9575          238.9458          271.8070
294.5559          304.5877          378.3775
406.3754          439.3287          443.8908
458.9902          460.4014          487.5816

```

522.1684	552.9629	563.9628
576.6224	577.8997	615.5967
637.9962	652.6553	660.7933
688.2238	756.3957	758.8792
775.7646	779.0306	781.8634
837.9316	838.7496	845.1230
875.0598	920.1563	924.3257
943.1755	970.0504	973.8785
977.1559	981.5609	981.6164
1042.9195	1043.6848	1063.3683
1145.6786	1157.3539	1168.8099
1184.8472	1188.4325	1214.7087
1233.2744	1249.7690	1264.7578
1302.7971	1345.1033	1391.1207
1407.0092	1413.6560	1432.3627
1444.4070	1461.2725	1493.4616
1499.5419	1505.8011	1534.6803
1620.8361	1621.6905	1642.7427
1666.0258	1670.8961	3158.2415
3158.4371	3160.6872	3161.0492
3171.2439	3172.1858	3176.8294
3177.8592	3183.7814	3184.5537

ZeroEnergy[kcal/mol] -37.6

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----fl_ts8-----

Barrier ts8 i3 i4

RRHO

Geometry[angstrom] 29

C	-0.7288615352	-1.2866004046	0.3004658366
C	-0.7592322446	-2.6611828116	0.0582911919
C	0.5520460274	-3.2707349162	-0.084991602
C	1.7332369625	-2.5726073377	0.0087923113
C	1.7414642403	-1.122485613	0.2199204021
C	0.4579668748	-0.5808987154	0.3878217634
C	-1.8302265764	-0.4269917182	0.5972157276
C	-3.0764708625	-1.0393616553	0.5846303467
C	-3.1589568771	-2.4257125507	0.301142964
C	-2.0457462037	-3.236003728	0.0521185276
C	0.1637281132	0.7401659413	0.7653360258
C	-1.2363786436	0.9054883534	0.896786312
C	-1.6603463502	2.1794084064	1.2930987768
C	-0.6860645735	3.1671899448	1.5372065144
C	0.6953824336	2.9489956346	1.4216458763
C	1.168059487	1.6778969035	1.027345355
C	2.5236383829	1.1840607378	0.8853850349
C	2.8192892914	-0.1432794319	0.514628781
H	0.6093840983	-4.3428129346	-0.2475229219
H	2.6733995203	-3.1041121778	-0.0920359171
H	2.3790109739	-0.5027233439	-0.7757764651
H	-3.988767302	-0.4921317087	0.7976610811

```

H -4.1411351804 -2.8855154551 0.2957175861
H -2.1849220979 -4.2965326909 -0.1298910046
H -2.7089606461 2.4228597099 1.4232688364
H -1.0234311399 4.151714889 1.8432061269
H 1.3856664585 3.7546036772 1.6470388584
H 3.3577083949 1.8559475425 1.0495098186
H 3.8476239741 -0.4863935465 0.5005278558
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1585.2839
WellDepth[kcal/mol] 41.6
WellDepth[kcal/mol] 25.2
End
Frequencies[1/cm] 80
75.6816 118.9189
181.2238 241.0157 273.4434
288.0002 298.1063 387.2782
414.7073 440.2177 446.3352
457.6140 520.6610 542.5423
549.6949 572.2414 573.2246
590.4730 629.4657 634.9446
646.6070 676.6580 734.9621
751.0621 752.7050 763.3355
773.1742 798.3015 811.9176
823.5768 865.8190 882.8019
898.9775 914.3129 930.4704
957.5147 961.5788 971.8127
975.5042 1040.8415 1050.5732
1059.6297 1070.0947 1120.8203
1145.0897 1164.0061 1182.0238
1197.2345 1219.6714 1225.8647
1245.1917 1267.6525 1292.0793
1338.6375 1360.8060 1390.0121
1405.8647 1412.3006 1435.1824
1437.7615 1470.3236 1494.4146
1504.1587 1524.4391 1551.9386
1575.4964 1604.6486 1623.5028
1632.1149 1672.5954 3154.9918
3158.0688 3158.4279 3167.7898
3171.6412 3173.5713 3174.8179
3181.8306 3183.0624 3187.7982
ZeroEnergy[kcal/mol] -33.4
ElectronicLevels[1/cm] 1
0 2
End
!-----
End

```

3.2. Output file of RRKM-ME calculations for the 7-fluoranthenyl + C₂H₂ reaction using MESS package

Wells (G - ground energy, D - dissociation limit, kcal/mol):

Name	G	D
i1	-39.2	-29.8
i2	-38.1	-30.8
i3	-75.0	-42.4
i4	-58.6	-37.6

Bimolecular Products (G - ground energy, kcal/mol):

Name	G
fl_p0	0.0
fl_p1	-46.7
fl_p2	-10.4

Well-to-Bimolecular Barriers (H/G - barrier height/well depth, kcal/mol)

Name	H	Well	G	Product
ts1	2.3	i1	-39.2	fl_p0
ts2	-3.7	i1	-39.2	fl_p2
ts5	-42.4	i3	-75.0	fl_p1
ts7	-37.6	i4	-58.6	fl_p1

Well-to-Well Barriers (H/G - barrier height/well depth, kcal/mol):

Name	H	Well	G1	Well	G2
ts3	-29.8	i1	-39.2	i2	-38.1
ts4	-30.8	i2	-38.1	i3	-75.0
ts6	-23.4	i1	-39.2	i4	-58.6
ts8	-33.4	i3	-75.0	i4	-58.6

Unimolecular Rate Units: 1/sec; Bimolecular Rate Units: cm³/sec

High Pressure Rate Coefficients (Temperature-Species Rate Tables):

T(K)	i1->i1	i1->i2	i1->i3	i1->i4	i1->fl_p0	i1->fl_p1	i1->fl_p2
300	***	2.68182e+06	***	7.01557	2.2051e-16	***	4.4662e-13
400	***	3.83646e+07	***	4527.92	1.33696e-08	***	1.60098e-06
500	***	2.44628e+08	***	224266	0.000674775	***	0.0158712
600	***	9.28099e+08	***	3.05705e+06	0.956284	***	7.90065
700	***	2.5246e+09	***	1.98829e+07	173.517	***	697.173

800	***	5.49975e+09	***	8.13121e+07	8649.29	***	20638.4
900	***	1.0262e+10	***	2.4384e+08	181465	***	293118
1000	***	1.71153e+10	***	5.88157e+08	2.07281e+06	***	2.4799e+06
1125	***	2.88952e+10	***	1.42127e+09	2.36555e+07	***	2.12369e+07
1250	***	4.43535e+10	***	2.88291e+09	1.65554e+08	***	1.19469e+08
1375	***	6.34102e+10	***	5.14712e+09	8.11411e+08	***	4.94125e+08
1500	***	8.58407e+10	***	8.34919e+09	3.04368e+09	***	1.62057e+09
1650	***	1.16767e+11	***	1.35522e+10	1.13813e+10	***	5.33819e+09
1750	***	1.39527e+11	***	1.78792e+10	2.41393e+10	***	1.05708e+10
1800	***	1.51478e+11	***	2.03019e+10	3.40533e+10	***	1.4465e+10
2000	***	2.02549e+11	***	3.16853e+10	1.13207e+11	***	4.34642e+10
2250	***	2.72098e+11	***	4.94809e+10	3.74186e+11	***	1.31117e+11
2500	***	3.45771e+11	***	7.07116e+10	9.68598e+11	***	3.18081e+11

T(K)	i2->i1	i2->i2	i2->i3	i2->i4	i2->fl_p0	i2->fl_p1	i2->fl_p2
300	6.82373e+06	***	4.86287e+06	***	***	***	***
400	6.15679e+07	***	9.38933e+07	***	***	***	***
500	3.01589e+08	***	5.62895e+08	***	***	***	***
600	9.6816e+08	***	1.87374e+09	***	***	***	***
700	2.35059e+09	***	4.44794e+09	***	***	***	***
800	4.71977e+09	***	8.53742e+09	***	***	***	***
900	8.28652e+09	***	1.42115e+10	***	***	***	***
1000	1.31869e+10	***	2.1401e+10	***	***	***	***
1125	2.12791e+10	***	3.22809e+10	***	***	***	***
1250	3.15454e+10	***	4.49059e+10	***	***	***	***
1375	4.38746e+10	***	5.88816e+10	***	***	***	***
1500	5.80881e+10	***	7.38442e+10	***	***	***	***
1650	7.7329e+10	***	9.26638e+10	***	***	***	***
1750	9.12983e+10	***	1.05528e+11	***	***	***	***
1800	9.85818e+10	***	1.12014e+11	***	***	***	***
2000	1.29388e+11	***	1.38067e+11	***	***	***	***
2250	1.70718e+11	***	1.70269e+11	***	***	***	***
2500	2.13944e+11	***	2.01439e+11	***	***	***	***

T(K)	i3->i1	i3->i2	i3->i3	i3->i4	i3->fl_p0	i3->fl_p1	i3->fl_p2
300	***	9.84011e-20	***	3.33945e-16	***	3.01742e-11	***
400	***	1.40303e-11	***	9.9584e-10	***	3.18258e-05	***
500	***	1.15841e-06	***	1.85802e-05	***	0.14427	***
600	***	0.00226005	***	0.0159303	***	41.7487	***
700	***	0.51416	***	2.13776	***	2475.53	***
800	***	30.3906	***	87.5818	***	54104.3	***
900	***	729.464	***	1608.66	***	605133	***
1000	***	9303.16	***	16755.2	***	4.22202e+06	***
1125	***	118970	***	176932	***	2.97767e+07	***
1250	***	915501	***	1.1782e+06	***	1.43295e+08	***
1375	***	4.86633e+06	***	5.59779e+06	***	5.21343e+08	***

1500	***	1.95926e+07	***	2.06166e+07	***	1.53612e+09	***
1650	***	7.89207e+07	***	7.62927e+07	***	4.54489e+09	***
1750	***	1.75001e+08	***	1.61494e+08	***	8.46366e+09	***
1800	***	2.521e+08	***	2.27855e+08	***	1.12598e+10	***
2000	***	9.04691e+08	***	7.62251e+08	***	3.06544e+10	***
2250	***	3.24721e+09	***	2.561e+09	***	8.37778e+10	***
2500	***	9.02724e+09	***	6.77382e+09	***	1.87792e+11	***

T(K)	i4->i1	i4->i2	i4->i3	i4->i4	i4->fl_p0	i4->fl_p1	i4->fl_p2
300	2.33677e-13	***	0.000216037	***	***	0.00852199	***
400	7.65779e-07	***	0.702325	***	***	49.9597	***
500	0.00672083	***	219.466	***	***	10665.5	***
600	2.97428	***	12318	***	***	409714	***
700	235.861	***	235620	***	***	5.7818e+06	***
800	6345.6	***	2.23738e+06	***	***	4.31882e+07	***
900	82751.9	***	1.31715e+07	***	***	2.0989e+08	***
1000	648690	***	5.51745e+07	***	***	7.52349e+08	***
1125	5.10549e+06	***	2.34178e+08	***	***	2.72777e+09	***
1250	2.66711e+07	***	7.51737e+08	***	***	7.71189e+09	***
1375	1.03336e+08	***	1.9653e+09	***	***	1.81617e+10	***
1500	3.19829e+08	***	4.39866e+09	***	***	3.72485e+10	***
1650	9.90836e+08	***	9.88942e+09	***	***	7.67213e+10	***
1750	1.89147e+09	***	1.57445e+10	***	***	1.1617e+11	***
1800	2.54412e+09	***	1.94946e+10	***	***	1.40569e+11	***
2000	7.18325e+09	***	4.12845e+10	***	***	2.74635e+11	***
2250	2.0295e+10	***	8.77873e+10	***	***	5.3869e+11	***
2500	4.66049e+10	***	1.6101e+11	***	***	9.26142e+11	***

T(K)	fl_p0->i1	fl_p0->i2	fl_p0->i3	fl_p0->i4	fl_p0->fl_p0	fl_p0->fl_p1	fl_p0->fl_p2
300	1.77273e-14	***	***	***	***	***	***
400	7.32052e-14	***	***	***	***	***	***
500	1.93371e-13	***	***	***	***	***	***
600	3.99329e-13	***	***	***	***	***	***
700	7.07631e-13	***	***	***	***	***	***
800	1.1311e-12	***	***	***	***	***	***
900	1.67972e-12	***	***	***	***	***	***
1000	2.36131e-12	***	***	***	***	***	***
1125	3.4096e-12	***	***	***	***	***	***
1250	4.68473e-12	***	***	***	***	***	***
1375	6.19395e-12	***	***	***	***	***	***
1500	7.94294e-12	***	***	***	***	***	***
1650	1.03644e-11	***	***	***	***	***	***
1750	1.21771e-11	***	***	***	***	***	***
1800	1.31436e-11	***	***	***	***	***	***
2000	1.74134e-11	***	***	***	***	***	***
2250	2.36688e-11	***	***	***	***	***	***

2500 3.09552e-11

*** **

T(K)	fl_p1->i1	fl_p1->i2	fl_p1->i3	fl_p1->i4	fl_p1->fl_p0	fl_p1->fl_p1	fl_p1->fl_p2
300	***	***	2.4195e-14	1.05628e-17	***	***	***
400	***	***	1.4398e-13	3.20475e-16	***	***	***
500	***	***	4.589e-13	2.87214e-15	***	***	***
600	***	***	1.05057e-12	1.33335e-14	***	***	***
700	***	***	1.97266e-12	4.18016e-14	***	***	***
800	***	***	3.25521e-12	1.01715e-13	***	***	***
900	***	***	4.91164e-12	2.08064e-13	***	***	***
1000	***	***	6.94464e-12	3.75803e-13	***	***	***
1125	***	***	1.0009e-11	6.92759e-13	***	***	***
1250	***	***	1.36397e-11	1.1505e-12	***	***	***
1375	***	***	1.78163e-11	1.76782e-12	***	***	***
1500	***	***	2.25172e-11	2.55914e-12	***	***	***
1650	***	***	2.88193e-11	3.75308e-12	***	***	***
1750	***	***	3.34044e-11	4.70293e-12	***	***	***
1800	***	***	3.58083e-11	5.22499e-12	***	***	***
2000	***	***	4.61373e-11	7.63178e-12	***	***	***
2250	***	***	6.05715e-11	1.1362e-11	***	***	***
2500	***	***	7.65831e-11	1.58896e-11	***	***	***

T(K)	fl_p2->i1	fl_p2->i2	fl_p2->i3	fl_p2->i4	fl_p2->fl_p0	fl_p2->fl_p1	fl_p2->fl_p2
300	7.27951e-16	***	***	***	***	***	***
400	1.05306e-14	***	***	***	***	***	***
500	5.8281e-14	***	***	***	***	***	***
600	1.9392e-13	***	***	***	***	***	***
700	4.76861e-13	***	***	***	***	***	***
800	9.64711e-13	***	***	***	***	***	***
900	1.70707e-12	***	***	***	***	***	***
1000	2.74352e-12	***	***	***	***	***	***
1125	4.49725e-12	***	***	***	***	***	***
1250	6.79648e-12	***	***	***	***	***	***
1375	9.66512e-12	***	***	***	***	***	***
1500	1.31151e-11	***	***	***	***	***	***
1650	1.8027e-11	***	***	***	***	***	***
1750	2.1767e-11	***	***	***	***	***	***
1800	2.37755e-11	***	***	***	***	***	***
2000	3.27187e-11	***	***	***	***	***	***
2250	4.58902e-11	***	***	***	***	***	***
2500	6.11836e-11	***	***	***	***	***	***

Capture/Escape Rate Coefficients:

T(K)	i1	i2	i3	i4	fl_p0	fl_p1	fl_p2
------	----	----	----	----	-------	-------	-------

300	2.68183e+06	1.16866e+07	3.01746e-11	0.00873802	1.77273e-14	2.42056e-14	7.27951e-16
400	3.83691e+07	1.55461e+08	3.18268e-05	50.662	7.32052e-14	1.44301e-13	1.05306e-14
500	2.44852e+08	8.64485e+08	0.14429	10884.9	1.93371e-13	4.61772e-13	5.8281e-14
600	9.31156e+08	2.8419e+09	41.7669	422035	3.99329e-13	1.0639e-12	1.9392e-13
700	2.54449e+09	6.79854e+09	2478.18	6.01766e+06	7.07631e-13	2.01446e-12	4.76861e-13
800	5.58109e+09	1.32572e+10	54222.2	4.5432e+07	1.1311e-12	3.35692e-12	9.64711e-13
900	1.05063e+10	2.2498e+10	607471	2.23144e+08	1.67972e-12	5.11971e-12	1.70707e-12
1000	1.7708e+10	3.45879e+10	4.24808e+06	8.08173e+08	2.36131e-12	7.32044e-12	2.74352e-12
1125	3.03614e+10	5.356e+10	3.00726e+07	2.96705e+09	3.4096e-12	1.07018e-11	4.49725e-12
1250	4.75214e+10	7.64513e+10	1.45389e+08	8.4903e+09	4.68473e-12	1.47902e-11	6.79648e-12
1375	6.98629e+10	1.02756e+11	5.31807e+08	2.02303e+10	6.19395e-12	1.95842e-11	9.66512e-12
1500	9.88541e+10	1.31932e+11	1.57633e+09	4.1967e+10	7.94294e-12	2.50763e-11	1.31151e-11
1650	1.47038e+11	1.69993e+11	4.7001e+09	8.76015e+10	1.03644e-11	3.25723e-11	1.8027e-11
1750	1.92116e+11	1.96826e+11	8.80016e+09	1.33806e+11	1.21771e-11	3.81074e-11	2.1767e-11
1800	2.20299e+11	2.10596e+11	1.17398e+10	1.62608e+11	1.31436e-11	4.10333e-11	2.37755e-11
2000	3.90906e+11	2.67454e+11	3.23214e+10	3.23102e+11	1.74134e-11	5.37691e-11	3.27187e-11
2250	8.26882e+11	3.40987e+11	8.95861e+10	6.46773e+11	2.36688e-11	7.19335e-11	4.58902e-11
2500	1.70316e+12	4.15383e+11	2.03593e+11	1.13376e+12	3.09552e-11	9.24727e-11	6.11836e-11

Temperature-Species Rate Tables:

Pressure = 0.0394737 atm

T(K) i1->i2 i1->i3 i1->i4 i1->fl_p0 i1->fl_p1 i1->fl_p2 i1-> Capture

300	1.79263e+06		315668	2.37554	4.31141e-22	1.83256	7.49363e-17
2.07461e+06	2.68183e+06						
400	***	1.05082e+07	362.729	2.18617e-15	394.86	1.56973e-11	1.05093e+07
3.83691e+07							
500	***	***	***	***	***	***	*** 2.44852e+08
600	***	***	***	***	***	***	*** 9.31156e+08
700	***	***	***	***	***	***	*** 2.54449e+09
800	***	***	***	***	***	***	*** 5.58109e+09
900	***	***	***	***	***	***	*** 1.05063e+10
1000	***	***	***	***	***	***	*** 1.7708e+10
1125	***	***	***	***	***	***	*** 3.03614e+10
1250	***	***	***	***	***	***	*** 4.75214e+10
1375	***	***	***	***	***	***	*** 6.98629e+10
1500	***	***	***	***	***	***	*** 9.88541e+10
1650	***	***	***	***	***	***	*** 1.47038e+11
1750	***	***	***	***	***	***	*** 1.92116e+11
1800	***	***	***	***	***	***	*** 2.20299e+11
2000	***	***	***	***	***	***	*** 3.90906e+11
2250	***	***	***	***	***	***	*** 8.26882e+11
2500	***	***	***	***	***	***	*** 1.70316e+12

Pressure = 1 atm

T(K)	i1->i2	i1->i3	i1->i4	i1->fl_p0	i1->fl_p1	i1->fl_p2	i1->	Capture
300	2.5843e+06		55820.8	6.39447	3.58536e-17	0.0319483		1.50926e-13
2.62601e+06	2.68183e+06							
400	2.85508e+07	4.18182e+06		3173.84	5.52991e-10	54.5821		1.84776e-07
3.27359e+07	3.83691e+07							
500	1.12633e+08	4.33767e+07		93793.6	4.94982e-06	5231.58		0.000419133
1.56108e+08	2.44852e+08							
600	***	3.16054e+08	716984	0.00185844	372223	0.0644829		3.17143e+08
9.31156e+08								
700	***	***	***	***	***	***	***	*** 2.54449e+09
800	***	***	***	***	***	***	***	*** 5.58109e+09
900	***	***	***	***	***	***	***	*** 1.05063e+10
1000	***	***	***	***	***	***	***	*** 1.7708e+10
1125	***	***	***	***	***	***	***	*** 3.03614e+10
1250	***	***	***	***	***	***	***	*** 4.75214e+10
1375	***	***	***	***	***	***	***	*** 6.98629e+10
1500	***	***	***	***	***	***	***	*** 9.88541e+10
1650	***	***	***	***	***	***	***	*** 1.47038e+11
1750	***	***	***	***	***	***	***	*** 1.92116e+11
1800	***	***	***	***	***	***	***	*** 2.20299e+11
2000	***	***	***	***	***	***	***	*** 3.90906e+11
2250	***	***	***	***	***	***	***	*** 8.26882e+11
2500	***	***	***	***	***	***	***	*** 1.70316e+12

Pressure = 10 atm

T(K)	i1->i2	i1->i3	i1->i4	i1->fl_p0	i1->fl_p1	i1->fl_p2	i1->	Capture
300	2.67214e+06	-780838		6.95589	1.65506e-16	0.000747094		3.76543e-13
2.67696e+06	2.68183e+06							
400	3.6659e+07	829653		4307.61	7.52754e-09	3.52557		1.08393e-06
3.74932e+07	3.83691e+07							
500	2.03298e+08	1.84023e+07		190017	0.000233519	1080.29		0.00723878
2.21891e+08	2.44852e+08							
600	6.13984e+08	1.18125e+08	2.08423e+06	0.166499		58488		2.02093
7.34251e+08	9.31156e+08							
700	***	***	***	***	***	***	***	2.54449e+09
800	***	***	***	***	***	***	***	5.58109e+09
900	***	***	***	***	***	***	***	1.05063e+10
1000	***	***	***	***	***	***	***	1.7708e+10
1125	***	***	***	***	***	***	***	3.03614e+10
1250	***	***	***	***	***	***	***	4.75214e+10
1375	***	***	***	***	***	***	***	6.98629e+10
1500	***	***	***	***	***	***	***	9.88541e+10
1650	***	***	***	***	***	***	***	1.47038e+11
1750	***	***	***	***	***	***	***	1.92116e+11
1800	***	***	***	***	***	***	***	2.20299e+11
2000	***	***	***	***	***	***	***	3.90906e+11
2250	***	***	***	***	***	***	***	8.26882e+11
2500	***	***	***	***	***	***	***	1.70316e+12

Pressure = 100 atm

T(K)	i1->i2	i1->i3	i1->i4	i1->fl_p0	i1->fl_p1	i1->fl_p2	i1->	Capture
300	2.68214e+06	1.93258e+07		7.02464	2.14091e-16	3.96322e-05		4.36052e-13
2.68263e+06	2.68183e+06							
400	3.82074e+07	91755.2		4512.36	1.24331e-08	0.236946		1.51536e-06
3.83057e+07	3.83691e+07							
500	2.38968e+08	2.79027e+06		220050	0.000574817	94.271		0.0140373
2.41979e+08	2.44852e+08							
600	8.65733e+08	2.77618e+07	2.89156e+06	0.705043		7807.46		6.20447
8.96394e+08	9.31156e+08							
700	2.18389e+09	1.35902e+08	1.75633e+07	104.716		226100		461.158
2.33758e+09	2.54449e+09							
800	4.32444e+09	4.11047e+08	6.39026e+07	4050.29	2.90558e+06			10935.4
4.80232e+09	5.58109e+09							
900	***	***	***	***	***	***	***	1.05063e+10
1000	***	***	***	***	***	***	***	1.7708e+10
1125	***	***	***	***	***	***	***	3.03614e+10
1250	***	***	***	***	***	***	***	4.75214e+10

1375	***	***	***	***	***	***	***	6.98629e+10
1500	***	***	***	***	***	***	***	9.88541e+10
1650	***	***	***	***	***	***	***	1.47038e+11
1750	***	***	***	***	***	***	***	1.92116e+11
1800	***	***	***	***	***	***	***	2.20299e+11
2000	***	***	***	***	***	***	***	3.90906e+11
2250	***	***	***	***	***	***	***	8.26882e+11
2500	***	***	***	***	***	***	***	1.70316e+12

Pressure = 0.0394737 atm

T(K)	i2->i1	i2->i3	i2->i4	i2->fl_p0	i2->fl_p1	i2->fl_p2	i2->	Capture
300	4.58298e+06	2.43718e+06		2.0589	4.56696e-22	7.73028	7.81422e-17	
7.2935e+06	1.16866e+07							
400	***	***	***	***	***	***	***	1.55461e+08
500	***	***	***	***	***	***	***	8.64485e+08
600	***	***	***	***	***	***	***	2.8419e+09
700	***	***	***	***	***	***	***	6.79854e+09
800	***	***	***	***	***	***	***	1.32572e+10
900	***	***	***	***	***	***	***	2.2498e+10
1000	***	***	***	***	***	***	***	3.45879e+10
1125	***	***	***	***	***	***	***	5.356e+10
1250	***	***	***	***	***	***	***	7.64513e+10
1375	***	***	***	***	***	***	***	1.02756e+11
1500	***	***	***	***	***	***	***	1.31932e+11
1650	***	***	***	***	***	***	***	1.69993e+11
1750	***	***	***	***	***	***	***	1.96826e+11
1800	***	***	***	***	***	***	***	2.10596e+11
2000	***	***	***	***	***	***	***	2.67454e+11
2250	***	***	***	***	***	***	***	3.40987e+11
2500	***	***	***	***	***	***	***	4.15383e+11

Pressure = 1 atm

T(K)	i2->i1	i2->i3	i2->i4	i2->fl_p0	i2->fl_p1	i2->fl_p2	i2->	Capture
300	6.57597e+06	4.5062e+06		1.30874	3.70618e-17	1.0099	1.45057e-13	
1.11603e+07	1.16866e+07							
400	4.58928e+07	7.10457e+07		1044.88	3.99998e-10	226.724	1.29427e-07	
1.16939e+08	1.55461e+08							
500	1.3794e+08	3.0619e+08		40169	3.96213e-06	13391.8	0.000318451	
4.44184e+08	8.64485e+08							
600	***	***	***	***	***	***	***	2.8419e+09
700	***	***	***	***	***	***	***	6.79854e+09
800	***	***	***	***	***	***	***	1.32572e+10
900	***	***	***	***	***	***	***	2.2498e+10
1000	***	***	***	***	***	***	***	3.45879e+10

1125	***	***	***	***	***	***	***	5.356e+10
1250	***	***	***	***	***	***	***	7.64513e+10
1375	***	***	***	***	***	***	***	1.02756e+11
1500	***	***	***	***	***	***	***	1.31932e+11
1650	***	***	***	***	***	***	***	1.69993e+11
1750	***	***	***	***	***	***	***	1.96826e+11
1800	***	***	***	***	***	***	***	2.10596e+11
2000	***	***	***	***	***	***	***	2.67454e+11
2250	***	***	***	***	***	***	***	3.40987e+11
2500	***	***	***	***	***	***	***	4.15383e+11

Pressure = 10 atm

T(K)	i2->i1	i2->i3	i2->i4	i2->fl_p0	i2->fl_p1	i2->fl_p2	i2->	Capture
300	6.79911e+06	4.59203e+06		0.188634	9.69249e-17	0.119086		1.36798e-13
400	5.88335e+07	8.96268e+07		323.425	4.23634e-09	44.3849		4.66368e-07
500	2.50561e+08	4.86293e+08		29513.5	0.000134931	3355.14		0.00361755
600	6.35219e+08	1.40337e+09		512706	0.113255	110760		1.23311
700	***	1.14533e+09	7.66625e+06	13.153	1.50967e+06	83.7544		1.1545e+09
800	***	2.1144e+09	1.26991e+07	323.569	3.37289e+07	1322.69		2.16083e+09
900	***	***	***	***	***	***	***	2.2498e+10
1000	***	***	***	***	***	***	***	3.45879e+10
1125	***	***	***	***	***	***	***	5.356e+10
1250	***	***	***	***	***	***	***	7.64513e+10
1375	***	***	***	***	***	***	***	1.02756e+11
1500	***	***	***	***	***	***	***	1.31932e+11
1650	***	***	***	***	***	***	***	1.69993e+11
1750	***	***	***	***	***	***	***	1.96826e+11
1800	***	***	***	***	***	***	***	2.10596e+11
2000	***	***	***	***	***	***	***	2.67454e+11
2250	***	***	***	***	***	***	***	3.40987e+11
2500	***	***	***	***	***	***	***	4.15383e+11

Pressure = 100 atm

T(K)	i2->i1	i2->i3	i2->i4	i2->fl_p0	i2->fl_p1	i2->fl_p2	i2->	Capture
300	6.82453e+06	1.73507e+07		0.0188566	1.83499e-17	0.0121541		2.02034e-14
400	6.13157e+07	9.31475e+07		40.1773	1.47854e-09	5.09833		1.14111e-07

500	2.94609e+08	5.50652e+08	5376.82	0.000105028	485.303	0.00183221
8.45267e+08	8.64485e+08					
600	9.02869e+08	1.78008e+09	151847	0.187763	17476	1.28568 2.68312e+09
2.8419e+09						
700	2.02911e+09	4.04654e+09	1.60341e+06	37.7942	330103	136.943
6.07759e+09	6.79854e+09					
800	3.67687e+09	7.38784e+09	8.99886e+06	1961.57	4.33269e+06	4483.34
1.10781e+10	1.32572e+10					
900	***	4.86655e+09	1.10847e+08	54909.1	2.78225e+07	99733.4
5.00537e+09	2.2498e+10					
1000	***	7.4358e+09	1.92661e+08	490959	1.67124e+08	676152
7.79675e+09	3.45879e+10					
1125	***	9.39633e+09	2.07658e+08	4.16607e+06	2.47134e+09	4.41395e+06
1.20839e+10	5.356e+10					
1250	***	***	***	***	***	*** 7.64513e+10
1375	***	***	***	***	***	*** 1.02756e+11
1500	***	***	***	***	***	*** 1.31932e+11
1650	***	***	***	***	***	*** 1.69993e+11
1750	***	***	***	***	***	*** 1.96826e+11
1800	***	***	***	***	***	*** 2.10596e+11
2000	***	***	***	***	***	*** 2.67454e+11
2250	***	***	***	***	***	*** 3.40987e+11
2500	***	***	***	***	***	*** 4.15383e+11

Pressure = 0.0394737 atm

T(K)	i3->i1	i3->i2	i3->i4	i3->fl_p0	i3->fl_p1	i3->fl_p2	i3->	Capture
300	1.40783e-20	5.52876e-20	3.07791e-16	1.0986e-41	3.00642e-11	2.2542e-38		
3.00645e-11	3.01746e-11							
400	4.09022e-12	***	9.88093e-10	2.85128e-27	3.16991e-05	3.62017e-25	3.17001e-05	3.17001e-05
05	3.18268e-05							
500	***	***	1.68509e-05	1.15408e-18	0.143631	3.25291e-17	0.143648	0.143648
0.14429								
600	***	***	0.00936058	4.24404e-13	41.3947	5.15224e-12	41.4041	41.4041
41.7669								
700	***	***	0.542994	2.18308e-09	2360.76	1.62052e-08	2361.3	2361.3
2478.18								
800	***	***	***	6.70684e-07	43067.8	3.63343e-06	43067.8	43067.8
54222.2								
900	***	***	***	3.09676e-05	313882	0.000134122	313881	313881
607471								
1000	***	***	***	0.000430622	1.17186e+06	0.00156746	1.17185e+06	1.17185e+06
4.24808e+06								
1125	***	***	***	***	***	***	*** 3.00726e+07	
1250	***	***	***	***	***	***	*** 1.45389e+08	
1375	***	***	***	***	***	***	*** 5.31807e+08	

1500	***	***	***	***	***	***	***	1.57633e+09
1650	***	***	***	***	***	***	***	4.7001e+09
1750	***	***	***	***	***	***	***	8.80016e+09
1800	***	***	***	***	***	***	***	1.17398e+10
2000	***	***	***	***	***	***	***	3.23214e+10
2250	***	***	***	***	***	***	***	8.95861e+10
2500	***	***	***	***	***	***	***	2.03593e+11

Pressure = 1 atm

T(K)	i3->i1	i3->i2	i3->i4	i3->fl_p0	i3->fl_p1	i3->fl_p2	i3->	Capture
300	2.13929e-21	9.27715e-20	3.07801e-16	8.72903e-42	3.00642e-11	1.20952e-38	3.00645e-11	3.01746e-11
400	9.91741e-13	1.06272e-11	9.93172e-10	2.97854e-27	3.16993e-05	3.14494e-25	3.17003e-05	3.18268e-05
500	1.11922e-07	6.28249e-07	1.84364e-05	1.6363e-18	0.143657	3.73532e-17	0.143676	0.14429
600	0.000397671	***	0.0150744	1.09229e-12	41.556	9.18192e-12	41.7669	41.5715
700	***	***	1.65027	1.43543e-08	2459.1	6.21505e-08	2478.18	2460.75
800	***	***	43.8763	1.40187e-05	52980.3	3.92062e-05	54222.2	53024.2
900	***	***	452.66	0.00209081	555335	0.00438895	607471	555788
1000	***	***	***	0.0766226	3.2495e+06	0.13222	4.24808e+06	3.24945e+06
1125	***	***	***	1.73361	1.52739e+07	2.51798	3.00726e+07	1.52733e+07
1250	***	***	***	14.918	4.32818e+07	19.0868	1.45389e+08	4.32784e+07
1375	***	***	***	***	***	***	***	5.31807e+08
1500	***	***	***	***	***	***	***	1.57633e+09
1650	***	***	***	***	***	***	***	4.7001e+09
1750	***	***	***	***	***	***	***	8.80016e+09
1800	***	***	***	***	***	***	***	1.17398e+10
2000	***	***	***	***	***	***	***	3.23214e+10
2250	***	***	***	***	***	***	***	8.95861e+10
2500	***	***	***	***	***	***	***	2.03593e+11

Pressure = 10 atm

T(K)	i3->i1	i3->i2	i3->i4	i3->fl_p0	i3->fl_p1	i3->fl_p2	i3->	Capture
300	2.47435e-22	9.74693e-20	3.07802e-16	9.11657e-43	3.00642e-11	7.0437e-40	3.00645e-11	3.01746e-11

400	1.98609e-13	1.33931e-11	9.9337e-10	7.72441e-28	3.16993e-05	5.11964e-26	
3.17003e-05	3.18268e-05						
500	4.68383e-08	1.00062e-06	1.8523e-05	8.3143e-19	0.143658	1.38975e-17	
0.143677	0.14429						
600	0.000154893	0.00168648	0.015792	8.30943e-13	41.5618	5.64768e-12	
41.5794	41.7669						
700	***	0.255904	2.04954	1.47739e-08	2463.55	5.25694e-08	2465.86
2478.18							
800	***	14.0812	74.8384	2.12714e-05	53757.3	4.80543e-05	53846.2
54222.2							
900	***	***	1081.36	0.00573003	596359	0.00968366	597440
607471							
1000	***	***	7964.72	0.396658	4.03195e+06	0.519164	4.03992e+06
4.24808e+06							
1125	***	***	***	20.0311	2.53535e+07	21.0687	2.53522e+07
3.00726e+07							
1250	***	***	***	323.43	9.63935e+07	293.116	9.6384e+07
1.45389e+08							
1375	***	***	***	2406.21	2.52203e+08	1957.59	2.52147e+08
5.31807e+08							
1500	***	***	***	***	***	***	*** 1.57633e+09
1650	***	***	***	***	***	***	*** 4.7001e+09
1750	***	***	***	***	***	***	*** 8.80016e+09
1800	***	***	***	***	***	***	*** 1.17398e+10
2000	***	***	***	***	***	***	*** 3.23214e+10
2250	***	***	***	***	***	***	*** 8.95861e+10
2500	***	***	***	***	***	***	*** 2.03593e+11

Pressure = 100 atm

T(K)	i3->i1	i3->i2	i3->i4	i3->fl_p0	i3->fl_p1	i3->fl_p2	i3->	Capture
300	2.51689e-23	9.80129e-20	3.07802e-16	1.50539e-44	3.00642e-11	9.75987e-42		
3.00645e-11	3.01746e-11							
400	2.24816e-14	1.39181e-11	9.9339e-10	2.12923e-29	3.16993e-05	1.11031e-27		
3.17003e-05	3.18268e-05							
500	7.08314e-09	1.13321e-06	1.8532e-05	4.54262e-20	0.143658	5.81987e-19		
0.143678	0.14429							
600	3.52072e-05	0.00214681	0.0158779	9.08211e-14	41.5624	4.77862e-13		
41.5804	41.7669							
700	0.0151065	0.467292	2.12266	2.89681e-09	2463.98	8.2517e-09	2466.58	
2478.18								
800	1.37217	26.187	85.5878	6.46987e-06	53835.9	1.17716e-05	53949	
54222.2								
900	***	453.26	1497	0.00206643	601582	0.00226725	603532	
607471								

1000	***	5768.25	14085.5	0.252954	4.1827e+06	0.237094	4.20256e+06
4.24808e+06							
1125	***	71644.1	120715	25.2203	2.90086e+07	19.3868	2.9201e+07
3.00726e+07							
1250	***	***	612347	1450.06	1.32979e+08	1092.39	1.33594e+08
1.45389e+08							
1375	***	***	***	18854.8	4.38112e+08	12396.1	4.38035e+08
5.31807e+08							
1500	***	***	***	132147	1.09647e+09	78663.1	1.09623e+09
1.57633e+09							
1650	***	***	***	765862	2.52133e+09	417564	2.51919e+09
4.7001e+09							
1750	***	***	***	1.92524e+06	3.89987e+09	1.00263e+06	3.89541e+09
8.80016e+09							
1800	***	***	***	***	***	***	1.17398e+10
2000	***	***	***	***	***	***	3.23214e+10
2250	***	***	***	***	***	***	8.95861e+10
2500	***	***	***	***	***	***	2.03593e+11

Pressure = 0.0394737 atm

T(K)	i4->i1	i4->i2	i4->i3	i4->fl_p0	i4->fl_p1	i4->fl_p2	i4->	Capture
300	8.03924e-14	2.6053e-14	0.000199117	1.38336e-32	0.00850162	4.19787e-29	0.00870074	0.00873802
400	1.154e-07	***	0.696862	1.05895e-21	49.6494	3.67082e-19	50.662	50.3463
500	***	***	199.038	1.34004e-15	9960.54	1.38404e-13	10884.9	10159.6
600	***	***	7232.26	7.92905e-12	272392	2.89679e-10	422035	279624
700	***	***	59091.6	3.82709e-09	1.89686e+06	4.75525e-08	6.01766e+06	1.95595e+06
800	***	***	***	***	***	***	***	4.5432e+07
900	***	***	***	***	***	***	***	2.23144e+08
1000	***	***	***	***	***	***	***	8.08173e+08
1125	***	***	***	***	***	***	***	2.96705e+09
1250	***	***	***	***	***	***	***	8.4903e+09
1375	***	***	***	***	***	***	***	2.02303e+10
1500	***	***	***	***	***	***	***	4.1967e+10
1650	***	***	***	***	***	***	***	8.76015e+10
1750	***	***	***	***	***	***	***	1.33806e+11
1800	***	***	***	***	***	***	***	1.62608e+11
2000	***	***	***	***	***	***	***	3.23102e+11
2250	***	***	***	***	***	***	***	6.46773e+11
2500	***	***	***	***	***	***	***	1.13376e+12

Pressure = 1 atm

T(K)	i4->i1	i4->i2	i4->i3	i4->fl_p0	i4->fl_p1	i4->fl_p2	i4->	Capture
300	2.13059e-13	1.7034e-14	0.000199124	4.79867e-32	0.00850212	4.20309e-29	0.00870124	0.00873802
400	5.41521e-07	1.04017e-07	0.700444	2.37297e-20	49.8179	1.89156e-18	50.5183	50.662
500	0.00304785	0.00082152	217.768	2.05151e-13	10597.2	4.6691e-12	10884.9	10815
600	0.826919	***	11656	4.98713e-09	393221	5.53892e-08	422035	404878
700	***	***	181805	3.40177e-06	4.72209e+06	2.40288e-05	6.01766e+06	4.90389e+06
800	***	***	1.11424e+06	0.00025953	2.45876e+07	0.00130506	4.5432e+07	2.57019e+07
900	***	***	3.58154e+06	0.00646983	7.3273e+07	0.0228285	2.23144e+08	7.68545e+07
1000	***	***	***	***	***	***	***	8.08173e+08
1125	***	***	***	***	***	***	***	2.96705e+09
1250	***	***	***	***	***	***	***	8.4903e+09
1375	***	***	***	***	***	***	***	2.02303e+10
1500	***	***	***	***	***	***	***	4.1967e+10
1650	***	***	***	***	***	***	***	8.76015e+10
1750	***	***	***	***	***	***	***	1.33806e+11
1800	***	***	***	***	***	***	***	1.62608e+11
2000	***	***	***	***	***	***	***	3.23102e+11
2250	***	***	***	***	***	***	***	6.46773e+11
2500	***	***	***	***	***	***	***	1.13376e+12

Pressure = 10 atm

T(K)	i4->i1	i4->i2	i4->i3	i4->fl_p0	i4->fl_p1	i4->fl_p2	i4->	Capture
300	2.31691e-13	2.46455e-15	0.000199125	1.0786e-32	0.00850213	7.25512e-30	0.00870126	0.00873802
400	7.28752e-07	3.36576e-08	0.700584	1.02585e-20	49.8243	5.79435e-19	50.5249	50.662
500	0.0057239	0.000668044	218.791	2.2512e-13	10629.9	3.30302e-12	10884.9	10848.7
600	2.09493	0.393408	12211.1	1.72911e-08	406648	1.11898e-07	422035	418861
700	***	169.987	225913	4.01127e-05	5.59342e+06	0.000153181	6.01766e+06	5.81951e+06
800	***	3372.24	1.91001e+06	0.00873929	3.80658e+07	0.0233699	3.99792e+07	4.5432e+07
900	***	***	8.82486e+06	0.409551	1.51331e+08	0.874996	2.23144e+08	1.60156e+08

1000	***	***	2.57847e+07	6.47856	4.05623e+08	11.3644	4.31408e+08
8.08173e+08							
1125	***	***	***	***	***	***	2.96705e+09
1250	***	***	***	***	***	***	8.4903e+09
1375	***	***	***	***	***	***	2.02303e+10
1500	***	***	***	***	***	***	4.1967e+10
1650	***	***	***	***	***	***	8.76015e+10
1750	***	***	***	***	***	***	1.33806e+11
1800	***	***	***	***	***	***	1.62608e+11
2000	***	***	***	***	***	***	3.23102e+11
2250	***	***	***	***	***	***	6.46773e+11
2500	***	***	***	***	***	***	1.13376e+12

Pressure = 100 atm

T(K)	i4->i1	i4->i2	i4->i3	i4->fl_p0	i4->fl_p1	i4->fl_p2	i4->	Capture
300	2.33971e-13	2.58209e-16	0.000199125	1.24697e-33	0.00850214	7.93646e-31	0.00870126	0.00873802
400	7.63151e-07	4.22775e-09	0.700598	1.42155e-21	49.825	7.34801e-20	50.5256	50.662
500	0.00659527	0.000129156	218.896	4.34605e-14	10633.3	5.59139e-13	10852.2	10884.9
600	2.81669	0.135056	12277.5	5.66156e-09	408217	3.03777e-08	422035	422035
700	209.736	18.0723	233956	2.75119e-05	5.74356e+06	8.13912e-05	5.97774e+06	6.01766e+06
800	5117.64	632.912	2.18649e+06	0.0148178	4.23638e+07	0.0287392	4.45561e+07	4.5432e+07
900	***	74607.2	1.22655e+07	1.64748	1.98126e+08	2.36945	2.23144e+08	2.10466e+08
1000	***	484545	4.63458e+07	54.7874	6.53462e+08	62.8265	8.08173e+08	7.00292e+08
1125	***	2.77862e+06	1.58191e+08	1280.01	1.98931e+09	1194.25	2.15028e+09	2.96705e+09
1250	***	***	3.76428e+08	29616.6	4.48447e+09	25001.9	8.4903e+09	4.86096e+09
1375	***	***	***	***	***	***	***	2.02303e+10
1500	***	***	***	***	***	***	***	4.1967e+10
1650	***	***	***	***	***	***	***	8.76015e+10
1750	***	***	***	***	***	***	***	1.33806e+11
1800	***	***	***	***	***	***	***	1.62608e+11
2000	***	***	***	***	***	***	***	3.23102e+11
2250	***	***	***	***	***	***	***	6.46773e+11
2500	***	***	***	***	***	***	***	1.13376e+12

Pressure = 0.0394737 atm

T(K)	fl_p0->i1	fl_p0->i2	fl_p0->i3	fl_p0->i4	fl_p0->fl_p1	fl_p0->fl_p2	fl_p0->
300	3.46867e-20	1.42871e-20	1.71537e-14	3.33886e-17	6.30453e-16	1.59746e-22	
400	1.65877e-20	***	6.51039e-14	3.42841e-17	8.51627e-15	1.26213e-20	7.36545e-14
500	***	***	1.30354e-13	1.2814e-17	6.43239e-14	4.0058e-19	1.94691e-13
600	***	***	1.40851e-13	3.39167e-18	2.61387e-13	6.43607e-18	4.02248e-13
700	***	***	8.27193e-14	1.23721e-18	6.30252e-13	6.20368e-17	7.13034e-13
800	***	***	2.86958e-14	***	1.1107e-12	4.05577e-16	1.1398e-12
900	***	***	6.83549e-15	***	1.68269e-12	1.96206e-15	1.69149e-12
1000	***	***	1.35198e-15	***	2.36297e-12	7.46496e-15	2.37179e-12
1125	***	***	***	***	3.3631e-12	3.01404e-14	3.39324e-12
1250	***	***	***	***	4.46576e-12	9.44245e-14	4.56018e-12
1375	***	***	***	***	5.54043e-12	2.38944e-13	5.77937e-12
1500	***	***	***	***	6.42197e-12	5.04963e-13	6.92694e-12
1650	***	***	***	***	7.03958e-12	1.01985e-12	8.05944e-12
1750	***	***	***	***	7.14693e-12	1.48096e-12	8.62789e-12
1800	***	***	***	***	7.11565e-12	1.74279e-12	8.85844e-12
2000	***	***	***	***	6.56523e-12	2.94999e-12	9.51521e-12
2250	***	***	***	***	5.42675e-12	4.67868e-12	1.01054e-11
2500	***	***	***	***	4.32972e-12	6.53322e-12	1.08629e-11

Pressure = 1 atm

T(K)	fl_p0->i1	fl_p0->i2	fl_p0->i3	fl_p0->i4	fl_p0->fl_p1	fl_p0->fl_p2	fl_p0->
300	2.88242e-15	1.17085e-15	1.36507e-14	1.1582e-16	1.88438e-17	8.13124e-23	
400	1.65877e-20	***	6.51039e-14	3.42841e-17	8.51627e-15	1.26213e-20	7.36545e-14

400	3.02879e-15	1.35292e-15	6.80206e-14	7.68268e-16	4.8387e-16	9.32395e-21
7.36545e-14	7.32052e-14					
500	1.40265e-15	8.36171e-16	1.84922e-13	1.96189e-15	5.56774e-15	3.50211e-19
1.94691e-13	1.93371e-13					
600	5.66766e-16	***	3.62717e-13	2.14125e-15	3.68171e-14	6.04225e-18
13	3.99329e-13					
700	***	***	5.43903e-13	1.16709e-15	1.67905e-13	6.0078e-17
7.07631e-13						
800	***	***	6.00119e-13	4.2203e-16	5.38865e-13	3.9856e-16
1.1311e-12						
900	***	***	4.66861e-13	1.51655e-16	1.22255e-12	1.94261e-15
1.67972e-12						
1000	***	***	2.59786e-13	***	2.10463e-12	7.4212e-15
2.36131e-12						
1125	***	***	8.87127e-14	***	3.27462e-12	3.00456e-14
3.4096e-12						
1250	***	***	2.45496e-14	***	4.44166e-12	9.42613e-14
4.68473e-12						
1375	***	***	***	***	5.54111e-12	2.38716e-13
6.19395e-12						
1500	***	***	***	***	6.42282e-12	5.04701e-13
7.94294e-12						
1650	***	***	***	***	7.04043e-12	1.01961e-12
1.03644e-11						
1750	***	***	***	***	7.14769e-12	1.48075e-12
1.21771e-11						
1800	***	***	***	***	7.11635e-12	1.7426e-12
1.31436e-11						
2000	***	***	***	***	6.56563e-12	2.94988e-12
1.74134e-11						
2250	***	***	***	***	5.42691e-12	4.67864e-12
2.36688e-11						
2500	***	***	***	***	4.32977e-12	6.5332e-12
3.09552e-11						

Pressure = 10 atm

T(K)	fl_p0->i1	fl_p0->i2	fl_p0->i3	fl_p0->i4	fl_p0->fl_p1	fl_p0->fl_p2	fl_p0->
300	1.33054e-14	3.06238e-15	1.28427e-14	2.60329e-17	2.70698e-19	1.56424e-23	
1.78176e-14	1.77273e-14						
400	4.12172e-14	1.44518e-14	1.76399e-14	3.32125e-16	1.39992e-17	2.87574e-21	
7.36545e-14	7.32052e-14						
500	6.69124e-14	3.12356e-14	9.40466e-14	2.15292e-15	3.43321e-16	1.66529e-19	
1.94691e-13	1.93371e-13						

600	6.93545e-14	4.37727e-14	2.77503e-13	7.42927e-15	4.18571e-15	3.91271e-18
4.02249e-13	3.99329e-13					
700	***	8.98692e-14	5.81117e-13	1.38588e-14	2.81505e-14	4.69402e-17
13	7.07631e-13					
800	***	6.64425e-14	9.35852e-13	1.50853e-14	1.22122e-13	3.45945e-16
12	1.1311e-12					
900	***	***	1.27968e-12	1.09851e-14	3.99221e-13	1.78676e-15
1.67972e-12						
1000	***	***	1.34906e-12	6.16637e-15	1.01004e-12	7.05224e-15
2.36131e-12						
1125	***	***	1.06146e-12	***	2.30395e-12	2.9209e-14
3.4096e-12						
1250	***	***	6.18256e-13	***	3.85202e-12	9.27847e-14
4.68473e-12						
1375	***	***	2.92631e-13	***	5.25471e-12	2.3663e-13
6.19395e-12						
1500	***	***	***	***	6.43059e-12	5.02287e-13
7.94294e-12						
1650	***	***	***	***	7.04832e-12	1.01731e-12
1.03644e-11						
1750	***	***	***	***	7.15473e-12	1.47878e-12
1.21771e-11						
1800	***	***	***	***	7.12279e-12	1.74084e-12
1.31436e-11						
2000	***	***	***	***	6.56943e-12	2.94892e-12
1.74134e-11						
2250	***	***	***	***	5.42838e-12	4.6783e-12
2.36688e-11						
2500	***	***	***	***	4.33024e-12	6.53311e-12
3.09552e-11						

Pressure = 100 atm

T(K)	fl_p0->i1	fl_p0->i2	fl_p0->i3	fl_p0->i4	fl_p0->fl_p1	fl_p0->fl_p2	fl_p0->
300	1.72113e-14	5.79771e-16	-3.50382e-13	3.00967e-18	2.46565e-21	1.77609e-24	
1.78176e-14	1.77273e-14						
400	6.80774e-14	5.04474e-15	4.88594e-16	4.60236e-17	1.46834e-19	3.87712e-22	
7.36545e-14	7.32052e-14						
500	1.64721e-13	2.44212e-14	5.12814e-15	4.15602e-16	4.98671e-18	2.91327e-20	
1.94691e-13	1.93371e-13						
600	2.94302e-13	7.52981e-14	3.01178e-14	2.43078e-15	1.00545e-16	9.42898e-19	
4.0225e-13	3.99329e-13						
700	4.26132e-13	1.66158e-13	1.10047e-13	9.47728e-15	1.23144e-15	1.57558e-17	
7.13061e-13	7.07631e-13						

800	5.2623e-13	2.98126e-13	2.81064e-13	2.50308e-14	9.39212e-15	1.56135e-16
1.14e-12	1.1311e-12					
900	***	9.80614e-13	6.18531e-13	4.55346e-14	4.67556e-14	1.02063e-15
1.67972e-12						
1000	***	1.08901e-12	1.05729e-12	6.12158e-14	1.62839e-13	4.79075e-15
2.36131e-12						
1125	***	1.13562e-12	1.76899e-12	7.10895e-14	4.05449e-13	2.29682e-14
3.4096e-12						
1250	***	***	2.82904e-12	7.98427e-14	1.59378e-12	8.12586e-14
4.68473e-12						
1375	***	***	2.50165e-12	***	3.09841e-12	2.19044e-13
6.19395e-12						
1500	***	***	1.86505e-12	***	4.63392e-12	4.80879e-13
7.94294e-12						
1650	***	***	1.10403e-12	***	6.01543e-12	9.96276e-13
1.03644e-11						
1750	***	***	7.19066e-13	***	6.49996e-12	1.4605e-12
1.21771e-11						
1800	***	***	***	***	7.18264e-12	1.72452e-12
1.31436e-11						
2000	***	***	***	***	6.60502e-12	2.93992e-12
1.74134e-11						
2250	***	***	***	***	5.4422e-12	4.67513e-12
2.36688e-11						
2500	***	***	***	***	4.33469e-12	6.53219e-12
3.09552e-11						

Pressure = 0.0394737 atm

T(K)	fl_p1->i1	fl_p1->i2	fl_p1->i3	fl_p1->i4	fl_p1->fl_p0	fl_p1->fl_p2	fl_p1->Capture
300	7.68064e-29	1.23081e-28	2.41068e-14	1.05375e-17	3.23762e-46	2.07342e-43	2.41174e-14
400	5.93614e-25	***	1.43407e-13	3.18485e-16	1.68735e-36	8.64596e-35	1.43726e-13
500	***	***	4.56868e-13	2.68226e-15	1.81145e-30	2.37734e-29	4.5955e-13
600	***	***	1.04166e-12	8.83449e-15	1.9819e-26	1.18851e-25	1.05049e-12
700	***	***	1.88122e-12	1.28783e-14	1.32543e-23	4.64705e-23	1.8941e-12
800	***	***	2.58982e-12	***	1.56103e-21	3.54712e-21	2.58983e-12
900	***	***	2.51805e-12	***	6.11562e-20	9.66917e-20	2.51806e-12

1000	***	***	1.77926e-12	***	1.14275e-18	1.34738e-18	1.77928e-12
7.32044e-12							
1125	***	***	***	***	2.12864e-17	1.89118e-17	4.01982e-17
1.07018e-11							
1250	***	***	***	***	2.17814e-16	1.56368e-16	3.74182e-16
1.47902e-11							
1375	***	***	***	***	1.41836e-15	8.65486e-16	2.28385e-15
1.95842e-11							
1500	***	***	***	***	6.47658e-15	3.48347e-15	9.96005e-15
2.50763e-11							
1650	***	***	***	***	2.76477e-14	1.32185e-14	4.08662e-14
3.25723e-11							
1750	***	***	***	***	6.06767e-14	2.72142e-14	8.7891e-14
3.81074e-11							
1800	***	***	***	***	8.58731e-14	3.74301e-14	1.23303e-13
4.10333e-11							
2000	***	***	***	***	2.68889e-13	1.06354e-13	3.75243e-13
5.37691e-11							
2250	***	***	***	***	7.42195e-13	2.67397e-13	1.00959e-12
7.19335e-11							
2500	***	***	***	***	1.53196e-12	5.13931e-13	2.04589e-12
9.24727e-11							

Pressure = 1 atm

T(K)	fl_p1->i1	fl_p1->i2	fl_p1->i3	fl_p1->i4	fl_p1->fl_p0	fl_p1->fl_p2	fl_p1->
300	1.3208e-30	1.63824e-29	2.41068e-14	1.05381e-17	9.67702e-48	3.73617e-45	
2.41174e-14	2.42056e-14						
400	6.02577e-26	1.50526e-25	1.43408e-13	3.19565e-16	9.58705e-38	3.74986e-36	
1.43727e-13	1.44301e-13						
500	4.5271e-23	7.52136e-23	4.5695e-13	2.85377e-15	1.56795e-31	1.74164e-30	
4.59804e-13	4.61772e-13						
600	8.62024e-21	***	1.04572e-12	1.27964e-14	2.79157e-27	1.3613e-26	1.05851e-12
1.0639e-12							
700	***	***	1.95957e-12	3.40705e-14	3.53108e-24	9.6854e-24	1.99364e-12
2.01446e-12							
800	***	***	3.18767e-12	5.61891e-14	7.5735e-22	1.40379e-21	3.24386e-12
3.35692e-12							
900	***	***	4.50735e-12	6.22311e-14	4.44328e-20	6.21316e-20	4.56958e-12
5.11971e-12							
1000	***	***	5.32803e-12	***	1.01781e-18	1.133e-18	5.32812e-12
7.32044e-12							
1125	***	***	4.94706e-12	***	2.07264e-17	1.80972e-17	4.9473e-12
1.07018e-11							

1250	***	***	3.47401e-12	***	2.16639e-16	1.54849e-16	3.47465e-12
1.47902e-11							
1375	***	***	***	***	1.41854e-15	8.65574e-16	2.28411e-15
1.95842e-11							
1500	***	***	***	***	6.47743e-15	3.48386e-15	9.96128e-15
2.50763e-11							
1650	***	***	***	***	2.76511e-14	1.32199e-14	4.08709e-14
3.25723e-11							
1750	***	***	***	***	6.06832e-14	2.72167e-14	8.78999e-14
3.81074e-11							
1800	***	***	***	***	8.58815e-14	3.74333e-14	1.23315e-13
4.10333e-11							
2000	***	***	***	***	2.68906e-13	1.0636e-13	3.75266e-13
5.37691e-11							
2250	***	***	***	***	7.42217e-13	2.67403e-13	1.00962e-12
7.19335e-11							
2500	***	***	***	***	1.53198e-12	5.13935e-13	2.04591e-12
9.24727e-11							

Pressure = 10 atm

T(K)	fl_p1->i1	fl_p1->i2	fl_p1->i3	fl_p1->i4	fl_p1->fl_p0	fl_p1->fl_p2	fl_p1->Capture
300	3.14292e-32	1.93237e-30	2.41068e-14	1.05382e-17	1.39014e-49	4.05113e-47	2.41174e-14
400	3.83165e-27	2.99881e-26	1.43408e-13	3.19607e-16	2.7737e-39	8.34569e-38	1.43727e-13
500	8.81312e-24	2.17077e-23	4.56953e-13	2.86257e-15	9.66838e-33	8.61724e-32	4.59816e-13
600	1.91818e-21	3.14413e-21	1.04586e-12	1.32337e-14	3.17371e-28	1.33692e-27	1.0591e-12
700	***	2.17624e-19	1.96312e-12	4.04379e-14	5.92011e-25	1.48848e-24	2.00355e-12
800	***	9.81576e-18	3.23435e-12	8.95144e-14	1.71636e-22	2.90188e-22	3.32387e-12
900	***	***	4.84058e-12	1.47521e-13	1.45094e-20	1.83281e-20	4.9881e-12
1000	***	***	6.63264e-12	1.86649e-13	4.8846e-19	4.90985e-19	6.81929e-12
1125	***	***	8.50353e-12	***	1.45827e-17	1.18549e-17	8.50398e-12
1250	***	***	8.98725e-12	***	1.8788e-16	1.29163e-16	8.98851e-12
1375	***	***	7.85198e-12	***	1.34522e-15	8.0542e-16	7.85601e-12

1500	***	***	***	***	6.48527e-15	3.48742e-15	9.97268e-15
2.50763e-11							
1650	***	***	***	***	2.7682e-14	1.32326e-14	4.09147e-14
3.25723e-11							
1750	***	***	***	***	6.0743e-14	2.72401e-14	8.7983e-14
3.81074e-11							
1800	***	***	***	***	8.59592e-14	3.74629e-14	1.23422e-13
4.10333e-11							
2000	***	***	***	***	2.69061e-13	1.06413e-13	3.75475e-13
5.37691e-11							
2250	***	***	***	***	7.42418e-13	2.67464e-13	1.00988e-12
7.19335e-11							
2500	***	***	***	***	1.53214e-12	5.1398e-13	2.04612e-12
9.24727e-11							

Pressure = 100 atm

T(K)	fl_p1->i1	fl_p1->i2	fl_p1->i3	fl_p1->i4	fl_p1->fl_p0	fl_p1->fl_p2	fl_p1->Capture
300	-1.38042e-32	1.93042e-31	2.41068e-14	1.05382e-17	1.26621e-51	3.54581e-49	2.41174e-14
400	2.57066e-28	3.44652e-27	1.43408e-13	3.19611e-16	2.90926e-41	8.13027e-40	1.43727e-13
500	7.61101e-25	3.17604e-24	4.56954e-13	2.86347e-15	1.40433e-34	1.12904e-33	4.59817e-13
600	2.47751e-22	5.29116e-22	1.04588e-12	1.32848e-14	7.6236e-30	2.84622e-29	1.05916e-12
700	1.95414e-20	3.00519e-20	1.96345e-12	4.15251e-14	2.58975e-26	5.7632e-26	2.00498e-12
800	5.49009e-19	8.93736e-19	3.23906e-12	9.97712e-14	1.32002e-23	2.01921e-23	3.33884e-12
900	***	1.82014e-17	4.88283e-12	1.96304e-13	1.6993e-21	1.94594e-21	5.07916e-12
1000	***	1.83193e-16	6.88011e-12	3.24881e-13	7.875e-20	7.12103e-20	7.20517e-12
1125	***	4.3466e-15	9.75347e-12	4.88631e-13	2.56625e-18	1.53879e-18	1.02464e-11
1250	***	***	1.26573e-11	5.89501e-13	7.77357e-17	5.01355e-17	1.32469e-11
1375	***	***	1.48811e-11	***	7.93199e-16	4.52002e-16	1.4886e-11
1500	***	***	1.56065e-11	***	4.67332e-15	2.3988e-15	1.562e-11
1650	***	***	1.42749e-11	***	2.36254e-14	1.09825e-14	1.43284e-11
3.25723e-11							

1750	***	***	1.23662e-11	***	5.5184e-14	2.42712e-14	1.24691e-11
3.81074e-11							
1800	***	***	***	***	8.66815e-14	3.77351e-14	1.24417e-13
4.10333e-11							
2000	***	***	***	***	2.70519e-13	1.0691e-13	3.77429e-13
5.37691e-11							
2250	***	***	***	***	7.44308e-13	2.68032e-13	1.01234e-12
7.19335e-11							
2500	***	***	***	***	1.53372e-12	5.14393e-13	2.04811e-12
9.24727e-11							

Pressure = 0.0394737 atm

T(K)	fl_p2->i1	fl_p2->i2	fl_p2->i3	fl_p2->i4	fl_p2->fl_p0	fl_p2->fl_p1	fl_p2->
Capture							
300	1.22223e-19	4.95715e-20	7.13612e-16	2.05419e-18	3.23875e-27	8.18583e-18	
7.24016e-16	7.27951e-16						
400	1.43079e-19	***	9.92988e-15	1.42767e-17	1.51618e-23	5.24208e-16	1.04685e-14
14	1.05306e-14						
500	***	***	4.7081e-14	1.69589e-17	5.13303e-21	1.08174e-14	5.79154e-14
5.8281e-14							
600	***	***	1.00506e-13	7.28322e-18	3.783e-19	9.2134e-14	1.92648e-13
1.9392e-13							
700	***	***	1.02986e-13	2.5769e-18	1.04049e-17	3.70613e-13	4.73613e-13
4.76861e-13							
800	***	***	5.55669e-14	***	1.44968e-16	9.02109e-13	9.57821e-13
9.64711e-13							
900	***	***	1.86264e-14	***	1.23446e-15	1.67386e-12	1.69372e-12
1.70707e-12							
1000	***	***	4.77919e-15	***	7.24952e-15	2.70571e-12	2.71774e-12
2.74352e-12							
1125	***	***	***	***	4.42825e-14	4.38988e-12	4.43416e-12
4.49725e-12							
1250	***	***	***	***	1.89832e-13	6.44527e-12	6.63511e-12
6.79648e-12							
1375	***	***	***	***	6.12265e-13	8.66284e-12	9.2751e-12
9.66512e-12							
1500	***	***	***	***	1.56596e-12	1.07117e-11	1.22776e-11
1.31151e-11							
1650	***	***	***	***	3.78194e-12	1.24809e-11	1.62628e-11
1.8027e-11							
1750	***	***	***	***	6.04524e-12	1.30847e-11	1.91299e-11
2.1767e-11							
1800	***	***	***	***	7.42172e-12	1.3208e-11	2.06297e-11
2.37755e-11							

2000	***	***	***	***	1.44369e-11	1.27082e-11	2.71451e-11
3.27187e-11							
2250	***	***	***	***	2.58878e-11	1.08181e-11	3.67058e-11
4.58902e-11							
2500	***	***	***	***	3.93219e-11	8.74228e-12	4.80642e-11
6.11836e-11							

Pressure = 1 atm

T(K)	fl_p2->i1	fl_p2->i2	fl_p2->i3	fl_p2->i4	fl_p2->fl_p0	fl_p2->fl_p1	fl_p2->
300	2.46e-16	9.2911e-17	3.84631e-16	2.05674e-18	1.64856e-27	1.47503e-19	
7.24016e-16	7.27951e-16						
400	1.21561e-15	5.26075e-16	8.63051e-15	7.35684e-17	1.12007e-23	2.27356e-17	
1.04685e-14	1.05306e-14						
500	1.51897e-15	8.64869e-16	5.41668e-14	5.72254e-16	4.4876e-21	7.92481e-16	
5.79154e-14	5.8281e-14						
600	1.15589e-15	***	1.7954e-13	1.39895e-15	3.55152e-19	1.05529e-14	1.92648e-13
13	1.9392e-13						
700	***	***	3.94977e-13	1.38267e-15	1.00763e-17	7.72434e-14	4.73613e-13
4.76861e-13							
800	***	***	5.99909e-13	7.5852e-16	1.4246e-16	3.57015e-13	9.57825e-13
9.64711e-13							
900	***	***	6.16596e-13	3.36244e-16	1.22223e-15	1.07558e-12	1.69374e-12
1.70707e-12							
1000	***	***	4.35351e-13	***	7.20703e-15	2.27521e-12	2.71778e-12
2.74352e-12							
1125	***	***	1.89308e-13	***	4.41431e-14	4.2008e-12	4.43426e-12
4.49725e-12							
1250	***	***	6.31469e-14	***	1.89504e-13	6.38264e-12	6.6353e-12
6.79648e-12							
1375	***	***	***	***	6.11682e-13	8.66372e-12	9.2754e-12
9.66512e-12							
1500	***	***	***	***	1.56515e-12	1.07129e-11	1.2278e-11
1.31151e-11							
1650	***	***	***	***	3.78102e-12	1.24822e-11	1.62632e-11
1.8027e-11							
1750	***	***	***	***	6.04437e-12	1.30859e-11	1.91303e-11
2.1767e-11							
1800	***	***	***	***	7.42091e-12	1.32091e-11	2.06301e-11
2.37755e-11							
2000	***	***	***	***	1.44364e-11	1.27089e-11	2.71453e-11
3.27187e-11							
2250	***	***	***	***	2.58876e-11	1.08183e-11	3.67059e-11
4.58902e-11							

2500 *** *** *** *** 3.93219e-11 8.74236e-12 4.80642e-11
6.11836e-11

Pressure = 10 atm

T(K)	fl_p2->i1	fl_p2->i2	fl_p2->i3	fl_p2->i4	fl_p2->fl_p0	fl_p2->fl_p1	fl_p2->Capture
300	6.13732e-16	8.76299e-17	5.24372e-16	3.55023e-19	3.17142e-28	1.59938e-21	7.24016e-16
400	7.12958e-15	1.91146e-15	1.40452e-15	2.25358e-17	3.45459e-24	5.06003e-19	1.04685e-14
500	2.65697e-14	1.07465e-14	2.01552e-14	4.04818e-16	2.1339e-21	3.92102e-17	5.79154e-14
600	4.93728e-14	2.81702e-14	1.1124e-13	2.8286e-15	2.29982e-19	1.03639e-15	1.92648e-13
700	***	9.59799e-14	3.56853e-13	8.90607e-15	7.87285e-18	1.1871e-14	4.73618e-13
800	***	9.70816e-14	7.72192e-13	1.46528e-14	1.23653e-16	7.38011e-14	9.57851e-13
900	***	***	1.36066e-12	1.47661e-14	1.12417e-15	3.17285e-13	1.69384e-12
1000	***	***	1.71477e-12	1.05036e-14	6.84871e-15	9.85959e-13	2.71808e-12
1125	***	***	1.64029e-12	***	4.2914e-14	2.75181e-12	4.43509e-12
1250	***	***	1.12645e-12	***	1.86535e-13	5.32391e-12	6.63701e-12
1375	***	***	6.10029e-13	***	6.06336e-13	8.06161e-12	9.27813e-12
1500	***	***	***	***	1.55766e-12	1.07238e-11	1.22815e-11
1650	***	***	***	***	3.77252e-12	1.24943e-11	1.62668e-11
1750	***	***	***	***	6.03634e-12	1.30971e-11	1.91335e-11
1800	***	***	***	***	7.41339e-12	1.32196e-11	2.0633e-11
2000	***	***	***	***	1.44317e-11	1.27153e-11	2.7147e-11
2250	***	***	***	***	2.58857e-11	1.08208e-11	3.67065e-11
2500	***	***	***	***	3.93213e-11	8.74311e-12	4.80644e-11

Pressure = 100 atm

T(K)	fl_p2->i1	fl_p2->i2	fl_p2->i3	fl_p2->i4	fl_p2->fl_p0	fl_p2->fl_p1	fl_p2->
Capture							
300	7.10727e-16	1.29419e-17	-1.43294e-14	3.88364e-20	3.60091e-29	1.39988e-23	
7.24016e-16	7.27951e-16						
400	9.96748e-15	4.67722e-16	3.08126e-17	2.85782e-18	4.65753e-25	4.92942e-21	
1.04685e-14	1.05306e-14						
500	5.15449e-14	5.4604e-15	8.41134e-16	6.85169e-17	3.73307e-22	5.13735e-19	
5.79154e-14	5.8281e-14						
600	1.52218e-13	3.03472e-14	9.29459e-15	7.66808e-16	5.54218e-20	2.20641e-17	
1.92649e-13	1.9392e-13						
700	3.14595e-13	1.01408e-13	5.24551e-14	4.70773e-15	2.64258e-18	4.59629e-16	
4.73628e-13	4.76861e-13						
800	5.06775e-13	2.4574e-13	1.82826e-13	1.74129e-14	5.58082e-17	5.13527e-15	
9.57944e-13	9.64711e-13						
900	***	1.12063e-12	4.98037e-13	4.13516e-14	6.42146e-16	3.36869e-14	1.69435e-12
1.70707e-12							
1000	***	1.45651e-12	1.04652e-12	6.92671e-14	4.65249e-15	1.42999e-13	2.71995e-12
2.74352e-12							
1125	***	1.76772e-12	2.18139e-12	1.01428e-13	3.37449e-14	3.57189e-13	4.44148e-12
4.49725e-12							
1250	***	***	4.28488e-12	1.35496e-13	1.63363e-13	2.06651e-12	6.65025e-12
6.79648e-12							
1375	***	***	4.2144e-12	***	5.61275e-13	4.52418e-12	9.3009e-12
9.66512e-12							
1500	***	***	3.44292e-12	***	1.49127e-12	7.37629e-12	1.23119e-11
1.31151e-11							
1650	***	***	2.2322e-12	***	3.69451e-12	1.03696e-11	1.62993e-11
1.8027e-11							
1750	***	***	1.52861e-12	***	5.96171e-12	1.16697e-11	1.91629e-11
2.1767e-11							
1800	***	***	***	***	7.34391e-12	1.33156e-11	2.06595e-11
2.37755e-11							
2000	***	***	***	***	1.43876e-11	1.27746e-11	2.71622e-11
3.27187e-11							
2250	***	***	***	***	2.58681e-11	1.08438e-11	3.67119e-11
4.58902e-11							
2500	***	***	***	***	3.93157e-11	8.75014e-12	4.80659e-11
6.11836e-11							

5.3. Input file for RRKM-ME calculations for the benzo[ghi]fluoranthene-5-yl + C₂H₂ reaction using MESS package

```

TemperatureList[K]          300. 400. 500. 600. 700. 800. 900.
1000. 1125. 1250. 1375. 1500. 1650. 1750. 1800. 2000. 2250. 2500.
PressureList[atm]          0.03947368 1. 10. 100.
EnergyStepOverTemperature  0.2          #Ratio of
discretization energy step to T
ExcessEnergyOverTemperature 100
ModelEnergyLimit[kcal/mol] 900
WellCutoff                 10
ChemicalEigenvalueMax     0.2
ChemicalEigenvalueMin     1.e-6          #only for direct
diagonalization method
CalculationMethod         direct
EigenvalueOutput          eigenvalue.out
Reactant p0               #ground energy of bimolecular species will be used as a
reference.
Model
EnergyRelaxation
Exponential
Factor[1/cm]              424      ! Jasper calc N2
Power                     0.62
ExponentCutoff            15
End
CollisionFrequency
LennardJones
!Epsilons[1/cm]           203.0 203.0 ! N2 pyrene-Frenklach
      Epsilons[1/cm]       101.5 866.4 ! N2 Frenklach correlation
with molecular weight
      Sigmas[angstrom]     3.6154 7.56 ! N2 Frenklach correlation
with molecular weight
Masses[amu]               28. 251.
End
OutputTemperatureStep[K]  100
OutputTemperatureSize     20
OutputReferenceEnergy[kcal/mol] 0.
!-----
!-----well_ip1-----
Well ip1
Species
RRHO
Geometry[angstrom]       31
C -0.1536227376 -1.1905535763 -0.0544566898
C -0.2833329374 -2.5739348999 -0.0620084383
C 0.9501004863 -3.2795646225 -0.0395618089
C 2.1404589528 -2.566170548 -0.0129195539
C 2.2145635446 -1.1423329589 -0.0063209597
C 1.0387696314 -0.414271599 -0.0275107408
C -1.2718587623 -0.3581078737 -0.0739137563
C -2.5848974138 -0.7763264968 -0.1018067881
C -2.7399850816 -2.210711738 -0.1101421085
C -1.645626025 -3.057089139 -0.0911771675
C 0.5869873694 1.0214976395 -0.0312617569
C -0.8342710635 0.9688743514 -0.0601036029

```

C	-1.7463285268	2.0181776283	-0.0745088473
C	-1.1492373164	3.3058767815	-0.0576115827
C	0.2302443877	3.4116477605	-0.0294337192
C	1.1431664588	2.3019067542	-0.0152506374
C	2.5773575125	2.6178743336	0.0149421112
C	3.6047218054	1.7966867322	0.0321781207
C	-3.5418769194	0.3040398735	-0.1170213181
C	-3.1370595556	1.6263524681	-0.1039496536
H	0.9725383666	-4.3643326649	-0.0429653436
H	3.0736065853	-3.1187371695	0.0040032816
H	3.1857713277	-0.6627065868	0.0150068445
H	-3.7348088703	-2.6437684039	-0.1317205392
H	-1.818388155	-4.1286083917	-0.0985244505
H	-1.7555096484	4.2055591725	-0.0664451051
H	0.6670847203	4.4050143546	-0.016868484
H	2.803726385	3.6911197734	0.0239974683
H	4.6804818521	1.8831095429	0.0542441097
H	-4.6039471316	0.0823068278	-0.1391479508
H	-3.8957492413	2.4023106746	-0.1162799327

Core RigidRotor

SymmetryFactor 1.0

End

Frequencies[1/cm] 87

59.6055	73.4364	107.3383
159.3553	168.2659	212.7712
271.3998	296.4052	299.8422
322.2266	396.5237	429.1202
439.9913	450.0487	471.0907
500.2310	525.9077	529.2397
561.4324	565.5378	580.5569
608.5805	647.1483	647.4991
657.8095	659.7622	697.9494
715.8589	767.5842	778.4761
779.7333	805.2169	806.0986
838.6801	841.6372	843.8490
862.2742	874.0991	906.2521
926.0585	958.7161	966.4985
972.2874	972.7186	982.0492
1041.8291	1062.2702	1079.5980
1147.8925	1159.0705	1162.2810
1181.4253	1197.7019	1216.4163
1231.4921	1239.9761	1257.1469
1276.4096	1308.4953	1351.8665
1377.2495	1400.5039	1419.2393
1430.8461	1451.5465	1457.8593
1486.4312	1497.0301	1517.0756
1533.5008	1600.9478	1623.5154
1648.0397	1652.2910	1674.4336
1699.8885	3013.1762	3156.3305
3156.7878	3157.1671	3160.3440
3173.4709	3174.3589	3174.8724
3175.9546	3185.7037	3243.8783

ZeroEnergy[kcal/mol] -39.24

```

ElectronicLevels[1/cm]      1
0 2
End
End
!-----
!-----well_ip2-----
Well      ip2
Species
RRHO
Geometry[angstrom]  31
C  -0.4530110751   -1.3986503836   -0.160007275
C  -0.7233981959   -2.7622925946   -0.1375728793
C   0.4208797074   -3.6051255794   -0.0918570439
C   1.6898367053   -3.0282062976   -0.0733901019
C   1.8440701762   -1.6328343704   -0.0993486892
C   0.8186894466   -0.7337993037   -0.1433682458
C  -1.4736498986   -0.4507468986   -0.2051448543
C  -2.8238279242   -0.7324078667   -0.2319100722
C  -3.128264187    -2.1418725446   -0.2092413424
C  -2.1297328481   -3.0981532287   -0.1645946054
C   0.5183015112    0.7365465565   -0.1820431004
C  -0.9003531227    0.8234377023   -0.2184112665
C  -1.7005399685    1.9600302577   -0.2622067991
C  -0.9739144943    3.178985258    -0.270740744
C   0.4090972122    3.1437266861   -0.2363991004
C   1.2111644344    1.9506853052   -0.1912618025
C   2.6656778428    2.1305869547   -0.1597561894
C   3.6128929307    1.1881153428   -0.1160646101
C  -3.663664119    0.4398861478   -0.2772784264
C  -3.1233602962    1.7129957247   -0.2914312609
H   0.3225255646   -4.6855922565   -0.0712556908
H   2.5662898653   -3.6662266884   -0.0385409507
H  -4.162921691    -2.4683116646   -0.2273970496
H  -2.4141939849   -4.1452906906   -0.1492045696
H  -1.4848044057    4.1355388022   -0.3036839295
H   0.943433033    4.0881524775   -0.2437136436
H   2.9856348867    3.170038301    -0.1746157192
H   4.6605000111    1.4654373223   -0.0966119995
H   3.3897141427    0.1276936284   -0.0982462829
H  -4.7427146281    0.3281966902   -0.3010215884
H  -3.7974786309    2.5628652107   -0.3259591669
Core RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  87
55.9246          71.7567          102.4406
151.8500         171.3659         222.1211
281.8090         292.3895         296.7099
311.5856         395.4961         429.1063
437.6798         454.0898         467.2335
503.5486         518.8605         524.3781
552.8878         562.3149         580.9597
606.8894         644.2322         647.6332

```


652.2388	660.8618	714.0770
723.4155	765.6181	775.6913
777.1401	820.2453	824.2203
835.6288	838.4354	853.9829
892.1891	947.3003	949.8065
950.0004	960.9328	968.6634
975.0374	1014.5807	1028.1314
1066.2563	1094.3530	1111.9298
1144.1882	1158.1568	1162.7825
1182.9350	1213.1963	1216.7849
1230.2812	1248.6597	1274.4580
1322.2429	1342.0233	1357.1841
1384.5501	1409.5287	1426.0066
1442.5009	1446.2645	1465.3739
1479.6861	1485.2549	1517.8398
1524.5712	1581.7183	1602.1180
1641.4802	1669.3373	1684.0739
1694.3105	3127.7801	3133.5974
3157.8538	3158.5962	3158.6411
3160.7927	3174.8822	3175.7983
3176.6425	3177.1948	3218.6282

ZeroEnergy[kcal/mol] -37.82

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_ip3-----

Well ip3

Species

RRHO

Geometry[angstrom] 31

C	-0.017673218	-1.3546393038	0.7008319847
C	-0.1457575335	-2.6265909266	0.162120267
C	1.0957484221	-3.2338709061	-0.2147984252
C	2.2965442195	-2.5180323156	-0.1920880516
C	2.3640911553	-1.1548425024	0.2245502022
C	1.1980107731	-0.6405187145	0.7256637833
C	-1.0790259785	-0.4195104159	0.7253497757
C	-2.3343789004	-0.6913662525	0.2158685305
C	-2.542163709	-2.0783214532	-0.1474659751
C	-1.5062110064	-2.9948956514	-0.1730364835
C	0.8786338495	0.7614217679	0.7638048157
C	-0.5209742259	0.8829988809	0.7581642203
C	-1.1974442273	1.9951935632	0.2714588789
C	-0.3384245303	3.1116311374	-0.0616994307
C	1.0374667549	2.9952407011	-0.0826479565
C	1.7188697285	1.7462876724	0.2334587475
C	3.011827112	1.3219605026	-0.1141206768
C	3.4829788442	-0.1339315387	0.0195361893
C	-3.1203360069	0.479388209	-0.0943228397
C	-2.5736139033	1.7574497617	-0.0716869424
H	1.1033475614	-4.2415577878	-0.6178693394

```

H 3.1867625168 -3.004164966 -0.5796481754
H -3.5210763583 -2.3956666712 -0.4928877574
H -1.7114853465 -3.996270081 -0.5382803739
H -0.7831214271 4.0471108451 -0.3869156276
H 1.6250131806 3.8410331678 -0.425018495
H 3.7232617219 2.0177559331 -0.5469019134
H 4.193003303 -0.1961416408 0.8623217311
H 4.0792934958 -0.3910979551 -0.8639890728
H -4.140448809 0.3601790642 -0.4451650775
H -3.1880744584 2.5854598761 -0.4112295125

```

```

Core RigidRotor
SymmetryFactor 0.5
End

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```

Frequencies[1/cm] 87
121.9214 137.6835 141.2942
210.1220 277.0644 299.5393
304.8244 329.3467 398.1015
404.0277 429.0642 435.5415
452.3133 490.3551 538.5589
546.3263 549.5083 572.1634
593.1238 605.9085 614.6802
637.3049 646.6811 650.8562
662.9895 696.3918 745.4680
753.5081 766.0119 776.2011
798.7437 813.6255 825.6382
843.2591 850.7098 856.0326
905.8822 939.7884 956.5168
959.4299 959.8103 970.6751
974.7715 1047.0416 1073.6215
1093.3909 1149.8290 1152.3406
1157.6144 1167.7535 1183.3822
1189.2244 1197.8003 1215.3928
1235.8857 1249.9255 1302.1565
1319.3274 1332.6072 1362.1130
1393.6499 1405.7932 1425.1401
1430.7111 1447.6710 1450.4774
1455.8754 1458.0406 1475.8669
1479.4177 1508.9741 1574.4775
1627.2427 1645.8851 1653.4316
1664.6758 2932.9170 3023.7983
3151.9625 3153.3466 3153.9675
3154.6047 3164.2806 3170.1536
3171.1447 3171.7768 3172.7105

```

```

ZeroEnergy[kcal/mol] -63.72
ElectronicLevels[1/cm] 1
0 2

```

```

End
End

```

```

!-----
!-----well_ip4-----
Well ip4
Species
RRHO

```

```

Geometry[angstrom] 31
C -0.2131442627 -1.0435982116 -0.8628221106
C -0.3344649523 -2.3883748541 -0.5319878418
C 0.9354181292 -3.0694028327 -0.2610352733
C 2.1275256184 -2.424280231 -0.2395599296
C 2.3252142896 -0.9559878963 -0.6340079505
C 1.0036354819 -0.3260840487 -0.8260579628
C -1.2801293685 -0.1365237771 -0.6193895105
C -2.5127642381 -0.5218721879 -0.1143691645
C -2.70764398 -1.9421627078 -0.0084653721
C -1.6485739245 -2.8296623463 -0.1869825283
C 0.6985420959 0.998278802 -0.4389353684
C -0.7142410686 1.1308635672 -0.3564658963
C -1.3497330398 2.0830577071 0.4261607598
C -0.4769485383 3.0537605427 1.0282834201
C 0.9067598843 2.8934712843 1.0004770578
C 1.5334748146 1.7950600231 0.3360269794
C 2.8449502026 1.2071744306 0.6260913613
C 3.1875598242 -0.0502372938 0.2528242225
C -3.2823616025 0.5454822506 0.4824621402
C -2.728581924 1.7861110258 0.7395411253
H 0.9094599483 -4.1201363735 0.0134865384
H 3.0232844858 -2.9841115045 0.0127287522
H 2.8698333724 -0.9980903806 -1.6034151203
H -3.6624851681 -2.330464114 0.3306100412
H -1.8119224061 -3.8792657013 0.0371423624
H -0.896934974 3.8639460067 1.6153854569
H 1.5168969602 3.5763662342 1.5835497154
H 3.5416904551 1.7748595029 1.236306902
H 4.1606664117 -0.4369118367 0.5409074466
H -4.2917486099 0.344761397 0.8275756129
H -3.3217149169 2.5191135237 1.2772391347

```

```

Core RigidRotor
SymmetryFactor 1.0
End

```

```

Frequencies[1/cm] 87
113.5482 132.4732 160.8483
250.2098 257.5097 290.9446
304.9282 389.0033 399.3270
418.9735 431.5921 433.6909
444.0386 513.0824 517.7153
542.2737 561.1469 585.0545
597.2934 599.4783 629.6372
636.2307 647.4117 651.4767
673.8147 733.7449 741.3618
750.1491 758.9015 798.6138
805.0032 816.0833 817.5237
838.7585 850.8880 864.1399
921.5836 946.9889 950.1190
971.0724 978.5962 982.8351
994.7089 1007.4237 1055.2148
1071.0808 1127.2056 1151.3635
1153.6306 1173.8293 1183.5924

```

1184.7616	1202.8676	1213.3076
1215.5413	1234.5987	1261.6173
1296.9569	1321.3404	1350.8446
1364.4477	1397.7649	1405.2539
1407.2431	1433.1777	1437.8738
1453.0551	1465.5725	1494.3663
1503.6626	1527.9349	1579.9173
1615.7920	1635.8307	1638.8200
1641.1212	2813.9357	3143.0083
3144.1048	3153.9123	3154.5286
3154.7490	3163.1207	3164.6039
3171.2825	3172.3709	3173.3142

ZeroEnergy[kcal/mol] -50.60

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----c2h2_c18h9_p0-----

Bimolecular p0

Fragment c18h9

RRHO

Geometry[angstrom] 27

C	-1.6714344227	0.7435386415	0.0407999711
C	-1.6666827272	-0.7576107723	0.0307466595
C	-0.2875223897	-1.1418714618	0.1077408108
C	0.5156560665	-0.0015911739	0.1623209927
C	-0.3057896757	1.1258814654	0.1227971092
C	0.2245595285	2.4096602814	0.1615673499
C	-0.7466332005	3.4452317979	0.11117814481
C	-2.0945339221	3.1159773945	0.0311108005
C	-2.5847503586	1.7786534942	-0.0061682051
C	0.2584895171	-2.419892055	0.1302476819
C	1.7029005804	-2.4544712245	0.2130201421
C	2.4808285304	-1.311217276	0.2657359508
C	1.8916416648	0.0061811043	0.241278728
C	-2.4895899798	-1.8428732294	-0.0238809232
C	-2.0480373089	-3.1762587311	-0.0075493427
C	-0.6883250744	-3.4791638556	0.0686129802
C	1.6678617984	2.4654524851	0.2450072873
C	2.4615036543	1.3325651963	0.2829768722
H	-0.4506218689	4.488718607	0.1355082334
H	-2.8204191368	3.9208846346	-0.0060845015
H	-3.6531265135	1.6060768767	-0.0696929025
H	2.1988292012	-3.4195005195	0.234679416
H	3.5589823441	-1.4171816214	0.3268949242
H	-2.7712892985	-3.9832799141	-0.0547237762
H	-0.3712714801	-4.5169485181	0.0795383921
H	2.1507075896	3.4368445225	0.2791377216
H	3.5381988821	1.4525618512	0.3455891798

Core RigidRotor

SymmetryFactor 1

End

```

Frequencies[1/cm] 75
68.4680          121.6609          189.9568
255.0591          281.0994          292.7914
296.9243          423.6986          432.2771
444.7833          451.8706          464.8133
511.9777          548.1120          558.5038
575.4590          580.1519          607.4851
635.9687          646.4537          666.9729
670.1416          755.1243          761.0664
770.7093          777.7764          780.8208
829.3704          840.2508          846.0823
881.3053          927.6504          930.6363
952.1689          966.5260          973.1626
974.9603          983.3169          1041.4231
1067.4839         1093.1375         1136.1651
1153.9630         1161.6953         1190.4416
1208.6275         1227.5532         1233.5603
1254.9956         1274.0067         1336.1406
1353.5140         1395.0457         1419.2376
1425.2496         1445.5117         1448.5834
1477.2820         1483.2974         1510.3245
1531.3235         1582.7235         1625.3391
1643.8875         1672.8030         1696.5347
3157.4984         3158.5174         3159.6962
3161.6833         3174.4845         3175.3515
3175.5244         3176.4633         3187.0159
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 2
End
Fragment          c2h2
RRHO
Geometry[angstrom] 4
C 0.0 0.0 0.5990703976
C 0.0 0.0 -0.5990703976
H 0.0 0.0 1.6619081422
H 0.0 0.0 -1.6619081422
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm] 7
642.0679          642.0679          772.6955
772.6955          2069.5209         3420.9273
3523.7963
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
GroundEnergy[kcal/mol] 0.00
End
!-----h_c20h10_p1-----
Bimolecular      p1
Fragment          c20h10

```

RRHO

Geometry[angstrom] 30

C	-0.9553401557	0.9048536981	0.0813041062
C	-1.0317964066	-0.5088526562	0.0792746372
C	0.0349372986	-1.0035940547	-0.7091566735
C	0.7706666051	0.1043368817	-1.1943901215
C	0.1586644913	1.2838486015	-0.7058789175
C	0.8534276725	2.462042337	-0.5052155473
C	0.2251839048	3.3760504328	0.4224960481
C	-0.8652335769	3.0050690699	1.1930336901
C	-1.441721279	1.6812530411	1.1165432476
C	0.5985905019	-2.2504672374	-0.5117996132
C	1.9360264287	-2.392970802	-1.0424425812
C	2.6562029349	-1.3084865006	-1.5174140635
C	2.1143108658	0.0320679805	-1.5115568265
C	2.1985880487	2.4608106586	-1.0355381064
C	2.7975765507	1.3063001473	-1.5137893314
C	-2.2261425094	0.9556562516	2.0906462953
C	-2.3009122731	-0.4280996077	2.0887025813
C	-1.5991809109	-1.2312606857	1.1124343232
C	-1.168471241	-2.6095762675	1.1854958476
C	-0.1243114923	-3.0938430193	0.4137358195
H	0.6688809494	4.3521248097	0.5915445972
H	-1.2342374199	3.7046173094	1.9364279501
H	2.4308123616	-3.3575186538	-0.9878003575
H	3.6877212955	-1.4647571897	-1.8169159093
H	2.7944627227	3.3662530946	-0.9785432097
H	3.8399504113	1.3512916161	-1.8131644228
H	-2.6999851034	1.497307434	2.9031963016
H	-2.8305378442	-0.9177430997	2.8998221838
H	-1.6104532632	-3.2671650186	1.9273679721
H	0.2119584321	-4.1123125711	0.5804790805

Core RigidRotor

SymmetryFactor 5

End

Frequencies[1/cm] 84

139.8628	140.3121	147.3140
279.5289	280.2974	311.6560
312.0266	411.0066	411.0327
439.9551	440.0089	455.1153
455.2850	543.4701	549.2172
549.4933	560.0198	605.1715
613.9523	614.4298	650.0013
650.2378	650.6653	673.8125
673.9455	760.7434	760.8108
767.1620	767.9532	813.6995
814.1964	832.3107	832.7107
854.8650	866.8752	866.9672
939.7872	961.5033	968.4527
968.8857	977.3301	978.0367
1048.4020	1088.9988	1089.1630
1161.7835	1161.7873	1162.6269
1162.6950	1185.6722	1185.8923

1214.5548	1214.8991	1238.1420
1259.1352	1334.1158	1334.4392
1377.4274	1377.5340	1425.4708
1425.5160	1442.8221	1443.2023
1464.9481	1470.4793	1470.6174
1484.2125	1484.2819	1512.3408
1653.4457	1653.9016	1654.3720
1654.5581	1655.4199	3154.1847
3154.7189	3155.0273	3155.5692
3155.5918	3171.5720	3171.6101
3172.4735	3172.7012	3173.7909
ZeroEnergy[kcal/mol]	0.0	
ElectronicLevels[1/cm]	1	
0 1		
End		
Fragment	H	
Atom		
Mass[amu]	1	
ElectronicLevels[1/cm]	1	
0 2		
End		
GroundEnergy[kcal/mol]	-34.30	
End		
!-----h_c20hh10_p2-----		
Bimolecular	p2	
Fragment	c20hh10	
RRHO		
Geometry[angstrom]	30	
C	-3.0806610335	-1.2612268458 0.0
C	-3.2127675276	-2.6435369025 0.0
C	-1.9775954456	-3.3475165413 0.0
C	-0.784812141	-2.6349960588 0.0
C	-0.7076495223	-1.2113947213 0.0
C	-1.8865374394	-0.4905808217 0.0
C	-4.1969621258	-0.4239516991 0.0
C	-5.5115765438	-0.8347777654 0.0
C	-5.6704629242	-2.2700418483 0.0
C	-4.5786903684	-3.1207211765 0.0
C	-2.3364966815	0.941485334 0.0
C	-3.7555423416	0.9007530458 0.0
C	-4.6531990498	1.9601514042 0.0
C	-4.0388160976	3.243164332 0.0
C	-2.6580931386	3.342378835 0.0
C	-1.7676587163	2.2117246622 0.0
C	-0.3592095292	2.4251427571 0.0
C	0.8307406353	2.6139386603 0.0
C	-6.4596626088	0.2547185106 0.0
C	-6.0469255545	1.5760926228 0.0
H	-1.9541228408	-4.4322262137 0.0
H	0.1467263932	-3.1903847212 0.0
H	0.2629934335	-0.7298561578 0.0
H	-6.6665357194	-2.7006584708 0.0
H	-4.7569376962	-4.1913045319 0.0

```

H -4.6361077064 4.1487518413 0.0
H -2.2020394024 4.3252333917 0.0
H 1.8796068536 2.7826911869 0.0
H -7.5236475461 0.041505083 0.0
H -6.8022876147 2.355247809 0.0
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm] 84
62.3559 77.4752 108.3685
132.1338 202.0971 260.3383
274.9219 295.0752 298.7608
382.2403 412.5145 434.2153
439.2445 439.6152 469.8069
484.8821 540.9394 549.5332
576.1986 586.5221 595.3368
616.2622 638.6002 647.9679
654.3565 656.7045 688.5269
689.3454 714.7693 768.2266
780.0242 780.6087 815.9687
825.0982 838.8870 841.2561
852.2474 889.5512 928.7795
963.5729 968.2530 969.5147
974.9126 983.6799 1038.9516
1046.5922 1075.0460 1148.9193
1160.1248 1161.0584 1191.4307
1198.3613 1215.0639 1231.9083
1241.3197 1258.3697 1293.8568
1347.0968 1377.4102 1400.7558
1418.6705 1428.5769 1450.2531
1457.1269 1484.5899 1494.1484
1514.3516 1529.6964 1612.5172
1626.7093 1653.1157 1676.0533
1700.7759 2201.1882 3157.1296
3158.6213 3161.3246 3168.1263
3174.2747 3175.9471 3177.2258
3190.2190 3192.7052 3476.1622
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
Fragment H
Atom
Mass[amu] 1
ElectronicLevels[1/cm] 1
0 2
End
GroundEnergy[kcal/mol] -8.71
End
!-----bar_ts1-----
Barrier ts1 ip1 p0
RRHO
Geometry[angstrom] 31

```



```

C 1.068924163 0.817824754 0.0282944288
C 2.357697102 1.3349979073 -0.0211705406
C 2.4224937259 2.7520435798 0.0568115447
C 1.2470050819 3.4849715062 0.1691892275
C -0.0525684576 2.9016602209 0.213571549
C -0.1576743232 1.5259351647 0.1441341261
C 0.8340795291 -0.5562623361 -0.0410426898
C 1.798249365 -1.5339320502 -0.1601754122
C 3.1453162499 -1.0152012395 -0.2107834878
C 3.4034623376 0.3426436609 -0.1446564567
C -1.2303422495 0.4727358995 0.1462401255
C -0.5426565893 -0.7761443169 0.0280620963
C -1.0774046369 -2.0581923896 -0.019300336
C -2.4961395916 -2.1155511551 0.0609125774
C -3.2223762464 -0.9314731942 0.1798716431
C -2.5870291769 0.3257543396 0.2297348742
C 1.2641985887 -2.8739908191 -0.2111120455
C -0.0970161871 -3.1150189696 -0.1442267915
H 3.3759848073 3.2690366917 0.0284199552
H 1.3172358813 4.5658880989 0.2252837483
H -0.9223007329 3.5433344309 0.296112742
H 3.981692682 -1.7004751804 -0.3037947558
H 4.4354624586 0.6760411889 -0.1881354309
H -3.0209361891 -3.0651662607 0.0291633099
H -4.3049466404 -0.9795784923 0.2359614815
H 1.9389154764 -3.7188027325 -0.3042038547
H -0.4431635239 -4.1427825547 -0.1874785586
C -3.9578884287 2.2081251706 0.5122096723
C -4.3179311744 2.6573669075 -0.5566195346
H -3.8433113916 2.0919133221 1.5648877302
H -4.539683909 2.9212058474 -1.5628429371
Core RigidRotor
SymmetryFactor 0.5
End
      Rotor      Hindered      ! C2H2      21.4605
      Group                29 30 31
      Axis                  16 28
      Symmetry                1
      Potential[kcal/mol]    12
0      0.100401534 0.414156329 0.847137947 0.38278085 0.087851343 0
      0.163152493 0.721636028 1.468372441 0.658885069 0.13805211
      End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 306.5415
WellDepth[kcal/mol] 43.61
WellDepth[kcal/mol] 4.37
End
Frequencies[1/cm] 85
      34.7121
      72.2245      73.6902      121.3654
      174.9122      212.2253      269.2699
      284.8418      296.2074      299.6392
      417.9028      432.8791      438.2260

```

455.3914	462.0026	515.9835
526.0508	548.4226	560.9624
576.9641	591.9867	608.3951
639.0298	649.8449	653.1465
665.4528	670.7455	729.1378
764.3375	768.8910	774.3254
775.5559	781.3890	788.3914
833.3385	840.9218	846.1497
881.2417	926.5398	928.7009
953.5836	965.4944	972.2340
973.1922	982.7795	1040.2929
1067.8059	1089.0287	1140.0326
1153.9344	1161.3996	1190.4398
1209.2487	1229.1677	1232.8739
1254.0083	1277.1329	1341.6519
1353.1283	1394.2701	1419.0266
1426.1230	1446.2682	1448.6405
1477.4733	1483.9059	1509.3247
1531.0919	1582.5349	1623.5777
1644.5412	1673.0755	1697.0403
1945.7010	3155.2920	3156.3559
3156.9567	3160.1212	3171.5369
3173.4820	3174.5822	3175.1822
3187.3073	3396.7239	3483.9202

ZeroEnergy[kcal/mol] 4.37

ElectronicLevels[1/cm] 1

0 1

End

!-----

!-----bar_ts2-----

Barrier ts2 ip1 p2

RRHO

Geometry[angstrom] 31

C	-4.6859067457	-1.2775564516	0.402364172
C	-4.8069681752	-2.6597281679	0.3445099071
C	-3.5670159171	-3.3550363816	0.3544879899
C	-2.3806355633	-2.6353102933	0.4188898116
C	-2.3148482925	-1.2122569021	0.4770979157
C	-3.4984587494	-0.499169165	0.4682057512
C	-5.8086945856	-0.4490959981	0.4027329852
C	-7.1192761942	-0.8692793579	0.3476950432
C	-7.2664486188	-2.304186629	0.2861986088
C	-6.1680859358	-3.1462825382	0.2852112524
C	-3.9599833724	0.9291775593	0.5112766119
C	-5.3786720146	0.8777058475	0.4686592932
C	-6.2858631892	1.9290844273	0.4851814117
C	-5.6843675594	3.2153180314	0.5565163323
C	-4.304805582	3.3249406228	0.6033571927
C	-3.4071584493	2.2023565579	0.5843276199
C	-1.9929812803	2.449172536	0.6633907522
C	-0.9069099324	2.8507795304	1.0400968386
C	-8.0765920257	0.2119143227	0.3629908824
C	-7.6757377748	1.5349050978	0.4279782257

```

H -3.5351077625 -4.4387154654 0.3125999725
H -1.4449643539 -3.1835765517 0.4252638036
H -1.3478212491 -0.726355784 0.5250018423
H -8.2585315361 -2.7413898337 0.2395297119
H -6.3372631095 -4.2172775165 0.2378508408
H -6.2891147527 4.1157238229 0.575497624
H -3.8571071503 4.3099078547 0.6580109903
H 0.1039755481 3.1259736344 1.2218448368
H -9.1382503514 -0.0091242247 0.3228903352
H -8.437453376 2.3077880292 0.4368013035
H -1.531245949 1.6131403865 -0.975778859
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 779.1538
WellDepth[kcal/mol] 37.49
WellDepth[kcal/mol] 6.97
End
Frequencies[1/cm] 86
62.1073 75.6062
89.2522 134.3212 172.6670
207.0347 269.4690 289.2184
295.4984 299.2279 372.4783
427.5822 434.1198 439.7452
443.3448 462.5756 481.5368
488.9645 543.1513 550.3168
576.8460 587.7190 598.2168
619.5391 633.7163 653.7334
655.6935 659.3442 686.2559
692.5905 716.7343 768.8628
780.3771 781.0590 818.1464
824.2891 839.7775 842.2741
852.4860 889.0953 929.8960
964.3371 968.4051 969.3809
975.5708 984.7898 1039.8368
1045.8521 1074.3458 1149.4659
1161.0751 1161.2571 1187.9140
1194.7049 1214.7701 1232.6744
1241.6727 1258.1903 1292.9869
1347.8911 1377.1534 1400.9870
1419.2762 1429.1215 1450.3541
1457.4555 1485.3584 1494.0462
1514.7439 1530.6220 1614.2133
1626.7113 1652.4324 1676.1227
1701.0618 2098.5953 3157.4436
3158.4209 3162.2015 3168.7490
3174.4913 3175.7692 3178.0328
3191.8628 3193.6987 3459.1347
ZeroEnergy[kcal/mol] -1.75
ElectronicLevels[1/cm] 1
0 2
End

```

```

!-----
!-----bar_ts3-----
Barrier      ts3  ip1  ip2
RRHO
Geometry[angstrom]  31
C  -0.3096779376   -1.1994206037    0.2713243292
C  -0.3670126484   -2.5692478997    0.0891942486
C   0.9159340577   -3.1890191471   -0.0457982905
C   2.0845971111   -2.421614279    -0.0398763327
C   2.0535270752   -1.005466876    0.0921350577
C   0.8490893112   -0.3866924125    0.2515959888
C  -1.4433425434   -0.3837452844    0.2821200345
C  -2.7353732841   -0.8195547302    0.1070475742
C  -2.8377510112   -2.2588320909   -0.0157750286
C  -1.7193109533   -3.0813473364   -0.0221267273
C   0.3853221738   1.0069527228    0.2469967334
C  -1.0248479528   0.9521885874    0.2707813358
C  -1.9094848184   2.0040434392    0.1038919467
C  -1.2652323808   3.2735901837   -0.0198707238
C   0.1232801854   3.3627453145   -0.0231274473
C   1.0036131047   2.2310907805    0.0796311814
C   2.4631237504   2.3240369935   -0.0450491207
C   3.3295270526   1.3053487377   -0.0736447761
C  -3.690344668    0.2642998875   -0.004850486
C  -3.2960697085   1.5947288606   -0.0016420546
H   0.9991036986   -4.2630222017   -0.1793495745
H   3.0349793045   -2.9298328252   -0.1604596429
H  -3.8134158202   -2.7187863198   -0.1356178318
H  -1.8703719053   -4.1490032756   -0.1455537437
H  -1.8484618914   4.180698597    -0.1398430031
H   0.5723404943   4.3440150213   -0.1412613607
H   2.8710758447   3.3332485885   -0.1374146692
H   4.4054794577   1.3955894082   -0.1779505203
H  -4.7459608586   0.041028871    -0.1214910038
H  -4.061640499    2.3558236891   -0.1141106794
H   2.9434462589   -0.0105184003   0.0016955865
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  1820.8859
WellDepth[kcal/mol]  15.78
WellDepth[kcal/mol]  14.36
End
Frequencies[1/cm]  86
42.7200          113.9742
136.9297         235.8815          252.6958
291.4467         298.9567          317.6534
355.0028         360.2753          400.1507
429.4365         438.7602          489.9332
493.9989         521.9848          528.9173
544.5163         566.5394          568.7456
599.0310         611.1730          643.9910

```

651.9060	656.6127	675.4220
708.0925	727.5020	771.4467
781.8434	794.0027	820.5252
830.8701	834.1089	839.3583
848.9686	904.8487	912.8449
956.6296	959.5258	967.5251
968.2923	973.9578	1010.3571
1044.5997	1079.7634	1097.7874
1109.3115	1148.5172	1155.8397
1159.2827	1184.0935	1202.1952
1224.8448	1230.4727	1236.4996
1287.4075	1290.4998	1341.8206
1354.9486	1390.2606	1417.2077
1423.4440	1439.5883	1446.4069
1473.2914	1478.1810	1500.2849
1513.9521	1527.6342	1618.1960
1639.0223	1651.1337	1662.7295
1682.5289	1698.7836	3073.9480
3155.2732	3156.2120	3156.6835
3158.6238	3173.0014	3173.5490
3174.4827	3176.7853	3177.3352

ZeroEnergy[kcal/mol] -23.46

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts4-----

Barrier ts4 ip2 ip3

RRHO

Geometry[angstrom] 31

C	-0.3084882683	-1.2889325102	-0.2820720327
C	-0.4737030028	-2.5990791132	0.1439407628
C	0.7412444633	-3.2734488914	0.4758621562
C	1.9684606798	-2.6000795432	0.4436617169
C	2.0432251303	-1.2306532165	0.095719778
C	0.9137694279	-0.5711379292	-0.2833053417
C	-1.3756358614	-0.3803742501	-0.3888734742
C	-2.677384678	-0.6817678032	-0.0448831806
C	-2.8979631756	-2.0779065629	0.2638163348
C	-1.8550358473	-2.9842982445	0.3472631766
C	0.5668338421	0.8492805117	-0.3758572556
C	-0.8435464499	0.9235600069	-0.4382786807
C	-1.6079686883	2.0348542519	-0.1054603437
C	-0.843290329	3.2065074644	0.2051393654
C	0.5383431599	3.1488245971	0.2979664737
C	1.2976244038	1.9491418344	0.0528972099
C	2.6662494416	1.695689671	0.4529784657
C	3.3954919593	0.6190111748	-0.0283866775
C	-3.5250150514	0.4765299161	0.1204317646
C	-3.0122703581	1.7639458966	0.0957615077
H	0.7230410979	-4.3097097149	0.799362677
H	2.8638851016	-3.1428574427	0.7274883307
H	-3.90138142	-2.4206275113	0.495376933

```

H -2.0807252094 -4.0052335537 0.6385764064
H -1.3472730638 4.1358060881 0.4504190206
H 1.0733990402 4.0401314625 0.6098112216
H 3.0629634104 2.2718432344 1.2852119922
H 4.3573559685 0.3879271057 0.4133276031
H 3.2689277776 0.3036558153 -1.0554798407
H -4.5795080671 0.3425478044 0.3395612762
H -3.6836654339 2.5912024515 0.3031606543
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 450.0772
WellDepth[kcal/mol] 14.14
WellDepth[kcal/mol] 40.04
End
Frequencies[1/cm] 86
106.8055 118.3946
135.7726 242.2322 247.7512
293.3245 295.9336 348.5725
361.7083 394.2185 429.9833
434.5902 445.2367 485.2961
502.6947 531.2513 544.7529
558.2111 580.4133 591.7221
610.7864 647.4491 651.0689
656.5426 661.5900 699.2834
734.3172 760.2542 766.5777
776.4370 808.6037 819.4957
829.5518 836.8196 845.5031
848.9639 898.4892 940.2448
952.5550 963.0333 964.3781
970.2069 975.3811 1009.1587
1076.3976 1094.4256 1107.5428
1145.0674 1159.6101 1160.7245
1189.1674 1203.9822 1221.1407
1228.1279 1234.6318 1250.7841
1291.3765 1326.2812 1345.3984
1384.0601 1410.9952 1422.5375
1424.8283 1438.1524 1452.7178
1465.5748 1472.8690 1491.6327
1506.9481 1522.4348 1604.2138
1605.2679 1638.8349 1655.9602
1672.1273 3138.9977 3146.5872
3153.7710 3155.4733 3156.0176
3156.7774 3170.7344 3172.5700
3173.4737 3174.4693 3229.7936
ZeroEnergy[kcal/mol] -23.68
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts5-----
Barrier ts5 ip3 ip4

```

RRHO

```
Geometry[angstrom] 31
C -0.9327724896 0.6937206687 -0.5763998201
C -0.93905043 -0.7257157892 -0.5807457573
C 0.4002832112 -1.1761184932 -0.5767033449
C 1.2341738455 -0.045229925 -0.5544500341
C 0.4002903896 1.1182706687 -0.5871786276
C 0.8080926171 2.3543339336 -0.0555426074
C -0.3054633583 3.2250831323 0.3445671389
C -1.6116922749 2.7842678289 0.3342884257
C -1.987334264 1.4395601458 -0.0515210414
C 0.7828881538 -2.4181326848 -0.07661342
C 2.1693284953 -2.5044729133 0.2855085285
C 2.9959021779 -1.3829525918 0.3120688536
C 2.5120163258 -0.0657851324 -0.0171795194
C -1.9870499162 -1.4773780245 -0.0789088358
C -1.635118936 -2.8456215651 0.2408192614
C -0.3209037075 -3.289898514 0.243813315
C 2.2329279063 2.3836276585 0.3628710977
C 3.0496694299 1.2306913197 0.3371012516
C -3.1514528755 0.6782524309 0.2932798791
C -3.1613993589 -0.7154171838 0.2706531694
H 1.745091104 2.9217458627 -0.8588430794
H -0.0887281097 4.2183411673 0.722629403
H -2.3729829048 3.4580010267 0.7165445219
H 2.5741815747 -3.4484440136 0.6370260482
H 4.0076546059 -1.4974325412 0.6872432325
H -2.4096842731 -3.5271960229 0.5781198681
H -0.1201358421 -4.3009178247 0.5846822732
H 2.6042698142 3.2922139252 0.8236609708
H 4.0726068999 1.3294505162 0.6795843256
H -4.0313361791 1.1913462978 0.6692958865
H -4.0482236315 -1.2315783638 0.6235586367
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1702.2231
WellDepth[kcal/mol] 41.79
WellDepth[kcal/mol] 28.67
End
Frequencies[1/cm] 86
134.1833 139.5802
145.8723 272.3031 278.4618
295.9589 308.7145 399.9807
405.4272 416.9472 429.2234
435.5088 453.6517 520.3135
544.0952 548.2091 562.2039
592.1942 595.3230 606.4266
636.7159 642.9271 648.0942
656.4578 668.3438 722.7414
745.2312 755.2975 756.6842
791.1974 797.2822 807.9293
```

814.2734	836.6471	849.4163
856.6634	888.4476	933.1637
946.2120	952.0464	965.5527
967.8935	1024.2673	1071.6121
1076.5936	1086.6857	1122.6211
1147.3310	1154.4600	1161.4657
1173.0107	1198.7482	1205.8811
1215.8065	1235.7117	1251.1656
1308.4327	1323.6835	1368.4567
1374.5787	1386.3319	1409.2874
1421.1561	1426.1771	1437.7090
1447.6749	1458.9008	1464.6559
1474.1063	1487.4856	1509.9266
1580.8086	1628.1633	1630.1892
1634.0596	1645.7257	3152.1283
3152.5347	3153.5667	3154.4044
3169.9378	3171.6525	3172.0494
3172.8769	3174.1292	3187.9891

ZeroEnergy[kcal/mol] -21.93

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts6-----

Barrier ts6 ip1 ip4

RRHO

Geometry[angstrom] 31

C	-0.1156769779	-1.2548701014	-0.3909590345
C	-0.1468517433	-2.5616571175	0.080114487
C	1.1496325573	-3.125977921	0.3312122677
C	2.2992521026	-2.3942817738	0.1090933677
C	2.3079209295	-1.0139288417	-0.350384645
C	1.0311184479	-0.444371727	-0.5364082758
C	-1.2711524516	-0.4507597186	-0.4376405107
C	-2.5165510615	-0.8620704214	-0.0042456768
C	-2.5893499786	-2.2578230727	0.3579053091
C	-1.4592523155	-3.0610600118	0.399225388
C	0.5599502174	0.9297681039	-0.5255847423
C	-0.8628497106	0.8922146858	-0.5261700244
C	-1.7023995872	1.9282366221	-0.141483719
C	-1.032626623	3.1581602654	0.1565098141
C	0.3504028744	3.1925573756	0.2481762326
C	1.1812785001	2.0469998401	0.0077019474
C	2.5217110674	1.8935478471	0.5879150168
C	3.1753164476	0.7379638016	0.6955605152
C	-3.4592487461	0.2129039962	0.1950691647
C	-3.0670419172	1.5385492648	0.1306300804
H	1.2360048773	-4.1447251096	0.6962004656
H	3.2569283289	-2.8814203289	0.2580159019
H	3.1649380832	-0.7016034012	-0.935767545
H	-3.5387384836	-2.6799118221	0.6713095177
H	-1.5642173154	-4.0846644417	0.7446869158
H	-1.6022333061	4.043924208	0.4180377008


```

H 0.8240802467 4.1039420675 0.5999539682
H 2.9460157984 2.7791988234 1.070204694
H 4.1392301238 0.5313334603 1.1418493252
H -4.4828416591 -0.0148170266 0.4747755197
H -3.7961907257 2.3070884755 0.3671375741
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 523.2349
WellDepth[kcal/mol] 21.14
WellDepth[kcal/mol] 32.5
End
Frequencies[1/cm] 86
107.3366 130.0228
142.2424 234.3077 242.3975
294.7907 306.1179 336.0197
344.5219 406.6015 423.8407
440.5552 449.8043 481.9841
519.8226 540.5401 555.3725
572.4412 577.3641 589.7970
610.8627 641.4829 642.5539
656.5650 669.8074 700.5353
721.2915 753.1885 769.7112
779.0403 797.9341 806.1296
818.3187 824.3848 838.3596
845.6569 885.0195 896.2980
953.4575 957.0969 959.3288
966.6378 972.5474 975.2797
1038.2954 1070.9616 1086.2514
1142.3968 1157.7210 1158.8744
1178.0659 1190.9583 1202.9027
1222.7255 1229.5722 1249.3374
1267.4048 1296.2386 1338.8508
1372.3610 1392.5754 1425.3542
1426.9070 1442.3734 1445.4116
1467.2620 1477.9431 1479.4777
1510.2039 1542.5618 1588.8263
1620.1821 1639.8309 1651.7222
1668.1283 3050.5258 3145.4647
3154.1904 3154.9675 3155.9783
3157.1683 3171.9865 3173.1717
3173.8924 3176.4733 3205.9862
ZeroEnergy[kcal/mol] -18.10
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts7-----
Barrier ts7 ip3 p1
RRHO
Geometry[angstrom] 31
C -0.0427572618 -1.254375079 0.7209000952

```

C -0.1673515684 -2.5135611885 0.1633120559
 C 1.0839450053 -3.1196960624 -0.2296765552
 C 2.2748584359 -2.4091124907 -0.2312964073
 C 2.335892159 -1.0217892086 0.1606702726
 C 1.1725539311 -0.5293963718 0.7177022977
 C -1.1081311965 -0.3228470724 0.7615606643
 C -2.3618725891 -0.5949024598 0.2468824653
 C -2.5653742244 -1.9743872599 -0.1362060128
 C -1.5228884219 -2.8860093291 -0.1760201131
 C 0.8577490458 0.852053783 0.7531673563
 C -0.5513391057 0.9789673352 0.781373754
 C -1.2162900113 2.0860667003 0.286229892
 C -0.3562342661 3.1950474397 -0.0630655176
 C 1.0226875273 3.0714125961 -0.093991515
 C 1.6872865085 1.8255946997 0.2232897213
 C 2.9883002213 1.3540602281 -0.1726221924
 C 3.3199101622 -0.0045657063 -0.1684912576
 C -3.1469928895 0.5774097258 -0.068221935
 C -2.6022867783 1.8517143494 -0.0496320368
 H 1.0865220921 -4.1323259821 -0.6202633528
 H 3.1649686403 -2.8930194844 -0.6203729127
 H -3.5417407616 -2.2902698085 -0.4897862224
 H -1.7215860411 -3.8818139673 -0.5593176817
 H -0.7992215 4.1274223398 -0.3984776953
 H 1.609765176 3.9109485189 -0.4523258123
 H 3.720528227 2.058060783 -0.5543048006
 H 4.4830815373 -0.095568412 1.5434637144
 H 4.2524795229 -0.3024074288 -0.6346554857
 H -4.1676694368 0.4568840836 -0.4171723141
 H -3.2165281395 2.6811467291 -0.3854624685

Core RigidRotor

SymmetryFactor 1

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 512.2347

WellDepth[kcal/mol] 33.12

WellDepth[kcal/mol] 3.71

End

Frequencies[1/cm] 86

135.7440	139.2672	
145.9976	228.3604	257.5094
286.5616	298.8591	311.3916
325.5355	411.0917	413.0531
439.6820	440.2201	455.5457
461.6903	543.4752	549.2677
549.8298	564.0122	605.1287
614.1759	616.3114	647.2589
650.2723	651.1643	671.7447
679.6134	759.6512	761.1893
767.6500	778.2802	811.9691
814.1896	831.8229	838.6109
857.6608	865.8447	866.8437
939.0251	962.9853	968.9548

970.9683	978.4298	978.8506
1047.3508	1087.4228	1089.7064
1150.2294	1161.7320	1162.2469
1162.5716	1183.7731	1186.4510
1212.7027	1213.7083	1237.3144
1257.9972	1332.6875	1334.7137
1370.3729	1377.0053	1423.7343
1425.5059	1433.6296	1442.0825
1460.2407	1468.9350	1470.1147
1480.2990	1484.3052	1511.1683
1642.4891	1649.6122	1653.3601
1653.9396	1654.7517	3155.3288
3156.0311	3156.5265	3157.0748
3162.0349	3172.4963	3173.1464
3173.9059	3174.4776	3178.6831

ZeroEnergy[kcal/mol] -30.60

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts8-----

Barrier ts8 ip4 p1

RRHO

Geometry[angstrom] 31

C	-0.2163584248	-1.0823125004	-0.5384030973
C	-0.2910799973	-2.4456661106	-0.3126409973
C	0.9921670461	-3.1049261746	-0.1800003056
C	2.1751407582	-2.4020226922	-0.1094292999
C	2.2301656543	-0.943238925	-0.2033985137
C	0.9923679841	-0.3504368687	-0.4558324323
C	-1.2846672194	-0.2032566023	-0.2325412693
C	-2.488003203	-0.6354432852	0.2960673022
C	-2.6534089906	-2.0698037761	0.3195472001
C	-1.6045905861	-2.9305500256	0.0344883171
C	0.6734247716	0.9742139127	-0.0722242385
C	-0.7345429213	1.068284099	0.0558385362
C	-1.3558347043	1.9809448362	0.8897102739
C	-0.4728627393	2.9694955647	1.4627790588
C	0.9054201369	2.8701536389	1.3502056412
C	1.5380120025	1.7816468263	0.6459479507
C	2.8729706075	1.2418692611	0.8056786152
C	3.1960527941	-0.0425387931	0.4257082913
C	-3.247035406	0.3880612947	0.9779090419
C	-2.7085825692	1.6324768255	1.2602567481
H	1.0233665314	-4.1810077559	-0.0410754603
H	3.0966682822	-2.94704037	0.065525132
H	-3.5925900556	-2.4931375459	0.6611531789
H	-1.7600971578	-3.996655338	0.1658488018
H	-0.8864612265	3.7605698144	2.0801006905
H	1.5210812351	3.5857906484	1.8857946726
H	3.6244462577	1.8307040033	1.322187532
H	4.1920250055	-0.4154612751	0.639762863
H	-4.2337142496	0.1514543959	1.3633177296

```

H -3.2927954531  2.326024594  1.8566969895
H  3.0695858367 -0.9326466764 -1.8509509527
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  833.1154
WellDepth[kcal/mol]  23.30
WellDepth[kcal/mol]  7.01
End
Frequencies[1/cm]  86
134.6871          138.1827
151.9417          272.6961          274.6460
305.9513          313.4044          354.8957
380.0012          416.7398          424.4424
439.8516          440.9156          458.9928
464.5369          541.2958          548.6619
549.6552          565.2039          603.3629
613.4672          615.9062          647.7643
651.4451          654.4067          672.8536
673.6251          759.2300          759.6339
767.2897          769.1926          812.8302
813.0605          831.4939          833.2502
852.8869          860.0860          864.3764
937.3613          961.7703          968.0075
972.5513          977.9871          981.8301
1046.5504         1084.3464         1086.1962
1161.0170         1161.4222         1163.0715
1165.5718         1176.8677         1186.6374
1208.0603         1215.6422         1236.7251
1259.5227         1328.0162         1333.4287
1375.9562         1381.7998         1422.0491
1424.6587         1439.1219         1448.2785
1460.1112         1467.9577         1473.8533
1479.0491         1487.6803         1507.2128
1623.2601         1644.3829         1650.0380
1650.2898         1651.7920         3155.4070
3156.1324         3156.3700         3157.2142
3157.4664         3172.5809         3173.2580
3174.0933         3175.5448         3176.8977
ZeroEnergy[kcal/mol] -27.3
ElectronicLevels[1/cm] 1
0 2
End
!-----
End

```

5.4. Output file of RRKM-ME calculations for the benzo[ghi]fluoranthene-5-yl + C₂H₂ reaction using MESS package

Wells (G - ground energy, D - dissociation limit, kcal/mol):

Name	G	D
------	---	---

ip1	-39.2	-23.5
ip2	-37.8	-23.7
ip3	-63.7	-30.6
ip4	-50.6	-27.3

Bimolecular Products (G - ground energy, kcal/mol):

Name	G
p0	0.0
p1	-34.3
p2	-8.7

Well-to-Bimolecular Barriers (H/G - barrier height/well depth, kcal/mol)

Name	H	Well	G	Product
ts1	4.4	ip1	-39.2	p0
ts2	-1.8	ip1	-39.2	p2
ts7	-30.6	ip3	-63.7	p1
ts8	-27.3	ip4	-50.6	p1

Well-to-Well Barriers (H/G - barrier height/well depth, kcal/mol):

Name	H	Well	G1	Well	G2
ts3	-23.5	ip1	-39.2	ip2	-37.8
ts4	-23.7	ip2	-37.8	ip3	-63.7
ts5	-21.9	ip3	-63.7	ip4	-50.6
ts6	-18.1	ip1	-39.2	ip4	-50.6

Unimolecular Rate Units: 1/sec; Bimolecular Rate Units: cm³/sec

High Pressure Rate Coefficients (Temperature-Species Rate Tables):

T(K)	ip1->ip1	ip1->ip2	ip1->ip3	ip1->ip4	ip1->p0	ip1->p1	ip1->p2
300	***	1061.73	***	0.000647328	5.93246e-18	***	1.88612e-14
400	***	75683.9	***	3.77823	8.73319e-10	***	1.56881e-07
500	***	1.73385e+06	***	699.691	7.45903e-05	***	0.00257383
600	***	1.67985e+07	***	22962.9	0.149536	***	1.79185
700	***	9.17919e+07	***	279757	34.6777	***	200.89
800	***	3.413e+08	***	1.83229e+06	2074.61	***	7116.42
900	***	9.70594e+08	***	7.92766e+06	50113.7	***	116219
1000	***	2.27473e+09	***	2.56452e+07	640327	***	1.09954e+06
1125	***	5.40981e+09	***	8.31365e+07	8.16932e+06	***	1.05304e+07
1250	***	1.09407e+10	***	2.13376e+08	6.24785e+07	***	6.47899e+07

1375	***	1.96206e+10	***	4.61942e+08	3.29179e+08	***	2.88372e+08
1500	***	3.21048e+10	***	8.80031e+08	1.3112e+09	***	1.00547e+09
1650	***	5.28179e+10	***	1.6779e+09	5.20549e+09	***	3.52136e+09
1750	***	7.03765e+10	***	2.4271e+09	1.14238e+10	***	7.22192e+09
1800	***	8.03213e+10	***	2.87481e+09	1.63694e+10	***	1.00426e+10
2000	***	1.27977e+11	***	5.20171e+09	5.74707e+10	***	3.1925e+10
2250	***	2.04956e+11	***	9.41935e+09	2.00585e+11	***	1.01899e+11
2500	***	2.99876e+11	***	1.51555e+10	5.4227e+11	***	2.58639e+11

T(K)	ip2->ip1	ip2->ip2	ip2->ip3	ip2->ip4	ip2->p0	ip2->p1	ip2->p2
300	10337.1	***	74.4086	***	***	***	***
400	414694	***	24066.8	***	***	***	***
500	6.8329e+06	***	784638	***	***	***	***
600	5.36821e+07	***	8.09306e+06	***	***	***	***
700	2.54179e+08	***	4.31569e+07	***	***	***	***
800	8.52349e+08	***	1.52163e+08	***	***	***	***
900	2.24308e+09	***	4.06789e+08	***	***	***	***
1000	4.95031e+09	***	8.95378e+08	***	***	***	***
1125	1.11065e+10	***	1.97515e+09	***	***	***	***
1250	2.14685e+10	***	3.72571e+09	***	***	***	***
1375	3.71384e+10	***	6.26931e+09	***	***	***	***
1500	5.90132e+10	***	9.68118e+09	***	***	***	***
1650	9.43441e+10	***	1.49617e+10	***	***	***	***
1750	1.23703e+11	***	1.91941e+10	***	***	***	***
1800	1.40158e+11	***	2.15175e+10	***	***	***	***
2000	2.17771e+11	***	3.21125e+10	***	***	***	***
2250	3.40307e+11	***	4.79584e+10	***	***	***	***
2500	4.88447e+11	***	6.61368e+10	***	***	***	***

T(K)	ip3->ip1	ip3->ip2	ip3->ip3	ip3->ip4	ip3->p0	ip3->p1	ip3->p2
300	***	7.37211e-17	***	5.77106e-16	***	3.34641e-12	***
400	***	1.84811e-09	***	6.8068e-10	***	4.83155e-06	***
500	***	5.40208e-05	***	1.08279e-05	***	0.0263612	***
600	***	0.0528449	***	0.00900794	***	8.62777	***
700	***	7.34847	***	1.20765	***	558.662	***
800	***	300.38	***	49.8521	***	13045.5	***
900	***	5413.13	***	924.959	***	153646	***
1000	***	54894.9	***	9736.14	***	1.11742e+06	***
1125	***	558255	***	104120	***	8.21636e+06	***
1250	***	3.5766e+06	***	701431	***	4.08877e+07	***
1375	***	1.6365e+07	***	3.36764e+06	***	1.52917e+08	***
1500	***	5.81521e+07	***	1.252e+07	***	4.61081e+08	***
1650	***	2.06744e+08	***	4.67971e+07	***	1.39619e+09	***
1750	***	4.26872e+08	***	9.96545e+07	***	2.63484e+09	***
1800	***	5.95152e+08	***	1.41001e+08	***	3.52681e+09	***
2000	***	1.90484e+09	***	4.7653e+08	***	9.80976e+09	***

2250	***	6.09784e+09	***	1.61831e+09	***	2.73944e+10	***
2500	***	1.54694e+10	***	4.31899e+09	***	6.24801e+10	***

T(K)	ip4->ip1	ip4->ip2	ip4->ip3	ip4->ip4	ip4->p0	ip4->p1	ip4->p2
300	5.30278e-11	***	4.90096e-06	***	***	0.000127445	***
400	5.73653e-05	***	0.0245624	***	***	2.34611	***
500	0.259177	***	14.7826	***	***	966.868	***
600	73.6768	***	1385.1	***	***	57132	***
700	4258.21	***	38985.6	***	***	1.09334e+06	***
800	90349.5	***	498623	***	***	1.02494e+07	***
900	979399	***	3.71578e+06	***	***	5.93969e+07	***
1000	6.62139e+06	***	1.88409e+07	***	***	2.45015e+08	***
1125	4.49398e+07	***	9.69943e+07	***	***	1.02204e+09	***
1250	2.08516e+08	***	3.63883e+08	***	***	3.23194e+09	***
1375	7.33152e+08	***	1.08174e+09	***	***	8.34109e+09	***
1500	2.09271e+09	***	2.6965e+09	***	***	1.84626e+10	***
1650	5.97899e+09	***	6.75605e+09	***	***	4.10398e+10	***
1750	1.08974e+10	***	1.14459e+10	***	***	6.49077e+10	***
1800	1.43498e+10	***	1.45827e+10	***	***	8.01234e+10	***
2000	3.76157e+10	***	3.41399e+10	***	***	1.67864e+11	***
2250	9.8665e+10	***	8.02938e+10	***	***	3.53079e+11	***
2500	2.1349e+11	***	1.59692e+11	***	***	6.41912e+11	***

T(K)	p0->ip1	p0->ip2	p0->ip3	p0->ip4	p0->p0	p0->p1	p0->p2
300	4.41869e-16	***	***	***	***	***	***
400	4.39123e-15	***	***	***	***	***	***
500	1.9549e-14	***	***	***	***	***	***
600	5.69914e-14	***	***	***	***	***	***
700	1.28933e-13	***	***	***	***	***	***
800	2.47195e-13	***	***	***	***	***	***
900	4.22487e-13	***	***	***	***	***	***
1000	6.64187e-13	***	***	***	***	***	***
1125	1.07187e-12	***	***	***	***	***	***
1250	1.60904e-12	***	***	***	***	***	***
1375	2.28646e-12	***	***	***	***	***	***
1500	3.11296e-12	***	***	***	***	***	***
1650	4.3116e-12	***	***	***	***	***	***
1750	5.24078e-12	***	***	***	***	***	***
1800	5.74535e-12	***	***	***	***	***	***
2000	8.03651e-12	***	***	***	***	***	***
2250	1.15307e-11	***	***	***	***	***	***
2500	1.57451e-11	***	***	***	***	***	***

T(K)	p1->ip1	p1->ip2	p1->ip3	p1->ip4	p1->p0	p1->p1	p1->p2
300	***	***	1.7083e-13	7.66095e-16	***	***	***
400	***	***	8.6206e-13	1.16004e-14	***	***	***

500	***	***	2.47599e-12	6.6519e-14	***	***	***
600	***	***	5.27914e-12	2.27347e-13	***	***	***
700	***	***	9.41436e-12	5.7073e-13	***	***	***
800	***	***	1.49396e-11	1.17352e-12	***	***	***
900	***	***	2.18614e-11	2.10375e-12	***	***	***
1000	***	***	3.01569e-11	3.41702e-12	***	***	***
1125	***	***	4.23988e-11	5.66146e-12	***	***	***
1250	***	***	5.6637e-11	8.62967e-12	***	***	***
1375	***	***	7.27772e-11	1.23585e-11	***	***	***
1500	***	***	9.0727e-11	1.68678e-11	***	***	***
1650	***	***	1.14533e-10	2.33195e-11	***	***	***
1750	***	***	1.31713e-10	2.82501e-11	***	***	***
1800	***	***	1.40682e-10	3.0903e-11	***	***	***
2000	***	***	1.78977e-10	4.27489e-11	***	***	***
2250	***	***	2.31999e-10	6.02666e-11	***	***	***
2500	***	***	2.90346e-10	8.06765e-11	***	***	***

T(K)	p2->ip1	p2->ip2	p2->ip3	p2->ip4	p2->p0	p2->p1	p2->p2
300	4.39189e-16	***	***	***	***	***	***
400	7.07967e-15	***	***	***	***	***	***
500	4.1744e-14	***	***	***	***	***	***
600	1.44791e-13	***	***	***	***	***	***
700	3.66657e-13	***	***	***	***	***	***
800	7.5813e-13	***	***	***	***	***	***
900	1.36433e-12	***	***	***	***	***	***
1000	2.22228e-12	***	***	***	***	***	***
1125	3.69173e-12	***	***	***	***	***	***
1250	5.63868e-12	***	***	***	***	***	***
1375	8.08831e-12	***	***	***	***	***	***
1500	1.10546e-11	***	***	***	***	***	***
1650	1.5304e-11	***	***	***	***	***	***
1750	1.85547e-11	***	***	***	***	***	***
1800	2.03047e-11	***	***	***	***	***	***
2000	2.81253e-11	***	***	***	***	***	***
2250	3.97051e-11	***	***	***	***	***	***
2500	5.32129e-11	***	***	***	***	***	***

Capture/Escape Rate Coefficients:

T(K)	ip1	ip2	ip3	ip4	p0	p1	p2
300	1061.73	10411.5	3.34706e-12	0.000132346	4.41869e-16	1.71596e-13	4.39189e-16
400	75687.6	438761	4.83408e-06	2.37073	4.39123e-15	8.7366e-13	7.07967e-15
500	1.73455e+06	7.61754e+06	0.0264261	981.91	1.9549e-14	2.54251e-12	4.1744e-14

600	1.68215e+07	6.17752e+07	8.68963	58590.8	5.69914e-14	5.50649e-12	
1.44791e-13	700	9.20719e+07	2.97335e+08	567.218	1.13658e+06	1.28933e-13	9.98509e-12
3.66657e-13	800	3.43141e+08	1.00451e+09	13395.7	1.08384e+07	2.47195e-13	1.61132e-11
7.5813e-13	900	9.78688e+08	2.64987e+09	159984	6.40921e+07	4.22487e-13	2.39651e-11
1.36433e-12	1000	2.30211e+09	5.84568e+09	1.18205e+06	2.70477e+08	6.64187e-13	3.35739e-11
2.22228e-12	1125	5.51165e+09	1.30816e+10	8.87873e+06	1.16397e+09	1.07187e-12	4.80602e-11
3.69173e-12	1250	1.12814e+10	2.51942e+10	4.51658e+07	3.80434e+09	1.60904e-12	6.52667e-11
5.63868e-12	1375	2.07e+10	4.34077e+10	1.7265e+08	1.0156e+10	2.28646e-12	8.51357e-11
8.08831e-12	1500	3.53015e+10	6.86944e+10	5.31753e+08	2.32518e+10	3.11296e-12	1.07595e-10
1.10546e-11	1650	6.32226e+10	1.09306e+11	1.64973e+09	5.37748e+10	4.3116e-12	1.37853e-10
1.5304e-11	1750	9.14493e+10	1.42897e+11	3.16137e+09	8.7251e+10	5.24078e-12	1.59964e-10
1.85547e-11	1800	1.09608e+11	1.61675e+11	4.26296e+09	1.09056e+11	5.74535e-12	1.71585e-10
2.03047e-11	2000	2.22575e+11	2.49884e+11	1.21911e+10	2.3962e+11	8.03651e-12	2.21726e-10
2.81253e-11	2250	5.16859e+11	3.88265e+11	3.51105e+10	5.32038e+11	1.15307e-11	2.92265e-10
3.97051e-11	2500	1.11594e+12	5.54583e+11	8.22685e+10	1.01509e+12	1.57451e-11	3.71023e-10
5.32129e-11							

Temperature-Species Rate Tables:

Pressure = 0.0394737 atm

T(K)	ip1->ip2	ip1->ip3	ip1->ip4	ip1->p0	ip1->p1	ip1->p2	ip1->
Capture							
300	996.647	0.158795	0.000635654	3.75767e-18	2.72415e-07	1.43657e-14	
996.79	1061.73						
400	64887.6	700.586	3.33809	3.52918e-10	0.027736	8.99123e-08	65591.5
75687.6							
500	814284	73432.9	455.614	1.0757e-05	37.0688	0.000703534	888209
1.73455e+06							

600	***	1.2505e+06	7454.2	0.00490259	3555.73	0.147785	1.26151e+06
1.68215e+07							
700	***	4.75179e+06	27196.6	0.212402	70424.5	3.83964	4.84941e+06
9.20719e+07							
800	***	***	***	***	***	***	*** 3.43141e+08
900	***	***	***	***	***	***	*** 9.78688e+08
1000	***	***	***	***	***	***	*** 2.30211e+09
1125	***	***	***	***	***	***	*** 5.51165e+09
1250	***	***	***	***	***	***	*** 1.12814e+10
1375	***	***	***	***	***	***	*** 2.07e+10
1500	***	***	***	***	***	***	*** 3.53015e+10
1650	***	***	***	***	***	***	*** 6.32226e+10
1750	***	***	***	***	***	***	*** 9.14493e+10
1800	***	***	***	***	***	***	*** 1.09608e+11
2000	***	***	***	***	***	***	*** 2.22575e+11
2250	***	***	***	***	***	***	*** 5.16859e+11
2500	***	***	***	***	***	***	*** 1.11594e+12

Pressure = 1 atm

T(K)	ip1->ip2	ip1->ip3	ip1->ip4	ip1->p0	ip1->p1	ip1->p2	ip1->
Capture							
300	1000.95	0.328409	0.000649134	5.49541e-18	8.35154e-09	1.83781e-14	
1000.96	1061.73						
400	74459.5	48.0151	3.75537	7.29896e-10	0.000984263	1.42451e-07	74511.3
75687.6							
500	1.56564e+06	14926.5	661.023	5.29318e-05	2.44223	0.00202017	
1.58123e+06	1.73455e+06						
600	1.13997e+07	536724	18760	0.0811642	611.553	1.11652	1.19558e+07
1.68215e+07							
700	3.97183e+07	4.76441e+06	166419	11.2105	27704.7	81.5364	4.46769e+07
9.20719e+07							
800	***	3.13876e+07	602407	392.001	477018	1827.37	3.24692e+07
3.43141e+08							
900	***	7.19827e+07	1.21427e+06	4642.8	3.7018e+06	16011.3	7.69195e+07
9.78688e+08							
1000	***	***	***	***	***	***	*** 2.30211e+09
1125	***	***	***	***	***	***	*** 5.51165e+09
1250	***	***	***	***	***	***	*** 1.12814e+10
1375	***	***	***	***	***	***	*** 2.07e+10
1500	***	***	***	***	***	***	*** 3.53015e+10
1650	***	***	***	***	***	***	*** 6.32226e+10
1750	***	***	***	***	***	***	*** 9.14493e+10
1800	***	***	***	***	***	***	*** 1.09608e+11
2000	***	***	***	***	***	***	*** 2.22575e+11
2250	***	***	***	***	***	***	*** 5.16859e+11

2500 *** *** *** *** *** *** *** 1.11594e+12

Pressure = 10 atm

T(K)	ip1->ip2	ip1->ip3	ip1->ip4	ip1->p0	ip1->p1	ip1->p2	ip1->
300	1001.12	-0.472371	0.000649719	5.84158e-18	8.23923e-10	1.88433e-14	
400	75038.3	4.99801	3.78912	8.4476e-10	9.65279e-05	1.55214e-07	75047.1
500	1.70043e+06	1935.18	696.879	6.84636e-05	0.249824	0.00245748	
600	1.5584e+07	116073	22181.9	0.123705	74.9668	1.57128	1.57223e+07
700	7.34331e+07	1.90316e+06	248858	24.7968	5404.5	154.157	7.55907e+07
800	2.15191e+08	1.26055e+07	1.37416e+06	1216.97	132411	4557.44	
900	***	1.0397e+08	3.88828e+06	23809	1.50369e+06	60527.1	1.09446e+08
1000	***	2.21695e+08	8.4014e+06	230040	9.12525e+06	449290	
1125	***	4.32514e+08	1.4924e+07	1.95854e+06	5.49509e+07	3.0077e+06	
1250	***	5.47851e+08	***	1.01172e+07	4.0558e+08	1.29523e+07	
1375	***	***	***	***	***	***	2.07e+10
1500	***	***	***	***	***	***	3.53015e+10
1650	***	***	***	***	***	***	6.32226e+10
1750	***	***	***	***	***	***	9.14493e+10
1800	***	***	***	***	***	***	1.09608e+11
2000	***	***	***	***	***	***	2.22575e+11
2250	***	***	***	***	***	***	5.16859e+11
2500	***	***	***	***	***	***	1.11594e+12

Pressure = 100 atm

T(K)	ip1->ip2	ip1->ip3	ip1->ip4	ip1->p0	ip1->p1	ip1->p2	ip1->
300	1001.14	5.98673e-05	0.000649778	5.88391e-18	8.22811e-11	1.88944e-14	
400	75098.4	0.0338345	3.79275	8.65263e-10	9.63149e-06	1.57052e-07	75102.7
500	1.71801e+06	200.667	701.947	7.34523e-05	0.0250587	0.00256643	

600	1.65343e+07	13704	22954.1	0.144532	7.78174	1.76284	1.6571e+07
1.68215e+07							
700	8.83119e+07	300244	276075	32.1526	618.112	191.246	8.88891e+07
9.20719e+07							
800	3.11219e+08	2.96062e+06	1.74868e+06		1794.94	18787.3	6385.66
3.15955e+08	3.43141e+08						
900	8.07426e+08	1.62188e+07	7.05279e+06		39567.1	276004	96007.4
8.31109e+08	9.78688e+08						
1000	1.67207e+09	5.75275e+07	2.00633e+07		452086	2.2253e+06	819149
1.75315e+09	2.30211e+09						
1125	3.32581e+09	1.82386e+08	4.96842e+07	4.30682e+06	-1.44741e+06		6.07011e+06
3.56681e+09	5.51165e+09						
1250	***	1.0596e+09	7.6753e+07	3.09676e+07	7.71301e+07		3.39891e+07
1.27844e+09	1.12814e+10						
1375	***	1.65338e+09	1.17956e+08	1.31393e+08	2.54033e+08		1.24844e+08
2.28161e+09	2.07e+10						
1500	***	2.20091e+09	***	3.98678e+08	8.98602e+08		3.40822e+08
3.72567e+09	3.53015e+10						
1650	***	***	***	***	***	***	6.32226e+10
1750	***	***	***	***	***	***	9.14493e+10
1800	***	***	***	***	***	***	1.09608e+11
2000	***	***	***	***	***	***	2.22575e+11
2250	***	***	***	***	***	***	5.16859e+11
2500	***	***	***	***	***	***	1.11594e+12

Pressure = 0.0394737 atm

T(K)	ip2->ip1	ip2->ip3	ip2->ip4	ip2->p0	ip2->p1	ip2->p2	ip2->
Capture							
300	9703.46	72.7593	0.000133728	1.10745e-17	7.11327e-06	3.43647e-14	
9776.38	10411.5						
400	355548	19737	2.07824	5.9976e-10	0.0802366	1.47762e-07	375287
438761							
500	3.21051e+06	404471	448.064	1.53674e-05		57.2537	0.000986803
3.61548e+06	7.61754e+06						
600	***	***	***	***	***	***	6.17752e+07
700	***	***	***	***	***	***	2.97335e+08
800	***	***	***	***	***	***	1.00451e+09
900	***	***	***	***	***	***	2.64987e+09
1000	***	***	***	***	***	***	5.84568e+09
1125	***	***	***	***	***	***	1.30816e+10
1250	***	***	***	***	***	***	2.51942e+10
1375	***	***	***	***	***	***	4.34077e+10
1500	***	***	***	***	***	***	6.86944e+10
1650	***	***	***	***	***	***	1.09306e+11
1750	***	***	***	***	***	***	1.42897e+11

1800	***	***	***	***	***	***	***	1.61675e+11
2000	***	***	***	***	***	***	***	2.49884e+11
2250	***	***	***	***	***	***	***	3.88265e+11
2500	***	***	***	***	***	***	***	5.54583e+11

Pressure = 1 atm

T(K)	ip2->ip1	ip2->ip3	ip2->ip4	ip2->p0	ip2->p1	ip2->p2	ip2->
Capture							
300	9745.38	71.1645	6.25031e-06	3.72388e-18	3.07257e-07	5.02264e-15	9819.7
10411.5							
400	407986	23765.1	0.199916	6.80278e-10	0.00467644	7.67237e-08	431751
438761							
500	6.17008e+06	715933	145.332	5.96325e-05	4.21989	0.00178132	
6.88616e+06	7.61754e+06						
600	3.64331e+07	5.96339e+06	9301.77	0.0949668	760.703	1.19482	
4.24065e+07	6.17752e+07						
700	1.09622e+08	2.43816e+07	124477	16.0765	43927.1	109.26	1.34172e+08
2.97335e+08							
800	***	***	***	***	***	***	*** 1.00451e+09
900	***	***	***	***	***	***	*** 2.64987e+09
1000	***	***	***	***	***	***	*** 5.84568e+09
1125	***	***	***	***	***	***	*** 1.30816e+10
1250	***	***	***	***	***	***	*** 2.51942e+10
1375	***	***	***	***	***	***	*** 4.34077e+10
1500	***	***	***	***	***	***	*** 6.86944e+10
1650	***	***	***	***	***	***	*** 1.09306e+11
1750	***	***	***	***	***	***	*** 1.42897e+11
1800	***	***	***	***	***	***	*** 1.61675e+11
2000	***	***	***	***	***	***	*** 2.49884e+11
2250	***	***	***	***	***	***	*** 3.88265e+11
2500	***	***	***	***	***	***	*** 5.54583e+11

Pressure = 10 atm

T(K)	ip2->ip1	ip2->ip3	ip2->ip4	ip2->p0	ip2->p1	ip2->p2	ip2->
Capture							
300	9746.99	79.0142	6.30553e-07	4.57063e-19	3.08484e-08	5.52244e-16	9821.37
10411.5							
400	411157	24027.7	0.0215522	1.24224e-10	0.000482801	1.11568e-08	435185
438761							
500	6.7012e+06	775552	21.1182	2.15494e-05	0.448036	0.000472732	
7.47677e+06	7.61754e+06						
600	4.98012e+07	7.65127e+06	2459.09	0.0710488	82.0029	0.660999	
5.7455e+07	6.17752e+07						

700	2.03336e+08	3.67152e+07	64710.8	20.2552	5232.67	105.091	2.40122e+08
2.97335e+08	800	5.36889e+08	1.116e+08	595311	1241.45	144458	4164.17 6.49234e+08
1.00451e+09	900	***	***	***	***	***	*** 2.64987e+09
1000	***	***	***	***	***	***	*** 5.84568e+09
1125	***	***	***	***	***	***	*** 1.30816e+10
1250	***	***	***	***	***	***	*** 2.51942e+10
1375	***	***	***	***	***	***	*** 4.34077e+10
1500	***	***	***	***	***	***	*** 6.86944e+10
1650	***	***	***	***	***	***	*** 1.09306e+11
1750	***	***	***	***	***	***	*** 1.42897e+11
1800	***	***	***	***	***	***	*** 1.61675e+11
2000	***	***	***	***	***	***	*** 2.49884e+11
2250	***	***	***	***	***	***	*** 3.88265e+11
2500	***	***	***	***	***	***	*** 5.54583e+11

Pressure = 100 atm

T(K)	ip2->ip1	ip2->ip3	ip2->ip4	ip2->p0	ip2->p1	ip2->p2	ip2->
Capture							
300	9747.15	74.385	6.30397e-08	4.67502e-20	3.08605e-09	5.57824e-17	9821.54
10411.5	400	411486	24057.8	0.00217313	1.35053e-11	4.8446e-05	1.17047e-09 435541
438761	500	6.77047e+06	783438	2.23049	2.80172e-06	0.0450053	5.66337e-05
7.55391e+06	7.61754e+06	600	5.28379e+07	8.03864e+06	306.964	0.0133174	7.90481 0.108066
6.08768e+07	6.17752e+07	700	2.44542e+08	4.21538e+07	11446.1	6.28386	475.376 27.5071 2.86708e+08
2.97335e+08	800	7.77211e+08	1.4324e+08	168527	621.903	13554.2	1754.59 9.20636e+08
1.00451e+09	900	1.86564e+09	3.60981e+08	1.23649e+06	20505.2	213866	41729.7
2.22813e+09	2.64987e+09	1000	3.63493e+09	7.38193e+08	5.40669e+06	314614	2.10289e+06 497065
4.38145e+09	5.84568e+09	1125	6.7586e+09	1.47234e+09	2.05492e+07	5.71051e+06	5.88766e+07 6.94301e+06
8.32302e+09	1.30816e+10	1250	***	***	***	***	*** 2.51942e+10
1375	***	***	***	***	***	***	*** 4.34077e+10
1500	***	***	***	***	***	***	*** 6.86944e+10
1650	***	***	***	***	***	***	*** 1.09306e+11
1750	***	***	***	***	***	***	*** 1.42897e+11
1800	***	***	***	***	***	***	*** 1.61675e+11
2000	***	***	***	***	***	***	*** 2.49884e+11

2250	***	***	***	***	***	***	***	3.88265e+11
2500	***	***	***	***	***	***	***	5.54583e+11

Pressure = 0.0394737 atm

T(K)	ip3->ip1	ip3->ip2	ip3->ip4	ip3->p0	ip3->p1	ip3->p2	ip3->
Capture							
300	1.36608e-18	7.22537e-17	4.78292e-16	9.45179e-36	3.34255e-12	9.58825e-33	
	3.3431e-12	3.34706e-12					
400	2.93989e-10	1.51642e-09	6.80184e-10	1.66822e-22	4.82447e-06	1.67262e-20	
	4.82696e-06	4.83408e-06					
500	1.98184e-05	2.79526e-05	1.05845e-05	1.53922e-14	0.026316	4.27753e-13	
	0.0263744	0.0264261					
600	0.0342565	***	0.00729309	2.57243e-09	8.60606	3.05916e-08	8.64761
	8.68963						
700	3.04884	***	0.54829	1.04076e-05	551.889	6.90997e-05	555.486
	567.218						
800	***	***	9.83297	0.00348209	12050.1	0.0160372	12060
	13395.7						
900	***	***	***	0.188335	112802	0.678936	112802
							159984
1000	***	***	***	2.84512	528481	8.66914	528480
	1.18205e+06						
1125	***	***	***	28.0954	1.88325e+06	73.4743	1.88267e+06
	8.87873e+06						
1250	***	***	***	***	***	***	***
							4.51658e+07
1375	***	***	***	***	***	***	***
							1.7265e+08
1500	***	***	***	***	***	***	***
							5.31753e+08
1650	***	***	***	***	***	***	***
							1.64973e+09
1750	***	***	***	***	***	***	***
							3.16137e+09
1800	***	***	***	***	***	***	***
							4.26296e+09
2000	***	***	***	***	***	***	***
							1.21911e+10
2250	***	***	***	***	***	***	***
							3.51105e+10
2500	***	***	***	***	***	***	***
							8.22685e+10

Pressure = 1 atm

T(K)	ip3->ip1	ip3->ip2	ip3->ip4	ip3->p0	ip3->p1	ip3->p2	ip3->
Capture							
300	5.75745e-20	7.36374e-17	4.78293e-16	9.73744e-38	3.34255e-12	5.38408e-35	
	3.3431e-12	3.34706e-12					
400	2.02147e-11	1.82495e-09	6.80716e-10	5.51147e-24	4.82448e-06	3.2611e-22	
	4.827e-06	4.83408e-06					
500	4.04311e-06	4.92973e-05	1.08222e-05	1.5916e-15	0.0263166	2.83974e-14	
	0.0263808	0.0264261					
600	0.0111746	0.038964	0.00888967	7.51973e-10	8.61156	6.12079e-09	8.67058
	8.68963						

700	2.30424	4.09405	1.09838	7.61273e-06	557.389	3.54447e-05	564.886
567.218							
800	216.707	***	34.9568	0.00637428	12976.7	0.0198091	13228.4
13395.7							
900	3185.93	***	413.873	0.933328	149918	2.15351	153521
159984							
1000	***	***	***	42.9567	1.01909e+06	84.4675	1.01918e+06
1.18205e+06							
1125	***	***	***	1107.51	5.96282e+06	1783.04	5.96521e+06
8.87873e+06							
1250	***	***	***	10240.8	2.02683e+07	14417.2	2.02897e+07
4.51658e+07							
1375	***	***	***	***	***	***	*** 1.7265e+08
1500	***	***	***	***	***	***	*** 5.31753e+08
1650	***	***	***	***	***	***	*** 1.64973e+09
1750	***	***	***	***	***	***	*** 3.16137e+09
1800	***	***	***	***	***	***	*** 4.26296e+09
2000	***	***	***	***	***	***	*** 1.21911e+10
2250	***	***	***	***	***	***	*** 3.51105e+10
2500	***	***	***	***	***	***	*** 8.22685e+10

Pressure = 10 atm

T(K)	ip3->ip1	ip3->ip2	ip3->ip4	ip3->p0	ip3->p1	ip3->p2	ip3->
300	5.77318e-21	7.36922e-17	4.78293e-16	1.18361e-39	3.34255e-12	5.97307e-37	
3.3431e-12	3.34706e-12						
400	2.10464e-12	1.84511e-09	6.80737e-10	1.00567e-25	4.82448e-06	4.96399e-24	
4.827e-06	4.83408e-06						
500	5.24926e-07	5.33953e-05	1.08328e-05	5.62822e-17	0.0263167	8.04527e-16	
0.0263814	0.0264261						
600	0.00241997	0.0499623	0.00900141	5.39076e-11	8.61171	3.59726e-10	
8.67309	8.68963						
700	0.897878	6.25113	1.19396	1.03786e-06	557.536	4.06191e-06	565.879
567.218							
800	63.0564	219.41	46.8934	0.00155781	13015.2	0.0040706	13344.6
13395.7							
900	4581.83	***	753.157	0.416704	153039	0.796788	158375
159984							
1000	43215.9	***	6138.59	31.0416	1.10367e+06	47.0799	1.1531e+06
1.18205e+06							
1125	379340	***	42821.8	1756.01	7.76729e+06	2151.35	8.19336e+06
8.87873e+06							
1250	1.92518e+06	***	***	30493.4	3.40059e+07	32138.5	3.61845e+07
4.51658e+07							

1375	***	***	***	404313	1.05869e+08	413142	1.06648e+08
1.7265e+08							
1500	***	***	***	1.78145e+06	2.41602e+08	1.67096e+06	2.44918e+08
5.31753e+08							
1650	***	***	***	***	***	***	1.64973e+09
1750	***	***	***	***	***	***	3.16137e+09
1800	***	***	***	***	***	***	4.26296e+09
2000	***	***	***	***	***	***	1.21911e+10
2250	***	***	***	***	***	***	3.51105e+10
2500	***	***	***	***	***	***	8.22685e+10

Pressure = 100 atm

T(K)	ip3->ip1	ip3->ip2	ip3->ip4	ip3->p0	ip3->p1	ip3->p2	ip3->
Capture							
300	5.77488e-22	7.36977e-17	4.78293e-16	1.20996e-41	3.34255e-12	6.04047e-39	
3.3431e-12	3.34706e-12						
400	2.11379e-13	1.84721e-09	6.80739e-10	1.09875e-27	4.82448e-06	5.25593e-26	
4.827e-06	4.83408e-06						
500	5.44177e-08	5.39381e-05	1.08339e-05	7.44913e-19	0.0263167	9.93859e-18	
0.0263815	0.0264261						
600	0.000285923	0.0524896	0.00901426	1.03802e-12	8.61172	6.23191e-12	
8.67351	8.68963						
700	0.141561	7.17768	1.20734	3.31998e-08	557.548	1.1535e-07	566.074
567.218							
800	14.6185	282.744	49.5427	8.42922e-05	13017.9	0.000196588	13364.8
13395.7							
900	502.624	4799.85	899.082	0.0358573	153291	0.061713	159493
159984							
1000	7859.69	45081.2	8924.98	4.18147	1.11409e+06	5.67076	1.17596e+06
1.18205e+06							
1125	112304	411436	81958.8	389.757	8.15732e+06	418.444	8.76383e+06
8.87873e+06							
1250	3.01804e+06	***	432752	14939.6	3.99479e+07	13443.6	4.34271e+07
4.51658e+07							
1375	1.25772e+07		***	1.55497e+06	214974	1.42875e+08	171959
1.57394e+08	1.7265e+08						
1500	3.85356e+07		***	***	1.54035e+06	3.9658e+08	1.12496e+06
4.38806e+08	5.31753e+08						
1650	***	***	***	3.04063e+07	1.03159e+09	2.28164e+07	1.08365e+09
1.64973e+09							
1750	***	***	***	7.03729e+07	1.7378e+09	5.03548e+07	1.80569e+09
3.16137e+09							
1800	***	***	***	9.99107e+07	2.16257e+09	7.00353e+07	2.2582e+09
4.26296e+09							
2000	***	***	***	***	***	***	1.21911e+10

2250	***	***	***	***	***	***	***	3.51105e+10
2500	***	***	***	***	***	***	***	8.22685e+10

Pressure = 0.0394737 atm

T(K)	ip4->ip1	ip4->ip2	ip4->ip3	ip4->p0	ip4->p1	ip4->p2	ip4->
Capture							
300	5.20718e-11	1.12487e-12	4.0618e-06	9.7419e-28	0.000127213	8.34663e-25	
0.000131275	0.000132346						
400	5.07069e-05	5.73352e-06	0.0245445	7.19584e-17	2.34011	6.8936e-15	
2.36471	2.37073						
500	0.170352	0.0405064	14.4502	1.57274e-10	949.996	5.48831e-09	964.657
981.91							
600	31.8735	***	1120.82	1.05515e-06	48697.3	2.09048e-05	49850
58590.8							
700	655.189	***	17533	0.000221025	579378	0.0029288	597566
1.13658e+06							
800	***	***	94661.3	0.00901181	2.57443e+06	0.0844835	2.6691e+06
1.08384e+07							
900	***	***	***	***	***	***	*** 6.40921e+07
1000	***	***	***	***	***	***	*** 2.70477e+08
1125	***	***	***	***	***	***	*** 1.16397e+09
1250	***	***	***	***	***	***	*** 3.80434e+09
1375	***	***	***	***	***	***	*** 1.0156e+10
1500	***	***	***	***	***	***	*** 2.32518e+10
1650	***	***	***	***	***	***	*** 5.37748e+10
1750	***	***	***	***	***	***	*** 8.7251e+10
1800	***	***	***	***	***	***	*** 1.09056e+11
2000	***	***	***	***	***	***	*** 2.3962e+11
2250	***	***	***	***	***	***	*** 5.32038e+11
2500	***	***	***	***	***	***	*** 1.01509e+12

Pressure = 1 atm

T(K)	ip4->ip1	ip4->ip2	ip4->ip3	ip4->p0	ip4->p1	ip4->p2	ip4->
Capture							
300	5.31757e-11	5.25924e-14	4.06181e-06	5.96198e-29	0.000127214	4.30184e-26	
0.000131276	0.000132346						
400	5.70184e-05	5.53773e-07	0.0245637	8.64989e-18	2.34135	5.65704e-16	
2.36597	2.37073						
500	0.244937	0.0135703	14.7748	7.60938e-11	964.168	1.36458e-09	979.201
981.91							
600	60.5144	8.9906	1366.94	3.502e-06	56434.8	2.95543e-05	57871.3
58590.8							
700	2612.9	606.616	35453.3	0.00522845	1.01132e+06	0.0277036	1.04999e+06
1.13658e+06							

800	42750.7	***	347771	0.680912	7.61016e+06	2.62387	8.00069e+06
1.08384e+07	900	241529	***	1.61008e+06	17.061	2.96707e+07	51.8507 3.15224e+07
6.40921e+07	1000	***	***	***	***	***	*** 2.70477e+08
1125	***	***	***	***	***	***	*** 1.16397e+09
1250	***	***	***	***	***	***	*** 3.80434e+09
1375	***	***	***	***	***	***	*** 1.0156e+10
1500	***	***	***	***	***	***	*** 2.32518e+10
1650	***	***	***	***	***	***	*** 5.37748e+10
1750	***	***	***	***	***	***	*** 8.7251e+10
1800	***	***	***	***	***	***	*** 1.09056e+11
2000	***	***	***	***	***	***	*** 2.3962e+11
2250	***	***	***	***	***	***	*** 5.32038e+11
2500	***	***	***	***	***	***	*** 1.01509e+12

Pressure = 10 atm

T(K)	ip4->ip1	ip4->ip2	ip4->ip3	ip4->p0	ip4->p1	ip4->p2	ip4->
Capture							
300	5.32237e-11	5.29997e-15	4.06181e-06	6.26678e-30	0.000127214	4.40959e-27	
0.000131276	0.000132346						
400	5.75307e-05	5.97189e-08	0.0245644	1.00724e-18	2.3414	6.25802e-17	
2.36602	2.37073						
500	0.258137	0.00198313	14.7893	1.09126e-11	964.757	1.79333e-10	979.807
981.91							
600	71.1899	2.44807	1384.09	7.65389e-07	56947.1	5.50829e-06	58404.8
58590.8							
700	3799.36	343.073	38545	0.00244161	1.08082e+06	0.0101051	1.12351e+06
1.13658e+06							
800	68819.8	10641.3	469049	0.902984	9.72889e+06	2.54547	1.02774e+07
1.08384e+07							
900	690986	***	3.01901e+06	64.3219	5.00144e+07	137.807	5.37246e+07
6.40921e+07							
1000	3.24153e+06		***	1.16982e+07	1304.28	1.6503e+08	2278.39
1.79974e+08	2.70477e+08						
1125	1.28059e+07		***	3.75282e+07	15189.3	4.70564e+08	22192
5.20936e+08	1.16397e+09						
1250	***	***	***	***	***	***	*** 3.80434e+09
1375	***	***	***	***	***	***	*** 1.0156e+10
1500	***	***	***	***	***	***	*** 2.32518e+10
1650	***	***	***	***	***	***	*** 5.37748e+10
1750	***	***	***	***	***	***	*** 8.7251e+10
1800	***	***	***	***	***	***	*** 1.09056e+11
2000	***	***	***	***	***	***	*** 2.3962e+11
2250	***	***	***	***	***	***	*** 5.32038e+11

2500 *** *** *** *** *** *** *** 1.01509e+12

Pressure = 100 atm

T(K)	ip4->ip1	ip4->ip2	ip4->ip3	ip4->p0	ip4->p1	ip4->p2	ip4->
300	5.32285e-11	5.30406e-16	4.06181e-06	6.30344e-31	0.000127214	4.42158e-28	
400	5.75858e-05	6.022e-09	0.0245645	1.03174e-19	2.3414	6.34869e-18	2.36602
500	0.260013	0.00020963	14.7908	1.18232e-12	964.816	1.89832e-11	979.868
600	73.6486	0.307871	1386.07	9.38803e-08	57001.2	6.4764e-07	58461.2
700	4202.52	62.5302	38975.7	0.000375348	1.08986e+06	0.00145133	
800	86293.5	3253.3	495535	0.204873	1.01688e+07	0.521057	1.07539e+07
900	874825	62256.2	3.61205e+06	26.6207	5.78928e+07	49.5608	6.2442e+07
1000	5.25609e+06	560118	1.72699e+07	1146.03	2.27596e+08	1685.87	
1125	2.81671e+07	3.98865e+06	7.61152e+07	37952.8	8.35907e+08	44873.6	
1250	1.13742e+08	***	2.19578e+08	397052	2.16302e+09	406305	
1375	2.89011e+08	***	4.68766e+08	1.53414e+06	4.37799e+09	1.44476e+06	
1500	***	***	***	***	***	***	2.32518e+10
1650	***	***	***	***	***	***	5.37748e+10
1750	***	***	***	***	***	***	8.7251e+10
1800	***	***	***	***	***	***	1.09056e+11
2000	***	***	***	***	***	***	2.3962e+11
2250	***	***	***	***	***	***	5.32038e+11
2500	***	***	***	***	***	***	1.01509e+12

Pressure = 0.0394737 atm

T(K)	p0->ip1	p0->ip2	p0->ip3	p0->ip4	p0->p1	p0->p2	p0->
300	2.79883e-16	8.47226e-17	7.29831e-17	8.85775e-19	1.36917e-19	1.19655e-23	
400	1.77477e-15	5.50146e-16	1.99361e-15	2.38305e-17	2.0822e-17	5.00068e-21	
500	2.83405e-15	1.00431e-15	1.48711e-14	1.11287e-16	6.17456e-16	3.63419e-19	

600	2.40686e-15	***	4.70308e-14	1.25807e-16	7.12875e-15	8.52476e-18	5.67007e-14
700	9.31626e-16	***	8.22092e-14	5.51034e-17	4.50082e-14	9.8933e-17	1.28303e-13
800	2.47195e-13	***	***	8.41537e-14	1.91108e-17	1.60898e-13	7.13415e-16
900	4.22487e-13	***	***	5.14935e-14	***	3.63349e-13	3.60292e-15
1000	6.64187e-13	***	***	2.14755e-14	***	6.15514e-13	1.3701e-14
1125	1.07187e-12	***	***	5.28397e-15	***	9.59193e-13	5.24731e-14
1250	1.60904e-12	***	***	***	***	1.28656e-12	1.48905e-13
1375	2.28646e-12	***	***	***	***	1.52598e-12	3.31854e-13
1500	3.11296e-12	***	***	***	***	1.63509e-12	6.12463e-13
1650	4.3116e-12	***	***	***	***	1.60114e-12	1.06327e-12
1750	5.24078e-12	***	***	***	***	1.51e-12	1.41654e-12
1800	5.74535e-12	***	***	***	***	1.45286e-12	1.60526e-12
2000	8.03651e-12	***	***	***	***	1.20146e-12	2.42229e-12
2250	1.15307e-11	***	***	***	***	9.26876e-13	3.56377e-12
2500	1.57451e-11	***	***	***	***	7.32553e-13	4.84774e-12

Pressure = 1 atm

T(K)	p0->ip1	p0->ip2	p0->ip3	p0->ip4	p0->p1	p0->p2	p0->
300	4.09316e-16	2.84885e-17	7.40043e-19	5.42089e-20	2.73295e-22	6.87308e-25	Capture
400	3.67007e-15	6.24274e-16	6.59062e-17	2.8646e-18	9.01725e-20	4.34889e-22	4.38611e-16
500	1.38733e-14	3.96511e-15	1.53751e-15	5.38396e-17	8.84784e-18	6.10048e-20	4.36316e-15
600	3.09851e-14	1.12638e-14	1.37453e-14	4.16059e-16	2.89e-16	2.80447e-18	4.39123e-15
700	4.25154e-14	2.04809e-14	6.02976e-14	1.28294e-15	3.68921e-15	5.31381e-17	1.94386e-14
	1.28319e-13	1.28933e-13					1.9549e-14

800	6.36744e-14	***	1.55741e-13	1.71156e-15	2.42471e-14	5.09864e-16	2.45884e-
13	2.47195e-13						
900	5.04761e-14	***	2.6135e-13	1.34297e-15	1.02666e-13	2.99787e-15	4.18833e-
13	4.22487e-13						
1000	***	***	3.33859e-13	***	3.05427e-13	1.24095e-14	6.51708e-13
6.64187e-13							
1125	***	***	2.48164e-13	***	7.20776e-13	5.0177e-14	1.01914e-12
1.07187e-12							
1250	***	***	1.31096e-13	***	1.16138e-12	1.46084e-13	1.43858e-12
1.60904e-12							
1375	***	***	***	***	1.5317e-12	3.29333e-13	1.86103e-12
2.28646e-12							
1500	***	***	***	***	1.63957e-12	6.10605e-13	2.25018e-12
3.11296e-12							
1650	***	***	***	***	1.60378e-12	1.06225e-12	2.66603e-12
4.3116e-12							
1750	***	***	***	***	1.51166e-12	1.41593e-12	2.9276e-12
5.24078e-12							
1800	***	***	***	***	1.45414e-12	1.6048e-12	3.05893e-12
5.74535e-12							
2000	***	***	***	***	1.20186e-12	2.42216e-12	3.62402e-12
8.03651e-12							
2250	***	***	***	***	9.26953e-13	3.56375e-12	4.49071e-12
1.15307e-11							
2500	***	***	***	***	7.32567e-13	4.84773e-12	5.5803e-12
1.57451e-11							

Pressure = 10 atm

T(K)	p0->ip1	p0->ip2	p0->ip3	p0->ip4	p0->p1	p0->p2	p0->
Capture							
300	4.351e-16	3.49663e-18	3.83671e-20	5.69802e-21	2.75573e-24	7.27467e-26	
4.38611e-16	4.41869e-16						
400	4.24763e-15	1.13998e-16	1.20184e-18	3.33569e-19	9.83297e-22	5.07763e-23	
4.36316e-15	4.39123e-15						
500	1.79433e-14	1.43316e-15	5.43602e-17	7.72117e-18	1.211e-19	8.07703e-21	
1.94386e-14	1.9549e-14						
600	4.71436e-14	8.47711e-15	9.8427e-16	9.09206e-17	6.26348e-18	4.45692e-19	
5.67026e-14	5.69914e-14						
700	9.21689e-14	2.72212e-14	8.18562e-15	5.96711e-16	1.51297e-16	1.13367e-17	
1.28335e-13	1.28933e-13						
800	1.45367e-13	5.87025e-14	3.78126e-14	2.19265e-15	1.8319e-15	1.57918e-16	
2.46065e-13	2.47195e-13						
900	2.85467e-13	***	1.16297e-13	4.52782e-15	1.2304e-14	1.32742e-15	4.19923e-
13	4.22487e-13						

1000	3.40736e-13	***	2.48643e-13	5.91984e-15	5.32059e-14	7.25717e-15	6.55762e-
13	6.64187e-13						
1125	3.53869e-13	***	4.26773e-13	5.63256e-15	2.0803e-13	3.71158e-14	1.03142e-
12	1.07187e-12						
1250	3.12945e-13	***	5.24545e-13	***	4.69278e-13	1.24231e-13	1.46195e-12
1.60904e-12							
1375	***	***	5.55672e-13	***	1.01952e-12	3.10136e-13	1.88553e-12
2.28646e-12							
1500	***	***	3.48121e-13	***	1.32946e-12	5.947e-13	2.27248e-12
3.11296e-12							
1650	***	***	***	***	1.62433e-12	1.05448e-12	2.67881e-12
4.3116e-12							
1750	***	***	***	***	1.52482e-12	1.4112e-12	2.93602e-12
5.24078e-12							
1800	***	***	***	***	1.46437e-12	1.6012e-12	3.06558e-12
5.74535e-12							
2000	***	***	***	***	1.20513e-12	2.42114e-12	3.62627e-12
8.03651e-12							
2250	***	***	***	***	9.27611e-13	3.56358e-12	4.49119e-12
1.15307e-11							
2500	***	***	***	***	7.32694e-13	4.84771e-12	5.5804e-12
1.57451e-11							

Pressure = 100 atm

T(K)	p0->ip1	p0->ip2	p0->ip3	p0->ip4	p0->p1	p0->p2	p0->
300	4.38253e-16	3.57649e-19	9.34278e-23	5.73136e-22	2.75797e-26	7.32678e-27	
4.38611e-16	4.41869e-16						
400	4.35072e-15	1.23934e-17	1.72652e-20	3.41683e-20	9.95353e-24	5.23155e-24	
4.36316e-15	4.39123e-15						
500	1.92507e-14	1.86327e-16	7.03962e-19	8.36538e-19	1.28314e-21	8.80456e-22	
1.94386e-14	1.9549e-14						
600	5.50841e-14	1.58842e-15	1.89437e-17	1.11517e-17	7.46192e-20	5.29878e-20	
5.67027e-14	5.69914e-14						
700	1.19538e-13	8.44504e-15	2.60958e-16	9.16996e-17	2.26665e-18	1.48701e-18	
1.28339e-13	1.28933e-13						
800	2.13757e-13	2.97975e-14	2.02434e-15	4.95563e-16	3.93854e-17	2.33132e-17	
2.46138e-13	2.47195e-13						
900	3.32843e-13	7.55948e-14	9.76264e-15	1.82504e-15	4.13244e-16	2.32199e-16	
4.20671e-13	4.22487e-13						
1000	4.66867e-13	1.52031e-13	3.24721e-14	4.68552e-15	2.74051e-15	1.60314e-15	
6.604e-13	6.64187e-13						
1125	5.78423e-13	3.48601e-13	9.15465e-14	9.76747e-15	1.65105e-14	1.15497e-14	
1.0564e-12	1.07187e-12						

1250	1.18932e-12	***	2.1832e-13	1.3022e-14	6.53411e-14	5.39515e-14	1.53995e-
12	1.60904e-12						
1375	1.34509e-12	***	3.4739e-13	1.28968e-14	1.72894e-13	1.72546e-13	2.05082e-
12	2.28646e-12						
1500	1.3209e-12	***	4.41532e-13		***	3.03692e-13	4.07447e-13
3.11296e-12							2.51419e-12
1650	***	***	1.01361e-12		***	7.59081e-13	9.97275e-13
4.3116e-12							2.77104e-12
1750	***	***	7.49444e-13		***	8.71319e-13	1.36724e-12
5.24078e-12							3.00993e-12
1800	***	***	6.35847e-13		***	9.09538e-13	1.56361e-12
5.74535e-12							3.12992e-12
2000	***	***	***		***	1.2241e-12	2.41564e-12
8.03651e-12							3.63974e-12
2250	***	***	***		***	9.31906e-13	3.56258e-12
1.15307e-11							4.49449e-12
2500	***	***	***		***	7.33625e-13	4.84756e-12
1.57451e-11							5.58118e-12

Pressure = 0.0394737 atm

T(K)	p1->ip1	p1->ip2	p1->ip3	p1->ip4	p1->p0	p1->p2	p1->
Capture							
300	1.34144e-25	3.59769e-25	1.70633e-13	7.64703e-16	9.05184e-40	2.79089e-37	
1.71398e-13	1.71596e-13						
400	2.08293e-21	1.09859e-21	8.60798e-13	1.15707e-14	3.10881e-31	1.35271e-29	
8.72368e-13	8.7366e-13						
500	9.50914e-19	3.62997e-19	2.47175e-12	6.53582e-14	6.00388e-26	9.06368e-25	
2.53711e-12	2.54251e-12						
600	5.86531e-17	***	5.26585e-12	1.93726e-13	2.38815e-22	1.6652e-21	5.45964e-
12	5.50649e-12						
700	6.72157e-16	***	9.30048e-12	2.97928e-13	9.61839e-20	3.92918e-19	9.59909e-
12	9.98509e-12						
800	***	***	1.38006e-11	2.58028e-13	7.62377e-18	2.18314e-17	1.40587e-11
1.61132e-11							
900	***	***	1.60076e-11		***	1.88587e-16	4.09046e-16
2.39651e-11							1.60084e-11
1000	***	***	1.38478e-11		***	2.13672e-15	3.63658e-15
3.35739e-11							1.38539e-11
1125	***	***	8.08308e-12		***	2.18901e-14	2.88628e-14
4.80602e-11							8.13676e-12
1250	***	***	***		***	1.30352e-13	1.40896e-13
6.52667e-11							2.71247e-13
1375	***	***	***		***	5.16611e-13	4.78036e-13
8.51357e-11							9.94647e-13

1500	***	***	***	***	1.49628e-12	1.22473e-12	2.72101e-12
1.07595e-10							
1650	***	***	***	***	3.91406e-12	2.84609e-12	6.76015e-12
1.37853e-10							
1750	***	***	***	***	6.43212e-12	4.37629e-12	1.08084e-11
1.59964e-10							
1800	***	***	***	***	7.96926e-12	5.26046e-12	1.32297e-11
1.71585e-10							
2000	***	***	***	***	1.58227e-11	9.4052e-12	2.52279e-11
2.21726e-10							
2250	***	***	***	***	2.88276e-11	1.5487e-11	4.43147e-11
2.92265e-10							
2500	***	***	***	***	4.46672e-11	2.22618e-11	6.69289e-11
3.71023e-10							

Pressure = 1 atm

T(K)	p1->ip1	p1->ip2	p1->ip3	p1->ip4	p1->p0	p1->p2	p1->
300	4.10303e-27	1.55497e-26	1.70633e-13	7.64708e-16	1.80681e-42	4.71622e-40	
1.71398e-13	1.71596e-13						
400	7.38921e-23	6.4073e-23	8.60798e-13	1.15768e-14	1.34631e-33	4.27245e-32	
8.72375e-13	8.7366e-13						
500	6.22494e-20	2.72759e-20	2.47181e-12	6.63332e-14	8.60326e-28	9.05243e-27	
2.53814e-12	2.54251e-12						
600	7.82847e-18	3.01789e-18	5.26922e-12	2.24573e-13	9.68159e-24	5.31308e-23	
5.4938e-12	5.50649e-12						
700	2.27118e-16	1.18638e-16	9.39292e-12	5.27812e-13	7.88396e-21	2.76038e-20	
9.92108e-12	9.98509e-12						
800	3.74524e-15	***	1.48612e-11	8.65706e-13	1.14889e-18	2.79947e-18	1.57307e-11
11	1.61132e-11						
900	2.17928e-14	***	2.13365e-11	9.92623e-13	5.32861e-17	9.74864e-17	2.2351e-11
11	2.39651e-11						
1000	***	***	2.74951e-11	***	1.06027e-15	1.59526e-15	2.74987e-11
3.35739e-11							
1125	***	***	3.0492e-11	***	1.64491e-14	2.01699e-14	3.05311e-11
4.80602e-11							
1250	***	***	2.62884e-11	***	1.17669e-13	1.22749e-13	2.6533e-11
6.52667e-11							
1375	***	***	***	***	5.18548e-13	4.79588e-13	9.98135e-13
8.51357e-11							
1500	***	***	***	***	1.50039e-12	1.22768e-12	2.72807e-12
1.07595e-10							
1650	***	***	***	***	3.92051e-12	2.8502e-12	6.77072e-12
1.37853e-10							

1750	***	***	***	***	6.43918e-12	4.38047e-12	1.08196e-11
1.59964e-10							
1800	***	***	***	***	7.97628e-12	5.26446e-12	1.32407e-11
1.71585e-10							
2000	***	***	***	***	1.58279e-11	9.40775e-12	2.52357e-11
2.21726e-10							
2250	***	***	***	***	2.883e-11	1.54879e-11	4.4318e-11
2.92265e-10							
2500	***	***	***	***	4.4668e-11	2.2262e-11	6.69301e-11
3.71023e-10							

Pressure = 10 atm

T(K)	p1->ip1	p1->ip2	p1->ip3	p1->ip4	p1->p0	p1->p2	p1->
Capture							
300	4.1962e-28	1.54623e-27	1.70633e-13	7.64709e-16	1.82187e-44	4.70557e-42	
1.71398e-13	1.71596e-13						
400	7.24665e-24	6.61498e-24	8.60798e-13	1.15771e-14	1.4681e-35	4.4978e-34	
8.72375e-13	8.7366e-13						
500	6.36657e-21	2.89723e-21	2.47181e-12	6.63738e-14	1.17753e-29	1.14761e-28	
2.53818e-12	2.54251e-12						
600	9.57318e-19	3.27479e-19	5.26931e-12	2.26611e-13	2.09829e-25	1.01562e-24	
5.49592e-12	5.50649e-12						
700	4.30105e-17	1.49647e-17	9.39539e-12	5.64194e-13	3.23326e-22	9.85101e-22	
9.95964e-12	9.98509e-12						
800	7.56164e-16	3.21306e-16	1.4905e-11	1.11371e-12	8.68007e-20	1.89585e-19	
1.60198e-11	1.61132e-11						
900	9.53431e-15	***	2.17756e-11	1.76491e-12	6.38607e-18	1.0714e-17	2.355e-11
2.39651e-11							
1000	4.91201e-14	***	2.97914e-11	2.23666e-12	1.84701e-16	2.49445e-16	3.20777e-11
11 3.35739e-11							
1125	2.42842e-13	***	4.01177e-11	2.24417e-12	4.74755e-15	5.18301e-15	4.26146e-11
11 4.80602e-11							
1250	1.30741e-12	***	4.73014e-11	***	4.75465e-14	4.27044e-14	4.88279e-11
6.52667e-11							
1375	***	***	4.92592e-11	***	3.45153e-13	2.99049e-13	4.99215e-11
8.51357e-11							
1500	***	***	4.32046e-11	***	1.2166e-12	9.54026e-13	4.53992e-11
1.07595e-10							
1650	***	***	***	***	3.97074e-12	2.88116e-12	6.8519e-12
1.37853e-10							
1750	***	***	***	***	6.49523e-12	4.41248e-12	1.09077e-11
1.59964e-10							
1800	***	***	***	***	8.03242e-12	5.29532e-12	1.33277e-11
1.71585e-10							

2000	***	***	***	***	1.5871e-11	9.42787e-12	2.52989e-11
2.21726e-10							
2250	***	***	***	***	2.88505e-11	1.54954e-11	4.43459e-11
2.92265e-10							
2500	***	***	***	***	4.46758e-11	2.2264e-11	6.69398e-11
3.71023e-10							

Pressure = 100 atm

T(K)	p1->ip1	p1->ip2	p1->ip3	p1->ip4	p1->p0	p1->p2	p1->
300	4.05172e-29	1.56084e-28	1.70633e-13	7.64709e-16	1.82335e-46	4.70407e-44	
1.71398e-13	1.71596e-13						
400	7.2309e-25	6.63747e-25	8.60798e-13	1.15771e-14	1.4861e-37	4.52825e-36	
8.72375e-13	8.7366e-13						
500	6.38595e-22	2.9103e-22	2.47181e-12	6.63778e-14	1.24767e-31	1.19693e-30	
2.53819e-12	2.54251e-12						
600	9.93568e-20	3.15809e-20	5.26932e-12	2.26827e-13	2.49977e-27	1.17089e-26	
5.49615e-12	5.50649e-12						
700	4.91239e-18	1.36308e-18	9.39559e-12	5.68914e-13	4.84391e-24	1.39697e-23	
9.96451e-12	9.98509e-12						
800	1.06226e-16	3.05411e-17	1.4908e-11	1.16429e-12	1.86619e-21	3.7902e-21	
1.60725e-11	1.61132e-11						
900	1.21522e-15	4.02063e-16	2.18109e-11	2.05032e-12	2.14484e-19	3.3349e-19	
2.38629e-11	2.39651e-11						
1000	8.19542e-15	3.43316e-15	3.00672e-11	3.17082e-12	9.51354e-18	1.19715e-17	
3.32497e-11	3.35739e-11						
1125	1.00332e-14	7.35054e-14	4.21002e-11	4.57688e-12	3.76793e-16	3.8547e-16	
4.67614e-11	4.80602e-11						
1250	3.24597e-13	***	5.53675e-11	5.43573e-12	6.62026e-15	5.72382e-15	6.11402e-11
6.52667e-11							
1375	9.80481e-13	***	6.80723e-11	5.3691e-12	5.85322e-14	4.45089e-14	7.45249e-11
8.51357e-11							
1500	2.82718e-12	***	7.76461e-11	***	2.77911e-13	1.87013e-13	8.10525e-11
1.07595e-10							
1650	***	***	8.40637e-11	***	1.85561e-12	1.2495e-12	8.72585e-11
1.37853e-10							
1750	***	***	7.8833e-11	***	3.71153e-12	2.36475e-12	8.72159e-11
1.59964e-10							
1800	***	***	7.54928e-11	***	4.98903e-12	3.10237e-12	8.60687e-11
1.71585e-10							
2000	***	***	***	***	1.61208e-11	9.53195e-12	2.56528e-11
2.21726e-10							
2250	***	***	***	***	2.89841e-11	1.55376e-11	4.45217e-11
2.92265e-10							

2500 *** *** *** *** 4.47325e-11 2.22764e-11 6.70089e-11
 3.71023e-10

Pressure = 0.0394737 atm

T(K)	p2->ip1	p2->ip2	p2->ip3	p2->ip4	p2->p0	p2->p1	p2->
Capture							
300	3.3451e-16	8.21881e-17	2.31459e-17	2.37254e-19	3.7407e-27	1.31973e-20	
400	4.058e-15	1.21647e-15	1.79401e-15	2.04893e-17	4.48806e-23	8.13138e-18	
500	1.14671e-14	3.99312e-15	2.55809e-14	2.40345e-16	2.24895e-20	5.76834e-16	
600	1.53826e-14	***	1.18759e-13	5.29573e-16	1.80742e-18	1.05388e-14	1.45212e-13
700	8.26721e-15	***	2.68727e-13	3.6298e-16	4.85658e-17	9.02567e-14	3.67662e-13
800	***	***	3.46531e-13	1.59975e-16	6.37855e-16	4.11946e-13	7.59275e-13
900	***	***	2.58485e-13	***	5.01696e-15	1.09741e-12	1.36092e-12
1000	***	***	1.27502e-13	***	2.66964e-14	2.04118e-12	2.19538e-12
1125	***	***	3.69222e-14	***	1.40205e-13	3.37927e-12	3.55641e-12
1250	***	***	***	***	5.03202e-13	4.69941e-12	5.20261e-12
1375	***	***	***	***	1.34005e-12	5.7019e-12	7.04195e-12
1500	***	***	***	***	2.8363e-12	6.19784e-12	9.03414e-12
1650	***	***	***	***	5.57902e-12	6.10895e-12	1.1688e-11
1750	***	***	***	***	7.93319e-12	5.7537e-12	1.36869e-11
1800	***	***	***	***	9.24717e-12	5.52451e-12	1.47717e-11
2000	***	***	***	***	1.52606e-11	4.49929e-12	1.97599e-11
2250	***	***	***	***	2.41562e-11	3.37519e-12	2.75313e-11
2500	***	***	***	***	3.43505e-11	2.58705e-12	3.69376e-11

Pressure = 1 atm

T(K)	p2->ip1	p2->ip2	p2->ip3	p2->ip4	p2->p0	p2->p1	p2->
Capture							
300	4.2794e-16	1.20124e-17	1.12718e-19	1.2228e-20	2.14869e-28	2.23016e-23	
400	6.42847e-15	6.31901e-16	3.5046e-17	1.6814e-18	3.90309e-24	2.56824e-20	
500	3.27643e-14	7.3311e-15	1.69755e-15	5.97485e-17	3.77517e-21	5.76118e-18	
600	9.03154e-14	3.00944e-14	2.37268e-14	7.44558e-16	5.94602e-19	3.36259e-16	
700	1.51212e-13	6.87349e-14	1.38079e-13	3.34291e-15	2.60852e-17	6.34084e-15	
800	2.65389e-13	***	4.35065e-13	5.95238e-15	4.55863e-16	5.28244e-14	7.59687e-13
900	2.42389e-13	***	8.48423e-13	5.82177e-15	4.17443e-15	2.61542e-13	1.36235e-12
1000	***	***	1.27915e-12	***	2.41798e-14	8.95406e-13	2.19878e-12
1125	***	***	1.06753e-12	***	1.3407e-13	2.3615e-12	3.56319e-12
1250	***	***	6.23697e-13	***	4.9367e-13	4.09415e-12	5.21161e-12
1375	***	***	***	***	1.32987e-12	5.7204e-12	7.05027e-12
1500	***	***	***	***	2.82769e-12	6.21276e-12	9.04045e-12
1650	***	***	***	***	5.57368e-12	6.11779e-12	1.16915e-11
1750	***	***	***	***	7.92977e-12	5.7592e-12	1.3689e-11
1800	***	***	***	***	9.24453e-12	5.52871e-12	1.47732e-11
2000	***	***	***	***	1.52598e-11	4.5005e-12	1.97603e-11
2250	***	***	***	***	2.4156e-11	3.37539e-12	2.75314e-11
2500	***	***	***	***	3.43505e-11	2.58708e-12	3.69376e-11

Pressure = 10 atm

T(K)	p2->ip1	p2->ip2	p2->ip3	p2->ip4	p2->p0	p2->p1	p2->
Capture							
300	4.38771e-16	1.32077e-18	3.18029e-20	1.25343e-21	2.27424e-29	2.22512e-25	
400	4.39189e-16						

400	7.00445e-15	9.18878e-17	5.32455e-19	1.86003e-19	4.55712e-25	2.7037e-22
7.09706e-15	7.07967e-15					
500	3.98569e-14	1.94562e-15	4.8077e-17	7.85211e-18	4.99832e-22	7.30367e-20
4.18585e-14	4.1744e-14					
600	1.26955e-13	1.67287e-14	1.39157e-15	1.38738e-16	9.44955e-20	6.42777e-18
1.4522e-13	1.44791e-13					
700	2.81137e-13	6.95053e-14	1.57092e-14	1.2128e-15	5.56515e-18	2.26286e-16
3.67796e-13	3.66657e-13					
800	4.85559e-13	1.77194e-13	8.83472e-14	5.53683e-15	1.41193e-16	3.57736e-15
7.60355e-13	7.5813e-13					
900	1.01053e-12	***	3.11456e-13	1.35939e-14	1.84839e-15	2.87441e-14
12	1.36433e-12					1.36617e-
1000	1.2967e-12	***	7.41015e-13	2.04822e-14	1.41406e-14	1.40011e-13
12	2.22228e-12					2.21235e-
1125	1.45199e-12	***	1.4218e-12	2.24749e-14	9.91712e-14	6.06828e-13
12	3.69173e-12					3.60227e-
1250	1.35365e-12	***	1.95226e-12	***	4.19819e-13	1.42435e-12
5.63868e-12						5.28398e-12
1375	***	***	2.29284e-12	***	1.25235e-12	3.56698e-12
8.08831e-12						7.11302e-12
1500	***	***	1.51215e-12	***	2.75403e-12	4.82792e-12
1.10546e-11						9.09494e-12
1650	***	***	***	***	5.53291e-12	6.18423e-12
1.5304e-11						1.17171e-11
1750	***	***	***	***	7.90324e-12	5.80129e-12
1.85547e-11						1.37045e-11
1800	***	***	***	***	9.22383e-12	5.56112e-12
2.03047e-11						1.4785e-11
2000	***	***	***	***	1.52533e-11	4.51013e-12
2.81253e-11						1.97634e-11
2250	***	***	***	***	2.41549e-11	3.37702e-12
3.97051e-11						2.75319e-11
2500	***	***	***	***	3.43503e-11	2.58731e-12
5.32129e-11						3.69376e-11

Pressure = 100 atm

T(K)	p2->ip1	p2->ip2	p2->ip3	p2->ip4	p2->p0	p2->p1	p2->
300	4.39961e-16	1.33412e-19	1.45814e-23	1.25684e-22	2.29053e-30	2.22442e-27	
4.40094e-16	4.39189e-16						
400	7.08739e-15	9.63999e-18	1.24283e-20	1.88697e-20	4.69526e-26	2.722e-24	
7.09706e-15	7.07967e-15						
500	4.1624e-14	2.33077e-16	5.60505e-19	8.31175e-19	5.44854e-23	7.61755e-22	
4.18585e-14	4.1744e-14						

600	1.42447e-13	2.73297e-15	2.40913e-17	1.6311e-17	1.12345e-20	7.41043e-20
	1.45221e-13	1.44791e-13				
700	3.49033e-13	1.81548e-14	4.43867e-16	1.74072e-16	7.29967e-19	3.20895e-18
	3.6781e-13	3.66657e-13				
800	6.79873e-13	7.5301e-14	4.20076e-15	1.12745e-15	2.0844e-17	7.15191e-17
	7.60594e-13	7.5813e-13				
900	1.12405e-12	2.15264e-13	2.32604e-14	4.73956e-15	3.23329e-16	8.94707e-16
	1.36853e-12	1.36433e-12				
1000	1.64525e-12	4.72373e-13	8.53902e-14	1.34958e-14	3.12371e-15	6.71949e-15
	2.22635e-12	2.22228e-12				
1125	2.15383e-12	1.15079e-12	2.62555e-13	3.12755e-14	3.08602e-14	4.5131e-14
	3.67445e-12	3.69173e-12				
1250	4.41126e-12	***	6.73305e-13	4.58269e-14	1.82321e-13	1.90911e-13
	5.63868e-12					
1375	5.1608e-12	***	1.14973e-12	4.92825e-14	6.96753e-13	5.3089e-13
	8.08831e-12					
1500	5.2291e-12	***	1.55848e-12	***	1.88688e-12	9.46394e-13
	1.10546e-11					
1650	***	***	3.99088e-12	***	5.23276e-12	2.68197e-12
	1.5304e-11					
1750	***	***	3.00325e-12	***	7.65706e-12	3.10905e-12
	1.85547e-11					
1800	***	***	2.56757e-12	***	9.00728e-12	3.25809e-12
	2.03047e-11					
2000	***	***	***	***	1.52187e-11	4.55992e-12
	2.81253e-11					
2250	***	***	***	***	2.41481e-11	3.38622e-12
	3.97051e-11					
2500	***	***	***	***	3.43492e-11	2.58874e-12
	5.32129e-11					

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