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

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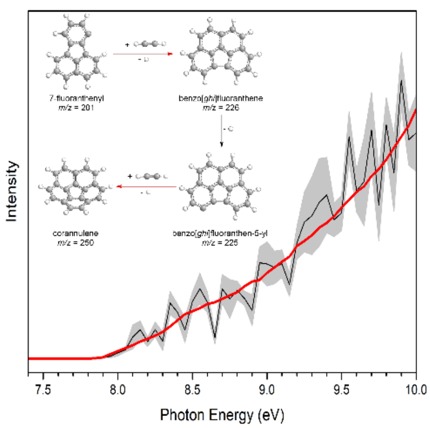
Abstract: Fullerenes (C_{60}, C_{70}) detected in planetary nebulae and carbonaceous chondrites have been implicated to play a key role in the astrochemical evolution of the interstellar medium. However, the formation mechanism of even their simplest molecular building block — the corannulene molecule ($C_{20}H_{10}$) — 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 star[5] 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 - fullerenes[11-14] 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 emissions[11] — 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 dicarbon[20-22] 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 electrons[29] 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 envelopes[25] 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-down[27] 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 ($C_{16}H_9^•$) and benzo[*ghi*]fluoranthen-5-yl ($C_{18}H_9^•$) radicals with acetylene (C_2H_2) involving the HACA mechanism[41] 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 ($C_{16}H_9^•$) 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 ($C_{18}H_9^•$) — 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 ($C_{16}H_9^•$) 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 ($C_{16}H_{10}Br_2$) 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 ($C_{16}H_{10}Br_2$) 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 $C_{18}H_{11}$ and $C_{20}H_{11}$ 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

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

The G3(MP2,CC) model chemistry approach normally provides chemical accuracy of 0.01–0.02 Å for bond lengths, 1–2º for bond angles, and 3–6 kJ mol^{-1} for relative energies of hydrocarbons, their radicals, reaction energies, and barrier heights in terms of average absolute deviations.[20] The adiabatic ionization energies were calculated using the same G3(MP2,CC)//B3LYP/6-311G(d,p) method with the expected accuracy of $\pm$0.1 eV. The GAUSSIAN 09[22] and MOLPRO 2010[23] program packages were employed for the ab initio calculations.

Pressure- and temperature-dependent rate constants and product branching ratios for the 7-fluoranthenyl + C_2H_2 and benzo[*ghi*]fluoranthen-5-yl + C_2H_2 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 Frenklach[26] and those for N_2 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 $\alpha_{300} = 424$ cm^{-1} derived by Jasper from classical trajectory calculations[29] and used earlier by us in the studies of the reactions of C_2H_2 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 ($C_{16}H_{10}Br_2$) precursor seeded in helium (Figure 1a) and in acetylene (Figure 1b) at a reactor temperature of 1450 ± 10 K. The 1-(2,6-dibromo-phenyl)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 ± 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 ($C_{18}H_{10}$) and corannulene ($C_{20}H_{10}$) represent distinct reaction products, which are absent in the control experiment when acetylene is absent. On the other hand, fluoranthene ($C_{16}H_{10}$) is formed in both systems suggesting that it is the hydrogen recombination product of the reaction of 7-fluoranthenyl radical ($C_{16}H_9^{\bullet}$) with atomic hydrogen in both systems.

Our experimental investigations reveal that corannulene ($C_{20}H_{10}$, 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 ($C_{16}H_9^{\bullet}$, 201 amu) and of the benzo[*ghi*]fluoranthen-5-yl radical ($C_{18}H_9^{\bullet}$, 225 amu) with acetylene (C_2H_2, 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 ($C_{18}H_{10}$) (Figure 3a) and corannulene ($C_{20}H_{10}$) (Figure 3b, Supplementary Figure 11). The 7-fluoranthenyl radical ($C_{16}H_9^{\bullet}$) 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 ($C_{18}H_{10}$) (**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 ($C_{18}H_{10}$). 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) mechanism[58] 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 HACA[51] 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 ($C_{20}H_{10}$) — though 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 model[59] 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 benzene[65] 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.

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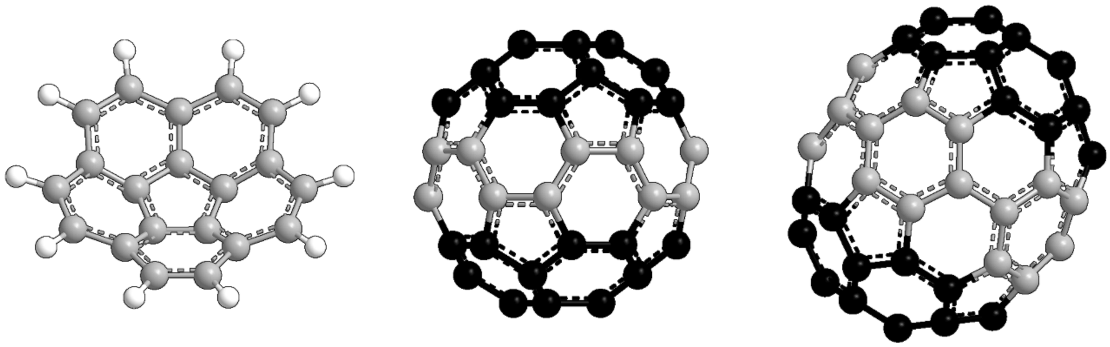
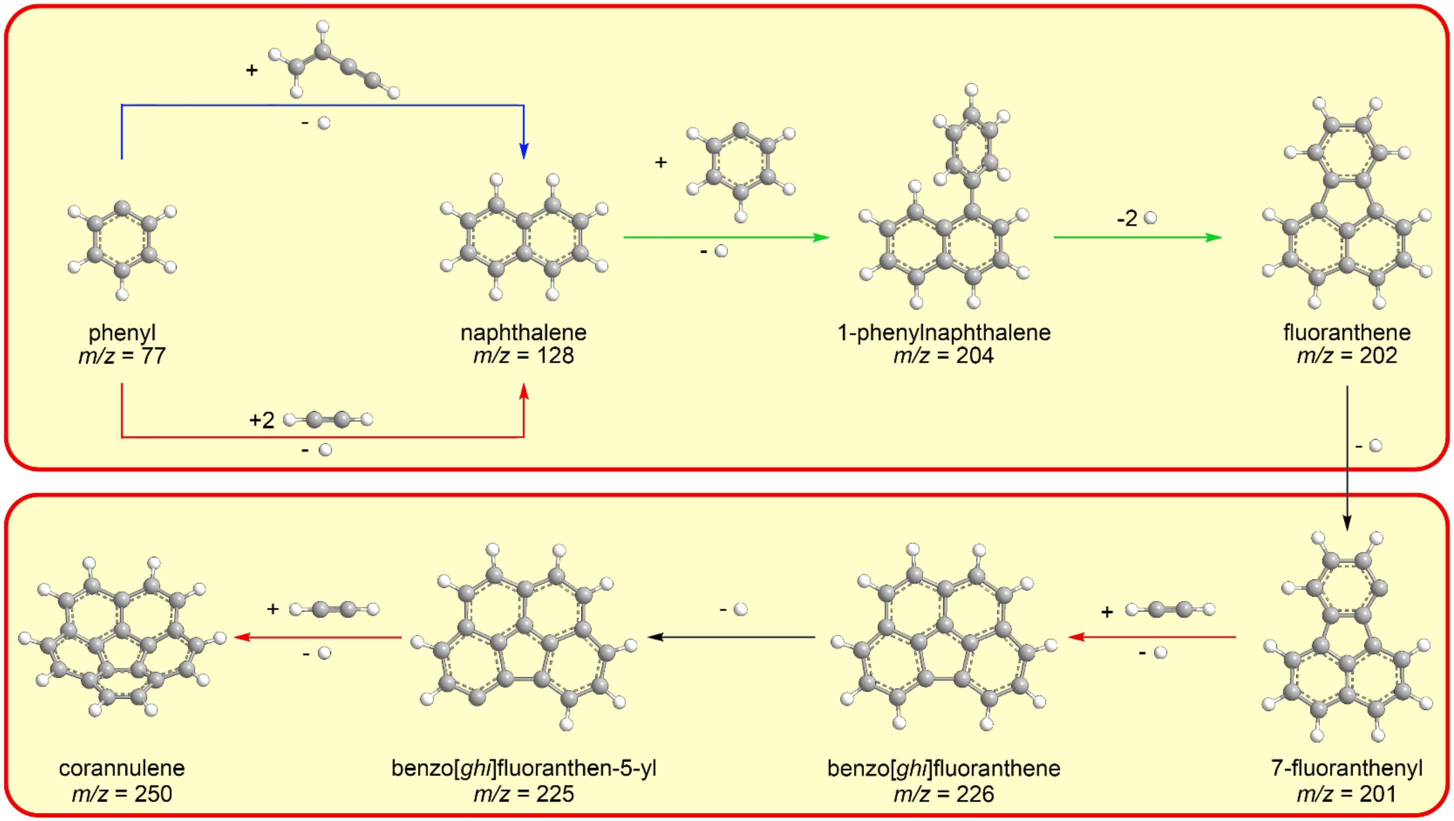


(1) (2) (3)

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.

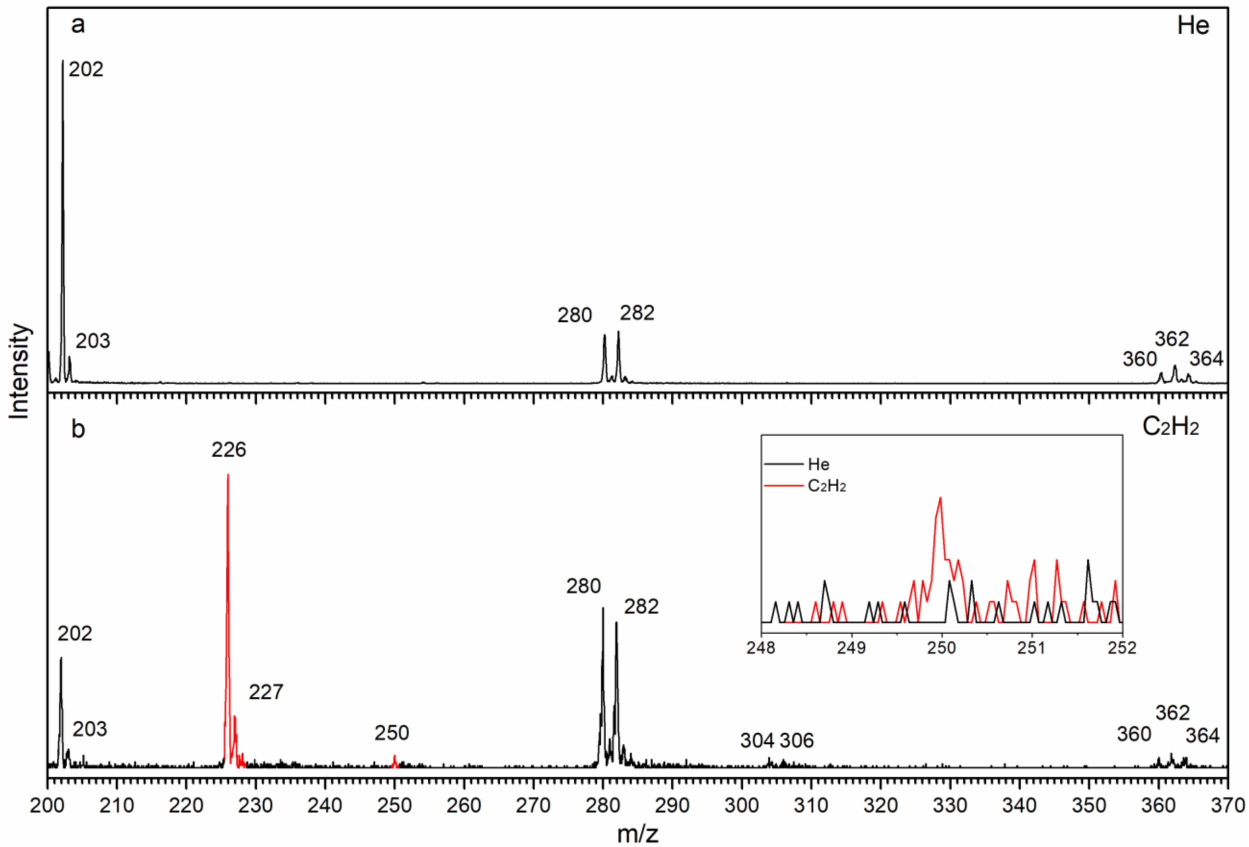


Figure 1. Photoionization mass spectra recorded at a photoionization energy of 9.5 eV at a reactor temperature of 1450 ± 10 K. (a) 1-(2,6-dibromophenyl)naphthalene ($C_{16}H_{10}Br_2$)–helium (He) system; (b) 1-(2,6-dibromophenyl)naphthalene ($C_{16}H_{10}Br_2$)–acetylene (C_2H_2) system. The mass peaks 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.

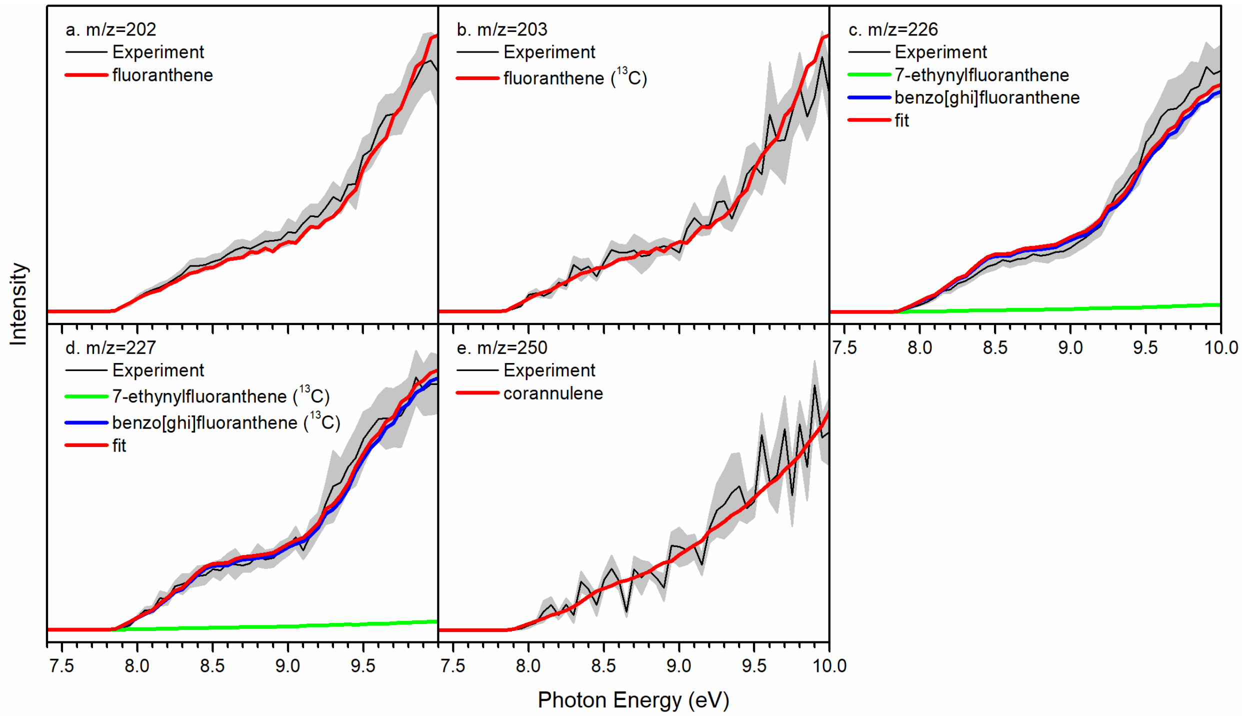


Figure 2. Photoionization efficiency (PIE) curves for *m/z* = 202, 203, 226, 227 and 250. Black: experimentally derived PIE curves with the error area presented in gray; red: reference PIE curve. The overall error bars consist of two parts: ±10% based on the accuracy of the photodiode and a 1 σ error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

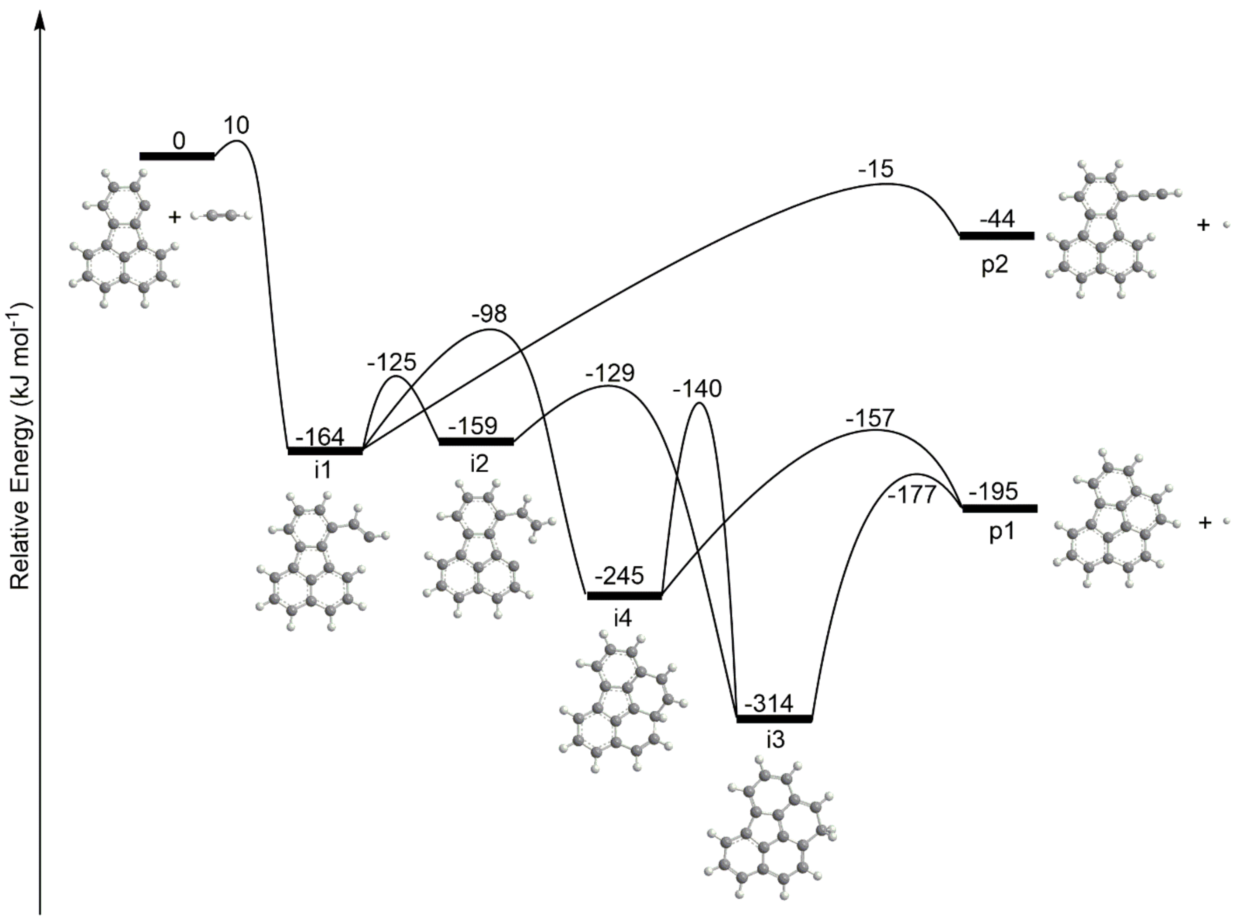


Figure 3a. Potential energy surface (PES) for the reaction of the 7-fluoranthenyl radical ($C_{16}H_9^{\bullet}$) with acetylene (C_2H_2) calculated at the G3(MP2,CC)//B3LYP/6-311G(d,p) level of theory. The relative energies are given in kJmol^{-1}. Cartesian coordinates of reactants, intermediates, products, and transition states are provided in the Supplementary Note 3.

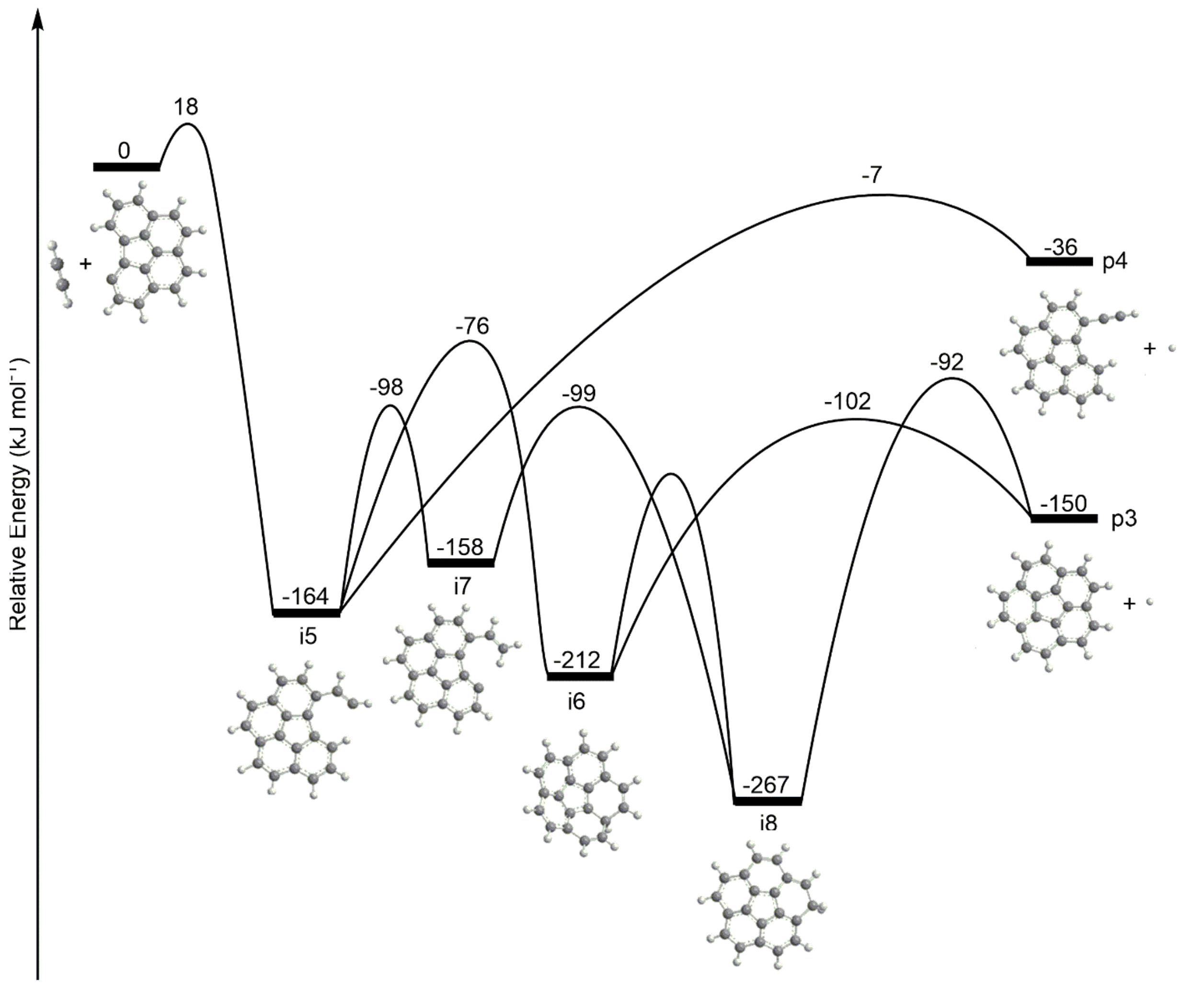


Figure 3b. Potential energy surface (PES) for the reaction of the benzofluoranthen-5-yl ($C_{18}H_9^{\bullet}$) with acetylene (C_2H_2) calculated at the G3(MP2,CC)//B3LYP/6-311G(d,p) level of theory. The relative energies are given in $kJmol^{-1}$. Cartesian coordinates of reactants, intermediates, 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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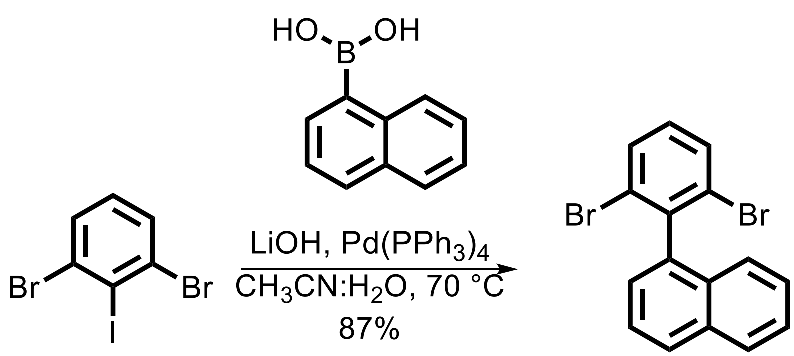
Supplementary Note 1. Materials and Synthetic Methods.

Unless otherwise stated, all manipulations of air and/or moisture sensitive compounds were carried out in oven-dried glassware, under an atmosphere of N_2. 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 N_2 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 ^{1}H and ^{13}C NMR spectra were recorded on Bruker AVB-400 and AVQ-400 MHz spectrometers, and are referenced to residual solvent peaks ($CDCl_3$ ^{1}H NMR = 7.26 ppm, ^{13}C NMR = 77.16 ppm). ESI mass spectrometry was performed on a Finnigan LTQFT (Thermo) spectrometer in positive ionization mode.

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



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

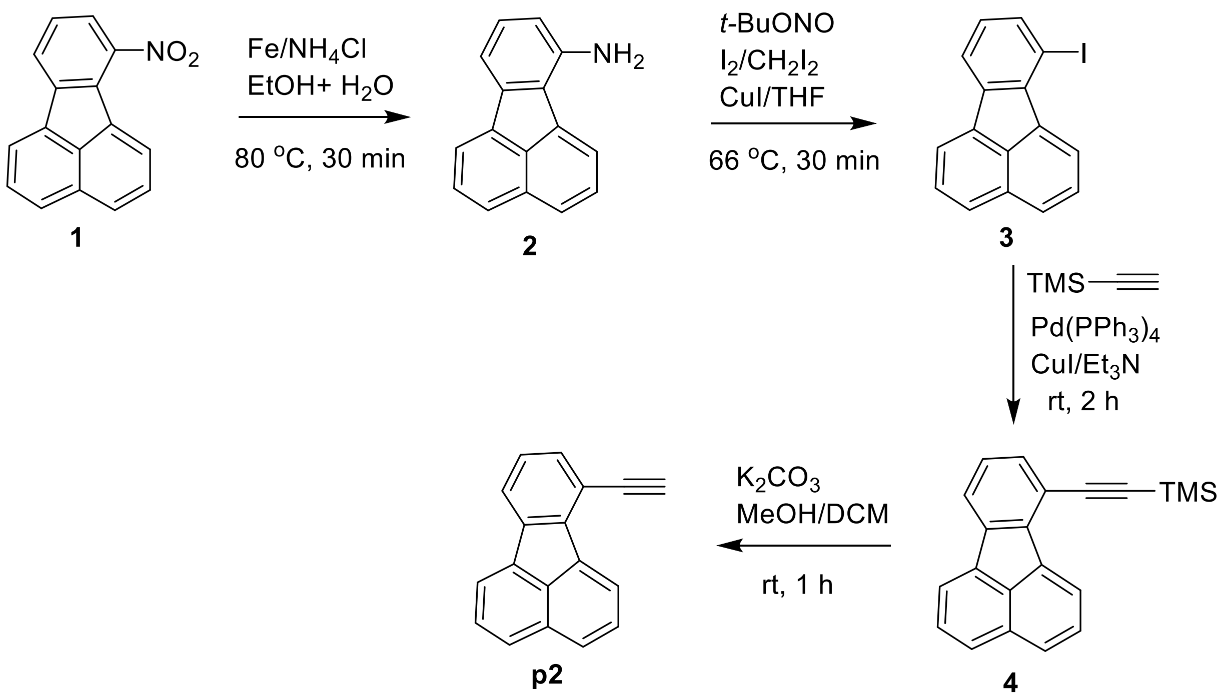
1-(2,6-dibromophenyl)naphthalene

1.2 g (3.36 mmol) of l,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 $Pd(PPh_3)_4$ in 3:1 N_2 degassed mixture of $CH_3CN:H_2O$ 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 $C_{16}H_{10}Br_2$, 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/CH_2I_2/I_2/CuI afforded 7-iodofluoranthene **3**. Sonogashira coupling of **3** with TMS-acetylene in presence of $Pd(PPh_3)_4$/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 NH_4Cl (1.05 g, 19.7 mmol) in H_2O/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 Na_2SO_4, filtered, and evaporated. The residue was purified by column chromatography (20 → 30% EtOAc/hexane) to give **2** (534 mg, 82%) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) 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; ^{13}C NMR (101 MHz, $CDCl_3$) 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

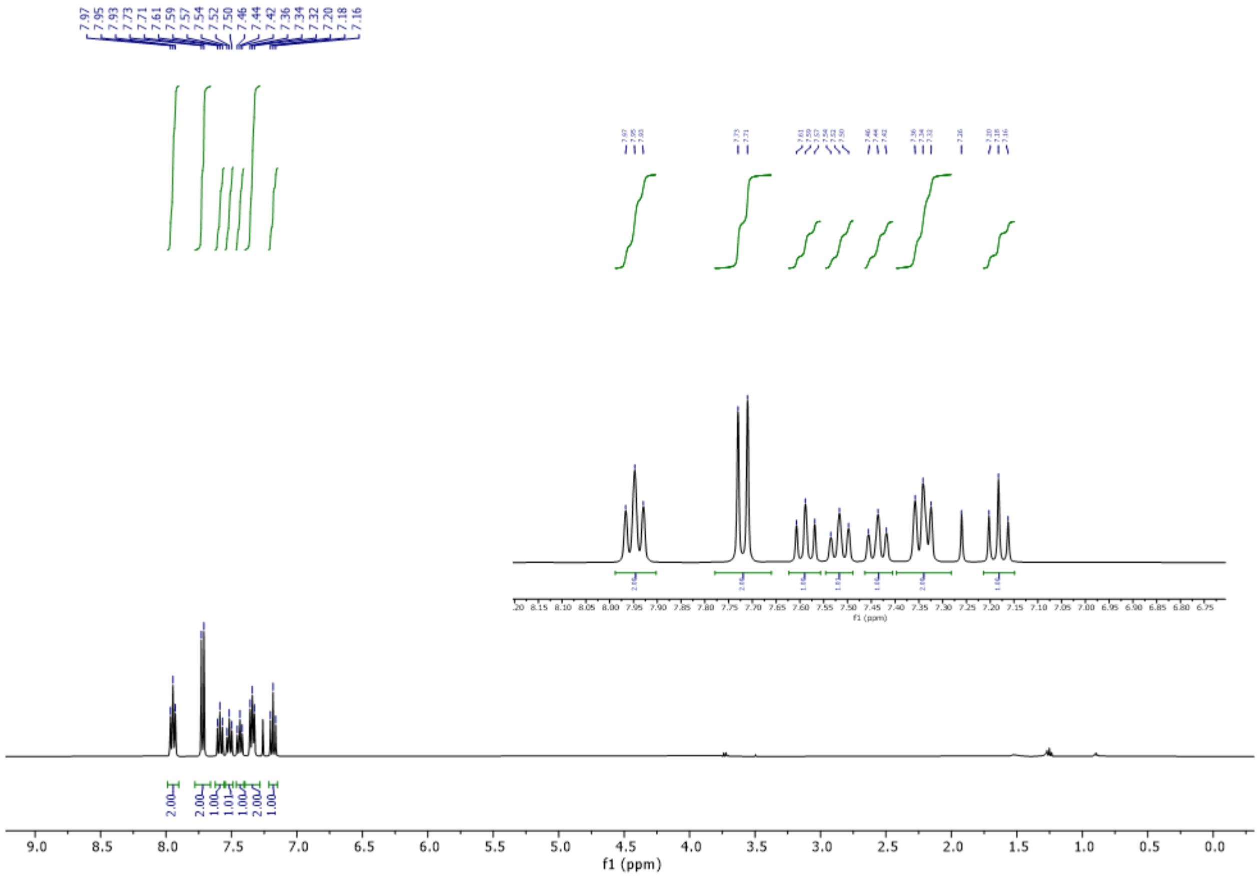
Iodine (467 mg, 1.84 mmol), CuI (420 g, 2.20 mmol), CH_2I_2 (445 µL, 5.52 mmol), and tert-butyl nitrite (660 µL, 5.55 mmol) were added to a solution of **2** (400 mg, 1.84 mmol) in dry THF (15 mL). The reaction mixture was stirred at 66 °C for 30 min, cooled to 24 °C, and filtered. The filtrate was concentrated under reduced pressure and extracted with EtOAc. The organic phase was separated, dried over anhydrous Na_2SO_4, 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. ^{1}H NMR (400 MHz, $CDCl_3$) 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; ^{13}C NMR (101 MHz, $CDCl_3$) 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

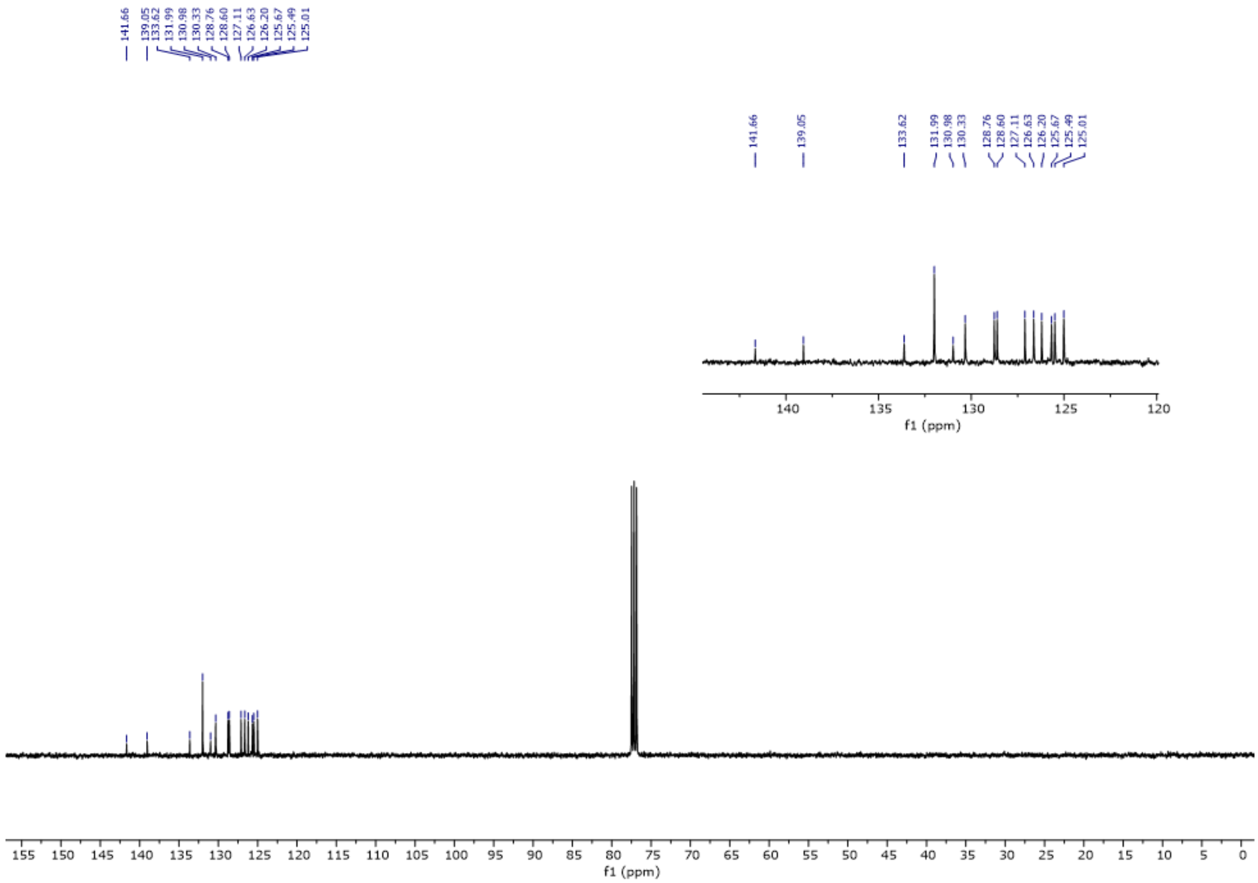
$Pd(PPh_3)_4$ (28.2 mg, 0.024 mmol) and Cu(I)I (9.1 mg, 0.048 mmol) were added to dry Et_3N (10 mL) in a flame-dried flask equipped with a stirring bar under N_2 at 24 °C. Then **3** (400 mg, 1.22 mmol) was added followed by TMS-acetylene (347 µL, 2.44 mmol). The resulting mixture was stirred for 2 h 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%). ^{1}H NMR (400 MHz, $CDCl_3$) 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; ^{13}C NMR (101 MHz, $CDCl_3$) 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

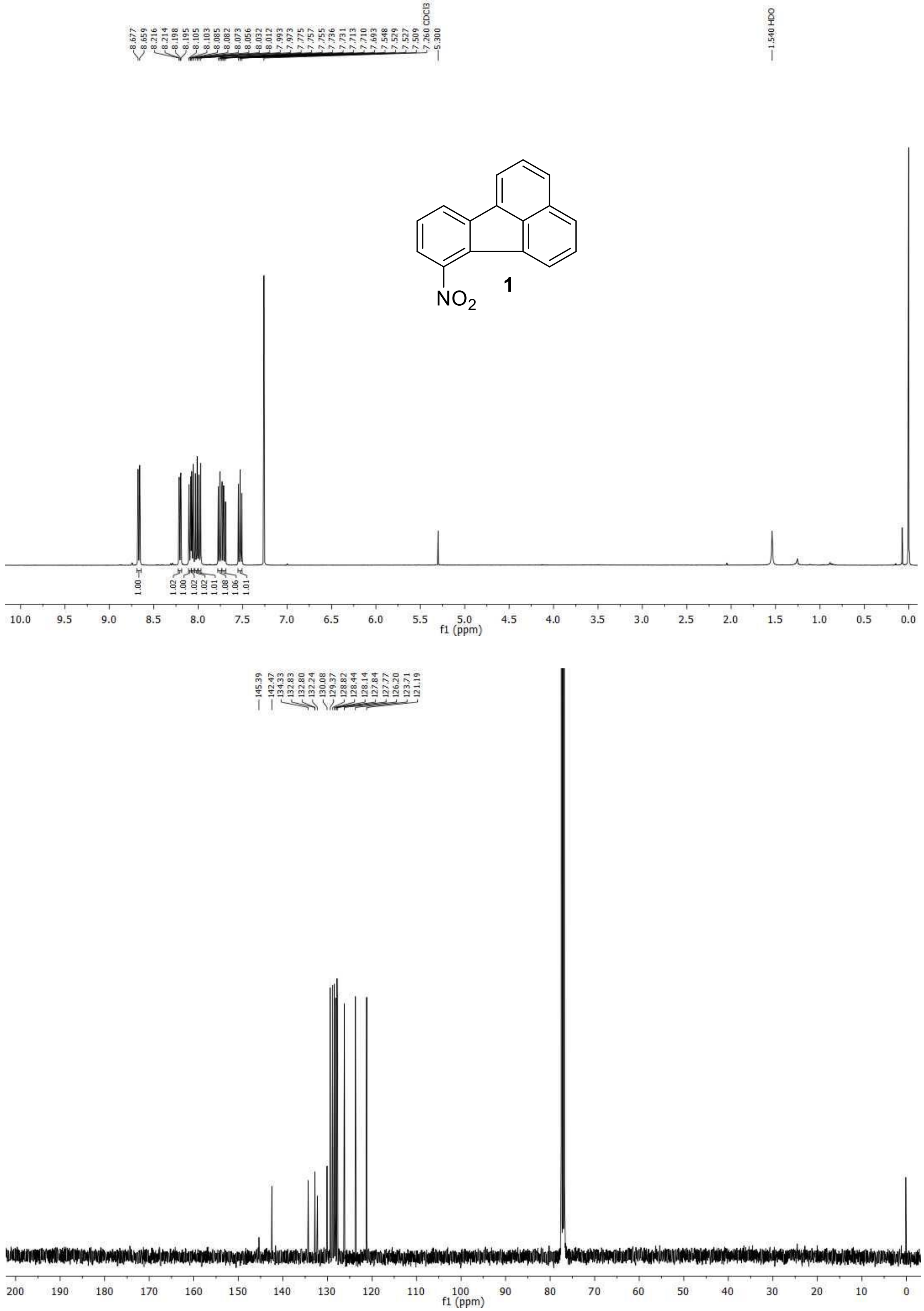
Anhydrous K_2CO_3 (370 mg, 2.68 mmol) was added to a stirred solution of mixture of **4** (200 mg, 0.67 mmol) in dry MeOH/DCM (10 mL, 1:1) at 24 °C. After 2 h, volatiles were evaporated and the residue was column chromatographed (0 → 5% EtOAc/hexane) to give **p2** as an off-white solid (140 mg, 92%). ^{1}H NMR (400 MHz, $CDCl_3$) 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; ^{13}C NMR (101 MHz, $CDCl_3$) 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.



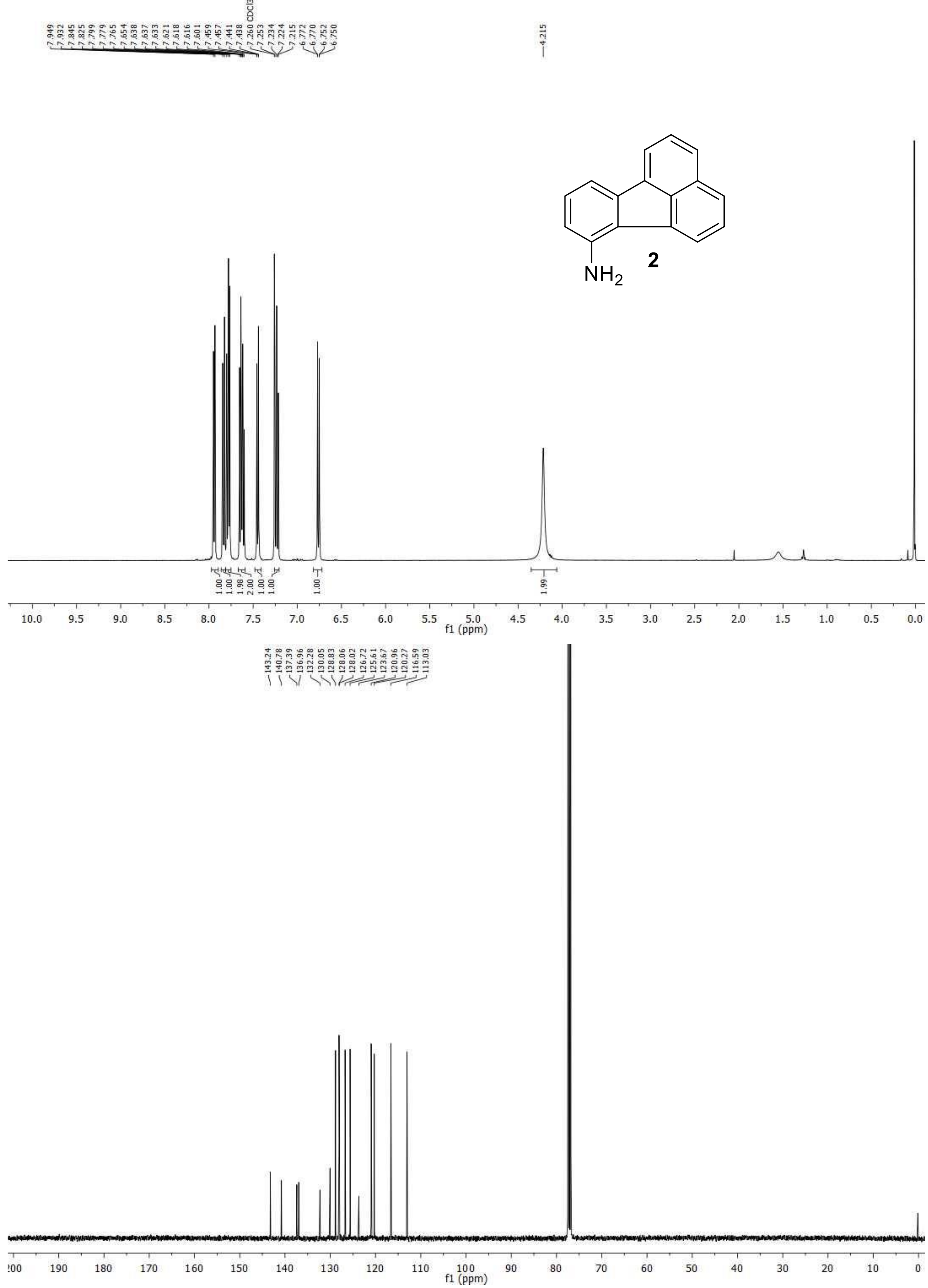
Supplementary Figure 1. ^{1}H NMR spectrum of 1-(2,6-dibromophenyl)naphthalene.



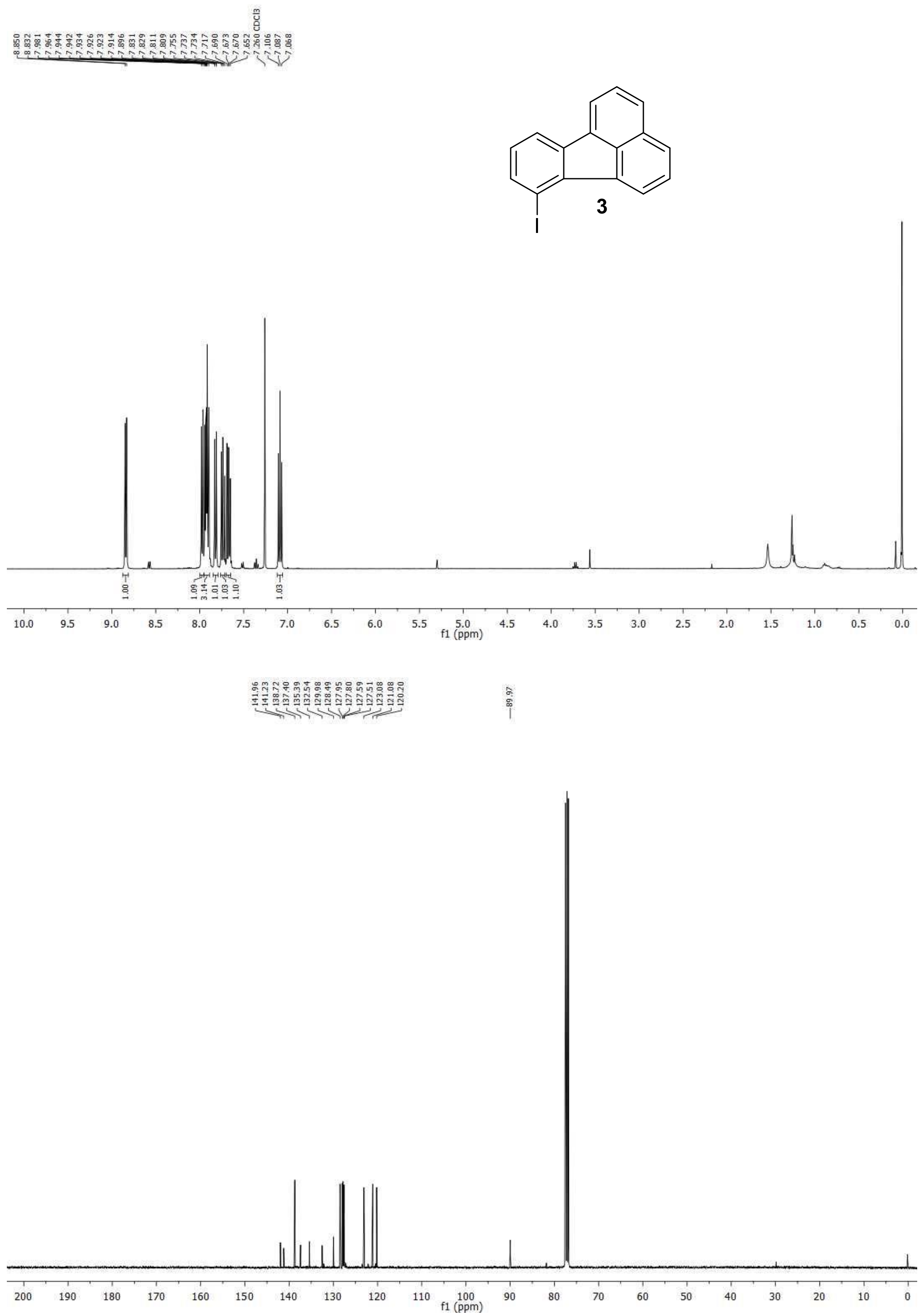
Supplementary Figure 2. ^{13}C NMR spectrum of 1-(2,6-dibromophenyl)naphthalene.



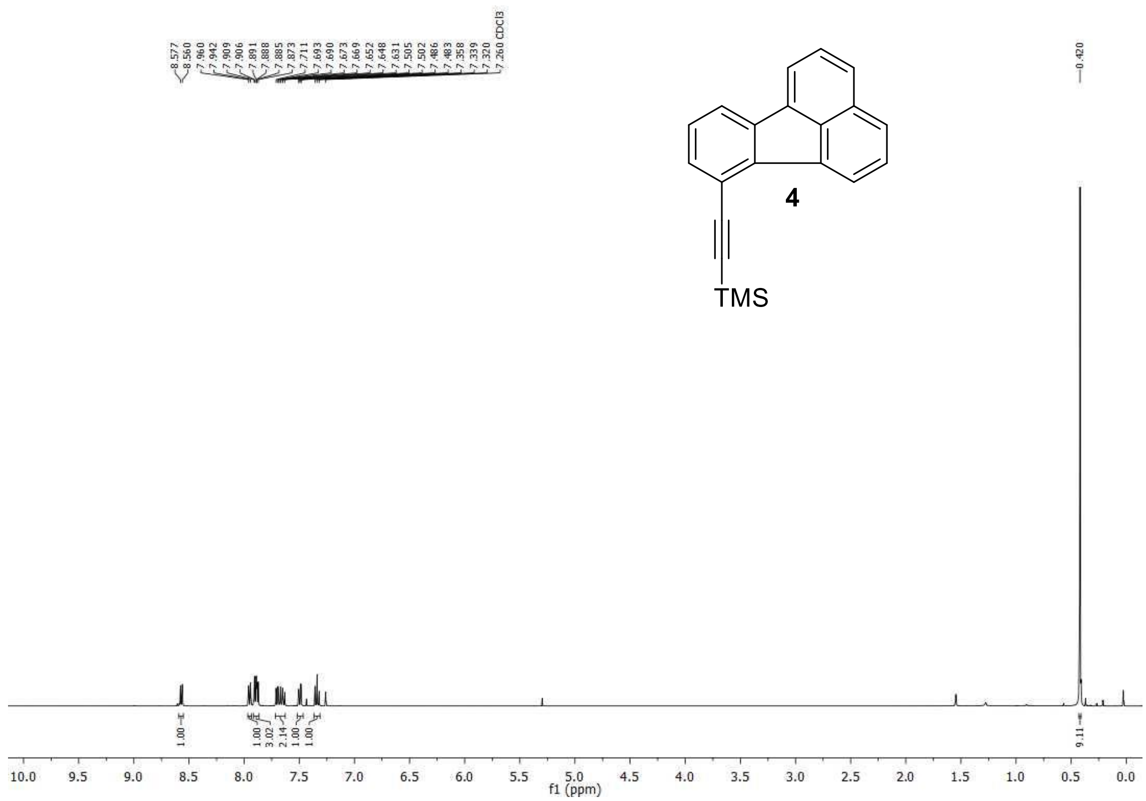
Supplementary Figure 3. ^{1}H NMR and ^{13}C NMR spectra of compound **1** in $CDCl_3$.

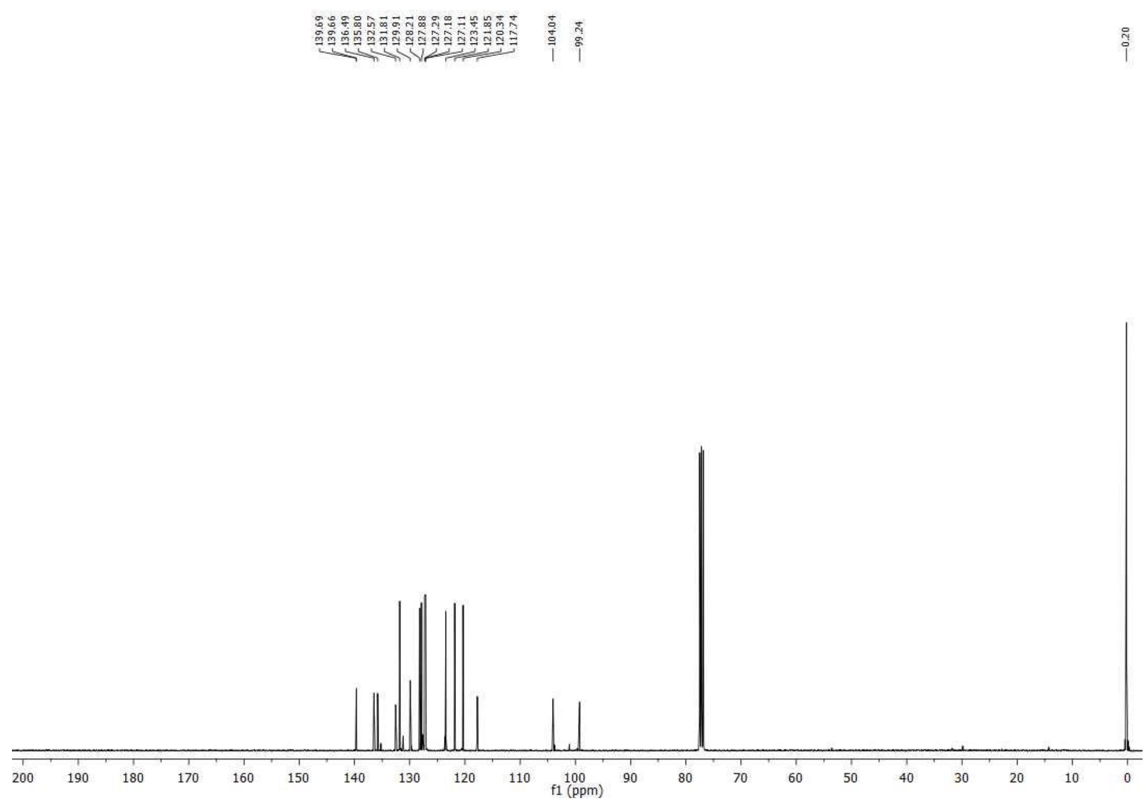


Supplementary Figure 4. ^{1}H NMR and ^{13}C NMR spectra of compound **2** in $CDCl_3$.

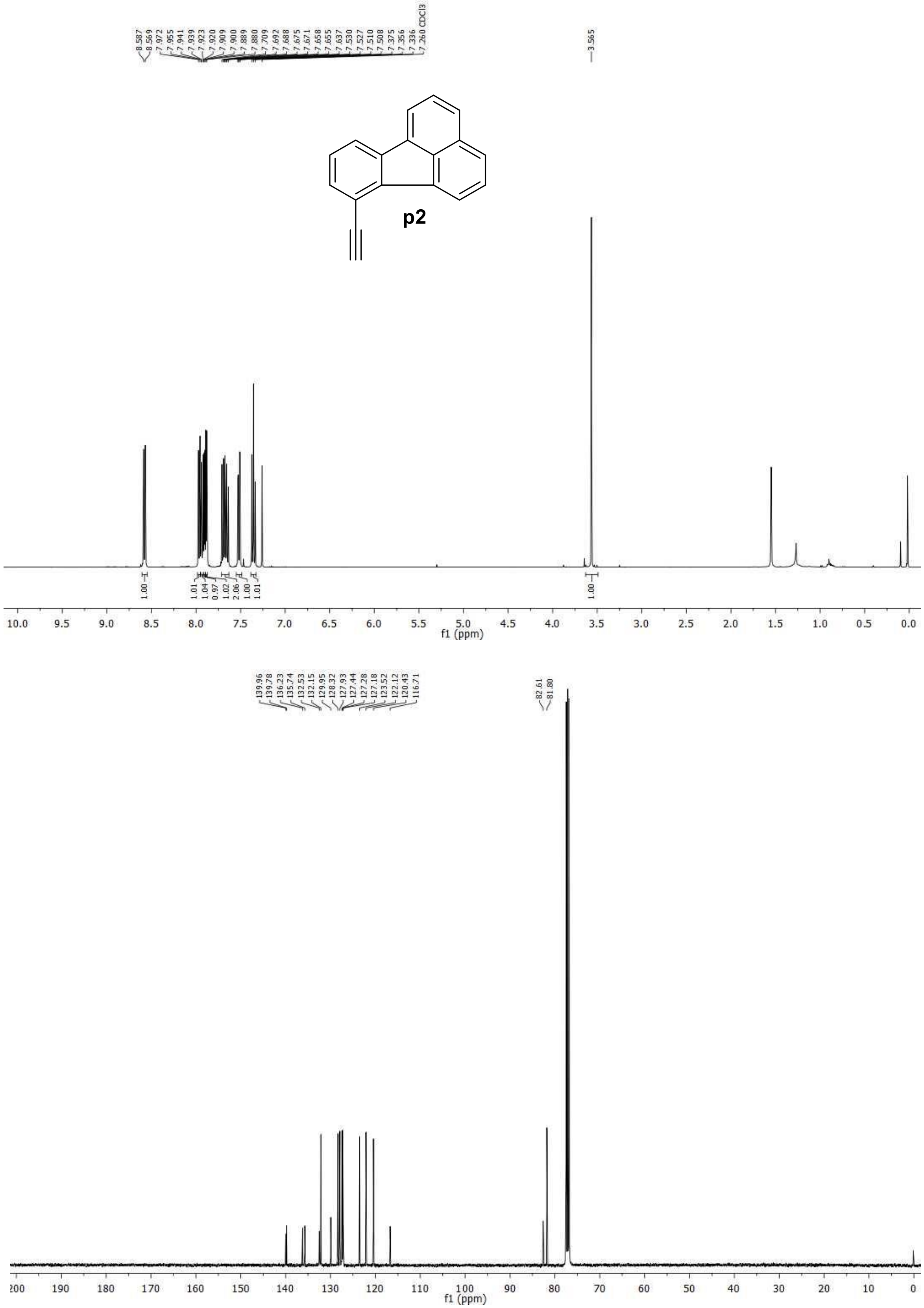


Supplementary Figure 5. ^{1}H NMR and ^{13}C NMR spectra of compound **3** in $CDCl_3$.

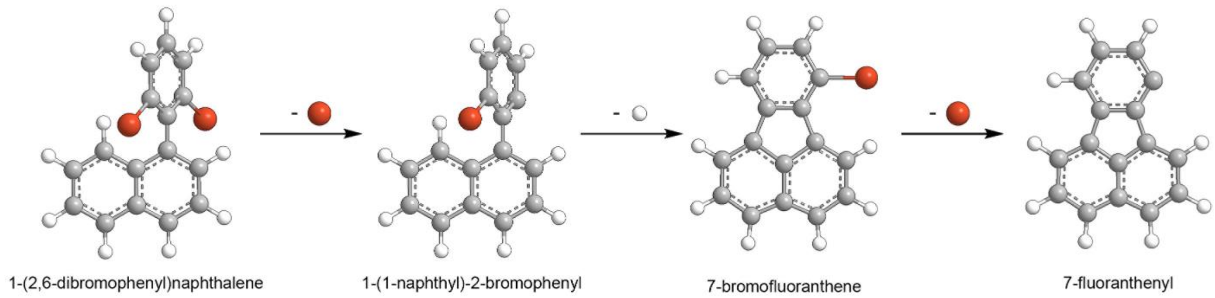




Supplementary Figure 6. ^{1}H NMR and ^{13}C NMR spectra of compound **4** in $CDCl_3$.

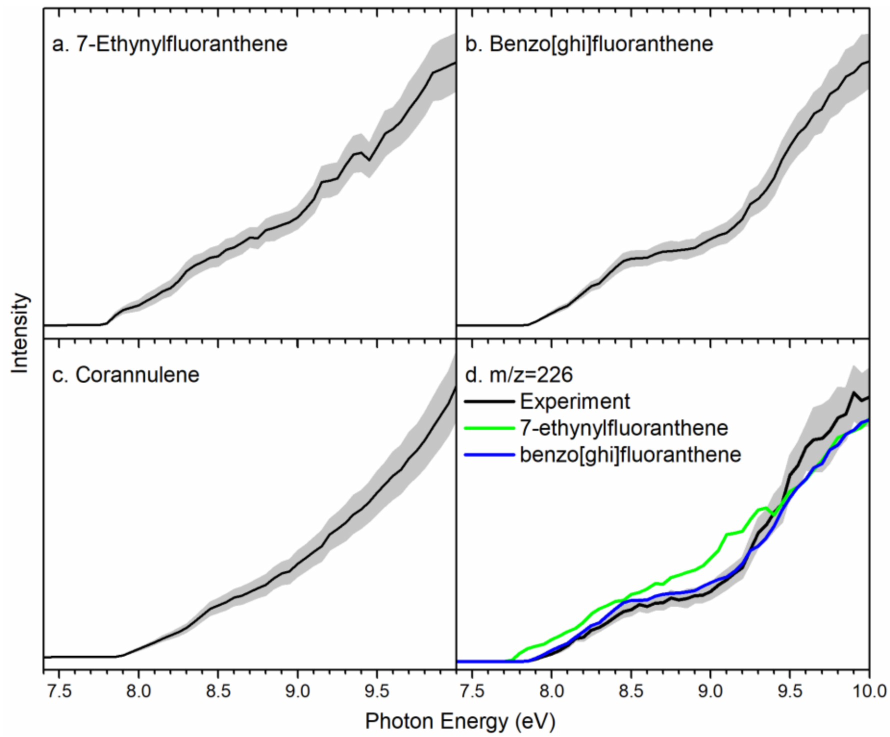


Supplementary Figure 7. ^{1}H NMR and ^{13}C NMR spectra of compound **p2** in $CDCl_3$.



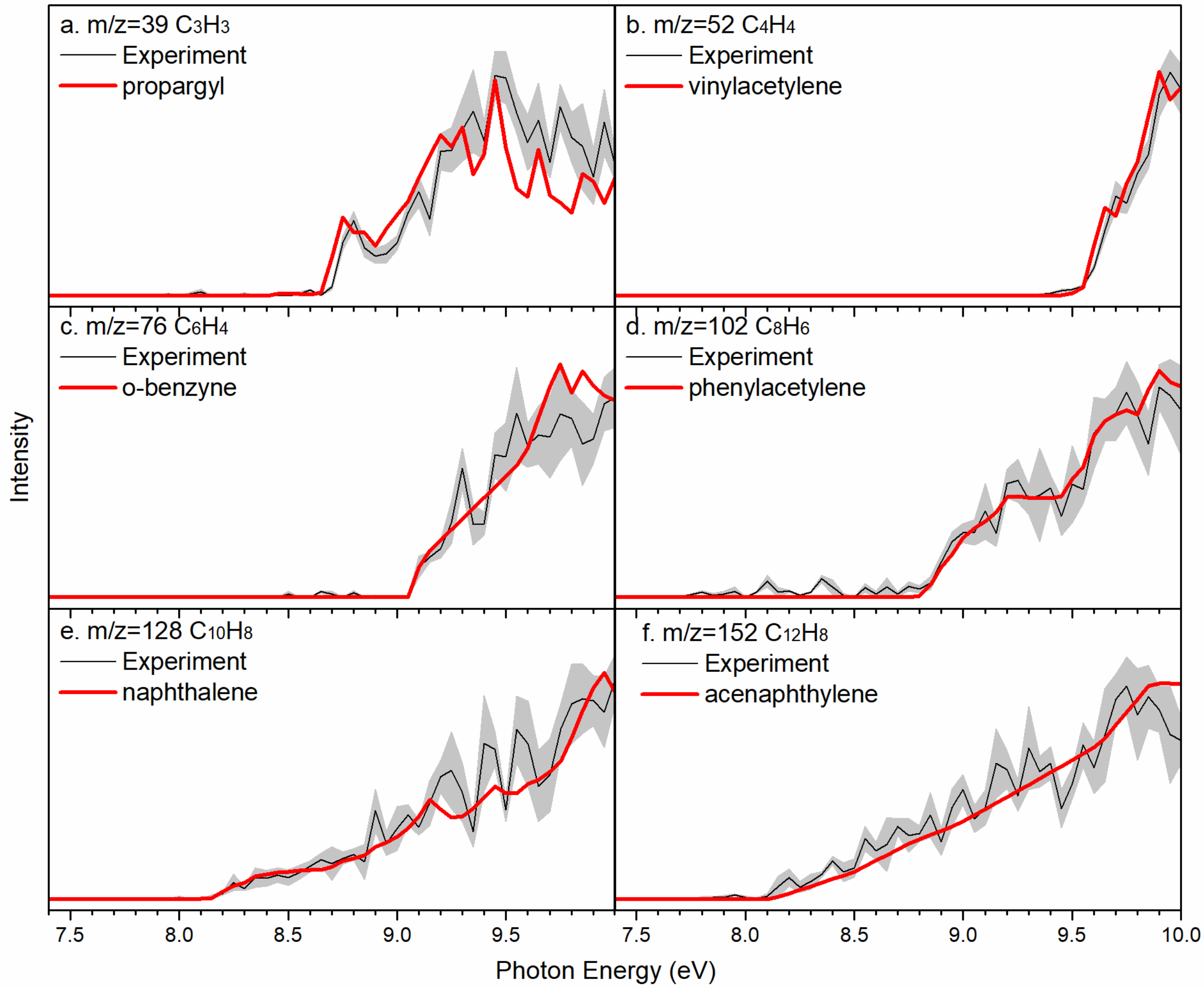
Supplementary Figure 8. Reaction scheme for the pyrolysis of the precursor 1-(2,6-dibromophenyl)naphthalene ($C_{16}H_{10}Br_2$) forming the 7-fluoranthenyl ($C_{16}H_9^{\bullet}$) radical via the 1-(1-naphthyl)-2-bromophenyl radical ($C_{16}H_{10}Br^{\bullet}$) and 7-bromofluoranthene ($C_{16}H_9Br$).

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*.



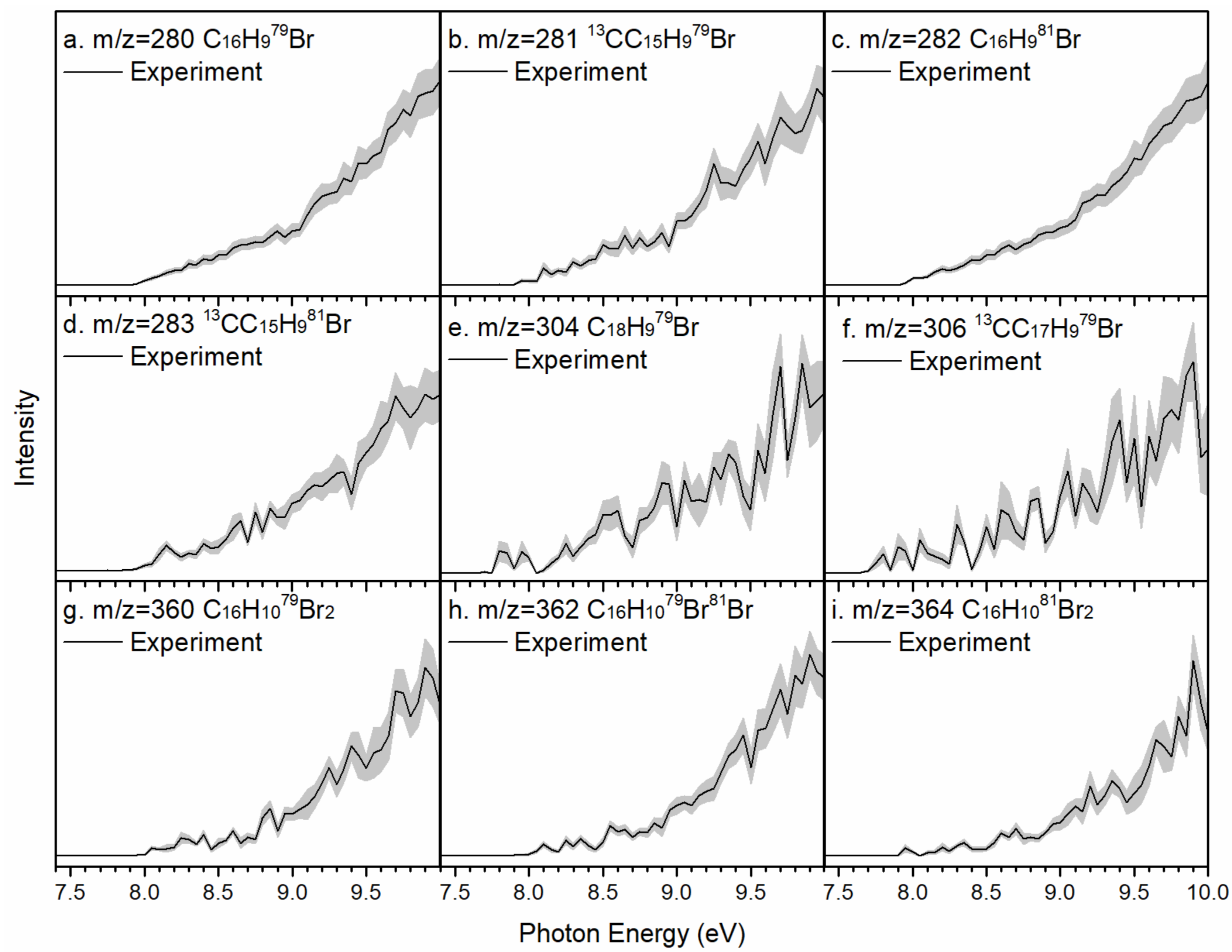
Supplementary Figure 9. PIE calibration curves for 7-ethynylfluorathene, benzo[*ghi*]-fluoranthene and corannulene, along with the comparison between the calibration curves and experimental measurement at m/z = 226.

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-ethynylfluorathene calibration curve alone and experiment data. Combined with Fig. 2 in the manuscript, it is concluded that 7-ethynylfluorathene is just a minor contributor while benzo[*ghi*]fluoranthene the major. The overall error bars consist of two parts: ±10% based on the accuracy of the photodiode and a 1 σ error of the PIE curve averaged over the individual scans.



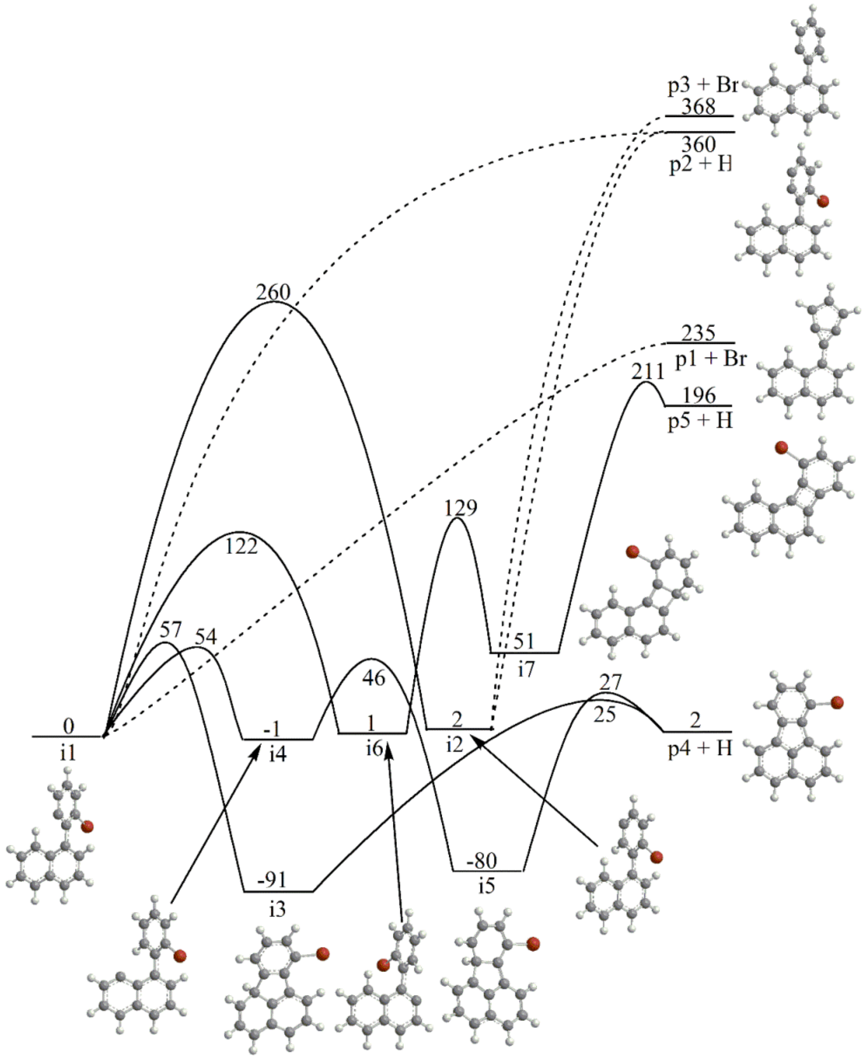
Supplementary Figure 10a. Photoionization efficiency (PIE) curves of distinct ions detected in 1-(2,6-dibromophenyl)naphthalene ($C_{16}H_{10}Br_2$)–acetylene (C_2H_2) system. The black lines shows the experimental measurements along with the error areas labelled in grey. The red lines present the calibration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

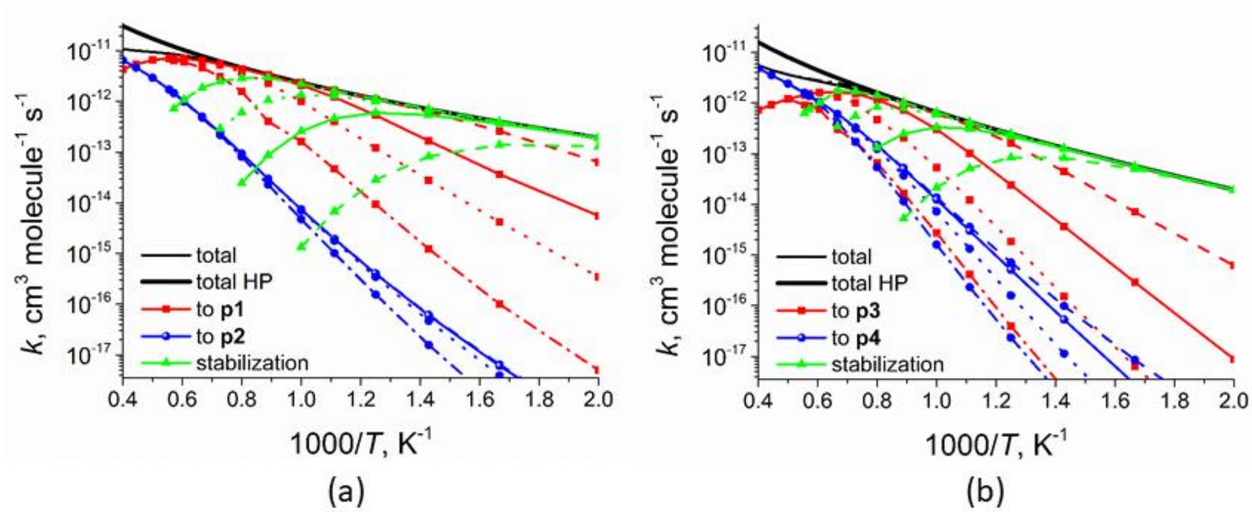


Supplementary Figure 11. B3LYP/6-311G** calculated potential energy diagram for various isomerization and dissociation pathways of the 1-(1-naphthyl)-2-bromophenyl radical produced via a C-Br bond cleavage in the 1-(2,6-dibromophenyl)naphthalene precursor. The energies are given in $kJmol^{-1}$ with 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) / 2.2E-6 (p5 + H) / 3.0E-7 (p1 + Br) / 9.5E-12 (p2 + H) / 4.9E-12 (p3 + Br). This reveals that 7-bromofluoanthene (p4) is the nearly exclusive product. Next, the weakest C-Br bond in 7-bromofluoranthene radical is cleaved in the reactor producing the fluoranthen-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]

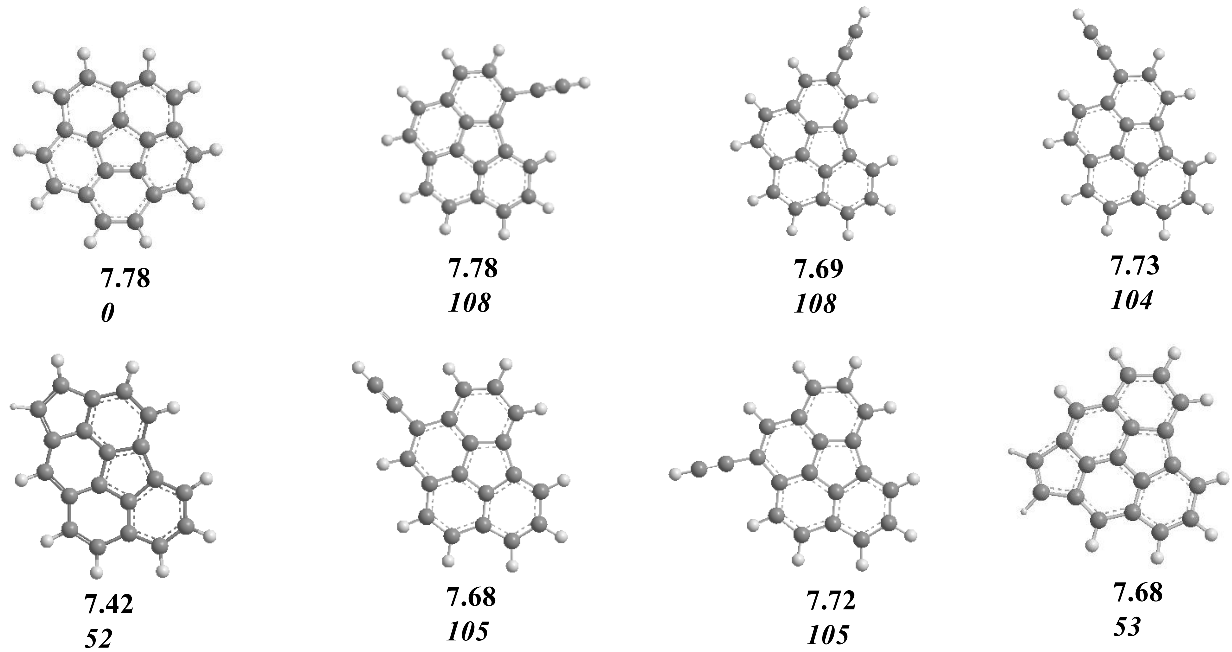
Supplementary Note 2. Rate constants and product branching ratios for C_2H_2 addition reactions

Computed rate constants for the 7-fluoranthenyl + C_2H_2 and benzo[*ghi*]fluoranthen-5-yl+ C_2H_2 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 + C_2H_2 (a) and benzo[*ghi*]fluoranthen-5-yl + C_2H_2 (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} cm^3 molecule^{-1} s^{-1} in the 500–2500 K temperature range for 7-fluoranthenyl + C_2H_2 and benzo[*ghi*]fluoranthen-5-yl + C_2H_2, 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 $C_{20}H_{10}$ isomers calculated at the G3(MP2,CC)//B3LYP level of theory. Distinct $C_{20}H_{10}$ isomers are distinguishable, which 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 + C_2H_2 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
```

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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
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H  2.6952707616   -3.0112688594   0.2218773203
H  -3.974644443   -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
Core  RigidRotor
SymmetryFactor  1.0
End
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
ZeroEnergy[kcal/mol] -75.0
ElectronicLevels[1/cm]        1
0  2
End
End
!-----------------------------------
!-------fl_i4------------
Well        i4
Species
RRHO
Geometry[angstrom]   29
C  -0.7554633883   -1.233079212   0.0526156337
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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
```

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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
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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
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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
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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
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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
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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
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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
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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
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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 + C_2H_2 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: cm^3/sec

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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	1.16159e+07	1.16866e+07
400	5.88335e+07	8.96268e+07	323.425	4.23634e-09	44.3849	4.66368e-07	1.48461e+08	1.55461e+08
500	2.50561e+08	4.86293e+08	29513.5	0.000134931	3355.14	0.00361755	7.36887e+08	8.64485e+08
600	6.35219e+08	1.40337e+09	512706	0.113255	110760	1.23311	2.03921e+09	2.8419e+09
700	***	1.14533e+09	7.66625e+06	13.153	1.50967e+06	83.7544	1.1545e+09	6.79854e+09
800	***	2.1144e+09	1.26991e+07	323.569	3.37289e+07	1322.69	2.16083e+09	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 = 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	1.16682e+07	1.16866e+07
400	6.13157e+07	9.31475e+07	40.1773	1.47854e-09	5.09833	1.14111e-07	1.54459e+08	1.55461e+08

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	3.18268e-05
500	***	***	1.68509e-05	1.15408e-18	0.143631	3.25291e-17	0.143648	0.14429
600	***	***	0.00936058	4.24404e-13	41.3947	5.15224e-12	41.4041	41.7669
700	***	***	0.542994	2.18308e-09	2360.76	1.62052e-08	2361.3	2478.18
800	***	***	***	6.70684e-07	43067.8	3.63343e-06	43067.8	54222.2
900	***	***	***	3.09676e-05	313882	0.000134122	313881	607471
1000	***	***	***	0.000430622	1.17186e+06	0.00156746	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	41.5715	41.7669
700	***	***	1.65027	1.43543e-08	2459.1	6.21505e-08	2460.75	2478.18
800	***	***	43.8763	1.40187e-05	52980.3	3.92062e-05	53024.2	54222.2
900	***	***	452.66	0.00209081	555335	0.00438895	555788	607471
1000	***	***	***	0.0766226	3.2495e+06	0.13222	3.24945e+06	4.24808e+06
1125	***	***	***	1.73361	1.52739e+07	2.51798	1.52733e+07	3.00726e+07
1250	***	***	***	14.918	4.32818e+07	19.0868	4.32784e+07	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 = 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	50.3463	50.662
500	***	***	199.038	1.34004e-15	9960.54	1.38404e-13	10159.6	10884.9
600	***	***	7232.26	7.92905e-12	272392	2.89679e-10	279624	422035
700	***	***	59091.6	3.82709e-09	1.89686e+06	4.75525e-08	1.95595e+06	6.01766e+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	10815	10884.9
600	0.826919	***	11656	4.98713e-09	393221	5.53892e-08	404878	422035
700	***	***	181805	3.40177e-06	4.72209e+06	2.40288e-05	4.90389e+06	6.01766e+06
800	***	***	1.11424e+06	0.00025953	2.45876e+07	0.00130506	2.57019e+07	4.5432e+07
900	***	***	3.58154e+06	0.00646983	7.3273e+07	0.0228285	7.68545e+07	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 = 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	10848.7	10884.9
600	2.09493	0.393408	12211.1	1.72911e-08	406648	1.11898e-07	418861	422035
700	***	169.987	225913	4.01127e-05	5.59342e+06	0.000153181	5.81951e+06	6.01766e+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	1.60156e+08	2.23144e+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	420498	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	2.10466e+08	2.23144e+08
1000	***	484545	4.63458e+07	54.7874	6.53462e+08	62.8265	7.00292e+08	8.08173e+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	4.86096e+09	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 = 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-> Capture	
300	3.46867e-20	1.42871e-20	1.71537e-14	3.33886e-17	6.30453e-16	1.59746e-22	1.78176e-14	1.77273e-14
400	1.65877e-20	***	6.51039e-14	3.42841e-17	8.51627e-15	1.26213e-20	7.36545e-14	7.32052e-14
500	***	***	1.30354e-13	1.2814e-17	6.43239e-14	4.0058e-19	1.94691e-13	1.93371e-13
600	***	***	1.40851e-13	3.39167e-18	2.61387e-13	6.43607e-18	4.02248e-13	3.99329e-13
700	***	***	8.27193e-14	1.23721e-18	6.30252e-13	6.20368e-17	7.13034e-13	7.07631e-13
800	***	***	2.86958e-14	***	1.1107e-12	4.05577e-16	1.1398e-12	1.1311e-12
900	***	***	6.83549e-15	***	1.68269e-12	1.96206e-15	1.69149e-12	1.67972e-12
1000	***	***	1.35198e-15	***	2.36297e-12	7.46496e-15	2.37179e-12	2.36131e-12
1125	***	***	***	***	3.3631e-12	3.01404e-14	3.39324e-12	3.4096e-12
1250	***	***	***	***	4.46576e-12	9.44245e-14	4.56018e-12	4.68473e-12
1375	***	***	***	***	5.54043e-12	2.38944e-13	5.77937e-12	6.19395e-12
1500	***	***	***	***	6.42197e-12	5.04963e-13	6.92694e-12	7.94294e-12
1650	***	***	***	***	7.03958e-12	1.01985e-12	8.05944e-12	1.03644e-11
1750	***	***	***	***	7.14693e-12	1.48096e-12	8.62789e-12	1.21771e-11
1800	***	***	***	***	7.11565e-12	1.74279e-12	8.85844e-12	1.31436e-11
2000	***	***	***	***	6.56523e-12	2.94999e-12	9.51521e-12	1.74134e-11
2250	***	***	***	***	5.42675e-12	4.67868e-12	1.01054e-11	2.36688e-11
2500	***	***	***	***	4.32972e-12	6.53322e-12	1.08629e-11	3.09552e-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-> Capture	
300	2.88242e-15	1.17085e-15	1.36507e-14	1.1582e-16	1.88438e-17	8.13124e-23	1.78176e-14	1.77273e-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	4.02248e-13	3.99329e-13
700	***	***	5.43903e-13	1.16709e-15	1.67905e-13	6.0078e-17	7.13035e-13	7.07631e-13
800	***	***	6.00119e-13	4.2203e-16	5.38865e-13	3.9856e-16	1.13981e-12	1.1311e-12
900	***	***	4.66861e-13	1.51655e-16	1.22255e-12	1.94261e-15	1.69151e-12	1.67972e-12
1000	***	***	2.59786e-13	***	2.10463e-12	7.4212e-15	2.37185e-12	2.36131e-12
1125	***	***	8.87127e-14	***	3.27462e-12	3.00456e-14	3.39338e-12	3.4096e-12
1250	***	***	2.45496e-14	***	4.44166e-12	9.42613e-14	4.56047e-12	4.68473e-12
1375	***	***	***	***	5.54111e-12	2.38716e-13	5.77983e-12	6.19395e-12
1500	***	***	***	***	6.42282e-12	5.04701e-13	6.92752e-12	7.94294e-12
1650	***	***	***	***	7.04043e-12	1.01961e-12	8.06004e-12	1.03644e-11
1750	***	***	***	***	7.14769e-12	1.48075e-12	8.62844e-12	1.21771e-11
1800	***	***	***	***	7.11635e-12	1.7426e-12	8.85895e-12	1.31436e-11
2000	***	***	***	***	6.56563e-12	2.94988e-12	9.51552e-12	1.74134e-11
2250	***	***	***	***	5.42691e-12	4.67864e-12	1.01056e-11	2.36688e-11
2500	***	***	***	***	4.32977e-12	6.5332e-12	1.0863e-11	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->Capture	
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	7.13043e-13	7.07631e-13
800	***	6.64425e-14	9.35852e-13	1.50853e-14	1.22122e-13	3.45945e-16	1.13985e-12	1.1311e-12
900	***	***	1.27968e-12	1.09851e-14	3.99221e-13	1.78676e-15	1.69167e-12	1.67972e-12
1000	***	***	1.34906e-12	6.16637e-15	1.01004e-12	7.05224e-15	2.37231e-12	2.36131e-12
1125	***	***	1.06146e-12	***	2.30395e-12	2.9209e-14	3.39468e-12	3.4096e-12
1250	***	***	6.18256e-13	***	3.85202e-12	9.27847e-14	4.56312e-12	4.68473e-12
1375	***	***	2.92631e-13	***	5.25471e-12	2.3663e-13	5.78404e-12	6.19395e-12
1500	***	***	***	***	6.43059e-12	5.02287e-13	6.93288e-12	7.94294e-12
1650	***	***	***	***	7.04832e-12	1.01731e-12	8.06564e-12	1.03644e-11
1750	***	***	***	***	7.15473e-12	1.47878e-12	8.63351e-12	1.21771e-11
1800	***	***	***	***	7.12279e-12	1.74084e-12	8.86363e-12	1.31436e-11
2000	***	***	***	***	6.56943e-12	2.94892e-12	9.51835e-12	1.74134e-11
2250	***	***	***	***	5.42838e-12	4.6783e-12	1.01067e-11	2.36688e-11
2500	***	***	***	***	4.33024e-12	6.53311e-12	1.08633e-11	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->Capture	
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	1.69246e-12	1.67972e-12
1000	***	1.08901e-12	1.05729e-12	6.12158e-14	1.62839e-13	4.79075e-15	2.37514e-12	2.36131e-12
1125	***	1.13562e-12	1.76899e-12	7.10895e-14	4.05449e-13	2.29682e-14	3.40411e-12	3.4096e-12
1250	***	***	2.82904e-12	7.98427e-14	1.59378e-12	8.12586e-14	4.58392e-12	4.68473e-12
1375	***	***	2.50165e-12	***	3.09841e-12	2.19044e-13	5.81972e-12	6.19395e-12
1500	***	***	1.86505e-12	***	4.63392e-12	4.80879e-13	6.98062e-12	7.94294e-12
1650	***	***	1.10403e-12	***	6.01543e-12	9.96276e-13	8.11719e-12	1.03644e-11
1750	***	***	7.19066e-13	***	6.49996e-12	1.4605e-12	8.68089e-12	1.21771e-11
1800	***	***	***	***	7.18264e-12	1.72452e-12	8.90716e-12	1.31436e-11
2000	***	***	***	***	6.60502e-12	2.93992e-12	9.54494e-12	1.74134e-11
2250	***	***	***	***	5.4422e-12	4.67513e-12	1.01173e-11	2.36688e-11
2500	***	***	***	***	4.33469e-12	6.53219e-12	1.08669e-11	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	2.42056e-14
400	5.93614e-25	***	1.43407e-13	3.18485e-16	1.68735e-36	8.64596e-35	1.43726e-13	1.44301e-13
500	***	***	4.56868e-13	2.68226e-15	1.81145e-30	2.37734e-29	4.5955e-13	4.61772e-13
600	***	***	1.04166e-12	8.83449e-15	1.9819e-26	1.18851e-25	1.05049e-12	1.0639e-12
700	***	***	1.88122e-12	1.28783e-14	1.32543e-23	4.64705e-23	1.8941e-12	2.01446e-12
800	***	***	2.58982e-12	***	1.56103e-21	3.54712e-21	2.58983e-12	3.35692e-12
900	***	***	2.51805e-12	***	6.11562e-20	9.66917e-20	2.51806e-12	5.11971e-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->Capture	
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	2.42056e-14
400	3.83165e-27	2.99881e-26	1.43408e-13	3.19607e-16	2.7737e-39	8.34569e-38	1.43727e-13	1.44301e-13
500	8.81312e-24	2.17077e-23	4.56953e-13	2.86257e-15	9.66838e-33	8.61724e-32	4.59816e-13	4.61772e-13
600	1.91818e-21	3.14413e-21	1.04586e-12	1.32337e-14	3.17371e-28	1.33692e-27	1.0591e-12	1.0639e-12
700	***	2.17624e-19	1.96312e-12	4.04379e-14	5.92011e-25	1.48848e-24	2.00355e-12	2.01446e-12
800	***	9.81576e-18	3.23435e-12	8.95144e-14	1.71636e-22	2.90188e-22	3.32387e-12	3.35692e-12
900	***	***	4.84058e-12	1.47521e-13	1.45094e-20	1.83281e-20	4.9881e-12	5.11971e-12
1000	***	***	6.63264e-12	1.86649e-13	4.8846e-19	4.90985e-19	6.81929e-12	7.32044e-12
1125	***	***	8.50353e-12	***	1.45827e-17	1.18549e-17	8.50398e-12	1.07018e-11
1250	***	***	8.98725e-12	***	1.8788e-16	1.29163e-16	8.98851e-12	1.47902e-11
1375	***	***	7.85198e-12	***	1.34522e-15	8.0542e-16	7.85601e-12	1.95842e-11

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	2.42056e-14
400	2.57066e-28	3.44652e-27	1.43408e-13	3.19611e-16	2.90926e-41	8.13027e-40	1.43727e-13	1.44301e-13
500	7.61101e-25	3.17604e-24	4.56954e-13	2.86347e-15	1.40433e-34	1.12904e-33	4.59817e-13	4.61772e-13
600	2.47751e-22	5.29116e-22	1.04588e-12	1.32848e-14	7.6236e-30	2.84622e-29	1.05916e-12	1.0639e-12
700	1.95414e-20	3.00519e-20	1.96345e-12	4.15251e-14	2.58975e-26	5.7632e-26	2.00498e-12	2.01446e-12
800	5.49009e-19	8.93736e-19	3.23906e-12	9.97712e-14	1.32002e-23	2.01921e-23	3.33884e-12	3.35692e-12
900	***	1.82014e-17	4.88283e-12	1.96304e-13	1.6993e-21	1.94594e-21	5.07916e-12	5.11971e-12
1000	***	1.83193e-16	6.88011e-12	3.24881e-13	7.875e-20	7.12103e-20	7.20517e-12	7.32044e-12
1125	***	4.3466e-15	9.75347e-12	4.88631e-13	2.56625e-18	1.53879e-18	1.02464e-11	1.07018e-11
1250	***	***	1.26573e-11	5.89501e-13	7.77357e-17	5.01355e-17	1.32469e-11	1.47902e-11
1375	***	***	1.48811e-11	***	7.93199e-16	4.52002e-16	1.4886e-11	1.95842e-11
1500	***	***	1.56065e-11	***	4.67332e-15	2.3988e-15	1.562e-11	2.50763e-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	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->Capture	
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	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 7.27951e-16
400 7.12958e-15 1.91146e-15 1.40452e-15 2.25358e-17 3.45459e-24 5.06003e-19
1.04685e-14 1.05306e-14
500 2.65697e-14 1.07465e-14 2.01552e-14 4.04818e-16 2.1339e-21 3.92102e-17
5.79154e-14 5.8281e-14
600 4.93728e-14 2.81702e-14 1.1124e-13 2.8286e-15 2.29982e-19 1.03639e-15
1.92648e-13 1.9392e-13
700 *** 9.59799e-14 3.56853e-13 8.90607e-15 7.87285e-18 1.1871e-14 4.73618e-
13 4.76861e-13
800 *** 9.70816e-14 7.72192e-13 1.46528e-14 1.23653e-16 7.38011e-14 9.57851e-
13 9.64711e-13
900 *** *** 1.36066e-12 1.47661e-14 1.12417e-15 3.17285e-13 1.69384e-12
1.70707e-12
1000 *** *** 1.71477e-12 1.05036e-14 6.84871e-15 9.85959e-13 2.71808e-12
2.74352e-12
1125 *** *** 1.64029e-12 *** 4.2914e-14 2.75181e-12 4.43509e-12
4.49725e-12
1250 *** *** 1.12645e-12 *** 1.86535e-13 5.32391e-12 6.63701e-12
6.79648e-12
1375 *** *** 6.10029e-13 *** 6.06336e-13 8.06161e-12 9.27813e-12
9.66512e-12
1500 *** *** *** *** 1.55766e-12 1.07238e-11 1.22815e-11
1.31151e-11
1650 *** *** *** *** 3.77252e-12 1.24943e-11 1.62668e-11
1.8027e-11
1750 *** *** *** *** 6.03634e-12 1.30971e-11 1.91335e-11
2.1767e-11
1800 *** *** *** *** 7.41339e-12 1.32196e-11 2.0633e-11
2.37755e-11
2000 *** *** *** *** 1.44317e-11 1.27153e-11 2.7147e-11
3.27187e-11
2250 *** *** *** *** 2.58857e-11 1.08208e-11 3.67065e-11
4.58902e-11
2500 *** *** *** *** 3.93213e-11 8.74311e-12 4.80644e-11
6.11836e-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*]fluoranthen-5-yl + C_2H_2 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
```

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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
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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
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   0.1117814481
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
```

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!-----------------------------------
!-------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
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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
```

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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
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```
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
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 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
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```
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*]fluoranthen-5-yl + C_2H_2 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: cm^3/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-> Capture	
300	1001.12	-0.472371	0.000649719	5.84158e-18	8.23923e-10	1.88433e-14	1001.12	1061.73
400	75038.3	4.99801	3.78912	8.4476e-10	9.65279e-05	1.55214e-07	75047.1	75687.6
500	1.70043e+06	1935.18	696.879	6.84636e-05	0.249824	0.00245748	1.70307e+06	1.73455e+06
600	1.5584e+07	116073	22181.9	0.123705	74.9668	1.57128	1.57223e+07	1.68215e+07
700	7.34331e+07	1.90316e+06	248858	24.7968	5404.5	154.157	7.55907e+07	9.20719e+07
800	2.15191e+08	1.26055e+07	1.37416e+06	1216.97	132411	4557.44	2.29309e+08	3.43141e+08
900	***	1.0397e+08	3.88828e+06	23809	1.50369e+06	60527.1	1.09446e+08	9.78688e+08
1000	***	2.21695e+08	8.4014e+06	230040	9.12525e+06	449290	2.39901e+08	2.30211e+09
1125	***	4.32514e+08	1.4924e+07	1.95854e+06	5.49509e+07	3.0077e+06	5.07355e+08	5.51165e+09
1250	***	5.47851e+08	***	1.01172e+07	4.0558e+08	1.29523e+07	8.88585e+08	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 = 100 atm

T(K)	ip1->ip2	ip1->ip3	ip1->ip4	ip1->p0	ip1->p1	ip1->p2	ip1-> Capture	
300	1001.14	5.98673e-05	0.000649778	5.88391e-18	8.22811e-11	1.88944e-14	1001.14	1061.73
400	75098.4	0.0338345	3.79275	8.65263e-10	9.63149e-06	1.57052e-07	75102.7	75687.6
500	1.71801e+06	200.667	701.947	7.34523e-05	0.0250587	0.00256643	1.71891e+06	1.73455e+06

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-> Capture	
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-> Capture	
300	5.32285e-11	5.30406e-16	4.06181e-06	6.30344e-31	0.000127214	4.42158e-28	0.000131276	0.000132346
400	5.75858e-05	6.022e-09	0.0245645	1.03174e-19	2.3414	6.34869e-18	2.36602	2.37073
500	0.260013	0.00020963	14.7908	1.18232e-12	964.816	1.89832e-11	979.868	981.91
600	73.6486	0.307871	1386.07	9.38803e-08	57001.2	6.4764e-07	58461.2	58590.8
700	4202.52	62.5302	38975.7	0.000375348	1.08986e+06	0.00145133	1.1331e+06	1.13658e+06
800	86293.5	3253.3	495535	0.204873	1.01688e+07	0.521057	1.07539e+07	1.08384e+07
900	874825	62256.2	3.61205e+06	26.6207	5.78928e+07	49.5608	6.2442e+07	6.40921e+07
1000	5.25609e+06	560118	1.72699e+07	1146.03	2.27596e+08	1685.87	2.50685e+08	2.70477e+08
1125	2.81671e+07	3.98865e+06	7.61152e+07	37952.8	8.35907e+08	44873.6	9.4426e+08	1.16397e+09
1250	1.13742e+08	***	2.19578e+08	397052	2.16302e+09	406305	2.49714e+09	3.80434e+09
1375	2.89011e+08	***	4.68766e+08	1.53414e+06	4.37799e+09	1.44476e+06	5.13875e+09	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 = 0.0394737 atm

T(K)	p0->ip1	p0->ip2	p0->ip3	p0->ip4	p0->p1	p0->p2	p0-> Capture	
300	2.79883e-16	8.47226e-17	7.29831e-17	8.85775e-19	1.36917e-19	1.19655e-23	4.38611e-16	4.41869e-16
400	1.77477e-15	5.50146e-16	1.99361e-15	2.38305e-17	2.0822e-17	5.00068e-21	4.36316e-15	4.39123e-15
500	2.83405e-15	1.00431e-15	1.48711e-14	1.11287e-16	6.17456e-16	3.63419e-19	1.94386e-14	1.9549e-14

600	2.40686e-15	***	4.70308e-14	1.25807e-16	7.12875e-15	8.52476e-18	5.67007e-14	5.69914e-14
700	9.31626e-16	***	8.22092e-14	5.51034e-17	4.50082e-14	9.8933e-17	1.28303e-13	1.28933e-13
800	***	***	8.41537e-14	1.91108e-17	1.60898e-13	7.13415e-16	2.45784e-13	2.47195e-13
900	***	***	5.14935e-14	***	3.63349e-13	3.60292e-15	4.18446e-13	4.22487e-13
1000	***	***	2.14755e-14	***	6.15514e-13	1.3701e-14	6.50691e-13	6.64187e-13
1125	***	***	5.28397e-15	***	9.59193e-13	5.24731e-14	1.01695e-12	1.07187e-12
1250	***	***	***	***	1.28656e-12	1.48905e-13	1.43546e-12	1.60904e-12
1375	***	***	***	***	1.52598e-12	3.31854e-13	1.85783e-12	2.28646e-12
1500	***	***	***	***	1.63509e-12	6.12463e-13	2.24755e-12	3.11296e-12
1650	***	***	***	***	1.60114e-12	1.06327e-12	2.66441e-12	4.3116e-12
1750	***	***	***	***	1.51e-12	1.41654e-12	2.92655e-12	5.24078e-12
1800	***	***	***	***	1.45286e-12	1.60526e-12	3.05811e-12	5.74535e-12
2000	***	***	***	***	1.20146e-12	2.42229e-12	3.62375e-12	8.03651e-12
2250	***	***	***	***	9.26876e-13	3.56377e-12	4.49065e-12	1.15307e-11
2500	***	***	***	***	7.32553e-13	4.84774e-12	5.58029e-12	1.57451e-11

Pressure = 1 atm

T(K)	p0->ip1	p0->ip2	p0->ip3	p0->ip4	p0->p1	p0->p2	p0-> Capture	
300	4.09316e-16	2.84885e-17	7.40043e-19	5.42089e-20	2.73295e-22	6.87308e-25	4.38611e-16	4.41869e-16
400	3.67007e-15	6.24274e-16	6.59062e-17	2.8646e-18	9.01725e-20	4.34889e-22	4.36316e-15	4.39123e-15
500	1.38733e-14	3.96511e-15	1.53751e-15	5.38396e-17	8.84784e-18	6.10048e-20	1.94386e-14	1.9549e-14
600	3.09851e-14	1.12638e-14	1.37453e-14	4.16059e-16	2.89e-16	2.80447e-18	5.6702e-14	5.69914e-14
700	4.25154e-14	2.04809e-14	6.02976e-14	1.28294e-15	3.68921e-15	5.31381e-17	1.28319e-13	1.28933e-13

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->Capture

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	2.51419e-12	3.11296e-12
1650	***	***	1.01361e-12	***	7.59081e-13	9.97275e-13	2.77104e-12	4.3116e-12
1750	***	***	7.49444e-13	***	8.71319e-13	1.36724e-12	3.00993e-12	5.24078e-12
1800	***	***	6.35847e-13	***	9.09538e-13	1.56361e-12	3.12992e-12	5.74535e-12
2000	***	***	***	***	1.2241e-12	2.41564e-12	3.63974e-12	8.03651e-12
2250	***	***	***	***	9.31906e-13	3.56258e-12	4.49449e-12	1.15307e-11
2500	***	***	***	***	7.33625e-13	4.84756e-12	5.58118e-12	1.57451e-11

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	1.60084e-11	2.39651e-11
1000	***	***	1.38478e-11	***	2.13672e-15	3.63658e-15	1.38539e-11	3.35739e-11
1125	***	***	8.08308e-12	***	2.18901e-14	2.88628e-14	8.13676e-12	4.80602e-11
1250	***	***	***	***	1.30352e-13	1.40896e-13	2.71247e-13	6.52667e-11
1375	***	***	***	***	5.16611e-13	4.78036e-13	9.94647e-13	8.51357e-11

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->Capture	
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	1.61132e-11
900	2.17928e-14	***	2.13365e-11	9.92623e-13	5.32861e-17	9.74864e-17	2.2351e-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 3.35739e-11
1125 2.42842e-13 *** 4.01177e-11 2.24417e-12 4.74755e-15 5.18301e-15 4.26146e-
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-> Capture	
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	4.40094e-16	4.39189e-16
400	4.058e-15	1.21647e-15	1.79401e-15	2.04893e-17	4.48806e-23	8.13138e-18	7.09706e-15	7.07967e-15
500	1.14671e-14	3.99312e-15	2.55809e-14	2.40345e-16	2.24895e-20	5.76834e-16	4.18583e-14	4.1744e-14
600	1.53826e-14	***	1.18759e-13	5.29573e-16	1.80742e-18	1.05388e-14	1.45212e-13	1.44791e-13
700	8.26721e-15	***	2.68727e-13	3.6298e-16	4.85658e-17	9.02567e-14	3.67662e-13	3.66657e-13
800	***	***	3.46531e-13	1.59975e-16	6.37855e-16	4.11946e-13	7.59275e-13	7.5813e-13
900	***	***	2.58485e-13	***	5.01696e-15	1.09741e-12	1.36092e-12	1.36433e-12
1000	***	***	1.27502e-13	***	2.66964e-14	2.04118e-12	2.19538e-12	2.22228e-12
1125	***	***	3.69222e-14	***	1.40205e-13	3.37927e-12	3.55641e-12	3.69173e-12
1250	***	***	***	***	5.03202e-13	4.69941e-12	5.20261e-12	5.63868e-12
1375	***	***	***	***	1.34005e-12	5.7019e-12	7.04195e-12	8.08831e-12
1500	***	***	***	***	2.8363e-12	6.19784e-12	9.03414e-12	1.10546e-11
1650	***	***	***	***	5.57902e-12	6.10895e-12	1.1688e-11	1.5304e-11
1750	***	***	***	***	7.93319e-12	5.7537e-12	1.36869e-11	1.85547e-11
1800	***	***	***	***	9.24717e-12	5.52451e-12	1.47717e-11	2.03047e-11
2000	***	***	***	***	1.52606e-11	4.49929e-12	1.97599e-11	2.81253e-11
2250	***	***	***	***	2.41562e-11	3.37519e-12	2.75313e-11	3.97051e-11
2500	***	***	***	***	3.43505e-11	2.58705e-12	3.69376e-11	5.32129e-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	4.40094e-16	4.39189e-16
400	6.42847e-15	6.31901e-16	3.5046e-17	1.6814e-18	3.90309e-24	2.56824e-20	7.09706e-15	7.07967e-15
500	3.27643e-14	7.3311e-15	1.69755e-15	5.97485e-17	3.77517e-21	5.76118e-18	4.18585e-14	4.1744e-14
600	9.03154e-14	3.00944e-14	2.37268e-14	7.44558e-16	5.94602e-19	3.36259e-16	1.45218e-13	1.44791e-13
700	1.51212e-13	6.87349e-14	1.38079e-13	3.34291e-15	2.60852e-17	6.34084e-15	3.67736e-13	3.66657e-13
800	2.65389e-13	***	4.35065e-13	5.95238e-15	4.55863e-16	5.28244e-14	7.59687e-13	7.5813e-13
900	2.42389e-13	***	8.48423e-13	5.82177e-15	4.17443e-15	2.61542e-13	1.36235e-12	1.36433e-12
1000	***	***	1.27915e-12	***	2.41798e-14	8.95406e-13	2.19878e-12	2.22228e-12
1125	***	***	1.06753e-12	***	1.3407e-13	2.3615e-12	3.56319e-12	3.69173e-12
1250	***	***	6.23697e-13	***	4.9367e-13	4.09415e-12	5.21161e-12	5.63868e-12
1375	***	***	***	***	1.32987e-12	5.7204e-12	7.05027e-12	8.08831e-12
1500	***	***	***	***	2.82769e-12	6.21276e-12	9.04045e-12	1.10546e-11
1650	***	***	***	***	5.57368e-12	6.11779e-12	1.16915e-11	1.5304e-11
1750	***	***	***	***	7.92977e-12	5.7592e-12	1.3689e-11	1.85547e-11
1800	***	***	***	***	9.24453e-12	5.52871e-12	1.47732e-11	2.03047e-11
2000	***	***	***	***	1.52598e-11	4.5005e-12	1.97603e-11	2.81253e-11
2250	***	***	***	***	2.4156e-11	3.37539e-12	2.75314e-11	3.97051e-11
2500	***	***	***	***	3.43505e-11	2.58708e-12	3.69376e-11	5.32129e-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	4.40094e-16	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	1.36617e-12	1.36433e-12
1000	1.2967e-12	***	7.41015e-13	2.04822e-14	1.41406e-14	1.40011e-13	2.21235e-12	2.22228e-12
1125	1.45199e-12	***	1.4218e-12	2.24749e-14	9.91712e-14	6.06828e-13	3.60227e-12	3.69173e-12
1250	1.35365e-12	***	1.95226e-12	***	4.19819e-13	1.42435e-12	5.28398e-12	5.63868e-12
1375	***	***	2.29284e-12	***	1.25235e-12	3.56698e-12	7.11302e-12	8.08831e-12
1500	***	***	1.51215e-12	***	2.75403e-12	4.82792e-12	9.09494e-12	1.10546e-11
1650	***	***	***	***	5.53291e-12	6.18423e-12	1.17171e-11	1.5304e-11
1750	***	***	***	***	7.90324e-12	5.80129e-12	1.37045e-11	1.85547e-11
1800	***	***	***	***	9.22383e-12	5.56112e-12	1.4785e-11	2.03047e-11
2000	***	***	***	***	1.52533e-11	4.51013e-12	1.97634e-11	2.81253e-11
2250	***	***	***	***	2.41549e-11	3.37702e-12	2.75319e-11	3.97051e-11
2500	***	***	***	***	3.43503e-11	2.58731e-12	3.69376e-11	5.32129e-11

Pressure = 100 atm

T(K)	p2->ip1	p2->ip2	p2->ip3	p2->ip4	p2->p0	p2->p1	p2-> Capture	
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	5.50362e-12	5.63868e-12
1375	5.1608e-12	***	1.14973e-12	4.92825e-14	6.96753e-13	5.3089e-13	7.58746e-12	8.08831e-12
1500	5.2291e-12	***	1.55848e-12	***	1.88688e-12	9.46394e-13	9.78158e-12	1.10546e-11
1650	***	***	3.99088e-12	***	5.23276e-12	2.68197e-12	1.19099e-11	1.5304e-11
1750	***	***	3.00325e-12	***	7.65706e-12	3.10905e-12	1.38572e-11	1.85547e-11
1800	***	***	2.56757e-12	***	9.00728e-12	3.25809e-12	1.49174e-11	2.03047e-11
2000	***	***	***	***	1.52187e-11	4.55992e-12	1.97786e-11	2.81253e-11
2250	***	***	***	***	2.41481e-11	3.38622e-12	2.75343e-11	3.97051e-11
2500	***	***	***	***	3.43492e-11	2.58874e-12	3.6938e-11	5.32129e-11

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