Supplementary Information

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

Long Zhao, Srinivas Doddipatla, Ralf I. Kaiser[*]

Department of Chemistry, University of Hawaii at Manoa, Honolulu, Hawaii, 96822

Wenchao Lu, Oleg Kostko, Musahid Ahmed

Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720

Lotefa Binta Tuli, Alexander N. Morozov, A. Hasan Howlader, Stanislaw F. Wnuk, Alexander M. Mebel

Department of Chemistry and Biochemistry, Florida International University, Miami, Florida 33199

Valeriy N. Azyazov

Samara National Research University, Samara 443086 and Lebedev Physical Institute, Samara 443011, Russian Federation


Rana K. Mohamed, Felix R. Fischer

Department of Chemistry, University of California, Berkeley, CA 94720
Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720
Kavli Energy Nano Sciences Institute at the University of California Berkeley and the Lawrence Berkeley National Laboratory, Berkeley, California 94720

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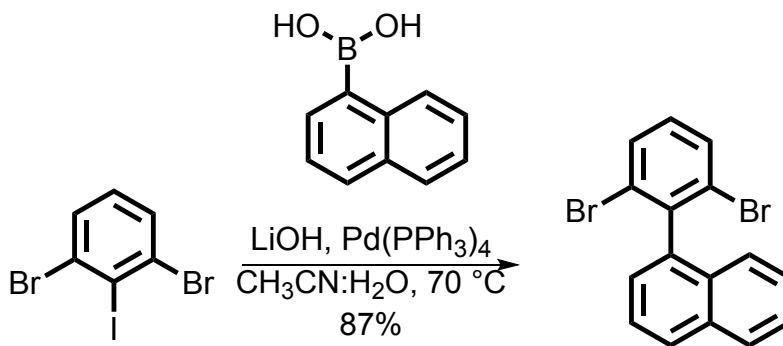
Supplementary Scheme 1. Synthetic pathway for 1-(2,6-dibromophenyl)naphthalene.

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$_3$CN:H$_2$O 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.

^{1}H 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$_4$Cl gave 7-aminofluoranthene **2** (Supplementary Scheme 2). Subsequent, diazotization-iodination of **2** with t-BuONO/CH$_2$I$_2$/I$_2$/CuI afforded 7-iodofluoranthene **3**. Sonogashira coupling of **3** with TMS-acetylene in presence of Pd(PPh$_3$)$_4$/CuI in Et$_3$N gave TMS protected 7-ethynylfluoranthene **4** which on desilylation with K$_2$CO$_3$ provided 7-ethynylfluoranthene **p2**.
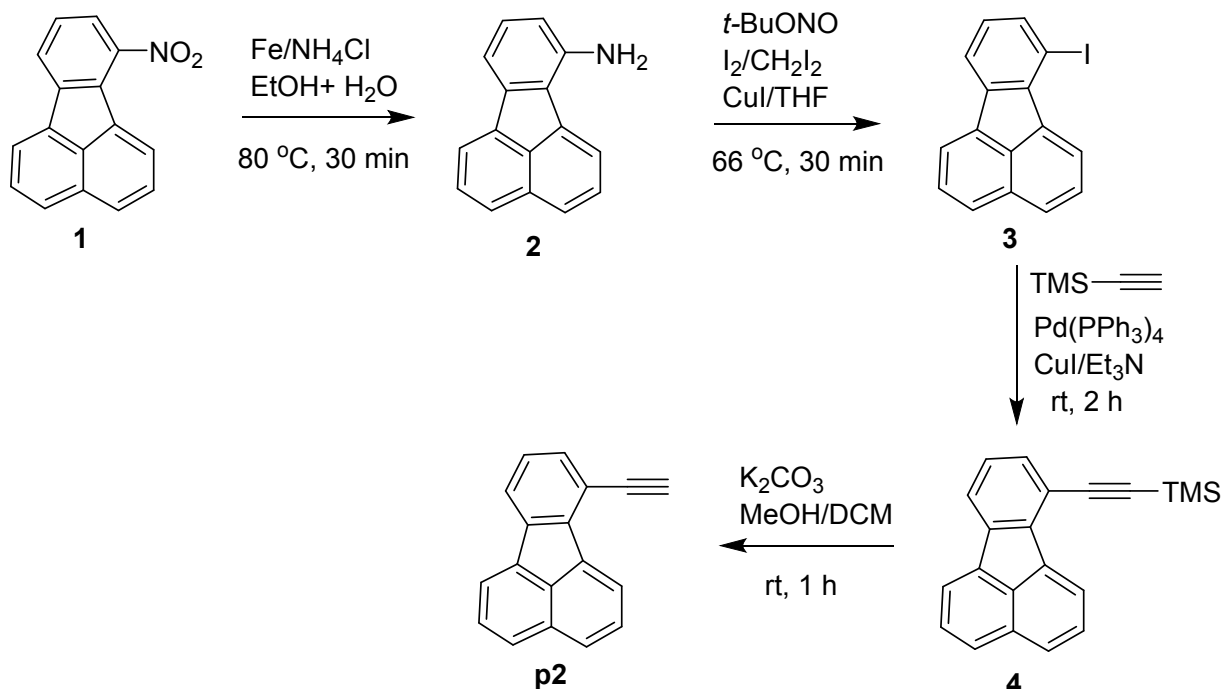
Supplementary Scheme 2. Synthesis of 7-Ethynylfluoranthene **p2**

7-Aminofluoranthene 2

Iron powder (1.10 g, 19.7 mmol) was added to the solution of NH$_4$Cl (1.05 g, 19.7 mmol) in H$_2$O/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$_2$SO$_4$, 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$_2$I$_2$ (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$_2$SO$_4$, 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$_3$N (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$_2$CO$_3$ (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.
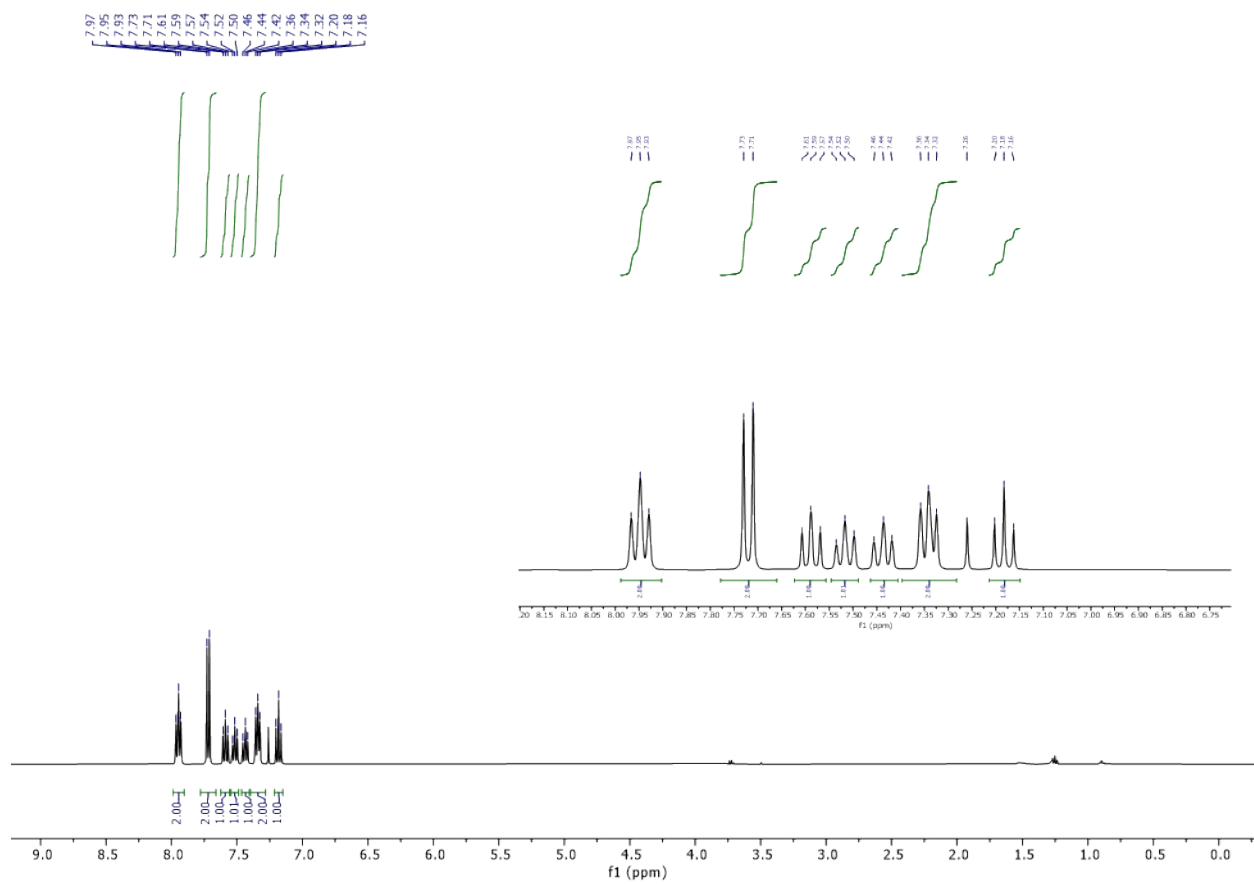
Supplementary Figure 1. ^{1}H NMR spectrum of 1-(2,6-dibromophenyl)naphthalene.
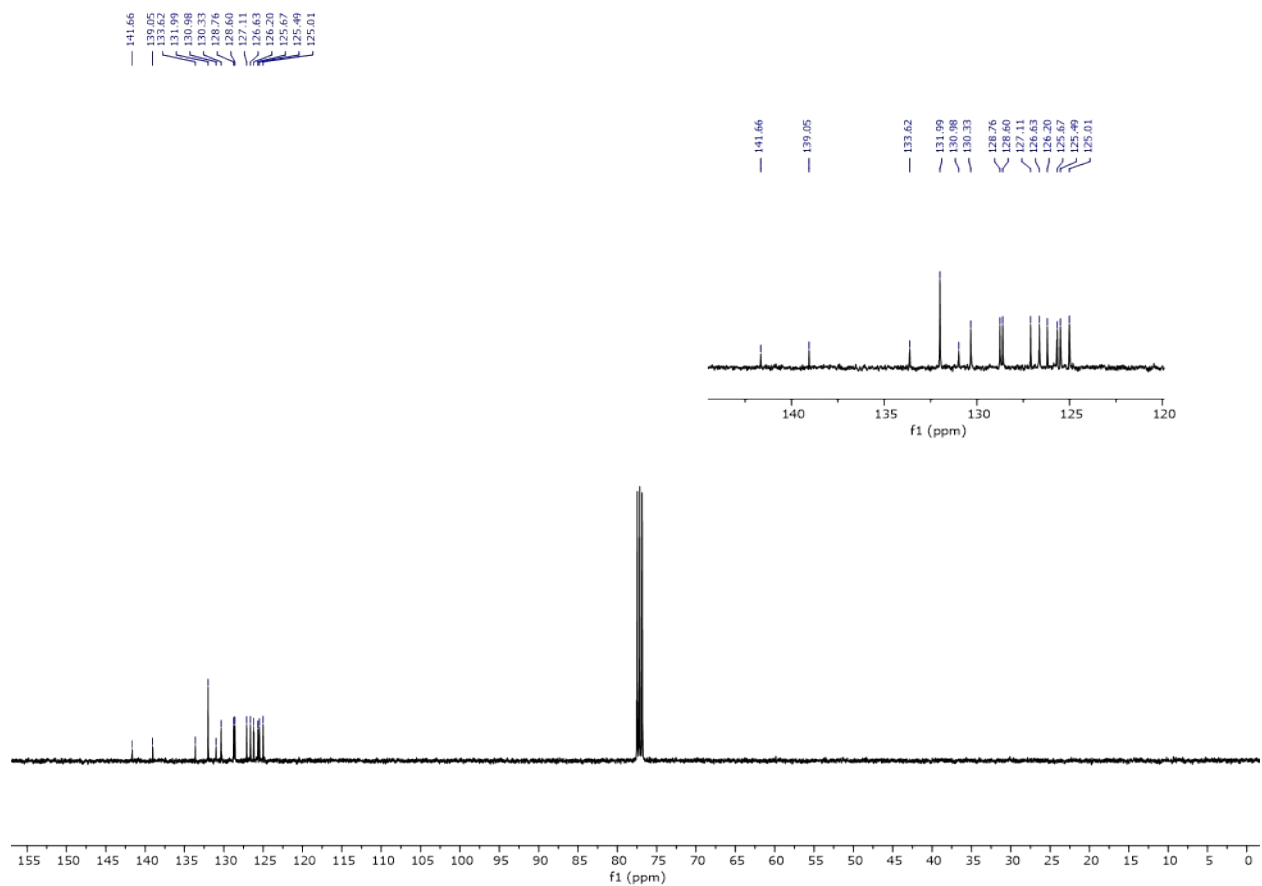
Supplementary Figure 2. ^{13}C NMR spectrum of 1-(2,6-dibromophenyl)naphthalene.
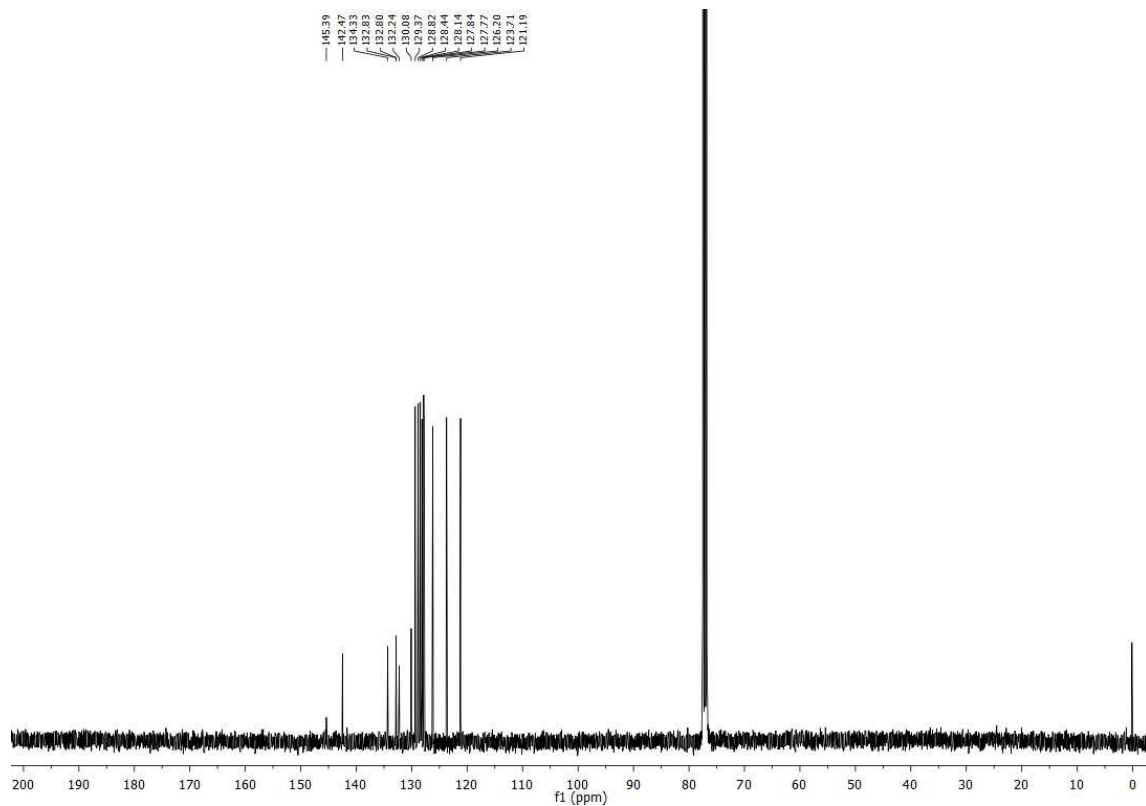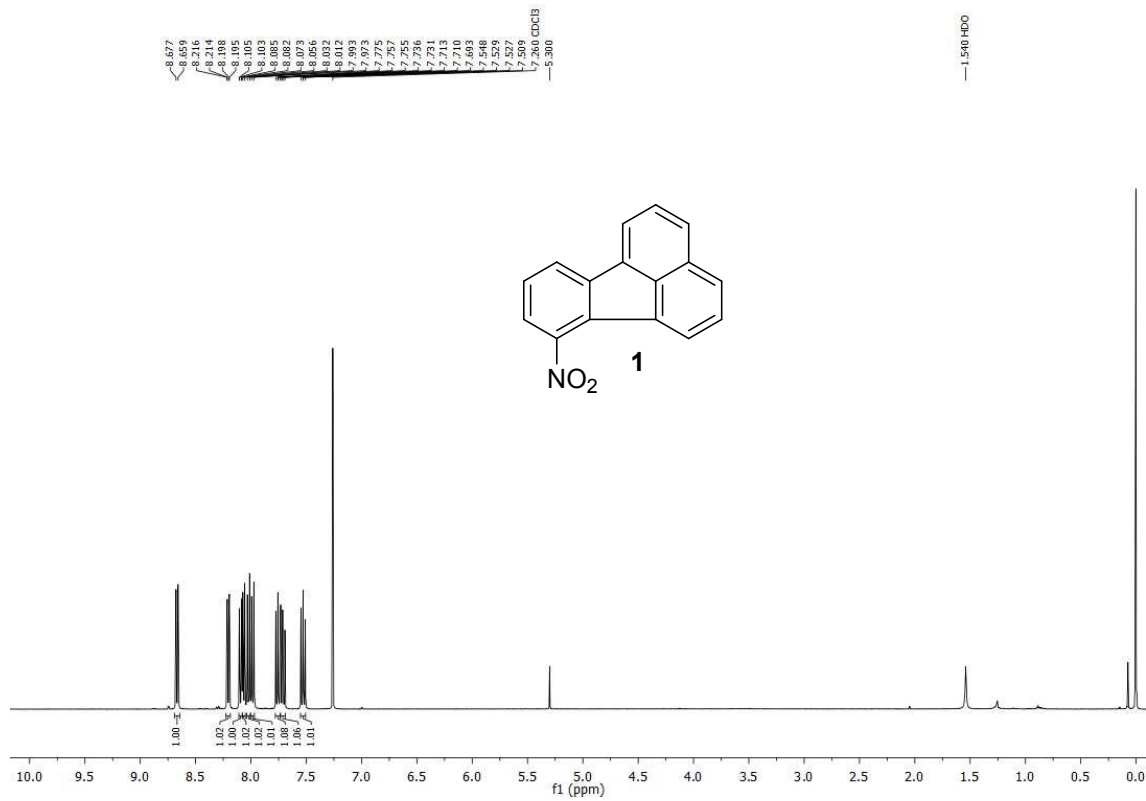
Supplementary Figure 3. ^{1}H NMR and ^{13}C NMR spectra of compound **1** in CDCl$_3$.
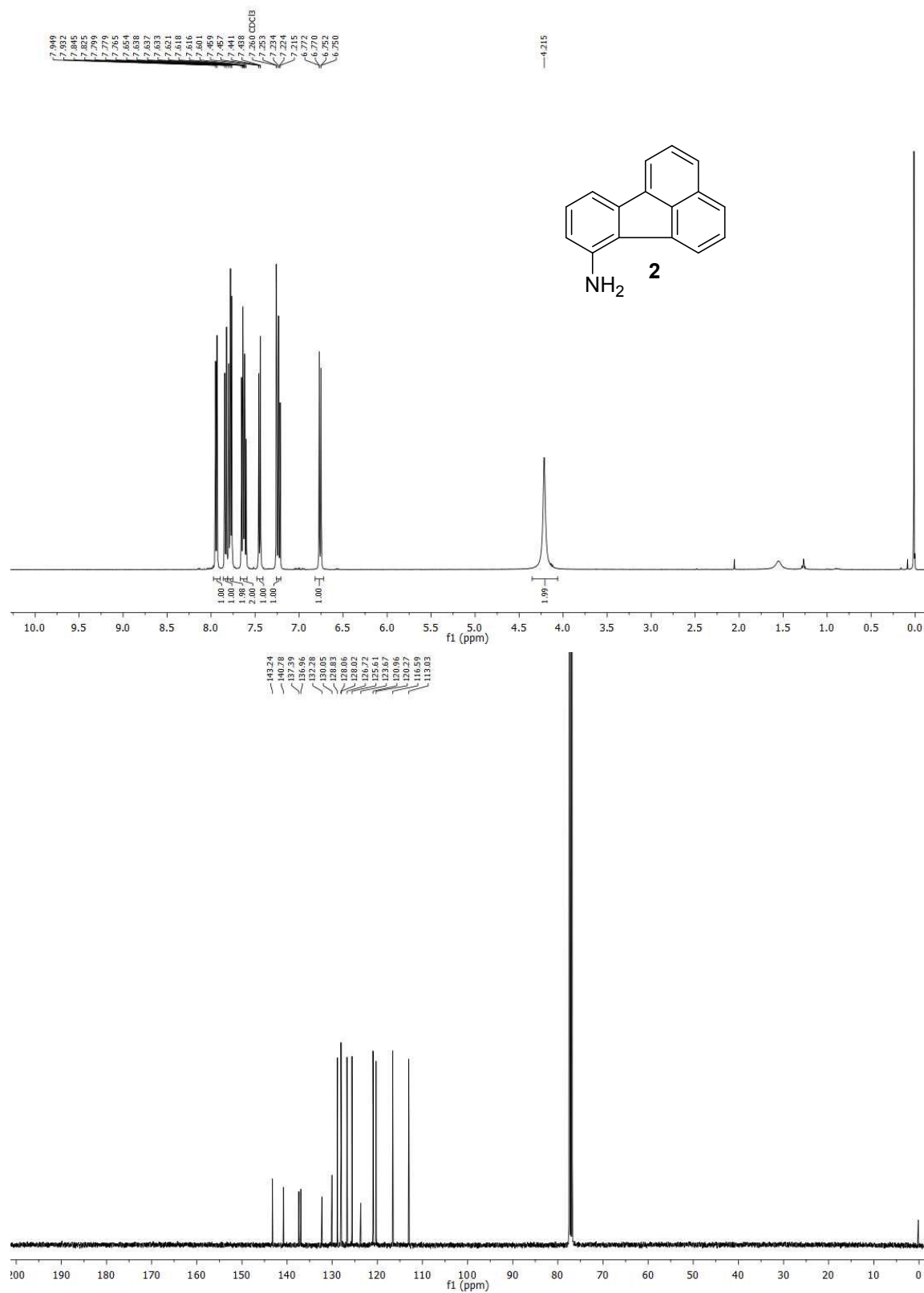
Supplementary Figure 4. ^{1}H NMR and ^{13}C NMR spectra of compound **2** in CDCl$_3$.

3
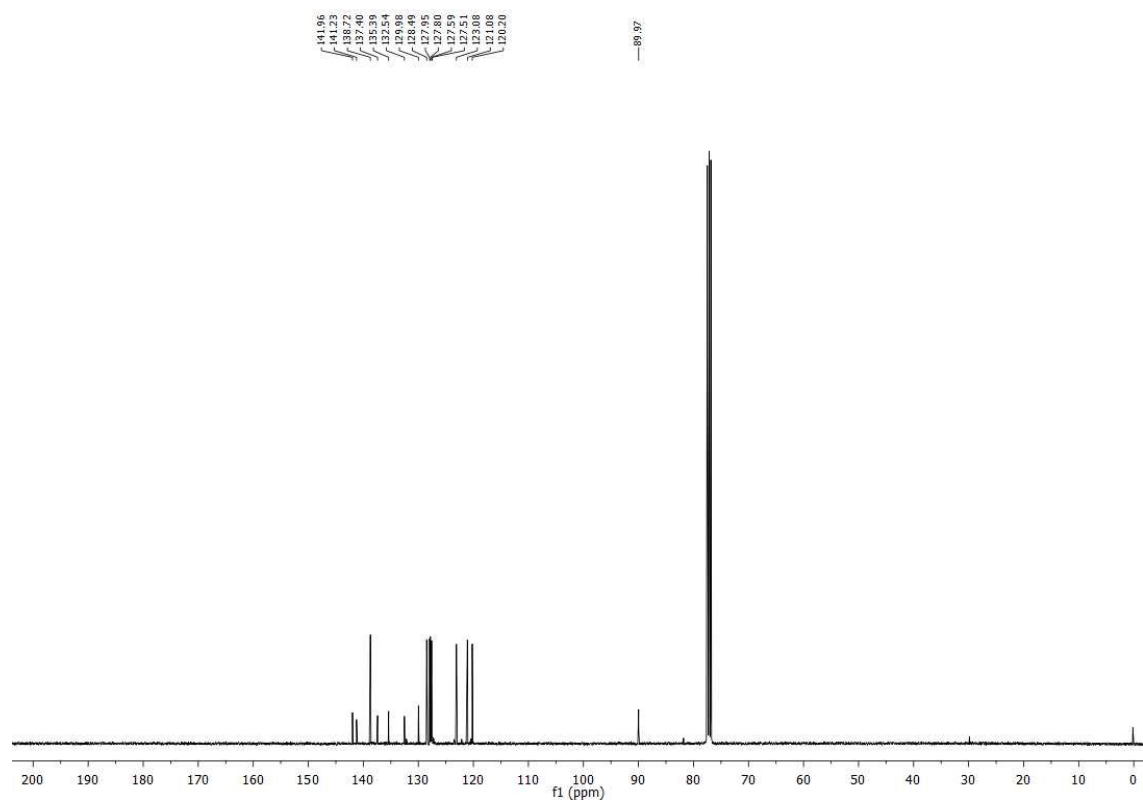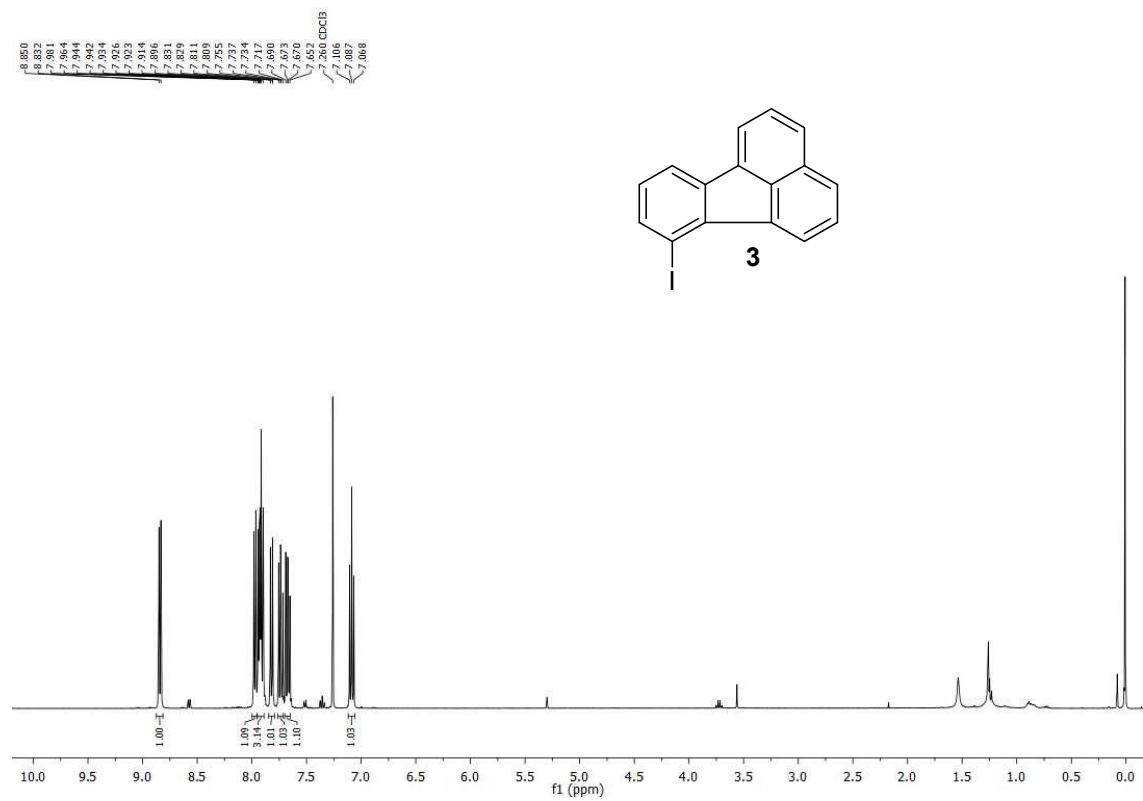
Supplementary Figure 5. ^{1}H NMR and ^{13}C NMR spectra of compound **3** in CDCl$_3$.
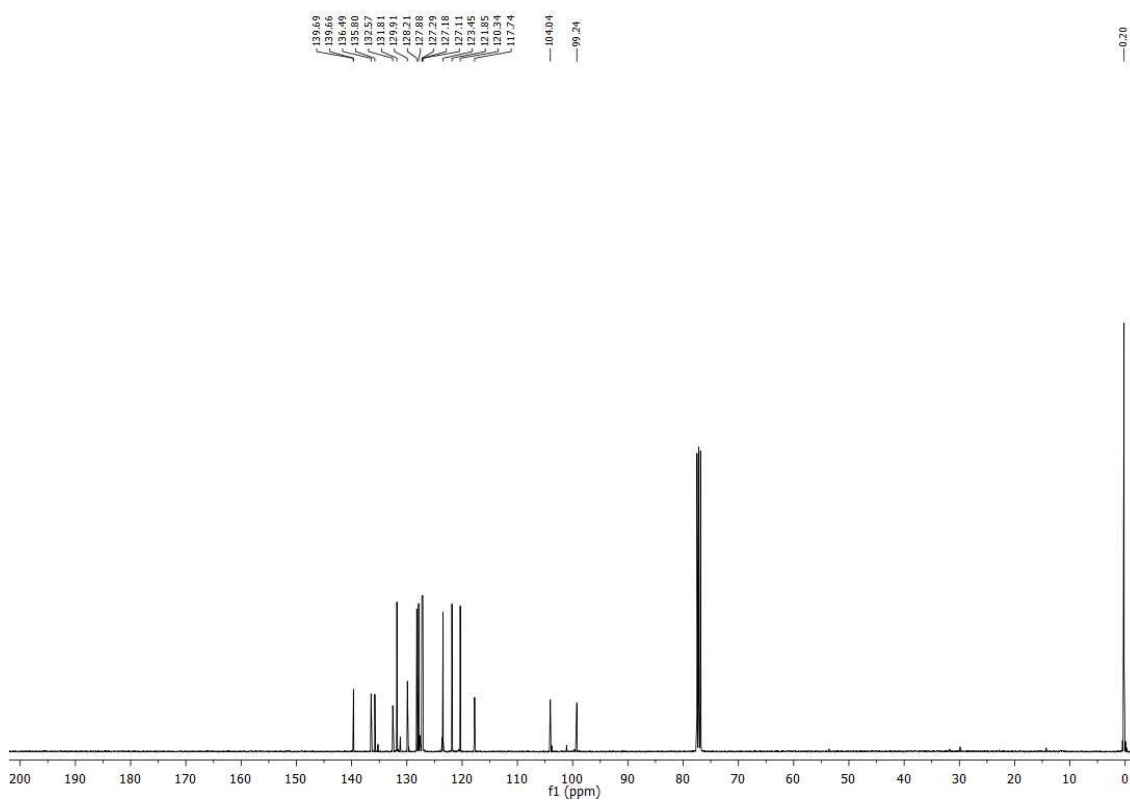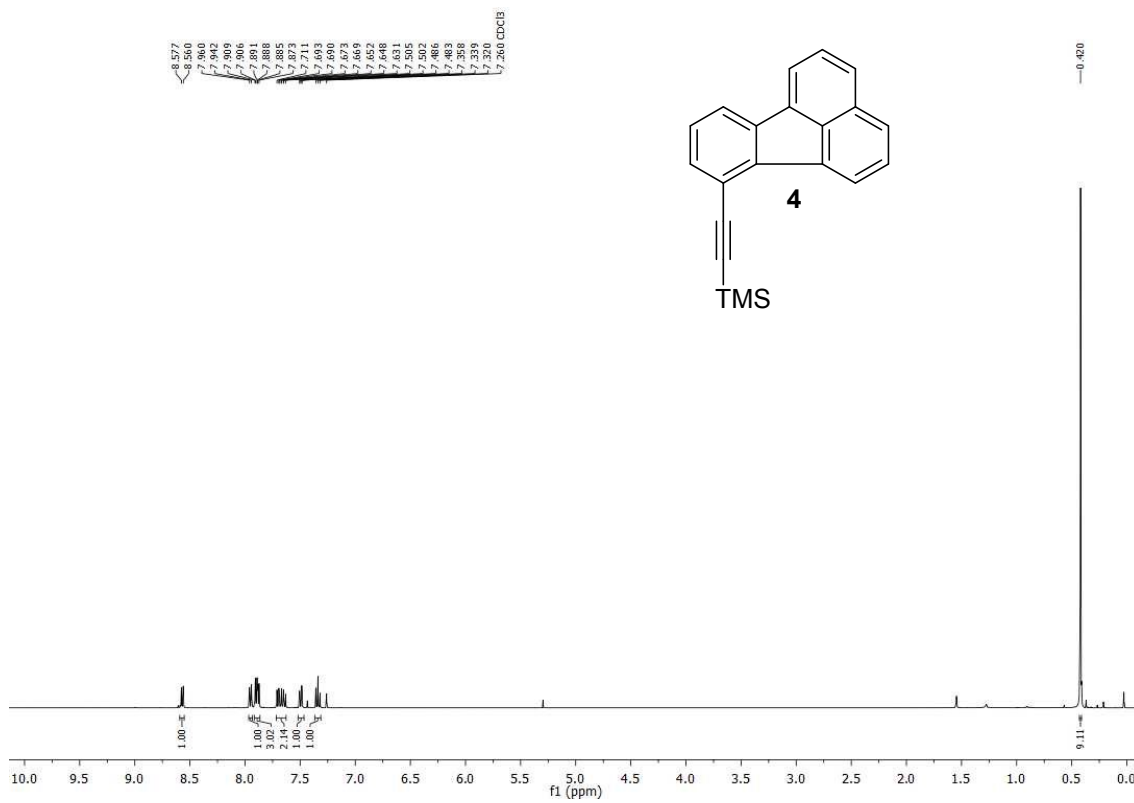
Supplementary Figure 6. ^{1}H NMR and ^{13}C NMR spectra of compound **4** in CDCl$_3$.
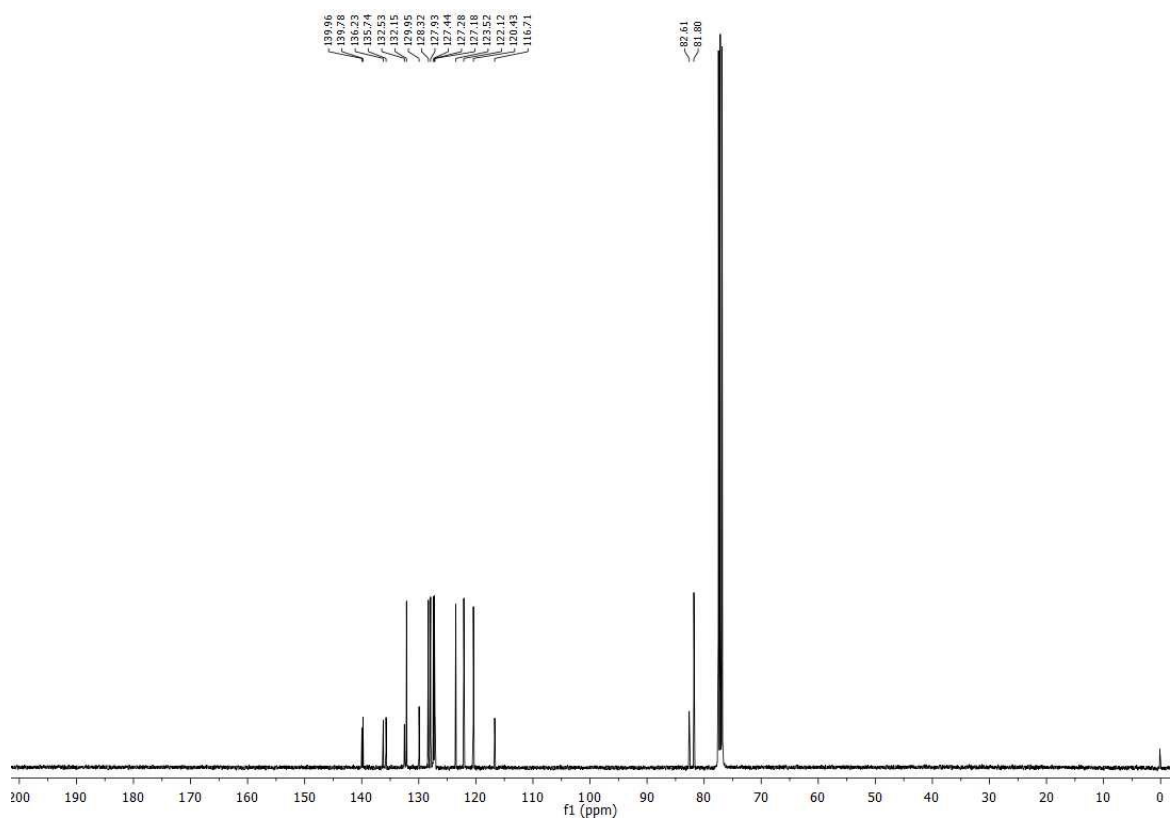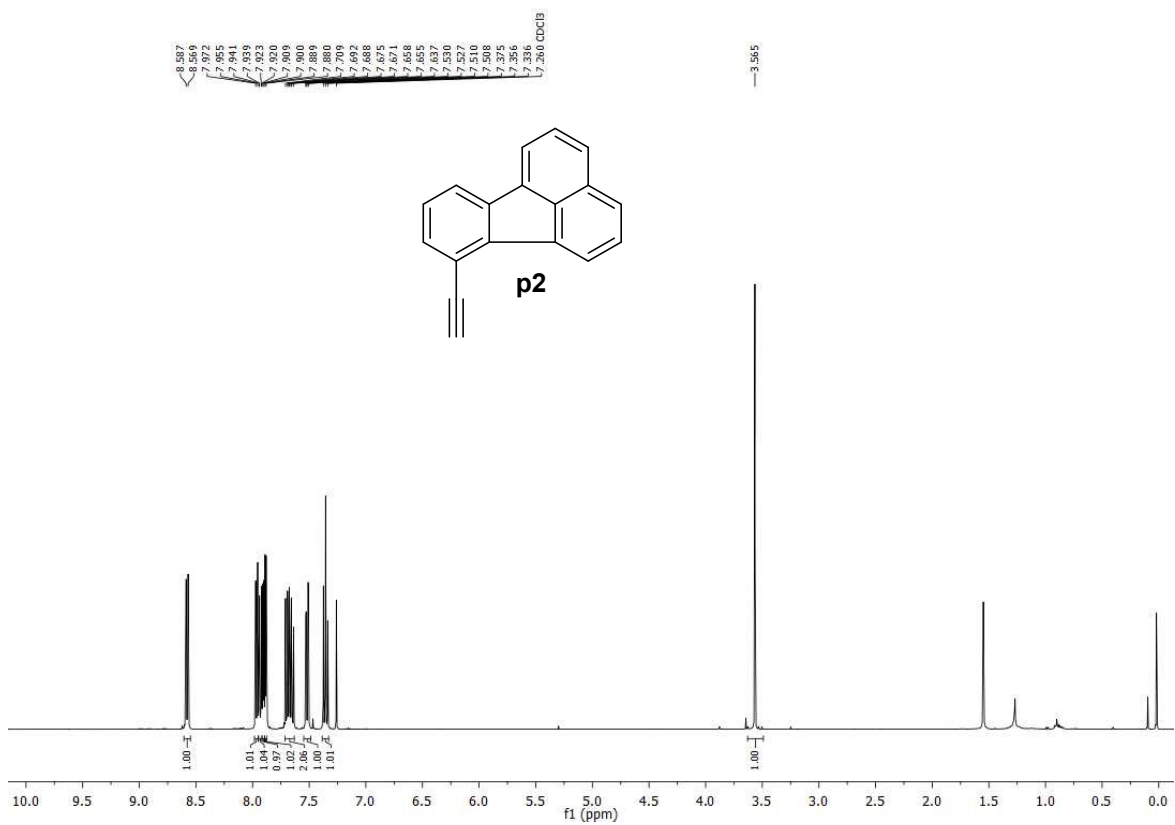
Supplementary Figure 7. ^{1}H NMR and ^{13}C NMR spectra of compound **p2** in CDCl$_3$.

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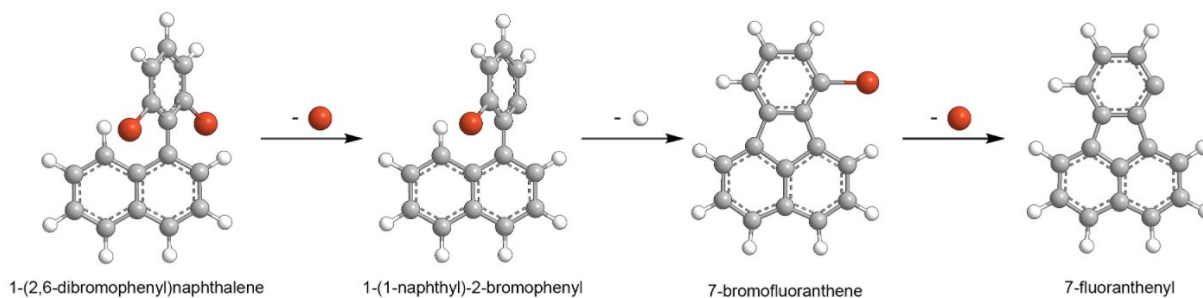
Supplementary Figure 8. Reaction scheme for the pyrolysis of the precursor 1-(2,6-dibromophenyl)naphthalene ($C_{16}H_{10}Br_2$) forming the 7-fluoranthenyl ($C_{16}H_9{}^{\bullet}$) radical via the 1-(1-naphthyl)-2-bromophenyl radical ($C_{16}H_{10}Br^{\bullet}$) and 7-bromofluoranthene ($C_{16}H_9Br$).

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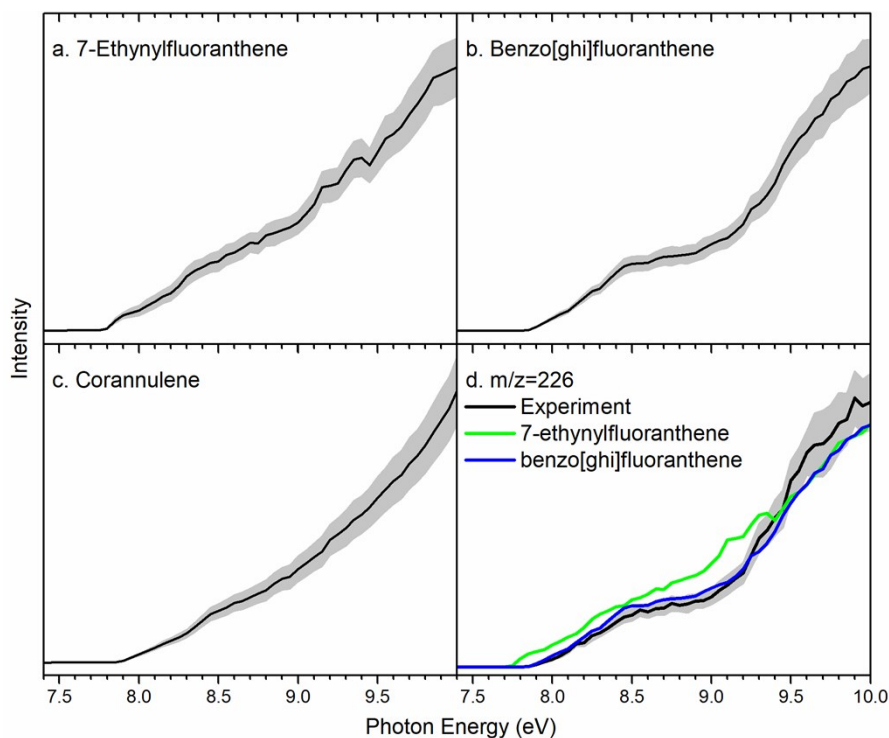
Supplementary Figure 9. PIE calibration curves for 7-ethynylfluorathene, benzo[*ghi*]-fluoranthene and corannulene, along with the comparison between the calibration curves and experimental measurement at m/z = 226.

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.
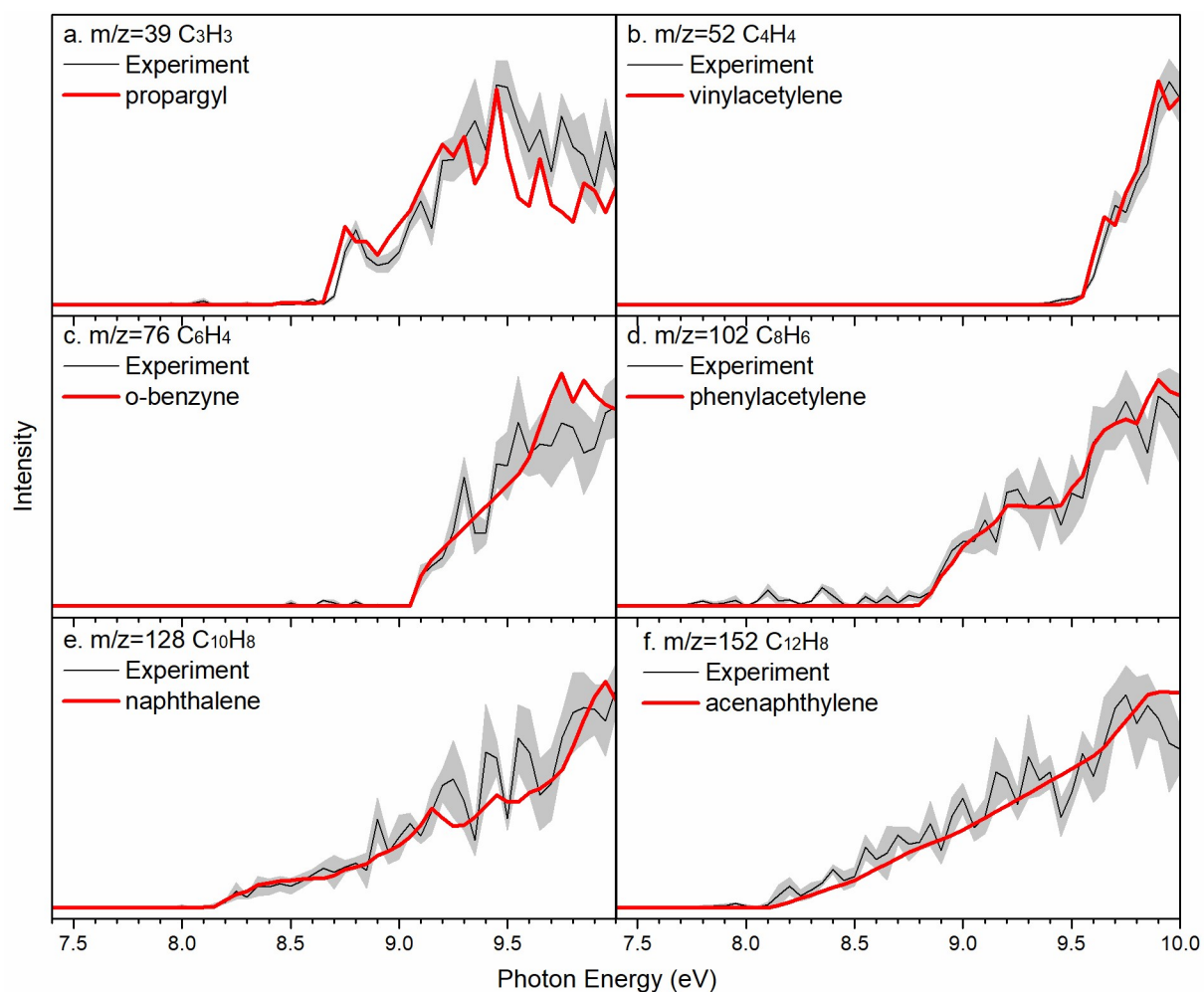
Supplementary Figure 10a. Photoionization efficiency (PIE) curves of distinct ions detected in 1-(2,6-dibromophenyl)naphthalene ($C_{16}H_{10}Br_2$)–acetylene (C_2H_2) system. The black lines shows the experimental measurements along with the error areas labelled in grey. The red lines present the calibration 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]
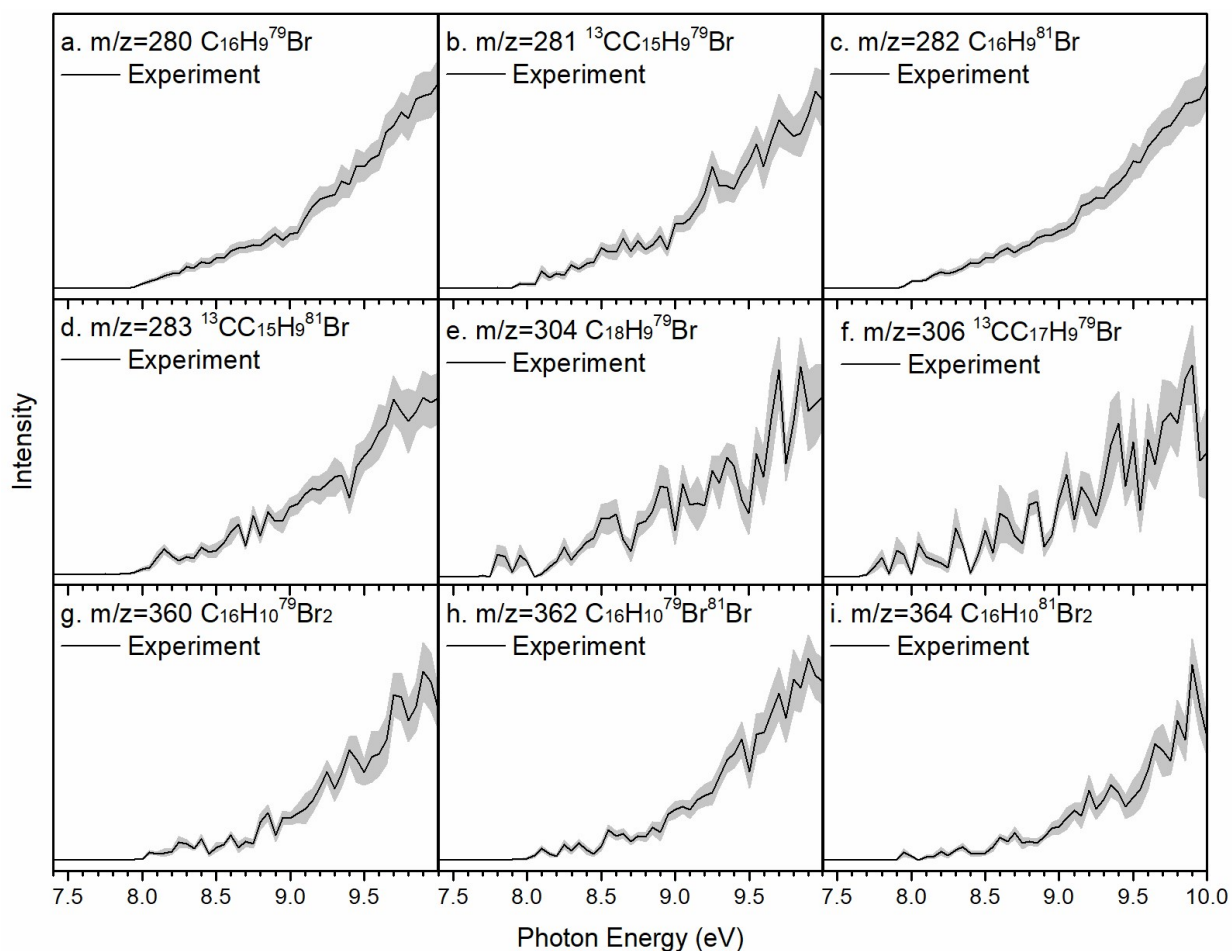
Supplementary Figure 10b. Photoionization efficiency (PIE) curves of distinct ions detected in 1-(2,6-dibromophenyl)naphthalene ($C_{16}H_{10}Br_2$)–acetylene (C_2H_2) system. The overall error bars consist of two parts: ±10% based on the accuracy of the photodiode and a 1 σ error of the PIE curve averaged 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.
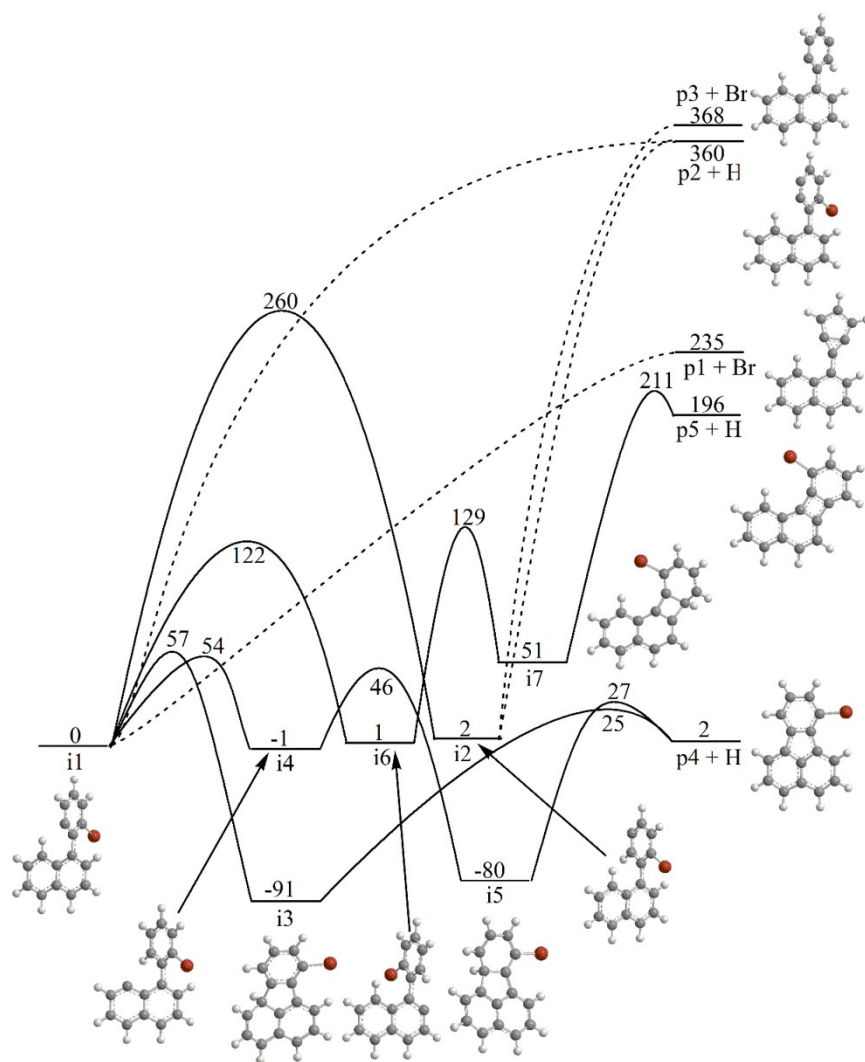
Supplementary Figure 11. B3LYP/6-311G** calculated potential energy diagram for various isomerization and dissociation pathways of the 1-(1-naphthyl)-2-bromophenyl radical produced via a C-Br bond cleavage in the 1-(2,6-dibromophenyl)naphthalene precursor. The energies are given in kJmol^{-1} with respect 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.
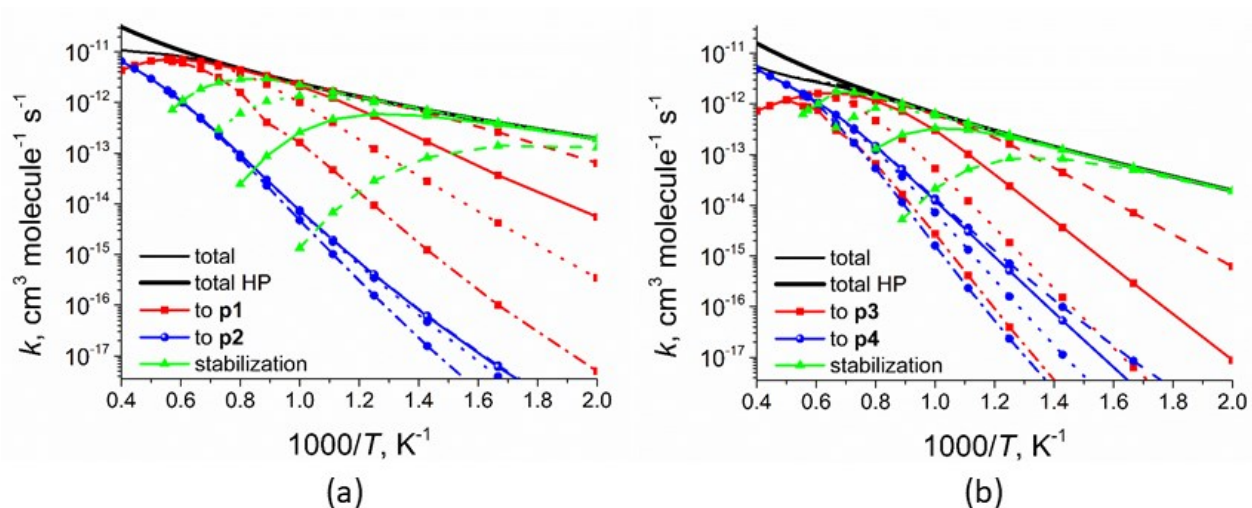
Supplementary Figure 12. Calculated total and individual channel rate constants for the 7-fluoranthenyl + C_2H_2 (a) and benzo[*ghi*]fluoranthen-5-yl + C_2H_2 (b) reactions. Individual channels include the formation of bimolecular products **p1** and **p2** (a), **p3** and **p4** (b), and overall collisional 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} cm³ 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.

7.78
0

7.78
108

7.69
108

7.73
104

7.42
52

7.68
105

7.72
105

7.68
53
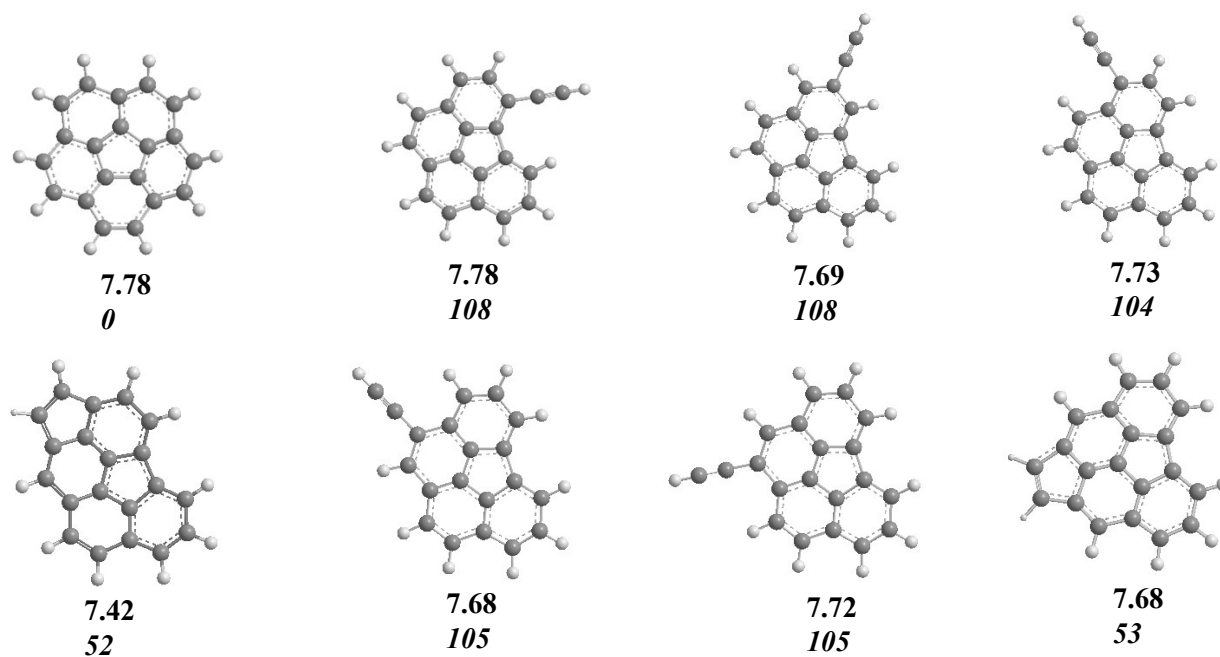
Supplementary Figure 13. Calculated structures, adiabatic ionization energies (eV), and relative energies (kJ mol^{-1}, in italics) of various $C_{20}H_{10}$ isomers calculated at the G3(MP2,CC)//B3LYP level of theory. Distinct $C_{20}H_{10}$ isomers are distinguishable, which the exception of ethynyl-benzo[ghi]fluoranthene (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
```

```
1639.8542                1641.9582                1657.0986
1659.8209                3004.0267                3148.1562
3160.5631                3161.4280                3163.9225
3170.3034                3172.1501                3181.2894
3184.5916                3187.7386                3237.4644
ZeroEnergy[kcal/mol] -39.2
ElectronicLevels[1/cm]        1
0  2
End
End
!--------------------------------
!-------fl_i2------------
Well       i2
Species
RRHO
Geometry[angstrom]   29
C  -0.6782458462   -1.2737605139   0.0202956166
C  -0.6972104237   -2.6762027154   0.027658191
C   0.5629241861   -3.3386382632   0.0391124672
C   1.7321639571   -2.5939993267   0.0403561542
C   1.6584386425   -1.1948831002   0.0285786205
C   0.5051917784   -0.4719890415   0.0171237158
C  -1.8350869873   -0.4637751    0.0152309873
C  -3.0679963152   -1.0816905229   0.0142209443
C  -3.1226975514   -2.4998822084   0.0178714636
C  -1.9838005473   -3.2826855524   0.0251438437
C   0.0617727098   0.9378900036   0.0162808466
C  -1.3667928211   0.9310546945   0.0240532516
C  -2.0934553549   2.1124792171   0.0701813761
C  -1.4002503015   3.3217846879   0.1289908778
C  -0.010985177   3.3348883939   0.1350546856
C   0.7615821206   2.1572585287   0.0597841377
C   2.2232391885   2.3234446473   0.0442120453
C   3.1533493501   1.4999736506   -0.4460837061
H   0.6091241711   -4.4227973121   0.0479236361
H   2.6953271302   -3.0925790401   0.0508346893
H  -3.9913500424   -0.5125518986   0.0114861697
H  -4.0940881793   -2.9815741709   0.0162372879
H  -2.0689269706   -4.3640778702   0.0298633774
H  -3.1775927842   2.0975074543   0.0767733801
H  -1.9452666213   4.2576266226   0.1774016666
H   0.5084000481   4.285940415   0.1864924667
H   2.5585371377   3.2737422163   0.4550515475
H   2.9145022518   0.5530863556   -0.9129911014
H   4.2022752515   1.7700907491   -0.4023486387
Core  RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]   81
46.2792                87.5061                107.6800
158.5739                171.0001                203.6578
242.2442                265.8166                297.8059
344.5362                432.7634                445.0316
```

```
454.2476                467.8911                487.2611
523.2452                539.7542                563.8073
578.4938                616.5200                627.2056
632.5180                636.4826                708.1789
753.0109                767.4992                772.5228
785.0953                803.4974                823.0663
825.8912                836.6068                913.8482
919.7216                937.9979                948.0368
954.7686                975.2611                982.1957
992.1317               1025.9045               1049.1073
1067.5129              1097.9764               1099.5354
1138.7678              1161.1768               1186.6242
1205.2709              1225.5607               1237.5251
1250.1765              1294.1243               1308.5732
1346.5559              1355.6352               1391.6886
1416.4052              1435.3891               1446.5843
1460.8962              1479.1282               1493.7553
1514.6981              1598.4076               1605.4641
1628.0816              1637.5202               1649.4571
1687.6223              3123.7963               3141.4836
3159.9553              3161.0323               3162.2839
3171.0189              3172.4768               3176.3612
3185.6783              3187.3031               3224.4390
ZeroEnergy[kcal/mol] -38.1
ElectronicLevels[1/cm]          1
0  2
End
End
!------------------------------
!-------fl_i3------------
Well       i3
Species
RRHO
Geometry[angstrom]   29
C  -0.7012180971   -1.2072199836   0.229018029
C  -0.7222528205   -2.5994526068   0.2036670863
C   0.571939824    -3.2213745895   0.2021147921
C   1.7489723987   -2.4788919938   0.2243979762
C   1.7374502117   -1.0502065706   0.2502024937
C   0.4944521394   -0.4912048306   0.2510057337
C  -1.8112640032   -0.3163614075   0.2367594655
C  -3.0561710281   -0.9095123901   0.2166595576
C  -3.1346459645   -2.3349248759   0.1902994512
C  -2.0273154964   -3.1686310486   0.1835657498
C   0.1699281745    0.891689623    0.2736251348
C  -1.2246206473    1.0664584096   0.2662453436
C  -1.6848379721    2.3834440065   0.2866413785
C  -0.7249734425    3.4260258857   0.3129409158
C   0.6504711022    3.2131139251   0.319585794
C   1.1628845799    1.8804294473   0.2991938197
C   2.4981367901    1.4128930878   0.3009244957
C   2.8976296121   -0.063534053    0.2764166338
H   0.6391452519   -4.3043082802   0.1830329729
```

```
H   2.6952707616   -3.0112688594    0.2218773203
H  -3.974644443    -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
```

```
C  -0.7745900476   -2.628456502    0.0052143609
C   0.5526800984   -3.2612495195  -0.0127570871
C   1.7147015817   -2.5649469064  -0.0223656597
C   1.772734743    -1.0483925424  -0.2042505235
C   0.4311672142   -0.4988221953   0.0309066449
C  -1.8502949924   -0.3919589624   0.4082924898
C  -3.0835194453   -1.0132665573   0.5477135062
C  -3.1593390396   -2.4159902758   0.3891600111
C  -2.0360980494   -3.2230489482   0.1580225622
C   0.1493912091    0.7886311619   0.4899965869
C  -1.2526819871    0.943277634    0.6971732081
C  -1.6654316848    2.1551410659   1.2332037918
C  -0.6854507018    3.1113873337   1.5849879775
C   0.6921188649    2.8725798088   1.4767700448
C   1.1453204857    1.6611841061   0.9332425623
C   2.5031941401    1.0967684517   0.9300564274
C   2.7936295649   -0.1543073191   0.4991503621
H   0.5974008055   -4.3450965284   0.042483755
H   2.6569542278   -3.1040955187  -0.0019999846
H   2.0199792202   -0.9252315559  -1.2850457704
H  -3.9793781562   -0.4601659399   0.8086838361
H  -4.1258381806   -2.8944961902   0.502475473
H  -2.149206452    -4.301932581    0.135357388
H  -2.7110160682    2.3737090985   1.4218038448
H  -1.0156049716    4.0546587072   2.0058991389
H   1.393249525     3.6129421439   1.8476830712
H   3.3029159842    1.6998140483   1.3502429748
H   3.8170035003   -0.5122073056   0.5587273738
Core  RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  81
90.3363            105.8798            184.2787
208.1437           254.9383            275.5309
296.4094           394.1259            404.7777
424.3205           442.9973            456.0702
479.4879           538.7268            539.4914
567.3763           569.4683            589.0460
621.3818           629.5629            632.6195
677.3564           732.6130            751.5327
753.8141           766.1517            769.8767
809.4824           822.2544            839.6533
861.6368           905.1072            910.4654
913.6768           959.0088            961.9533
963.3979           981.6585            987.0756
1018.3440          1032.8386           1046.7619
1050.5167          1111.0438           1134.3293
1157.6795          1172.7368           1178.1546
1207.1437          1211.9609           1223.8541
1244.6461          1271.5675           1285.6522
1322.7767          1366.3093           1381.2019
1390.0443          1416.7142           1419.6335
1429.6340          1496.7316           1505.6988
```

```
1535.2498              1552.6935              1582.6891
1596.9374              1605.0714              1637.3244
1649.5440              2783.5580              3145.6366
3146.4432              3158.7719              3159.2070
3165.5353              3167.0285              3168.2828
3169.3757              3182.5791              3183.3999
ZeroEnergy[kcal/mol] -58.6
ElectronicLevels[1/cm]        1
0   2
End
End
!--------------------------------
!-------c2h2_c16h9_fl_p0------------
Bimolecular    fl_p0
Fragment         c16h9
RRHO
Geometry[angstrom]    25
C  0.002979243   -1.2242687746   0.0
C  0.002927131   -2.625290378    0.0
C  1.2804201651  -3.2521834629   0.0
C  2.4295235094  -2.484850224    0.0
C  2.399259978   -1.0638171069   0.0
C  1.1759217869  -0.4314156414   0.0
C  -1.1677046206  -0.4272702325   0.0
C  -2.3911245603  -1.0618962694   0.0
C  -2.4231727914  -2.4826265394   0.0
C  -1.2746488757  -3.2510339572   0.0
C  0.7204653547   0.9691772575   0.0
C  -0.7151126344  0.9773328182   0.0
C  -1.4103313867  2.1813107224   0.0
C  -0.705828709  3.389270637     0.0
C  0.697670027   3.404386394     0.0
C  1.344822846   2.1880747675    0.0
H  1.3510489887  -4.3347117916   0.0
H  3.3938638383  -2.9808574969   0.0
H  3.3282232827  -0.5050325848   0.0
H  -3.3235319598  -0.5079706134  0.0
H  -3.388090729  -2.977467472    0.0
H  -1.3464584441  -4.3334961311  0.0
H  -2.4946223621  2.1906915881   0.0
H  -1.2467582987  4.3295520947   0.0
H  1.2395052211   4.3435473967   0.0
Core  RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]   69
99.7431               125.9431              167.1969
207.6710              256.0968              293.5303
358.2715              431.9756              459.4859
470.2009              478.8379              495.1143
558.6415              569.5332              573.3931
618.4091              632.4881              642.3197
681.8167              729.6749              754.2886
```

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

28

```
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
```
31

```
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 1.299918796 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
```

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

```
415.5305              436.7948              465.7811
468.5801              481.6739              520.0629
550.8899              552.7460              586.9453
600.8773              607.1880              633.5685
640.3058              646.3144              662.9600
692.5351              751.1348              774.5555
775.7447              790.8321              815.7269
822.7636              825.6002              843.2900
918.6186              921.7191              931.2693
955.2090              978.0642              980.2987
990.3295             1008.0876             1051.2904
1063.1073            1081.3356             1137.7485
1164.9455            1185.3030             1201.7450
1208.3207            1237.6451             1254.5704
1266.0949            1295.4806             1342.8345
1397.9567            1401.8090             1419.0808
1453.7784            1467.3706             1476.4439
1507.1755            1524.2862             1610.7458
1628.7651            1640.9313             1641.9151
1659.1698            2097.7229             3161.4061
3163.2097            3168.1997             3171.7568
3180.1185            3182.4192             3185.1663
3197.1588            3206.1581             3459.9939
ZeroEnergy[kcal/mol]  -3.7
ElectronicLevels[1/cm] 1
0  2
End
!------------------------------
!-------fl_ts3------------
Barrier      ts3  i1  i2
RRHO
Geometry[angstrom]   29
C  -1.3472323463   -1.1941113717   -0.0060284311
C  -1.2792031996   -2.591015176    -0.007055374
C   0.031637137    -3.1579852619   -0.0161569339
C   1.1560778993   -2.3462356334   -0.0234437676
C   1.0285467189   -0.9368798683   -0.0220125089
C  -0.2081846989   -0.3569941332   -0.0133956019
C  -2.5372853615   -0.4292430154    0.002328135
C  -3.7350319786   -1.1129669931    0.0101431697
C  -3.7086471633   -2.534807288     0.0093876721
C  -2.5325639571   -3.2639386967    0.0011440443
C  -0.687713791     1.019767004    -0.0095905179
C  -2.1124932803    0.9894748768    3.59419E-5
C  -2.8284436775    2.1782239988    0.0053750718
C  -2.1219002107    3.3878052463    0.0010990366
C  -0.7310214057    3.4098097942   -0.0083055677
C   0.0285949235    2.2221757353   -0.0139381299
C   1.4953609466    2.2901628162   -0.0238538809
C   2.3750928013    1.288814767    -0.0302092371
H   0.1505534939   -4.2368636295   -0.0174022216
H   2.1401448541   -2.8020741838   -0.0303116719
H   1.942325037     0.0231782399   -0.027801424
```

34

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

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

```
 1140.6690              1159.8029             1185.9991
 1213.5369              1230.3179             1240.8913
 1251.1126              1267.3097             1282.7259
 1327.0109              1363.7808             1392.8791
 1407.3380              1431.9140             1434.2209
 1447.7442              1476.8342             1494.8895
 1507.7204              1542.0874             1607.5026
 1618.1753              1623.3205             1637.6715
 1645.2715              3136.0253             3144.1219
 3153.6301              3159.9040             3161.0257
 3169.6953              3170.7088             3171.5903
 3183.4390              3185.0481             3226.8231
ZeroEnergy[kcal/mol]  -30.8
ElectronicLevels[1/cm] 1
0   2
End
!--------------------------------
!-------fl_ts5------------
Barrier      ts5  i3  fl_p1
RRHO
Geometry[angstrom]   29
C  -0.7066088264   -1.2012227186    0.2336914036
C  -0.7117477756   -2.5905496394    0.2371788397
C   0.5974520665   -3.2003991634    0.3024978387
C   1.7667729279   -2.4608260255    0.3584618277
C   1.7481084857   -1.0199096457    0.3560751413
C   0.4863158935   -0.4785399212    0.2896514584
C  -1.8178083919   -0.3164209067    0.1888606644
C  -3.0589369358   -0.9198388894    0.1358494273
C  -3.1239367581   -2.3442182507    0.1315257501
C  -2.0083805987   -3.170258104     0.1806223074
C   0.1757888826    0.8848778318    0.2867566119
C  -1.2308394209    1.0692540432    0.2272322084
C  -1.6624355251    2.3824042211    0.2381311051
C  -0.6873766226    3.4195798236    0.3105796951
C   0.6811363804    3.1916908583    0.3762197824
C   1.1684520316    1.8556195973    0.3669100388
C   2.512121919    1.3421031985    0.4486713301
C   2.8074147651   -0.0241270206    0.3981539567
H   0.6692455913   -4.2832768622    0.3082131773
H   2.7147314328   -2.9868393978    0.4020268238
H  -3.9815445176   -0.3508625776    0.0988792249
H  -4.1049796132   -2.8046476603    0.0889398657
H  -2.1380740929   -4.2473819598    0.1766012623
H  -2.7128409532    2.6493656952    0.1981849046
H  -1.0403062218    4.445036344     0.3177766746
H   1.3633877523    4.0331170393    0.4344865773
H   3.3378987133    2.0411382792    0.5292640849
H   3.8301476339   -0.3368490367    0.5741851625
H   3.4091207781   -0.1824291521   -1.4988501449
Core  RigidRotor
SymmetryFactor  0.5
End
```

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

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

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

```
522.1684                552.9629                563.9628
576.6224                577.8997                615.5967
637.9962                652.6553                660.7933
688.2238                756.3957                758.8792
775.7646                779.0306                781.8634
837.9316                838.7496                845.1230
875.0598                920.1563                924.3257
943.1755                970.0504                973.8785
977.1559                981.5609                981.6164
1042.9195               1043.6848               1063.3683
1145.6786               1157.3539               1168.8099
1184.8472               1188.4325               1214.7087
1233.2744               1249.7690               1264.7578
1302.7971               1345.1033               1391.1207
1407.0092               1413.6560               1432.3627
1444.4070               1461.2725               1493.4616
1499.5419               1505.8011               1534.6803
1620.8361               1621.6905               1642.7427
1666.0258               1670.8961               3158.2415
3158.4371               3160.6872               3161.0492
3171.2439               3172.1858               3176.8294
3177.8592               3183.7814               3184.5537
ZeroEnergy[kcal/mol]  -37.6
ElectronicLevels[1/cm] 1
0  2
End
!-------------------------------
!-------fl_ts8------------
Barrier      ts8  i3  i4
RRHO
Geometry[angstrom]   29
C  -0.7288615352  -1.2866004046   0.3004658366
C  -0.7592322446  -2.6611828116   0.0582911919
C   0.5520460274  -3.2707349162  -0.084991602
C   1.7332369625  -2.5726073377   0.0087923113
C   1.7414642403  -1.122485613    0.2199204021
C   0.4579668748  -0.5808987154   0.3878217634
C  -1.8302265764  -0.4269917182   0.5972157276
C  -3.0764708625  -1.0393616553   0.5846303467
C  -3.1589568771  -2.4257125507   0.301142964
C  -2.0457462037  -3.236003728    0.0521185276
C   0.1637281132   0.7401659413   0.7653360258
C  -1.2363786436   0.9054883534   0.896786312
C  -1.6603463502   2.1794084064   1.2930987768
C  -0.6860645735   3.1671899448   1.5372065144
C   0.6953824336   2.9489956346   1.4216458763
C   1.168059487    1.6778969035   1.027345355
C   2.5236383829   1.1840607378   0.8853850349
C   2.8192892914  -0.1432794319   0.514628781
H   0.6093840983  -4.3428129346  -0.2475229219
H   2.6733995203  -3.1041121778  -0.0920359171
H   2.3790109739  -0.5027233439  -0.7757764651
H  -3.988767302   -0.4921317087   0.7976610811
```

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

3.2. Output file of RRKM-ME calculations for the 7-fluoranthenyl + 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

_____

_____

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

T(K)							
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	***	***	***	***	***	***

T(K)							
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 |

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

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

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

T(K)								
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

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

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

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

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	
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

T(K)								
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

T(K)								
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

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	
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

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	
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

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
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

T(K)								
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

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_p3	fl_p2->Capture
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->fl_p3	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

T(K)							
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$_2$H$_2$ 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
```

69

```
C  -1.7463285268    2.0181776283   -0.0745088473
C  -1.1492373164    3.3058767815   -0.0576115827
C   0.2302443877    3.4116477605   -0.0294337192
C   1.1431664588    2.3019067542   -0.0152506374
C   2.5773575125    2.6178743336    0.0149421112
C   3.6047218054    1.7966867322    0.0321781207
C  -3.5418769194    0.3040398735   -0.1170213181
C  -3.1370595556    1.6263524681   -0.1039496536
H   0.9725383666   -4.3643326649   -0.0429653436
H   3.0736065853   -3.1187371695    0.0040032816
H   3.1857713277   -0.6627065868    0.0150068445
H  -3.7348088703   -2.6437684039   -0.1317205392
H  -1.818388155    -4.1286083917   -0.0985244505
H  -1.7555096484    4.2055591725   -0.0664451051
H   0.6670847203    4.4050143546   -0.016868484
H   2.803726385     3.6911197734    0.0239974683
H   4.6804818521    1.8831095429    0.0542441097
H  -4.6039471316    0.0823068278   -0.1391479508
H  -3.8957492413    2.4023106746   -0.1162799327
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  87
59.6055              73.4364              107.3383
159.3553             168.2659             212.7712
271.3998             296.4052             299.8422
322.2266             396.5237             429.1202
439.9913             450.0487             471.0907
500.2310             525.9077             529.2397
561.4324             565.5378             580.5569
608.5805             647.1483             647.4991
657.8095             659.7622             697.9494
715.8589             767.5842             778.4761
779.7333             805.2169             806.0986
838.6801             841.6372             843.8490
862.2742             874.0991             906.2521
926.0585             958.7161             966.4985
972.2874             972.7186             982.0492
1041.8291            1062.2702            1079.5980
1147.8925            1159.0705            1162.2810
1181.4253            1197.7019            1216.4163
1231.4921            1239.9761            1257.1469
1276.4096            1308.4953            1351.8665
1377.2495            1400.5039            1419.2393
1430.8461            1451.5465            1457.8593
1486.4312            1497.0301            1517.0756
1533.5008            1600.9478            1623.5154
1648.0397            1652.2910            1674.4336
1699.8885            3013.1762            3156.3305
3156.7878            3157.1671            3160.3440
3173.4709            3174.3589            3174.8724
3175.9546            3185.7037            3243.8783
ZeroEnergy[kcal/mol]  -39.24
```

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

```
 652.2388               660.8618                714.0770
 723.4155               765.6181                775.6913
 777.1401               820.2453                824.2203
 835.6288               838.4354                853.9829
 892.1891               947.3003                949.8065
 950.0004               960.9328                968.6634
 975.0374              1014.5807               1028.1314
1066.2563              1094.3530               1111.9298
1144.1882              1158.1568               1162.7825
1182.9350              1213.1963               1216.7849
1230.2812              1248.6597               1274.4580
1322.2429              1342.0233               1357.1841
1384.5501              1409.5287               1426.0066
1442.5009              1446.2645               1465.3739
1479.6861              1485.2549               1517.8398
1524.5712              1581.7183               1602.1180
1641.4802              1669.3373               1684.0739
1694.3105              3127.7801               3133.5974
3157.8538              3158.5962               3158.6411
3160.7927              3174.8822               3175.7983
3176.6425              3177.1948               3218.6282
ZeroEnergy[kcal/mol] -37.82
ElectronicLevels[1/cm]        1
0  2
End
End
!-------------------------------
!-------well_ip3------------
Well        ip3
Species
RRHO
Geometry[angstrom]   31
C  -0.017673218   -1.3546393038   0.7008319847
C  -0.1457575335  -2.6265909266   0.162120267
C   1.0957484221  -3.2338709061  -0.2147984252
C   2.2965442195  -2.5180323156  -0.1920880516
C   2.3640911553  -1.1548425024   0.2245502022
C   1.1980107731  -0.6405187145   0.7256637833
C  -1.0790259785  -0.4195104159   0.7253497757
C  -2.3343789004  -0.6913662525   0.2158685305
C  -2.542163709   -2.0783214532  -0.1474659751
C  -1.5062110064  -2.9948956514  -0.1730364835
C   0.8786338495   0.7614217679   0.7638048157
C  -0.5209742259   0.8829988809   0.7581642203
C  -1.1974442273   1.9951935632   0.2714588789
C  -0.3384245303   3.1116311374  -0.0616994307
C   1.0374667549   2.9952407011  -0.0826479565
C   1.7188697285   1.7462876724   0.2334587475
C   3.011827112    1.3219605026  -0.1141206768
C   3.4829788442  -0.1339315387   0.0195361893
C  -3.1203360069   0.479388209   -0.0943228397
C  -2.5736139033   1.7574497617  -0.0716869424
H   1.1033475614  -4.2415577878  -0.6178693394
```

72

```
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
```

81

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

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

```
651.9060                 656.6127                   675.4220
708.0925                 727.5020                   771.4467
781.8434                 794.0027                   820.5252
830.8701                 834.1089                   839.3583
848.9686                 904.8487                   912.8449
956.6296                 959.5258                   967.5251
968.2923                 973.9578                  1010.3571
1044.5997               1079.7634                  1097.7874
1109.3115               1148.5172                  1155.8397
1159.2827               1184.0935                  1202.1952
1224.8448               1230.4727                  1236.4996
1287.4075               1290.4998                  1341.8206
1354.9486               1390.2606                  1417.2077
1423.4440               1439.5883                  1446.4069
1473.2914               1478.1810                  1500.2849
1513.9521               1527.6342                  1618.1960
1639.0223               1651.1337                  1662.7295
1682.5289               1698.7836                  3073.9480
3155.2732               3156.2120                  3156.6835
3158.6238               3173.0014                  3173.5490
3174.4827               3176.7853                  3177.3352
ZeroEnergy[kcal/mol]  -23.46
ElectronicLevels[1/cm] 1
0  2
End
!--------------------------------
!-------bar_ts4-----------
Barrier      ts4  ip2  ip3
RRHO
Geometry[angstrom]    31
C  -0.3084882683   -1.2889325102   -0.2820720327
C  -0.4737030028   -2.5990791132    0.1439407628
C   0.7412444633   -3.2734488914    0.4758621562
C   1.9684606798   -2.6000795432    0.4436617169
C   2.0432251303   -1.2306532165    0.095719778
C   0.9137694279   -0.5711379292   -0.2833053417
C  -1.3756358614   -0.3803742501   -0.3888734742
C  -2.677384678    -0.6817678032   -0.0448831806
C  -2.8979631756   -2.0779065629    0.2638163348
C  -1.8550358473   -2.9842982445    0.3472631766
C   0.5668338421    0.8492805117   -0.3758572556
C  -0.8435464499    0.9235600069   -0.4382786807
C  -1.6079686883    2.0348542519   -0.1054603437
C  -0.843290329     3.2065074644    0.2051393654
C   0.5383431599    3.1488245971    0.2979664737
C   1.2976244038    1.9491418344    0.0528972099
C   2.6662494416    1.695689671     0.4529784657
C   3.3954919593    0.6190111748   -0.0283866775
C  -3.5250150514    0.4765299161    0.1204317646
C  -3.0122703581    1.7639458966    0.0957615077
H   0.7230410979   -4.3097097149    0.799362677
H   2.8638851016   -3.1428574427    0.7274883307
H  -3.90138142     -2.4206275113    0.495376933
```

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

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

```
814.2734                  836.6471                  849.4163
856.6634                  888.4476                  933.1637
946.2120                  952.0464                  965.5527
967.8935                 1024.2673                 1071.6121
1076.5936                1086.6857                 1122.6211
1147.3310                1154.4600                 1161.4657
1173.0107                1198.7482                 1205.8811
1215.8065                1235.7117                 1251.1656
1308.4327                1323.6835                 1368.4567
1374.5787                1386.3319                 1409.2874
1421.1561                1426.1771                 1437.7090
1447.6749                1458.9008                 1464.6559
1474.1063                1487.4856                 1509.9266
1580.8086                1628.1633                 1630.1892
1634.0596                1645.7257                 3152.1283
3152.5347                3153.5667                 3154.4044
3169.9378                3171.6525                 3172.0494
3172.8769                3174.1292                 3187.9891
ZeroEnergy[kcal/mol]  -21.93
ElectronicLevels[1/cm] 1
0  2
End
!-------------------------------
!-------bar_ts6-----------
Barrier       ts6  ip1  ip4
RRHO
Geometry[angstrom]   31
C  -0.1156769779   -1.2548701014   -0.3909590345
C  -0.1468517433   -2.5616571175    0.080114487
C   1.1496325573   -3.125977921     0.3312122677
C   2.2992521026   -2.3942817738    0.1090933677
C   2.3079209295   -1.0139288417   -0.350384645
C   1.0311184479   -0.444371727    -0.5364082758
C  -1.2711524516   -0.4507597186   -0.4376405107
C  -2.5165510615   -0.8620704214   -0.0042456768
C  -2.5893499786   -2.2578230727    0.3579053091
C  -1.4592523155   -3.0610600118    0.399225388
C   0.5599502174    0.9297681039   -0.5255847423
C  -0.8628497106    0.8922146858   -0.5261700244
C  -1.7023995872    1.9282366221   -0.141483719
C  -1.032626623     3.1581602654    0.1565098141
C   0.3504028744    3.1925573756    0.2481762326
C   1.1812785001    2.0469998401    0.0077019474
C   2.5217110674    1.8935478471    0.5879150168
C   3.1753164476    0.7379638016    0.6955605152
C  -3.4592487461    0.2129039962    0.1950691647
C  -3.0670419172    1.5385492648    0.1306300804
H   1.2360048773   -4.1447251096    0.6962004656
H   3.2569283289   -2.8814203289    0.2580159019
H   3.1649380832   -0.7016034012   -0.935767545
H  -3.5387384836   -2.6799118221    0.6713095177
H  -1.5642173154   -4.0846644417    0.7446869158
H  -1.6022333061    4.043924208     0.4180377008
```

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

```
C  -0.1673515684  -2.5135611885   0.1633120559
C   1.0839450053  -3.1196960624  -0.2296765552
C   2.2748584359  -2.4091124907  -0.2312964073
C   2.335892159   -1.0217892086   0.1606702726
C   1.1725539311  -0.5293963718   0.7177022977
C  -1.1081311965  -0.3228470724   0.7615606643
C  -2.3618725891  -0.5949024598   0.2468824653
C  -2.5653742244  -1.9743872599  -0.1362060128
C  -1.5228884219  -2.8860093291  -0.1760201131
C   0.8577490458   0.852053783    0.7531673563
C  -0.5513391057   0.9789673352   0.781373754
C  -1.2162900113   2.0860667003   0.286229892
C  -0.3562342661   3.1950474397  -0.0630655176
C   1.0226875273   3.0714125961  -0.093991515
C   1.6872865085   1.8255946997   0.2232897213
C   2.9883002213   1.3540602281  -0.1726221924
C   3.3199101622  -0.0045657063  -0.1684912576
C  -3.1469928895   0.5774097258  -0.068221935
C  -2.6022867783   1.8517143494  -0.0496320368
H   1.0865220921  -4.1323259821  -0.6202633528
H   3.1649686403  -2.8930194844  -0.6203729127
H  -3.5417407616  -2.2902698085  -0.4897862224
H  -1.7215860411  -3.8818139673  -0.5593176817
H  -0.7992215    4.1274223398  -0.3984776953
H   1.609765176   3.9109485189  -0.4523258123
H   3.720528227   2.058060783   -0.5543048006
H   4.4830815373  -0.095568412   1.5434637144
H   4.2524795229  -0.3024074288  -0.6346554857
H  -4.1676694368   0.4568840836  -0.4171723141
H  -3.2165281395   2.6811467291  -0.3854624685
Core   RigidRotor
SymmetryFactor  1
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]   512.2347
WellDepth[kcal/mol]   33.12
WellDepth[kcal/mol]   3.71
End
Frequencies[1/cm]   86
 135.7440              139.2672
 145.9976              228.3604              257.5094
 286.5616              298.8591              311.3916
 325.5355              411.0917              413.0531
 439.6820              440.2201              455.5457
 461.6903              543.4752              549.2677
 549.8298              564.0122              605.1287
 614.1759              616.3114              647.2589
 650.2723              651.1643              671.7447
 679.6134              759.6512              761.1893
 767.6500              778.2802              811.9691
 814.1896              831.8229              838.6109
 857.6608              865.8447              866.8437
 939.0251              962.9853              968.9548
```

```
  970.9683              978.4298              978.8506
 1047.3508             1087.4228             1089.7064
 1150.2294             1161.7320             1162.2469
 1162.5716             1183.7731             1186.4510
 1212.7027             1213.7083             1237.3144
 1257.9972             1332.6875             1334.7137
 1370.3729             1377.0053             1423.7343
 1425.5059             1433.6296             1442.0825
 1460.2407             1468.9350             1470.1147
 1480.2990             1484.3052             1511.1683
 1642.4891             1649.6122             1653.3601
 1653.9396             1654.7517             3155.3288
 3156.0311             3156.5265             3157.0748
 3162.0349             3172.4963             3173.1464
 3173.9059             3174.4776             3178.6831
ZeroEnergy[kcal/mol]  -30.60
ElectronicLevels[1/cm] 1
0  2
End
!--------------------------------
!-------bar_ts8------------
Barrier      ts8  ip4  p1
RRHO
Geometry[angstrom]   31
C  -0.2163584248  -1.0823125004  -0.5384030973
C  -0.2910799973  -2.4456661106  -0.3126409973
C   0.9921670461  -3.1049261746  -0.1800003056
C   2.1751407582  -2.4020226922  -0.1094292999
C   2.2301656543  -0.943238925   -0.2033985137
C   0.9923679841  -0.3504368687  -0.4558324323
C  -1.2846672194  -0.2032566023  -0.2325412693
C  -2.488003203   -0.6354432852   0.2960673022
C  -2.6534089906  -2.0698037761   0.3195472001
C  -1.6045905861  -2.9305500256   0.0344883171
C   0.6734247716   0.9742139127  -0.0722242385
C  -0.7345429213   1.068284099    0.0558385362
C  -1.3558347043   1.9809448362   0.8897102739
C  -0.4728627393   2.9694955647   1.4627790588
C   0.9054201369   2.8701536389   1.3502056412
C   1.5380120025   1.7816468263   0.6459479507
C   2.8729706075   1.2418692611   0.8056786152
C   3.1960527941  -0.0425387931   0.4257082913
C  -3.247035406    0.3880612947   0.9779090419
C  -2.7085825692   1.6324768255   1.2602567481
H   1.0233665314  -4.1810077559  -0.0410754603
H   3.0966682822  -2.94704037    0.065525132
H  -3.5925900556  -2.4931375459   0.6611531789
H  -1.7600971578  -3.996655338    0.1658488018
H  -0.8864612265   3.7605698144   2.0801006905
H   1.5210812351   3.5857906484   1.8857946726
H   3.6244462577   1.8307040033   1.322187532
H   4.1920250055  -0.4154612751   0.639762863
H  -4.2337142496   0.1514543959   1.3633177296
```

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

5.4. Output file of RRKM-ME calculations for the benzo[*ghi*]fluoranthen-5-yl + C$_2$H$_2$ 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	***	***	***

T(K)							
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

T(K)								
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

T(K)	ip1->ip2	ip1->ip3	ip1->ip4	ip1->p0	ip1->p1	ip1->p2	ip1->	Capture
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

T(K)	ip2->ip1	ip2->ip3	ip2->ip4	ip2->p0	ip2->p1	ip2->p2	ip2->Capture	
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

T(K)								
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

T(K)	ip3->ip1	ip3->ip2	ip3->ip4	ip3->p0	ip3->p1	ip3->p2	ip3->Capture	Capture
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	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	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

T(K)	ip3->ip1	ip3->ip2	ip3->ip4	ip3->p0	ip3->p1	ip3->p2		ip3->Capture
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

T(K)	ip4->ip1	ip4->ip2	ip4->ip3	ip4->p0	ip4->p1	ip4->p2	ip4->Capture
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

T(K)	ip4->ip1	ip4->ip2	ip4->ip3	ip4->p0	ip4->p1	ip4->p2	ip4->	Capture
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

T(K)	ip4->ip1	ip4->ip2	ip4->ip3	ip4->p0	ip4->p1	ip4->p2	ip4->Capture
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

T(K)								
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

T(K)	p0->ip1	p0->ip2	p0->ip3	p0->ip4	p0->p1	p0->p2	p0->Capture	
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

T(K)	p0->ip1	p0->ip2	p0->ip3	p0->ip4	p0->p1	p0->p2		p0->Capture
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

T(K)	p1->ip1	p1->ip2	p1->ip3	p1->ip4	p1->p0	p1->p2	p1->Capture	
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

T(K)								
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

T(K)	p1->ip1	p1->ip2	p1->ip3	p1->ip4	p1->p0	p1->p2	p1->Capture	
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

T(K)					p1->p0	p1->p2	p1->Capture	
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->p2	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

	p2->ip1	p2->ip2	p2->ip3	p2->ip4	p2->p0	p2->p1	p2->Capture	
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

References

1. L. Zhao, M. B. Prendergast, R. I. Kaiser, B. Xu, U. Ablikim, M. Ahmed, B. J. Sun, Y. L. Chen, A. H. Chang and R. K. Mohamed, *Angew. Chem. Int. Ed.*, 2019, **58**, 17442-17450.
2. L. Zhao, R. I. Kaiser, B. Xu, U. Ablikim, M. Ahmed, M. M. Evseev, E. K. Bashkirov, V. N. Azyazov and A. M. Mebel, *Nat. Astron.*, 2018, **2**, 973.
3. L. Zhao, R. I. Kaiser, B. Xu, U. Ablikim, M. Ahmed, D. Joshi, G. Veber, F. R. Fischer and A. M. Mebel, *Nat. Astron.*, 2018, **2**, 413-419.
4. L. Zhao, R. I. Kaiser, B. Xu, U. Ablikim, M. Ahmed, M. V. Zagidullin, V. N. Azyazov, A. H. Howlader, S. F. Wnuk and A. M. Mebel, *J. Phys. Chem. Lett.*, 2018, **9**, 2620-2626.
5. L. Zhao, R. I. Kaiser, W. Lu, B. Xu, M. Ahmed, A. N. Morozov, A. M. Mebel, A. H. Howlader and S. F. Wnuk, *Nat. Commun.*, 2019, **10**, 1-7.
6. L. Zhao, R. I. Kaiser, B. Xu, U. Ablikim, W. Lu, M. Ahmed, M. M. Evseev, E. K. Bashkirov, V. N. Azyazov, M. V. Zagidullin, A. N. Morozov, A. H. Howlader, S. F. Wnuk, A. M. Mebel, D. Joshi, G. Veber and F. R. Fischer, *Nat. Commun.*, 2019, **10**, 1510.
7. L. Zhao, M. Prendergast, R. I. Kaiser, B. Xu, U. Ablikim, W. Lu, M. Ahmed, A. D. Oleinikov, V. N. Azyazov and A. H. Howlader, *Phys. Chem. Chem. Phys.*, 2019, **21**, 16737-16750.
8. L. Zhao, B. Xu, U. Ablikim, W. Lu, M. Ahmed, M. M. Evseev, E. K. Bashkirov, V. N. Azyazov, A. H. Howlader and S. F. Wnuk, *ChemPhysChem*, 2019, **20**, 791-797.