Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supplementary Information

The intermolecular anthracene-transfer in a regiospecific antipodal C_{60} difunctionalization

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Computational Methodology

On all obtained stationary points, energy minima and transition states, an energy decomposition analysis (EDA)[1] was performed using Turbomole, as to quantify the non-covalent interactions between the anthracene and fullerenes. It divides the total energy into several contributions: the electrostatic interaction energy (E_{ele}), which represents a combination of the nuclear repulsion energy along with the 1-electron and 2-electron Coulomb integrals, the exchange-repulsion ($E_{xc\text{-}rep}$) term, which sums up the fragments exchange interaction ($E_{xc\text{-}int}$) along with the repulsion term (E_{rep}), the polarization energy, which contains the orbital relaxation (E_{orb}) term, the correlation interaction (E_{cor}), which represents a correction to the Hartree-Fock (HF) energy, due to the utilization of Kohn-Sham orbitals, and the dispersion term of the interaction energy (E_{disp}), which denotes the empirical dispersion corrections. Alongside the DFT EDA, an analysis of the non-covalent interactions is performed at the CCSD(T) level using the Domain-based Local Pair Natural Orbital – Local Energy Decomposition (DLPNO-LED)[2] method, as implemented in ORCA 4.0.1. It is used in combination with the cc-pVDZ basis set.[3] In this scheme, the sum of electrostatic interactions (E_{ele}) along with the 2-electron exchange (E_{xc}) make up the Hartree-Fock interactions, while summing up the CCSD pair energies (E_{CCSDP}) along with the, triples contribution (E_{trp}) and the PNO and local corrections (E_{PNO}) provides the equivalent of the E_{disp}.

Bis-Adduct Energetics

Out of all potential C_{60}:anthracene bis-adducts only edge and trans adducts were found in experiment and no cis adducts were observed. In total 5 bis-adducts were investigated with the anthracene located in the following positions: “edge” (Figure S1), “trans-2” (Figure S2), “trans-3” (Figure S3), “trans-4” (Figure S4) and “trans-1” (Figure S5). For details about the nomenclature, see e.g. Ref. 4.

When looking at the reaction energies in Table S1, it can be seen that bis-adduct “edge” is the most stable thermodynamically, with a reaction energy of -115.0 kJ mol^{-1}. It is followed by bis adducts “trans-3” and “trans-2”, which are slightly less stable, being 1.4 kJ mol^{-1} and 5.9 kJ mol^{-1} higher in energy, respectively. Finally, bis-adducts “trans-4” and the antipodal bis-adduct “trans-1” are the least stable of the group, with relative energies of 8.7 and 9.2 kJ mol^{-1}. However, bis-adduct “trans-1” is the only one that was found in the solid-state experiment.

Table S1. Electronic reaction energies of the formation of the various trans bis-adducts, calculated using BP86/def2-TZVP/D3// BP86/def2-SVP/D3. ΔE_{rel} represents the relative energy difference compared to the most stable bis-adduct, while ΔE_r is the reaction energy compared to free educt molecules.

Structure	Reaction Energies	
	ΔE_r	ΔE_{rel}
Bis adduct “edge” / e	-115.0	0.0
Bis adduct “trans-3” / t3	-113.5	1.4
Bis adduct “trans-2” / t2	-109.1	5.9
Bis adduct “trans-4” / t4	-106.3	8.7
Bis adduct “trans-1” / t1 /antipodal	-105.8	9.2

As the reaction energies only offer information on the thermodynamics of the formation of bis-adducts, it is necessary to look at the transition state barriers in order to obtain information about the kinetics to examine difference along the reaction pathway for the various conformers. The optimized structures of the intermediates and transition states leading to the bis-adducts formation are depicted in Figures S6-S10.

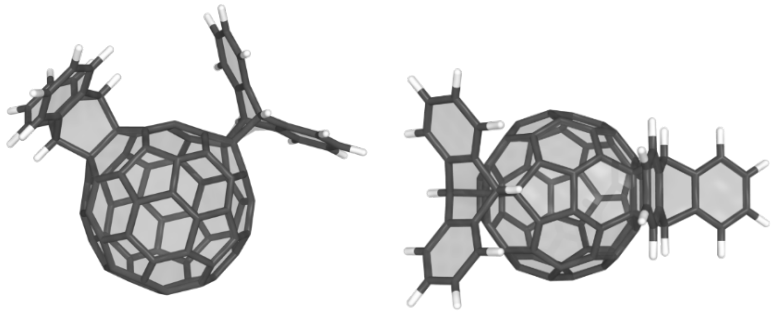

Figure S1. Bis adduct “edge”; 2 views of the structure optimized with BP86/def2-TZVP/D3 are shown.

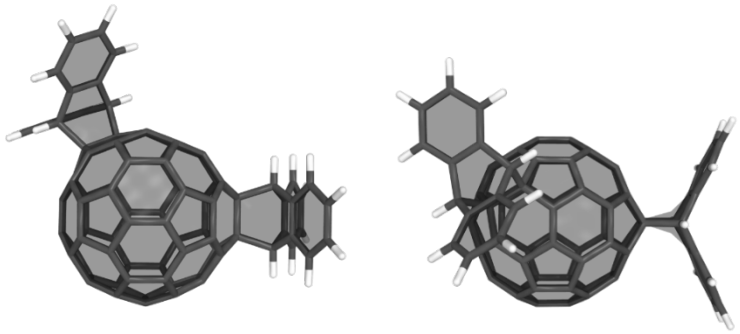

Figure S2. Bis adduct “trans-3”; 2 views of the structure optimized with BP86/def2-TZVP/D3 are shown.

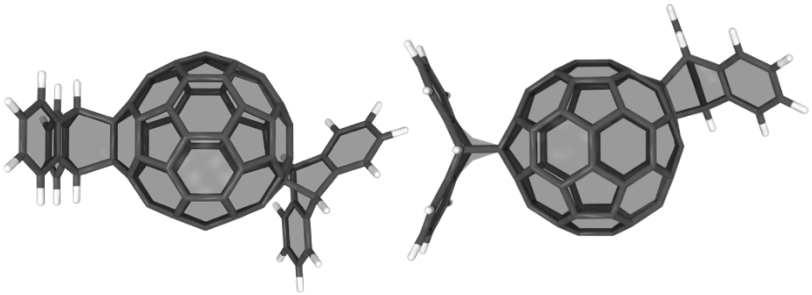

Figure S3. Bis adduct “trans-2”; 2 views of the structure optimized with BP86/def2-TZVP/D3 are shown.

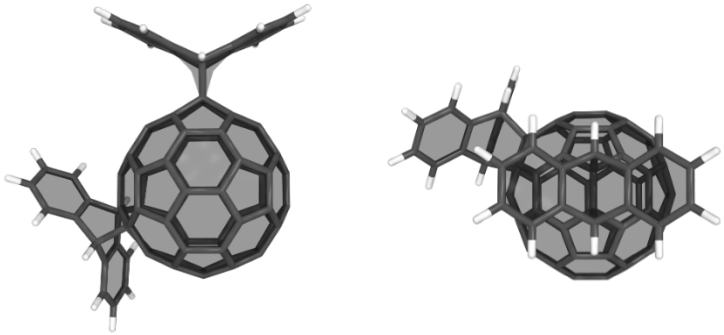

Figure S4 Bis adduct “trans-4”; 2 views of the structure optimized with BP86/def2-TZVP/D3 are shown.

Figure S5. Bis adduct “trans-1”, also termed as antipodal; 2 views of the structure optimized with BP86/def2-TZVP/D3 are shown.

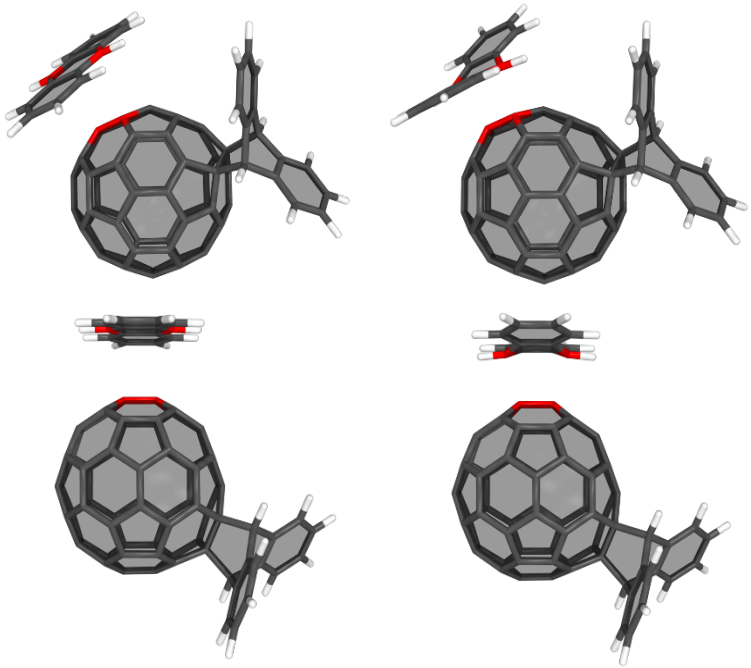

Figure 6. Bis adduct ”edge”; intermediate structure(left) and transition state (right) optimized at the BP86/def2-TZVP/D3 level of theory.

Figure S7. Bis adduct ”trans-3”; intermediate structure(left) and transition state (right) optimized at the BP86/def2-TZVP/D3 level of theory.

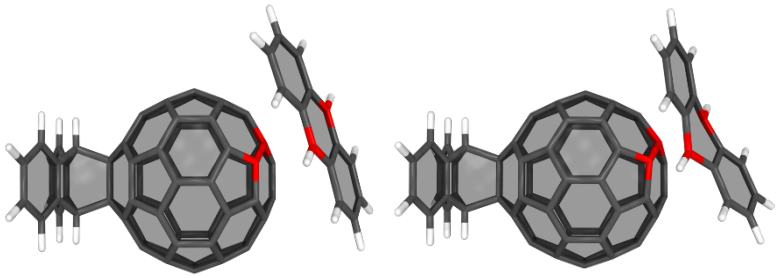

Figure S8. Bis adduct ”trans-2”; intermediate structure(left) and transition state (right) optimized at the BP86/def2-TZVP/D3 level of theory.

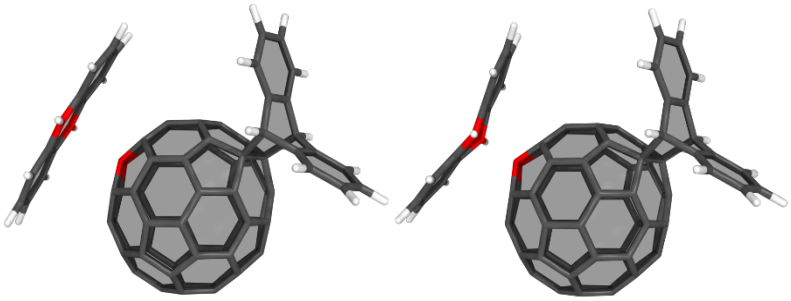

Figure S9. Bis adduct ”trans-4”; intermediate structure(left) and transition state (right) optimized at the BP86/def2-TZVP/D3 level of theory.

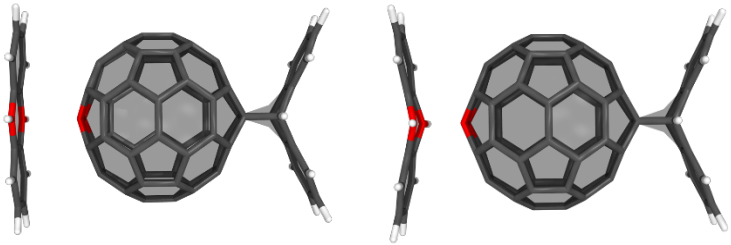

Figure S10. Bis adduct ”trans-1”; intermediate structure(left) and transition state (right) optimized at the BP86/def2-TZVP/D3 level of theory. $d_{C1\text{-}C10'}$= 2.153 Å and $d_{C9\text{-}C9'}$= 2.150 Å.

While examining the energies for the formation of the intermediate and transition state structures shown in Table S2, as well as the relative energies presented in Table S3, we can see that not only the product energy varies, but the intermediate and transition state energies too. The energy barriers can be calculated from the difference between the transition states and their respective intermediates. The energy barriers for all adducts are relatively similar, varying between 61.7 and 67.2 kJ mol^{-1} depending on the position of the anthracene. The order of the amount of activation energy required for the creation of the bis-adducts matches the stability of the adducts. Notably, the antipodal bis-adduct is the least stable out of all bis-adducts investigated, while also exhibiting the highest energy barrier.

Table S2. Relative energies of various bis-adducts for the formation of the intermediate, transition state and product from the separated educts as well as transition barriers. All energy values are in kJ mol^{-1}, calculated using BP86/def2-TZVP/D3//BP86/def2-SVP/D3.

Structure	ΔE_r Intermediate	ΔE_r Transition State	ΔE_r Product	$\Delta E_{Barrier}$
Bis adduct “edge’	-98.6	-36.9	-115.0	61.7
Bis adduct “trans-3“	-97.7	-34.7	-113.5	62.9
Bis adduct “trans-2”	-96.7	-31.6	-109.1	65.2
Bis adduct “trans-4”	-96.0	-28.9	-106.3	67.1
Bis adduct “trans-1”	-95.8	-28.6	-105.8	67.2

Table S3. Relative energy differences when comparing all intermediates and transition states and products with each other All energy values are in kJ mol^{-1}, calculated using BP86/def2-TZVP/D3//BP86/def2-SVP/D3.

Structure	ΔE_{rel} Intermediate	ΔE_{rel} Transition State	ΔE_{rel} Product
Bis adduct “edge”	0.0	0.0	0.0
Bis adduct “trans-3“	0.9	1.3	1.4
Bis adduct “trans-2“	1.9	3.5	5.9
Bis adduct “trans-4“	2.6	5.5	8.7
Bis adduct “trans-1“	2.8	5.5	9.2

Comparison with Experimental Data and Validation of Computational Methodology

The optimized structures of two bis-adducts ("edge" and "trans-4") were compared with crystal structures[5] in order to validate the accuracy of the methods employed. The consistent numbering of the atoms is given in Figure S11.

As it can be seen from Table S4, the structures obtained from the optimization are very close to their crystal counterparts, with the error in bond lengths being lower than 0.01 Å. In the case of angles and dihedrals, the errors are again small, deviating less than 2°.

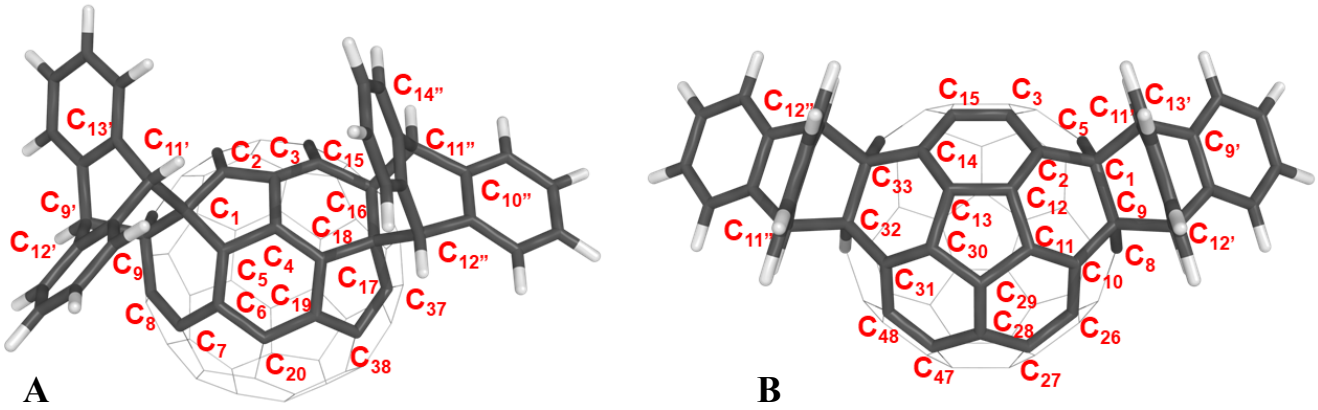

Figure S11. Labelling of the C_{60}:anthracene bis-adduct "edge" (A) and **"**trans-4" (B).

Table S4. Relevant structural parameters of the bis adducts "edge" (left) and "trans-4" (right) as seen in Figure S11; bond lengths are in Å; angles are in degrees; the structures were optimized with BP86/def2-SVP/D3.

Bonds	Crystal structure	Optimized "edge"
C(1)-C(9)	1.595	1.604
C(1)-C(11')	1.597	1.602
C(9)-C(12')	1.600	1.601
C(1)-C(2)	1.529	1.528
C(1)-C(5)	1.530	1.528
C(3)-C(4)	1.466	1.470
C(15)-C(16)	1.519	1.530
C(16)-C(17)	1.604	1.602
C(17)-C(18)	1.523	1.530
C(16)-C(11")	1.592	1.600
C(17)-C(12")	1.591	1.600
Angle		
C(9)-C(1)-C(11')	108.2	107.9
C(2)-C(1)-C(11')	110.4	109.8
C(5)-C(1)-C(11')	109.5	109.8
C(17)-C(16)-C(11")	107.6	108.0
C(15)-C(16)-C(11")	110.7	109.8
C(18)-C(17)-C(12")	110.3	110.0
Dihedral		
C(2)-C(1)-C(11')-C(9')	176.6	176.5
C(2)-C(1)-C(11')-C(13')	67.0	67.0
C(2)-C(1)-C(9)-C(8)	114.7	114.1

Bonds	Crystal structure	Optimized "trans-4"
C(1)-C(9)	1.597	1.604
C(1)-C(11')	1.596	1.600
C(9)-C(12')	1.598	1.601
C(1)-C(2)	1.529	1.530
C(9)-C(10)	1.530	1.530
C(11)-C(12)	1.471	1.474
C(12)-C(13)	1.437	1.446
C(13)-C(30)	1.477	1.474
C(14)-C(33)	1.520	1.530
C(32)-C(11")	1.586	1.601
C(33)-C(12")	1.589	1.600
Angle		
C(9)-C(1)-C(11')	107.8	108.0
C(2)-C(1)-C(11')	111.2	109.8
C(5)-C(1)-C(11')	109.5	109.8
C(32)-C(33)-C(12")	107.7	107.9
C(14)-C(33)-C(12")	109.7	110.0
C(34)-C(33)-C(12")	110.9	109.9
Dihedral		
C(2)-C(1)-C(11')-C(9')	177.0	176.6
C(2)-C(1)-C(11')-C(13')	66.4	66.8
C(2)-C(1)-C(9)-C(8)	114.9	114.4

To validate further our computational methodology, we tested the effect of the crystal environment by modelling it with an implicit solvent and tested the effect of a different density functional on our investigated model reaction A as listed Table S5. In agreement with Ref. 6, we chose a dielectric constant of ε=4 to account for the crystal environment.

Table S5. Relative electronic energies, enthalpies and Gibbs energies. The reference energy has been set to 0.0 for the intermediate **INT_{Mono}** in all cases. The electronic energies are computed with BP86/def2-TZVP/D3//BP86/def2-SVP/D3 as well as B3LYP/def2-TZVP/D3//BP86/def2-SVP/D3 in the case of "B3LYP". The thermal and zero-point energy corrections are obtained with BP86/def2-SVP/D3.

	ΔE	ΔH	ΔG	
BP86 + implicit solvent	0.0	0.0	0.0	**INT_{Mono}**
	59.4	54.7	63.9	**TS(INT_{Mono}-1')**
	-22.2	-19.5	-1.2	**1'**
BP86	0.0	0.0	0.0	**INT_{Mono}**
	57.6	52.9	62.0	**TS(INT_{Mono}-1')**
	-21.8	-19.0	-0.8	**1'**
B3LYP	0.0	0.0	0.0	**INT_{Mono}**
	85.0	80.3	89.5	**TS(INT_{Mono}-1')**
	-9.6	-6.9	11.4	**1'**

The inclusion of an implicit solvent resembling the crystal environment of the reaction does not have a significant and only slightly stabilizing effect on the reaction energetics, as seen in Table S5. However, switching from the BP86 to B3LYP functional results in a large increase in the energy barrier for the C_{60}:anthracene and in a decrease in the stability of **1'**.

Sarova *et al*.[7] reported activation energies for the cycloaddution and the cycloreversion as well as reaction energies for the addition of anthracene to C60 in toluene (listed in Table S6).

Table S6. Experimental C_{60}:anthracene mono-adduct reaction barriers for the cycloaddition as well as the cycloreversion, whereas Δ_{exp} denotes the reaction energy for the cycloaddition. Enthalpies and Gibbs energies are given in kJ mol^{-1}, whereas entropies are given in J K^{-1} mol^{-1}.

	Cycloaddition	Cycloreversion	Δ_{exp}
ΔH	57.0	138.0	-81.0
ΔS	-123.0	71.0	
ΔG	93.7	116.8	-23.2

Calculated energies for the formation of the of the educts (C_{60} and anthracene), product (C_{60}:anthracene), the noncovalently bound intermediate as well as the barrier to the cycloaddition for the formation of the C_{60}:anthracene mono-adduct are listed in Table S7, where the energy of the separated educts, C_{60} and anthracene were arbitrarily set to zero. First entry block lists BP86/def2-TZVP/D3//BP86/def2-SVP/D3 values, the 2nd block B3LYP/def2-TZVP/D3//BP86/def2-SVP/D3, in both cases, thermodynamic corrections were calculated with BP86/def2-SVP/D3. In the last block, structures and thermodynamic corrections were obtained with BP86/def2-TZVP/D3. Full reoptimisation with the lager triple-zeta def2-TZVP basis set cures the inadequacies of the smaller def2-SVP basis in the calculation of thermodynamic corrections and correctly predicts the formation of the C_{60}:anthracene mono-adduct to be exergonic.

Table S7. Relative electronic energies, enthalpies and Gibbs energies for the formation of C_{60}:anthracene mono-adduct. The reference energy has been set to 0 for the C_{60} and anthracene. The electronic energies were computed with BP86/def2-TZVP/D3//BP86/def2-SVP/D3 as well as B3LYP/def2-TZVP/D3//BP86/def2-SVP/D3 in the case of "B3LYP". In these two cases, thermal and zero-point energy corrections were obtained with BP86/def2-SVP/D3. In the last case, structures as well as thermal and zero-point corrections were obtained with BP86/def2-TZVP/D3. Energies are in kJ mol^{-1}.

	ΔE	ΔH	ΔG	
C_{60}:anthracene (BP86)	0.0	0.0	0.0	C_{60} + Anthracene
	-46.9	-43.7	9.1	Intermediate
	15.4	15.7	72.6	TS
	-62.4	-54.5	7.4	Product
	62.3	59.4	72.6	Barrier Cycloaddition
C_{60}:anthracene (B3LYP)	0.0	0.0	0.0	C_{60} + Anthracene
	-31.7	-28.5	24.2	Intermediate
	57.4	57.7	114.6	TS
	-39.3	-31.4	31.7	Product
	89.1	86.2	114.6	Barrier Cycloaddition
C_{60}:anthracene (opt def2-TZVP)	0.0	0.0	0.0	C_{60} + Anthracene
	-65.6	-55.0	-5.2	Product

Minimum Energy Structure of 1

As initial investigations of the educt **1** in reaction "A" pointed to a shallow potential energy surface, we performed a 2D potential energy scan for this educt to determine the most stable conformation. As depicted in Figure S12, the C_{60} fullerene can freely rotate over a large space (~90° along the X-axis and ~135° along the Y axis) without having to surpass any energy barriers higher than 10.0 kJ mol^{-1}, passing through multiple energy minima that are identical due to symmetry considerations. It is worth noting here, that due to computational costs the PES was generated by calculation of single point energies of the distorted structures. This is only an approximation of the true PES and re-optimization of the involved structures should further decrease the energy differences, making it even flatter.

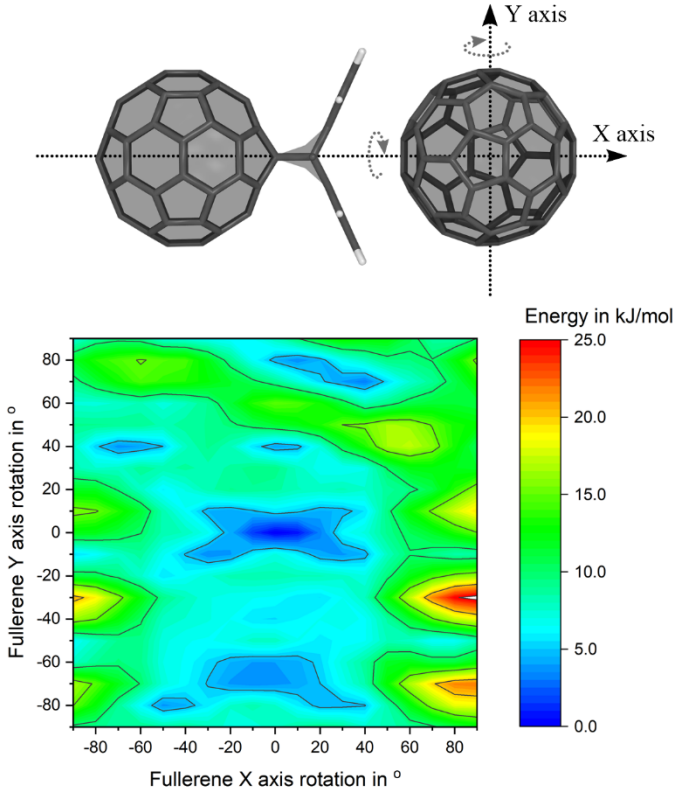

Figure S12: Energy surface scan of the C_{60} fullerene rotation along the X and Y axes. Top: complex 1 with chosen rotation axes plotted; Bottom: 2D projection of the energy surface scan results.

Distortion Interaction Analysis

The distortion of the transition state **TS(1-INT$_{Mono}$)** is visualized in Figure S13, both anthracene and fullerene are significantly deformed. The anthracene is bent by ca. 32° and the fullerene exhibits a deformation involving the two carbon atoms taking part in the Retro Diels-Alder reaction.

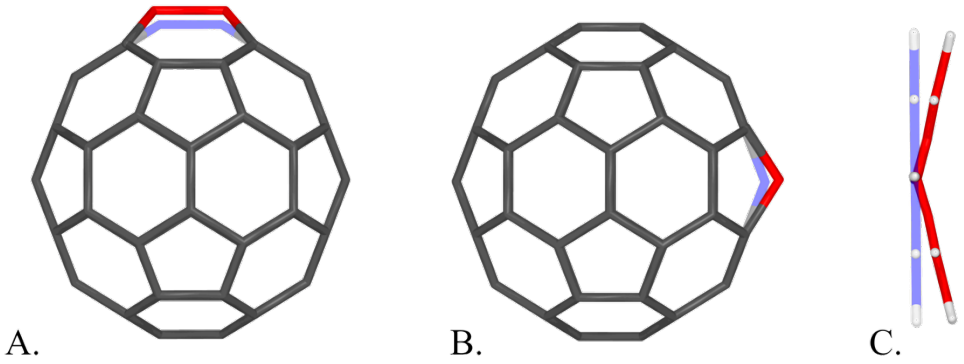

Figure S13. Distortion of the fullerene and anthracene molecules in the transition state. A: Top view of the C_{60} fullerene; B: side view of the C_{60} fulerene; C: side view of the anthracene. The blue coloring denotes an isolated C_{60} and an isolated anthracene molecule, while the red coloring marks the **TS(1-INT$_{Mono}$)** structure deformations.

Energy Decomposition Analysis

To further elucidate the driving forces of this reaction we performed an Energy Decomposition Analysis (EDA) along the reaction coordinates at the DFT level, where the individual contributions to the total interaction energy are dissected. We intended to quantify the contribution of non-covalent interactions between the substituents along the reaction coordinate by dividing the complex into two subfragments and evaluating the interaction energy. Due to computational cost (and as the results are expected to be similar), we restrict our EDA analysis to reaction A only.

In our analysis, we divided **1** into two fragments, a C_{60}:anthracene mono-adduct and a C_{60} fullerene, as displayed in Figure S14 in blue and red, and studied the interaction between these fragments along the reaction coordinate.

Based on the data displayed in Table S8 for the DFT EDA, the reaction is – as expected – totally symmetric. The interaction energies between the fragments varying only by about 6 kJ mol^{-1} along the reaction, being between -52.0 and -58.2 kJ mol^{-1}. The total interaction energy is governed mainly by repulsive electrostatic interactions (E_{ele}) that are compensated by attractive correlation (E_{cor}) and dispersive interactions (E_{disp}), whereas all other contributions, such as exchange-repulsion ($E_{xc\text{-}rep}$) and orbital relaxation (E_{orb}), are small. All three contributions, E_{ele}, E_{cor} and E_{disp}, are most pronounced in **1** and sum up to a total interaction energy of E= -58.2 kJ mol^{-1}. They decrease going to the transition states, (**TS(1-INT$_{Mono}$)** and **TS(INT$_{Mono}$-1')**, respectively, to around ~-56 kJ mol^{-1} and are smallest in the intermediate **INT$_{Mono}$,** with only -52.0 kJ mol^{-1}. It should be noted here that in **INT$_{Mono}$**, the non-covalent interactions are only depicted with one fullerene, whereas in reality the anthracene is noncovalently bound to both fullerenes. Looking at the trend in interaction energy, it can be seen that the shape of the anthracene has an influence on the total interaction strength. **1**, where the anthracene molecule distorted towards the 2nd fullerene, shows the strongest intermolecular interactions of all.

Considering the DLPNO-EDA, the total interaction energy is with $E_{\mathbf{disp+\ total\ SCF}}$=-441.1 kJ mol^{-1} most favorable in **1** and **1'** and smallest in the two transition-states ($E_{\mathbf{disp\ +\ total\ SCF}}$=-389.5 kJ mol^{-1}). The electrostatic and exchange interactions E_{disp} follow the trend of $E_{\mathbf{total\ int\ +\ total\ SCF}}$ and are least attractive in the transition states. The energy of the transition state is dominated by less favorable electrostatic interactions (compared to **1** and **INT$_{Mono}$**). Regardless the differences in the decomposition scheme that give rise to different electrostatic contributions, we can see a general trend in both interaction analyses methods for the non-covalent interactions. In both DFT EDA and DLPNO-LED approaches, the dispersion interactions (E_{disp}) follow the same relative energy pattern, with the intermediate structure providing the lowest non-covalent interactions. Again, due to the decomposition into two fragments, these analyses only evaluate the interaction for the anthracene with one fullerene, where in reality it interacts with both.

Table S8. Energy decomposition analysis contributions of various reaction species of reaction "A" according to DFT-EDA and DLPNO-LED. All energies are in kJ mol^{-1}.

Structure	**1**	**TS(1-INT$_{Mono}$)**	**INT$_{Mono}$ A**	**INT$_{Mono}$ B**	**TS(INT$_{Mono}$-1')**
DFT-EDA					
$E_{\text{total int}}$	-58.2	-56.3	-52.0	-52.0	-56.3
E_{ele}	102.4	90.3	84.6	84.6	90.3
$E_{\text{xc-rep}}$	-6.1	-1.8	-4.3	-4.3	-1.8
E_{orb}	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1
E_{cor}	-65.9	-59.8	-55.3	-55.3	-59.8
E_{disp}	-88.6	-85.0	-77.0	-77.0	-85.0
DLPNO-EDA					
Hartree-Fock Energy					
S_{ele}	-208.8	-176.5	-196.8	-196.8	-176.5
E_{xc}	-95.1	-81.2	-90.1	-90.1	-81.2
$E_{\text{total SCF}}$	-303.9	-257.7	-286.9	-286.9	-257.7
Correlations Energy					
E_{CCSDT}	-92.6	-85.8	-82.8	-82.8	-85.8
E_{trp}	-17.6	-16.6	-16.3	-16.3	-16.6
$E_{\text{PNO-}}$	-27.1	-29.7	-26.3	-26.3	-29.7
$E_{\text{disp.}}$	-137.3	-132.2	-125.2	-125.4	-132.2
$\boldsymbol{E_{\text{disp+ total SCF}}}$	-441.1	-389.9	-412.3	-412.3	-389.9

The two different energy decomposition analysis methods show very similar results in relative dispersion interactions (when the intermediate structure is taken as a baseline for comparison), as can be seen in Figure S14, where the half reaction is depicted. The electrostatic interactions on the other hand, show very different results, likely due to the different theoretical approaches. As evident from Table S8 the reaction is totally symmetric but the 2nd half was omitted to increase readability.

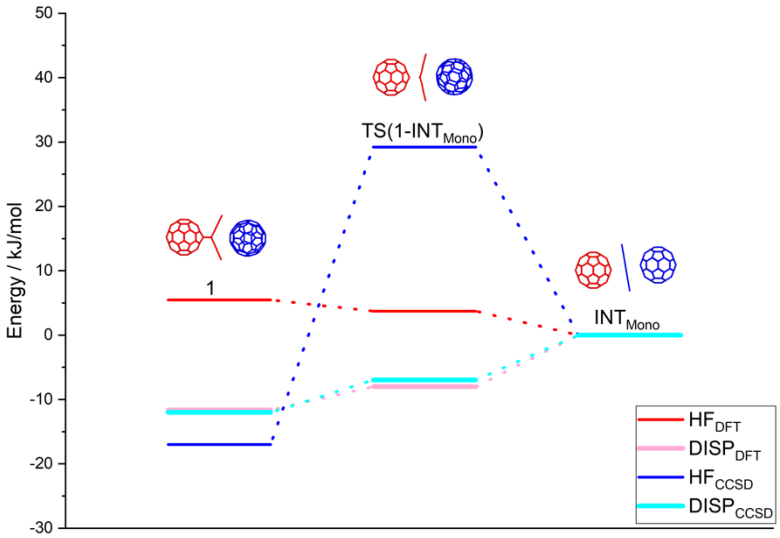

Figure S14. Energy Decomposition Analysis for the Half Reaction A. Each complex structure was divided into two fragments, displayed in blue and red. The interactions are separated into electrostatic and dispersive and are plotted for both the DFT approach, as well as for DLPNO-LED. The energy contributions of the intermediate **INT$_{Mono}$**, where arbitrarily set to zero and for all other species given relative to **INT$_{Mono}$**.

Intermediates with Smaller Rings

Apart from anthracene, smaller rings, such as naphthalene or benzene also form a noncovalently bound intermediate with two C_{60} fullerene molecules, as depicted in Figure S15. Figure S15 shows that the orientation that is seen in the anthracene of the $\mathbf{INT_{Mono}}$ structure is largely identical in the case of replacing anthracene with naphthalene or benzene. Notably, the orientation of the aromatic ring over the curved fullerene surface differs.

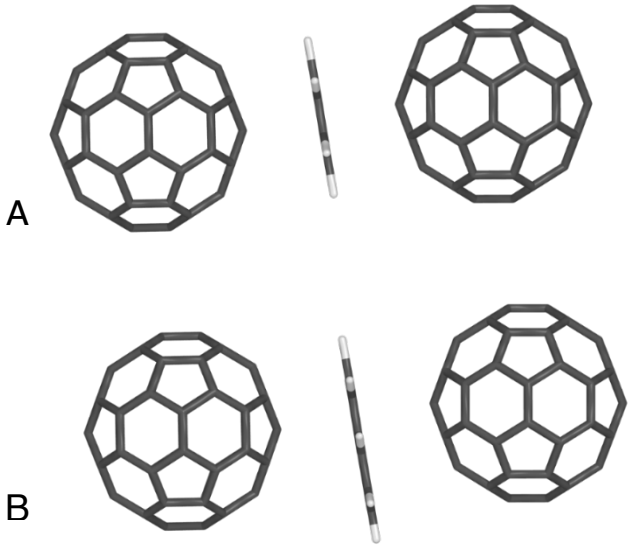

Figure S15. The intermediate states of benzene (A) and naphthalene (B) transfer reactions. Structures optimized with BP86/def2-SVP/D3. The naphthalene and benzene molecules have a similar orientation compared to the fullerenes as the anthracene molecule in **INT**.

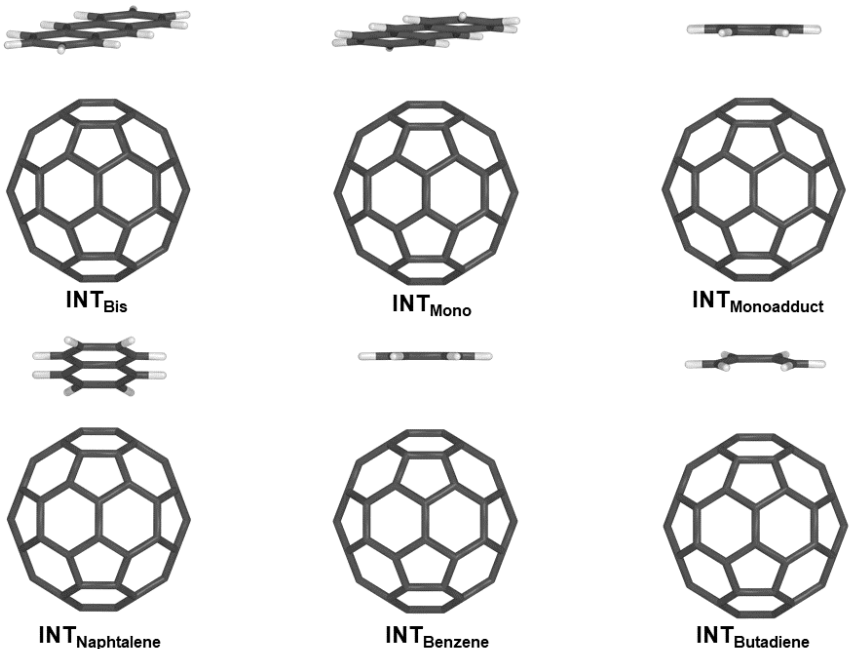

Figure S16. The intermediate states of transfer reaction B, transfer teaction A, mono-adduct addition, naphtalene addition, benzene addition and butadiene addition. Structures optimized with BP86/def2-SVP/D3.

Comparison of Energy Barriers

The energetics for the formation of mono-adducts with benzene, naphthalene and anthracene are as well as for the complexes **1'**, **2**, and **3** were shown in Table S9.

Table S9. Relative electronic energies, enthalpies and Gibbs energies of the C_{60}:acene mono-adduct complexes, as well as of **1'**, **2**, and **3**, their intermediates and TS to cycloaddition. The energy of the intermediates has been set to 0 in all cases. The electronic energies are computed with BP86/def2-TZVP/D3//BP86/def2-SVP/D3 as well as B3LYP/def2-TZVP/D3//BP86/def2-SVP/D3 in the case of C_{60}:anthracene (B3LYP). The thermal and zero-point energy corrections are obtained with BP86/def2-SVP/D3.

	ΔE	ΔH	ΔG	Structure
C_{60}:benzene	0.0	0.0	0.0	**Intermediate**
	128.1	123.0	140.7	**TS**
	88.5	88.2	113.5	**Product**
C_{60}:naphthalene	0.0	0.0	0.0	**Intermediate**
	100.9	98.6	103.8	**TS**
	44.4	48.4	60.6	**Product**
C_{60}:anthracene	0.0	0.0	0.0	**Intermediate**
	62.3	59.4	63.5	**TS**
	-15.5	-10.8	-1.7	**Product**
C_{60}:anthracene (B3LYP)	0.0	0.0	0.0	**Intermediate**
	89.1	86.2	90.3	**TS**
	-7.6	-2.9	7.5	**Product**
INT_{Mono} to **1**	0.0	0.0	0.0	**INT_{Mono}**
	57.6	52.9	62.0	**TS(INT_{Mono}-1')**
	-21.8	-19.0	-0.8	**1'**
INT_{Bis} to **2**	0.0	-2.6	0.0	**INT_{Bis}**
	57.7	52.8	61.7	**TS(INT_{Bis}-2)**
	-19.1	-16.4	-2.8	**2**
INT_{Bis} to **3**	0.0	0.0	-16.2	**INT_{Bis}**
	65.6	60.3	52.9	**TS(INT_{Bis}-3)**
	-11.2	-9.1	-11.8	**3**

Curvature of Planar Surfaces and Bowl Depth

In Figure S17 it can be seen that the anthracene in the INT_{Mono} with two neighboring fullerenes is close to being perfectly planar (left hand side of Figure S17 depicted in blue), whereas in the monoadduct structure adopts a conformation that slightly follows the curvature of the fullerene (right hand side of Figure S17 depicted in red).

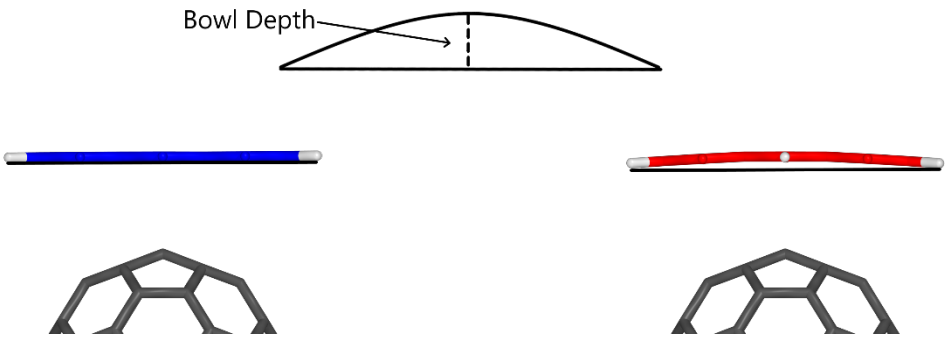

Figure S17. Difference in the anthracene deformation illustrated via differences in the bowl depth. On the left, in blue, the anthracene of **INT_{Mono}** is shown, while on the right side the anthracene of the C_{60}:anthracene intermediate is depicted in red.

XYZ Structure Coordinates

1

C	-2.4728409	0.0456403	-0.7457961
C	-2.5197732	-0.0801925	0.8571730
C	-3.2701588	1.0586016	1.5582668
C	-3.6587450	2.2403554	0.9414331
C	-3.6155204	2.3559394	-0.5349071
C	-3.1865091	1.2825879	-1.3040932
C	-3.9034613	0.9391604	-2.5077835
C	-3.9274506	-0.5132569	-2.6224835
C	-3.2238172	-1.0652583	-1.4897456
C	-3.6926782	-2.2298176	-0.8958622
C	-3.7360416	-2.3454265	0.5806885
C	-3.3081908	-1.2892089	1.3742717
C	-4.0787625	-0.9167043	2.5361869
C	-4.0545776	0.5358100	2.6501859
C	-5.1848905	1.2266442	3.1361240
C	-5.5877776	2.4634944	2.4962912
C	-4.8369993	2.9528593	1.4053201
C	-5.5225301	3.5045087	0.2423488
C	-4.7679887	3.1371867	-0.9503708
C	-5.4517696	2.8265416	-2.1459507
C	-5.0066729	1.7022671	-2.9456192
C	-6.1832305	1.0305494	-3.4902587
C	-6.2070481	-0.3716947	-3.6004652
C	-5.0553072	-1.1600115	-3.1710007
C	-5.5406371	-2.3795987	-2.5554993
C	-4.8707751	-2.8962931	-1.4250942
C	-5.6407876	-3.4194735	-0.3026017

C	-4.9398711	-3.0805534	0.9304936
C	-5.6767426	-2.7425326	2.0864119
C	-5.2336410	-1.6356125	2.9109280
C	-6.4120057	-0.9182609	3.3899536
C	-6.3881560	0.4839488	3.5003977
C	-7.5402640	1.2703813	3.0753692
C	-7.0435425	2.4948523	2.4528180
C	-7.7031677	3.0270428	1.3273050
C	-6.9283505	3.5475755	0.2045225
C	-7.6340843	3.2111396	-1.0286935
C	-6.9077116	2.8572181	-2.1828227
C	-7.3617033	1.7466781	-3.0157764
C	-8.5233752	1.0324727	-2.6650346
C	-8.5481276	-0.4228321	-2.7794900
C	-7.4104720	-1.1125275	-3.2405798
C	-6.9967403	-2.3544357	-2.5928193
C	-7.7378863	-2.8593243	-1.5062652
C	-7.0472314	-3.4082092	-0.3429007
C	-7.8069814	-3.0435432	0.8494597
C	-7.1326286	-2.7168750	2.0424775
C	-7.5890516	-1.5887669	2.8500538
C	-8.7011771	-0.8306663	2.4363862
C	-8.6764051	0.6246120	2.5510417
C	-9.3583347	1.1794642	1.3878425
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C	-8.9154008	-2.1474648	-1.0324682

C	-8.9581443	-2.2613895	0.4243377
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C	-9.8055456	0.0687674	0.5547503
C	-0.9315113	0.0635982	-1.1952181
H	-0.8835630	0.1509650	-2.2968230
C	-0.3271165	-1.2242679	-0.6850849
C	0.1751022	-2.2751292	-1.4656800
H	0.1982735	-2.1858717	-2.5622957
C	0.6564900	-3.4345037	-0.8318873
H	1.0720768	-4.2553438	-1.4349131
C	0.6238311	-3.5411937	0.5693284
H	1.0130558	-4.4465701	1.0582774
C	0.1037143	-2.4932060	1.3528161
H	0.0702065	-2.5781957	2.4496397
C	-0.3667490	-1.3347549	0.7220788
C	-1.0075857	-0.1411172	1.3926281
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C	0.6966413	3.4419184	-0.2846300
H	1.1222838	4.3426449	-0.7510266
C	0.2070352	2.4005500	-1.0932559
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C	-0.3072547	1.2452705	-0.4883957
C	6.6509386	3.3809962	0.9655624
C	8.0389580	2.9457899	0.8557283
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C	7.7645642	2.7731764	-1.6056916
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C	5.8574712	3.5010160	-0.1918715
C	6.0892722	2.7925340	2.1765524
C	7.1302751	1.9945023	2.8162949
C	8.3354986	2.0894262	1.9996880
C	9.1680841	0.9657343	1.8402965
C	9.4493662	1.4832950	-0.5713823
C	8.1203240	1.6862678	-2.5119959
C	7.1232636	1.0562954	-3.2806773
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C	5.3915384	2.5395384	-2.2979921
C	4.1852509	2.4464244	-1.4825961
C	4.4734192	3.0409586	-0.1803274
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C	6.7993615	0.7790029	3.4445125
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C	3.0859217	1.2869042	0.8984674
C	2.8102446	0.7137576	-0.3546155
C	3.3704100	1.3026197	-1.5660952
C	3.7231287	0.2159400	-2.4736163
C	4.8853883	0.3080970	-3.2631238
C	9.1612391	0.8889049	-1.8725146
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C	8.1359074	-1.1636573	-2.8207967
C	9.4648985	-1.3667059	-0.8803755
C	9.7431783	-0.7932734	0.3745936
C	9.1808726	-1.3812056	1.5858063
C	8.3608109	-2.5219167	1.4996259
C	7.1555849	-2.6171997	2.3160322
C	6.1224527	-3.2707265	1.5189199
C	4.7826693	-2.8514679	1.6242767
C	3.9625447	-2.7241352	0.4245866
C	3.3815388	-1.0442315	-1.8209972
C	2.8164933	-0.7348056	-0.5116895
C	3.1007399	-1.5598123	0.5901601
C	3.3845433	-0.9670877	1.8920328
C	4.4261641	-1.7643345	2.5315030
C	5.4233116	-1.1342426	3.3005395
C	6.8122631	-1.5682474	3.1897756
C	7.6623422	-0.3858985	3.2790734
C	8.8254632	-0.2941463	2.4915604
C	9.1689392	-0.5105319	-2.0242353
C	9.7353020	0.6572470	0.5318983
C	5.8954478	-3.4580381	-0.9463753

TS(1-INT$_{Mono}$)

C	-1.4011648	1.2803257	4.1581428

C	0.0607485	1.1926966	4.3511369
C	0.7864465	2.4357120	4.7088833
C	0.1591347	3.6850293	4.7379054
C	-1.2988648	3.7730255	4.5482113
C	-2.0415716	2.6068131	4.3404067
C	-3.3196099	2.4360848	5.0049157
C	-3.4519012	1.0314199	5.3687982
C	-2.2550426	0.3409944	4.9273040
C	-1.7193054	-0.6901459	5.7047888
C	-0.2614177	-0.7785253	5.8945106
C	0.5731332	0.1702903	5.2955910
C	1.6912759	0.7205136	6.0386276
C	1.8235700	2.1252297	5.6747050
C	2.2130830	3.0736389	6.6413819
C	1.5540153	4.3688671	6.6812200
C	0.5376265	4.6630837	5.7464678
C	-0.6722070	5.3538330	6.1823594
C	-1.8036984	4.8045806	5.4416243
C	-3.0525194	4.6472891	6.0811444
C	-3.8281056	3.4387628	5.8544574
C	-4.4728790	3.0646056	7.1102378
C	-4.6006193	1.7076705	7.4618320
C	-4.0888527	0.6686901	6.5722041
C	-3.5273571	-0.3956083	7.3877749
C	-2.3558097	-1.0572041	6.9605031
C	-1.3056545	-1.3703632	7.9246173
C	-0.0146469	-1.1989688	7.2653539
C	1.0788998	-0.6741895	7.9878584
C	1.9520674	0.3034507	7.3591092
C	2.3389559	1.2881616	8.3658862

C	2.4667902	2.6450921	8.0142947
C	1.9562581	3.6812769	8.9045217
C	1.3904478	4.7453564	8.0794540
C	0.2229271	5.4123855	8.4982753
C	-0.8256333	5.7238757	7.5319028
C	-2.1155070	5.5538890	8.1936650
C	-3.2080618	5.0234906	7.4804147
C	-4.0877075	4.0467654	8.1172107
C	-3.8429599	3.6363350	9.4414634
C	-3.9755071	2.2290565	9.8061282
C	-4.3481290	1.2817366	8.8336216
C	-3.6828902	-0.0177205	8.7865920
C	-2.6689283	-0.3210177	9.7159063
C	-1.4601370	-1.0116159	9.2771048
C	-0.3304343	-0.4625041	10.0205916
C	0.9156607	-0.2956909	9.3856057
C	1.6958964	0.9164859	9.6209202
C	1.2022730	1.9161251	10.4804770
C	1.3347798	3.3232563	10.1158353
C	0.1266691	4.0163567	10.5483864
C	-0.4183538	5.0426372	9.7529697
C	-1.8642168	5.1301275	9.5647193
C	-2.7118838	4.1879740	10.1786979
C	-2.1458743	3.1229264	10.9991802
C	-2.9262238	1.9123641	10.7683465
C	-2.2854052	0.6592268	10.7232951
C	-0.8395805	0.5717534	10.9117037
C	-0.0877146	1.7407781	11.1381916
C	-0.7521217	3.0386662	11.1807134
C	-1.7880369	0.7796509	2.0804840

H	-2.8853615	0.8685303	2.0281067
C	-1.2240329	-0.5499455	2.1324833
C	-1.9956644	-1.7358791	2.1006536
H	-3.0861962	-1.6670963	1.9716690
C	-1.3678263	-2.9784346	2.1929929
H	-1.9647771	-3.9000001	2.1250628
C	0.0341011	-3.0624420	2.3810583
H	0.5155326	-4.0485161	2.4586888
C	0.8044427	-1.9037431	2.4721757
H	1.8917815	-1.9633853	2.6298701
C	0.1943563	-0.6351886	2.3167302
C	0.9074876	0.6169387	2.4218610
H	1.9846259	0.5756981	2.6512678
C	0.4181371	1.7639216	1.6933656
C	1.2428002	2.8293989	1.2548971
H	2.3305649	2.7664283	1.4083328
C	0.6785417	3.9303755	0.6108595
H	1.3253959	4.7399548	0.2414263
C	-0.7240354	4.0151667	0.4333273
H	-1.1579696	4.8904405	-0.0725479
C	-1.5575488	3.0000723	0.9023167
H	-2.6490564	3.0697793	0.7807319
C	-1.0001919	1.8501931	1.5137184
C	1.5828088	-2.5775886	-7.2688489
C	2.7930680	-2.2695520	-6.6196131
C	3.1829730	-0.8769362	-6.4257981
C	2.3487861	0.1583327	-6.8879605
C	1.0942738	-0.1610554	-7.5609938
C	0.7181389	-1.5045034	-7.7479526
C	-0.6665856	-1.9111287	-7.5331043

C	-0.6576286	-3.2355428	-6.9210781
C	0.7325927	-3.6473758	-6.7577827
C	1.1224647	-4.3713791	-5.6155585
C	2.3769903	-4.0520599	-4.9422510
C	3.1973197	-3.0199691	-5.4354736
C	3.8366992	-2.0910994	-4.5096357
C	3.8280076	-0.7668448	-5.1216787
C	3.6169173	0.3751471	-4.3259169
C	2.7521711	1.4488604	-4.8054434
C	2.1294975	1.3421185	-6.0636111
C	0.7394199	1.7541253	-6.2270364
C	0.0994432	0.8250198	-7.1523538
C	-1.2363216	0.4327373	-6.9446796
C	-1.6261815	-0.9600129	-7.1383297
C	-2.6120048	-1.2983723	-6.1173025
C	-2.6035136	-2.5761240	-5.5267803
C	-1.6087314	-3.5622143	-5.9362090
C	-1.2045487	-4.3131593	-4.7525170
C	0.1365182	-4.7106768	-4.5952240
C	0.7823211	-4.6009594	-3.2911027
C	2.1668847	-4.1942173	-3.5054912
C	2.7840770	-3.2978934	-2.6115135
C	3.6342563	-2.2272994	-3.1231674
C	3.4168565	-1.0440489	-2.2979693
C	3.4077670	0.2345089	-2.8890406
C	2.4136765	1.2218970	-2.4805810
C	2.0082036	1.9727785	-3.6652361
C	0.6666615	2.3702010	-3.8231527
C	0.0208586	2.2584424	-5.1264947
C	-1.3644593	1.8513410	-4.9108427

C	-1.9815068	0.9549138	-5.8040097
C	-2.8312987	-0.1150963	-5.2926210
C	-3.0353592	-0.2510372	-3.9062601
C	-3.0271399	-1.5760803	-3.2938025
C	-2.8151837	-2.7181303	-4.0903543
C	-1.9505597	-3.7914944	-3.6117451
C	-1.3278919	-3.6851847	-2.3536539
C	0.0634835	-4.0975989	-2.1904555
C	0.7035833	-3.1684024	-1.2655567
C	2.0407567	-2.7777243	-1.4692675
C	2.4313206	-1.3832520	-1.2761663
C	1.4698973	-0.4325649	-0.8882336
C	1.4608703	0.8928623	-1.4990658
C	0.0709006	1.3010122	-1.6674587
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C	-1.5761022	1.7118401	-3.4740783
C	-2.3968741	0.6786416	-2.9804323
C	-1.9935621	-0.0725414	-1.7962681
C	-2.3839557	-1.4664306	-1.9887543
C	-1.5472947	-2.5016181	-1.5292004
C	-0.2916300	-2.1826627	-0.8602454
C	0.0852833	-0.8410462	-0.6801494
C	-0.7780614	0.2318981	-1.1580874

INT_{Mono}

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C	0.8433837	-1.0799829	4.5572071
C	1.5063103	-0.1801630	3.7005683
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C	-2.3632243	4.1129117	4.3828895
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C	-3.4300250	1.3209735	6.3860647
C	-2.9601806	0.1955576	5.5842557
C	-2.1894390	-0.6880864	6.4530427
C	-1.0387656	-1.3341456	5.9604944
C	0.1586699	-1.4236608	6.7903339
C	1.3218091	-1.2655204	5.9228441
C	2.4482190	-0.5534087	6.3792006
C	3.1373792	0.3735143	5.4870923
C	3.5678218	1.5246506	6.2745256
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C	0.1632231	-0.8647890	8.0824394
C	1.3304165	-0.1277574	8.5551449
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C	2.6406789	3.7325084	7.8499496
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C	-0.7521571	5.2108093	7.5438510
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C	-3.5678218	-1.5246506	-6.2745256
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C	-2.2796873	-4.8239702	-5.6487354
C	-1.1291973	-5.4686998	-6.1411814
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C	2.3568372	-4.6893186	-5.7229007
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C	3.4770865	-2.6133785	-5.8291409
C	3.4300250	-1.3209735	-6.3860647
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C	2.1894390	0.6880864	-6.4530427
C	1.0387656	1.3341456	-5.9604944
C	-0.1586699	1.4236608	-6.7903339
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C	-2.4482190	0.5534087	-6.3792006
C	-3.1373792	-0.3735143	-5.4870923
C	-2.6752568	-0.5566486	-4.1702744
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C	-3.0449595	-3.0077179	-4.3508015
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C	1.2401484	-4.2657778	-3.5457668
C	2.3632243	-4.1129117	-4.3828895
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C	1.3576116	0.2644968	-3.7452979

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C	-1.4285915	-1.9894952	-2.7680511
C	-0.6905478	-3.1855195	-2.7195786
C	0.7691553	-3.1439080	-2.7421421
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H	-3.4252965	-0.8472439	0.2258094
H	-3.4244404	-3.2707571	0.8157248
H	-1.2561129	-4.5064713	1.1045576
H	0.9187448	-3.3196987	0.8062616
H	2.1691648	-1.2325308	0.2948705
H	3.4252965	0.8472439	-0.2258094
H	3.4244404	3.2707571	-0.8157248
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C	-1.3056545	-1.3703632	7.9246173
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C	-2.1458743	3.1229264	10.9991802
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C	-0.7521217	3.0386662	11.1807134
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2

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C	2.6266136	0.7964496	-2.1457689
C	1.4500412	1.2037359	-1.4029952
C	0.7205575	2.3244947	-1.8148702
C	-0.7530903	2.2812086	-1.8021976
C	-1.4093907	1.1210630	-1.3774858
C	-0.6800385	-0.0368964	-0.7997843
C	-1.3411460	-1.2276279	-1.3926136
C	-0.6190569	-2.3427877	-1.8306356
C	0.8547379	-2.3002296	-1.8431843
C	1.5180705	-1.1440734	-1.4176082
C	0.7990154	0.0063964	-0.8175979
C	-1.3185251	-0.0008204	-9.7507234
H	-2.4243076	-0.0326612	-9.7540543
C	-0.6973228	-1.2154923	-10.4030150
C	-1.3776864	-2.3330596	-10.9033880
H	-2.4779003	-2.3671201	-10.8769746
C	-0.6399522	-3.4083091	-11.4327915
H	-1.1667755	-4.2873482	-11.8342317
C	0.7654156	-3.3677995	-11.4452965
H	1.3347348	-4.2152572	-11.8565002
C	1.4493281	-2.2515851	-10.9285550
H	2.5499684	-2.2222542	-10.9217820
C	0.7147826	-1.1747679	-10.4155759
C	1.2764920	0.0741131	-9.7739008
H	2.3820338	0.1060898	-9.7970737
C	0.6436144	1.2958470	-10.4013278
C	1.3147902	2.4188288	-10.9019826
H	2.4152981	2.4527330	-10.8953432

C	0.5675833	3.4995966	-11.4062780
H	1.0870474	4.3829416	-11.8078329
C	-0.8377815	3.4590597	-11.3936019
H	-1.4144600	4.3107886	-11.7852568
C	-1.5122238	2.3372577	-10.8765230
H	-2.6125702	2.3076404	-10.8500762
C	-0.7684912	1.2550940	-10.3886466

3

C	-4.2995552	0.4615871	-1.5461528
C	-3.9831044	0.4581365	-0.1752090
C	-4.4121735	1.5587196	0.6767084
C	-5.1444446	2.6273622	0.1307181
C	-5.4769217	2.6331137	-1.2885957
C	-5.0630519	1.5671638	-2.1121204
C	-5.9782552	1.0189638	-3.1088076
C	-5.7781515	-0.4260584	-3.1592604
C	-4.7405074	-0.7702558	-2.1931934
C	-4.8441162	-1.9579088	-1.4456546
C	-4.5088475	-1.9585948	-0.0260230
C	-4.0815059	-0.7739658	0.5977366
C	-4.5698658	-0.4345086	1.9298779
C	-4.7731082	1.0102760	1.9786034
C	-5.8642646	1.5461995	2.6877107
C	-6.6295103	2.6528341	2.1205150
C	-6.2756473	3.1833201	0.8652898
C	-7.3125916	3.5286046	-0.1011827
C	-6.8194615	3.1870712	-1.4322567
C	-7.7010178	2.6586386	-2.3942240

C	-7.2728366	1.5548151	-3.2470720
C	-8.4136697	0.6656898	-3.4404139
C	-8.2204346	-0.7278983	-3.4889885
C	-6.8792987	-1.2840410	-3.3464691
C	-6.9830715	-2.5171189	-2.5738613
C	-5.9826308	-2.8478798	-1.6400848
C	-6.3502977	-3.4001024	-0.3394345
C	-5.4374204	-2.8510384	0.6578190
C	-5.9091472	-2.5253733	1.9432378
C	-5.4671495	-1.2937849	2.5918919
C	-6.6015991	-0.7384038	3.3230708
C	-6.7961904	0.6557556	3.3714352
C	-8.1375512	1.2109008	3.2258319
C	-8.0345111	2.4446933	2.4529845
C	-9.0357175	2.7772364	1.5206461
C	-8.6682340	3.3288168	0.2207462
C	-9.5814597	2.7806171	-0.7765369
C	-9.1062616	2.4512385	-2.0598778
C	-9.5466473	1.2197622	-2.7068186
C	-10.4467093	0.3611768	-2.0476994
C	-10.2460640	-1.0830980	-2.0974331
C	-9.1532341	-1.6179677	-2.8052470
C	-8.3885475	-2.7240404	-2.2391387
C	-8.7431816	-3.2560459	-0.9851250
C	-7.7057519	-3.6008708	-0.0180596
C	-8.1968874	-3.2595024	1.3126634
C	-7.3149844	-2.7308039	2.2749908
C	-7.7428936	-1.6266982	3.1278285
C	-9.0371878	-1.0905752	2.9883852
C	-9.2382294	0.3535901	3.0384422

C	-10.2757846	0.6982781	2.0723762
C	-10.1761274	1.8880750	1.3268579
C	-10.5133748	1.8901434	-0.0928914
C	-10.9386024	0.7023517	-0.7170851
C	-11.0416244	-0.5310890	0.0557241
C	-10.6137770	-1.6345712	-0.7975284
C	-9.8754979	-2.7012674	-0.2512211
C	-9.5379144	-2.7033354	1.1684310
C	-9.9509346	-1.6387144	1.9915491
C	-10.7163082	-0.5332102	1.4252156
C	-0.3613712	0.0481894	-1.0388687
H	-0.4213893	0.0588669	-2.1431258
C	-0.9621796	-1.1999914	-0.4349035
C	-1.4293636	-2.3190541	-1.1344208
H	-1.4584125	-2.3110157	-2.2344371
C	-1.8649392	-3.4476880	-0.4150268
H	-2.2502588	-4.3240733	-0.9572239
C	-1.8171314	-3.4594990	0.9906251
H	-2.1640530	-4.3455775	1.5427737
C	-1.3338262	-2.3417091	1.6931884
H	-1.2792973	-2.3505219	2.7924072
C	-0.9113791	-1.2122588	0.9779493
C	-0.2604112	0.0232820	1.5559537
H	-0.2307792	0.0130656	2.6615355
C	-0.9080050	1.2701725	1.0003731
C	-1.3468654	2.3796871	1.7362788
H	-1.2986877	2.3671938	2.8358288
C	-1.8425316	3.5049565	1.0541583
H	-2.2024706	4.3746399	1.6239893
C	-1.8901768	3.5213029	-0.3515495

H	-2.2882163	4.4023965	-0.8764177
C	-1.4413215	2.4125270	-1.0901091
H	-1.4733804	2.4215320	-2.1900957
C	-0.9574300	1.2860374	-0.4104265
C	8.7773522	0.0235042	-0.9176783
C	8.8415546	0.0102778	0.6906841
C	8.1195453	1.1840101	1.3633345
C	7.6609733	2.3118671	0.6935776
C	7.6007289	2.3236623	-0.7874002
C	8.0028354	1.2069686	-1.5102863
C	7.2135261	0.7691525	-2.6347344
C	7.2101959	-0.6884847	-2.6461711
C	7.9974479	-1.1473677	-1.5288214
C	7.5901877	-2.2735695	-0.8236760
C	7.6502157	-2.2854140	0.6573015
C	8.1130655	-1.1699589	1.3443921
C	7.4208115	-0.7295210	2.5298013
C	7.4244370	0.7280914	2.5413958
C	6.3171482	1.4344510	3.0598867
C	5.8421861	2.6158931	2.3644661
C	6.5025340	3.0344153	1.1887343
C	5.7245192	3.4849365	0.0403120
C	6.4061378	3.0532531	-1.1748038
C	5.6519452	2.6528917	-2.2992318
C	6.0679792	1.4828738	-3.0497683
C	4.8720169	0.7555677	-3.4615051
C	4.8687705	-0.6512219	-3.4725578
C	6.0613924	-1.3904047	-3.0723800
C	5.6399901	-2.5701664	-2.3404219
C	6.3923655	-2.9916078	-1.2224656

C	5.7086812	-3.4392476	-0.0142403
C	6.4886193	-3.0104261	1.1411798
C	5.8302267	-2.6071973	2.3233772
C	6.3105068	-1.4389844	3.0373069
C	5.1549306	-0.7069194	3.5450716
C	5.1581632	0.6998235	3.5560545
C	3.9653485	1.4388579	3.1558927
C	4.3867699	2.6185813	2.4238390
C	3.6343264	3.0402143	1.3060762
C	4.3180114	3.4879494	0.0978617
C	3.5381423	3.0592077	-1.0575522
C	4.1966165	2.6557081	-2.2395892
C	3.7164017	1.4875142	-2.9536493
C	2.6058472	0.7782910	-2.4465915
C	2.6023979	-0.6793464	-2.4580766
C	3.7097132	-1.3856918	-2.9762526
C	4.1846245	-2.5671616	-2.2807256
C	3.5242458	-2.9859942	-1.1051507
C	4.3021722	-3.4365601	0.0433199
C	3.6206345	-3.0047623	1.2584450
C	4.3748768	-2.6040769	2.3827216
C	3.9588447	-1.4340554	3.1332779
C	2.8130073	-0.7204596	2.7188807
C	2.8161379	0.7372356	2.7304378
C	2.0286157	1.1964677	1.6132435
C	2.4363753	2.3221426	0.9073747
C	2.3765075	2.3341638	-0.5736611
C	1.9137960	1.2190280	-1.2612574
C	1.1866168	0.0385875	-0.6072277
C	1.9078786	-1.1353333	-1.2799116

C	2.3659652	-2.2631846	-0.6099188
C	2.4261027	-2.2749942	0.8710866
C	2.0240175	-1.1584645	1.5943414
C	1.2498366	0.0251222	1.0017410
C	10.2836417	0.0239363	-1.4715802
H	10.2525998	0.0343443	-2.5773360
C	10.9408195	-1.2200928	-0.9172580
C	11.4075775	-2.3157706	-1.6546484
H	11.3511245	-2.3056282	-2.7542018
C	11.9424047	-3.4257335	-0.9745261
H	12.3175575	-4.2880876	-1.5463133
C	11.9935180	-3.4410151	0.4304891
H	12.4072526	-4.3159190	0.9546024
C	11.5126736	-2.3455410	1.1716872
H	11.5368959	-2.3591914	2.2723786
C	10.9950959	-1.2340424	0.4943334
C	10.3864652	-0.0002056	1.1223268
H	10.4434425	-0.0106707	2.2270437
C	11.0089152	1.2377441	0.5170698
C	11.5457036	2.3275004	1.2145457
H	11.5709725	2.3203168	2.3152770
C	12.0463465	3.4274601	0.4933707
H	12.4774719	4.2842699	1.0331598
C	11.9939285	3.4391482	-0.9116267
H	12.3849512	4.3047483	-1.4676655
C	11.4386974	2.3518152	-1.6117513
H	11.3822239	2.3630522	-2.7112940
C	10.9537868	1.2505746	-0.8945233

Naphthalene Transfer Intermediate

C	-0.667000	0.667000	2.865000
C	0.736000	0.707000	2.840000
C	1.429000	1.989000	2.768000
C	0.690000	3.185000	2.719000
C	-0.769000	3.143000	2.742000
C	-1.434000	1.905000	2.814000
C	-2.599000	1.744000	3.676000
C	-2.551000	0.404000	4.254000
C	-1.358000	-0.265000	3.746000
C	-0.616000	-1.122000	4.581000
C	0.843000	-1.080000	4.558000
C	1.506000	-0.180000	3.701000
C	2.675000	0.556000	4.171000
C	2.627000	1.897000	3.592000
C	3.045000	3.007000	4.351000
C	2.277000	4.248000	4.308000
C	1.121000	4.334000	3.507000
C	-0.072000	5.003000	4.018000
C	-1.240000	4.266000	3.545000
C	-2.364000	4.113000	4.383000
C	-3.055000	2.829000	4.449000
C	-3.477000	2.613000	5.829000
C	-3.429000	1.321000	6.386000
C	-2.960000	0.196000	5.584000
C	-2.190000	-0.688000	6.453000
C	-1.039000	-1.334000	5.961000
C	0.159000	-1.424000	6.790000

C	1.322000	-1.266000	5.923000
C	2.448000	-0.554000	6.379000
C	3.137000	0.373000	5.487000
C	-1.219000	0.670000	-0.163000
C	3.567000	1.525000	6.274000
C	-1.255000	-0.699000	0.185000
C	3.521000	2.817000	5.717000
C	3.049000	3.940000	6.519000
C	-0.003000	-1.416000	0.358000
C	2.280000	4.824000	5.649000
C	1.212000	-0.723000	0.177000
C	1.248000	0.646000	-0.171000
C	1.129000	5.469000	6.141000
C	2.478000	1.355000	-0.352000
C	2.479000	2.699000	-0.685000
C	-0.068000	5.560000	5.312000
C	1.249000	3.405000	-0.852000
C	0.039000	2.753000	-0.685000
C	-1.231000	5.400000	6.179000
C	-0.004000	1.363000	-0.345000
C	-0.751000	-3.411000	-9.279000
C	-2.357000	4.689000	5.723000
C	0.655000	-3.364000	-9.300000
C	1.341000	-2.078000	-9.342000
C	-3.045000	3.763000	6.616000
C	0.597000	-0.883000	-9.362000
C	-0.861000	-0.932000	-9.340000
C	-2.583000	3.581000	7.933000

C	-1.523000	-2.174000	-9.299000
C	-2.685000	-2.353000	-8.436000
C	-2.535000	2.242000	8.511000
C	-2.631000	-3.701000	-7.881000
C	-1.436000	-4.355000	-8.402000
C	-2.950000	1.132000	7.751000
C	-0.691000	-5.219000	-7.577000
C	0.767000	-5.170000	-7.599000
C	-2.184000	-0.109000	7.792000
C	1.428000	-4.260000	-8.445000
C	2.592000	-3.526000	-7.960000
C	-1.029000	-0.196000	8.593000
C	2.538000	-2.177000	-8.514000
C	2.948000	-1.079000	-7.734000
C	0.163000	-0.865000	8.083000
C	2.177000	0.159000	-7.755000
C	1.022000	0.255000	-8.554000
C	1.330000	-0.128000	8.556000
C	-0.173000	0.910000	-8.033000
C	-1.337000	0.176000	-8.519000
C	2.452000	0.025000	7.718000
C	-2.459000	0.004000	-7.685000
C	-3.145000	-1.284000	-7.643000
C	3.144000	1.309000	7.653000
C	-3.568000	-1.525000	-6.268000
C	-3.516000	-2.826000	-5.733000
C	2.689000	2.394000	8.427000
C	-3.040000	-3.934000	-6.554000

C	-2.267000	-4.829000	-5.699000
C	2.640000	3.732000	7.850000
C	-1.113000	-5.460000	-6.202000
C	0.084000	-5.560000	-5.374000
C	1.448000	4.401000	8.360000
C	1.246000	-5.381000	-6.238000
C	2.369000	-4.674000	-5.769000
C	0.706000	5.253000	7.520000
C	3.054000	-3.729000	-6.646000
C	3.480000	-2.591000	-5.839000
C	-0.752000	5.211000	7.544000
C	3.428000	-1.290000	-6.373000
C	2.954000	-0.180000	-5.552000
C	-1.416000	4.318000	8.406000
C	2.180000	0.715000	-6.406000
C	1.026000	1.348000	-5.903000
C	-0.647000	3.434000	9.275000
C	-0.172000	1.447000	-6.731000
C	-1.335000	1.269000	-5.867000
C	-1.338000	2.151000	9.341000
C	-2.458000	0.560000	-6.336000
C	-3.143000	-0.386000	-5.461000
C	-0.599000	0.954000	9.380000
C	-2.681000	-0.590000	-4.147000
C	-2.627000	-1.940000	-3.593000
C	0.859000	0.996000	9.357000
C	-3.040000	-3.038000	-4.370000
C	-2.267000	-4.276000	-4.349000

C	1.526000	2.234000	9.295000
C	-1.111000	-4.372000	-3.549000
C	0.085000	-5.026000	-4.071000
C	0.760000	3.475000	9.253000
C	1.250000	-4.292000	-3.585000
C	2.373000	-4.120000	-4.419000
C	3.059000	-2.833000	-4.463000
C	2.598000	-1.763000	-3.672000
C	2.545000	-0.413000	-4.226000
C	1.348000	0.241000	-3.707000
C	0.603000	1.109000	-4.527000
C	-0.856000	1.061000	-4.505000
C	-1.515000	0.144000	-3.665000
C	-0.742000	-0.755000	-2.820000
C	-1.429000	-2.041000	-2.769000
C	-0.686000	-3.234000	-2.741000
C	0.774000	-3.186000	-2.762000
C	1.433000	-1.944000	-2.813000
C	0.661000	-0.709000	-2.843000
H	-2.199000	-1.205000	0.320000
H	-0.003000	-2.463000	0.621000
H	-2.169000	1.213000	-0.291000
H	2.163000	-1.266000	0.305000
H	3.427000	0.809000	-0.220000
H	3.434000	3.233000	-0.819000
H	1.268000	4.475000	-1.112000
H	-0.912000	3.295000	-0.809000

Benzene Transfer Intermediate

C	-0.667000	0.667000	2.865000
C	0.736000	0.707000	2.840000
C	1.429000	1.989000	2.768000
C	0.690000	3.185000	2.719000
C	-0.769000	3.143000	2.742000
C	-1.434000	1.905000	2.814000
C	-2.599000	1.744000	3.676000
C	-2.551000	0.404000	4.254000
C	-1.358000	-0.265000	3.746000
C	-0.616000	-1.122000	4.581000
C	0.843000	-1.080000	4.558000
C	1.506000	-0.180000	3.701000
C	2.675000	0.556000	4.171000
C	2.627000	1.897000	3.592000
C	3.045000	3.007000	4.351000
C	2.277000	4.248000	4.308000
C	1.121000	4.334000	3.507000
C	-0.072000	5.003000	4.018000
C	-1.240000	4.266000	3.545000
C	-2.364000	4.113000	4.383000
C	-3.055000	2.829000	4.449000
C	-3.477000	2.613000	5.829000
C	-3.429000	1.321000	6.386000
C	-2.960000	0.196000	5.584000
C	-2.190000	-0.688000	6.453000
C	-1.039000	-1.334000	5.961000
C	0.159000	-1.424000	6.790000

C	1.322000	-1.266000	5.923000
C	2.448000	-0.554000	6.379000
C	3.137000	0.373000	5.487000
C	-1.219000	0.670000	-0.163000
C	3.567000	1.525000	6.274000
C	-1.255000	-0.699000	0.185000
C	3.521000	2.817000	5.717000
C	3.049000	3.940000	6.519000
C	-0.003000	-1.416000	0.358000
C	2.280000	4.824000	5.649000
C	1.212000	-0.723000	0.177000
C	1.248000	0.646000	-0.171000
C	1.129000	5.469000	6.141000
C	-0.068000	5.560000	5.312000
C	-1.231000	5.400000	6.179000
C	-0.004000	1.363000	-0.345000
C	-0.751000	-3.411000	-9.279000
C	-2.357000	4.689000	5.723000
C	0.655000	-3.364000	-9.300000
C	1.341000	-2.078000	-9.342000
C	-3.045000	3.763000	6.616000
C	0.597000	-0.883000	-9.362000
C	-0.861000	-0.932000	-9.340000
C	-2.583000	3.581000	7.933000
C	-1.523000	-2.174000	-9.299000
C	-2.685000	-2.353000	-8.436000
C	-2.535000	2.242000	8.511000
C	-2.631000	-3.701000	-7.881000

C	-1.436000	-4.355000	-8.402000
C	-2.950000	1.132000	7.751000
C	-0.691000	-5.219000	-7.577000
C	0.767000	-5.170000	-7.599000
C	-2.184000	-0.109000	7.792000
C	1.428000	-4.260000	-8.445000
C	2.592000	-3.526000	-7.960000
C	-1.029000	-0.196000	8.593000
C	2.538000	-2.177000	-8.514000
C	2.948000	-1.079000	-7.734000
C	0.163000	-0.865000	8.083000
C	2.177000	0.159000	-7.755000
C	1.022000	0.255000	-8.554000
C	1.330000	-0.128000	8.556000
C	-0.173000	0.910000	-8.033000
C	-1.337000	0.176000	-8.519000
C	2.452000	0.025000	7.718000
C	-2.459000	0.004000	-7.685000
C	-3.145000	-1.284000	-7.643000
C	3.144000	1.309000	7.653000
C	-3.568000	-1.525000	-6.268000
C	-3.516000	-2.826000	-5.733000
C	2.689000	2.394000	8.427000
C	-3.040000	-3.934000	-6.554000
C	-2.267000	-4.829000	-5.699000
C	2.640000	3.732000	7.850000
C	-1.113000	-5.460000	-6.202000
C	0.084000	-5.560000	-5.374000

C	1.448000	4.401000	8.360000
C	1.246000	-5.381000	-6.238000
C	2.369000	-4.674000	-5.769000
C	0.706000	5.253000	7.520000
C	3.054000	-3.729000	-6.646000
C	3.480000	-2.591000	-5.839000
C	-0.752000	5.211000	7.544000
C	3.428000	-1.290000	-6.373000
C	2.954000	-0.180000	-5.552000
C	-1.416000	4.318000	8.406000
C	2.180000	0.715000	-6.406000
C	1.026000	1.348000	-5.903000
C	-0.647000	3.434000	9.275000
C	-0.172000	1.447000	-6.731000
C	-1.335000	1.269000	-5.867000
C	-1.338000	2.151000	9.341000
C	-2.458000	0.560000	-6.336000
C	-3.143000	-0.386000	-5.461000
C	-0.599000	0.954000	9.380000
C	-2.681000	-0.590000	-4.147000
C	-2.627000	-1.940000	-3.593000
C	0.859000	0.996000	9.357000
C	-3.040000	-3.038000	-4.370000
C	-2.267000	-4.276000	-4.349000
C	1.526000	2.234000	9.295000
C	-1.111000	-4.372000	-3.549000
C	0.085000	-5.026000	-4.071000
C	0.760000	3.475000	9.253000

C	1.250000	-4.292000	-3.585000
C	2.373000	-4.120000	-4.419000
C	3.059000	-2.833000	-4.463000
C	2.598000	-1.763000	-3.672000
C	2.545000	-0.413000	-4.226000
C	1.348000	0.241000	-3.707000
C	0.603000	1.109000	-4.527000
C	-0.856000	1.061000	-4.505000
C	-1.515000	0.144000	-3.665000
C	-0.742000	-0.755000	-2.820000
C	-1.429000	-2.041000	-2.769000
C	-0.686000	-3.234000	-2.741000
C	0.774000	-3.186000	-2.762000
C	1.433000	-1.944000	-2.813000
C	0.661000	-0.709000	-2.843000
H	-2.199000	-1.205000	0.320000
H	-0.003000	-2.463000	0.621000
H	2.192000	1.152000	-0.306000
H	-0.004000	2.410000	-0.610000
H	-2.169000	1.213000	-0.291000
H	2.163000	-1.266000	0.305000

Anthracene

C	3.6844493	0.7153920	-0.0000206
C	2.4921155	1.4151871	0.0000366
C	1.2323468	0.7278603	0.0000414
C	1.2323508	-0.7278659	0.0000245
C	2.4921192	-1.4151889	-0.0000257
C	3.6844568	-0.7153889	-0.0000603
C	-0.0000005	1.4127535	0.0000394
C	-0.0000007	-1.4127590	0.0000408
C	-1.2323522	-0.7278657	0.0000364
C	-1.2323478	0.7278605	0.0000177
C	-2.4921165	1.4151875	-0.0000345
H	-2.4912306	2.5166453	-0.0000665
C	-3.6844502	0.7153927	-0.0000557
C	-3.6844582	-0.7153883	-0.0000128
C	-2.4921206	-1.4151886	0.0000332
H	-0.0000004	2.5149292	0.0000403
H	4.6425316	1.2575625	-0.0000394
H	2.4912299	2.5166449	0.0000718
H	2.4912336	-2.5166493	-0.0000475
H	4.6425440	-1.2575509	-0.0001192
H	-0.0000007	-2.5149363	0.0000421
H	-4.6425325	1.2575634	-0.0001062
H	-4.6425454	-1.2575500	-0.0000201
H	-2.4912353	-2.5166489	0.0000634

C_{60}

C	-4.5612818	1.2447477	3.8673553
C	-3.1026153	1.2447809	3.8673096
C	-2.3988017	2.4638603	3.8674839
C	-3.1282955	3.7271146	3.8673278
C	-4.5357355	3.7270815	3.8673737
C	-5.2651605	2.4637906	3.8675759
C	-5.0122806	0.1416981	3.0252499
C	-3.8319522	-0.5398252	2.5045658
C	-2.6516232	0.1417517	3.0251726
C	-1.5126246	0.2969390	2.2123668
C	-1.2181663	2.6247797	3.0248356
C	-2.3988022	4.6690053	3.0249168
C	-3.1026167	5.5776217	2.2121200
C	-4.5616385	5.5775917	2.2121727
C	-5.2653443	4.6689389	3.0250198
C	-6.4455874	3.9874400	2.5042977
C	-6.4458711	2.6246513	3.0250163
C	-6.8807395	1.5607152	2.2123214
C	-6.1513474	0.2968260	2.2125292
C	-3.8319898	-1.0420846	1.1894630
C	-5.0124253	-0.8811074	0.3471211
C	-6.1513814	-0.2238169	0.8494193
C	-6.8806901	0.7182699	0.0070318
C	-7.3310196	1.8210103	0.8493462
C	-7.3310670	3.1357998	0.3473224
C	-6.8807342	4.2385562	1.1896078
C	-6.1515451	5.1806833	0.3471631

C	-5.0125935	5.8380408	0.8493797
C	-1.2185653	3.9875621	2.5041125
C	-2.6519151	4.8152884	-1.8288351
C	-1.5128625	4.6601467	-1.0161058
C	-0.7834783	3.3962591	-1.0158946
C	-1.2183324	2.3323304	-1.8285932
C	-2.3990399	2.4931865	-2.6711632
C	-4.5615866	3.7121998	-2.6708971
C	-5.0125920	4.8152347	-1.8287550
C	-3.8322504	5.4968154	-1.3081579
C	-3.8322174	5.9990790	0.0069550
C	-2.6517783	5.8380887	0.8492955
C	-1.5128329	5.1807828	0.3469978
C	-0.3332114	3.1359700	0.3470735
C	-0.3331504	1.8211816	0.8491002
C	-0.7834785	0.7184261	0.0068184
C	-1.2186261	0.9695436	-1.3078816
C	-2.3988643	0.2880405	-1.8285948
C	-3.1284676	1.2298998	-2.6709556
C	-4.5359098	1.2298649	-2.6709038
C	-5.2654029	2.4931158	-2.6710618
C	-6.1515829	4.6600432	-1.0159465
C	-6.8809052	3.3961122	-1.0156833
C	-6.4460473	2.3322030	-1.8284092
C	-6.4456459	0.9694115	-1.3076972
C	-5.2654044	0.2879694	-1.8284917
C	-4.5615905	-0.6206381	-1.0156955
C	-3.1025718	-0.6206020	-1.0157475

C	-2.6516265	-0.8810483	0.3470373
C	-1.5126691	-0.2236995	0.8492574
C	-0.7835360	4.2386964	1.1893876
C	-0.7833052	1.5608647	2.2121054
C	-3.1029190	3.7122347	-2.6709472

$INT_{Butadiene}$

C	-4.4133605	1.1776388	1.4353493
C	-3.6815862	0.7308880	2.6153863
C	-3.9847480	2.3184940	0.7315732
C	-4.8584837	-0.0055408	0.7057619
C	-2.5467672	1.4408162	3.0501942
C	-3.6738632	-0.7286688	2.6155694
C	-2.8086580	3.0541354	1.1820260
C	-3.9851398	2.3184398	-0.7281845
C	-4.4009158	-1.1834972	1.4355318
C	-4.8588834	-0.0055914	-0.7019018
C	-2.1021379	2.6233889	2.3205766
C	-1.3625835	0.7174555	3.5017957
C	-2.5315773	-1.4262330	3.0506953
C	-2.0814483	3.5089120	0.0012587
C	-2.8092565	3.0540831	-1.1791511
C	-4.4141391	1.1775709	-1.4317343
C	-3.9593434	-2.3195908	0.7316491
C	-4.4017110	-1.1836248	-1.4318101
C	-0.6429115	2.6319469	2.3209111
C	-0.1860612	1.4543409	3.0498605
C	-1.3551888	-0.6900441	3.5020721

C	-2.0737355	-2.6039632	2.3210259
C	-0.6737720	3.5168893	0.0009739
C	-2.1032928	2.6232113	-2.3179946
C	-3.6829720	0.7307259	-2.6121217
C	-3.9597467	-2.3196492	-0.7280473
C	-2.7754326	-3.0424032	1.1823797
C	-3.6752613	-0.7288597	-2.6122488
C	0.0589866	3.0704891	1.1817332
C	0.9551665	0.7560621	2.6127896
C	-0.1709727	-1.4144723	3.0504865
C	-0.6145799	-2.5968238	2.3222994
C	0.0583810	3.0703494	-1.1800818
C	-2.5483149	1.4406212	-3.0473842
C	-0.6440827	2.6317247	-2.3188850
C	-2.7760487	-3.0425416	-1.1792321
C	-2.0430979	-3.4886453	0.0014239
C	-2.5331374	-1.4264701	-3.0477985
C	1.2434961	2.3490015	0.7309733
C	1.6821754	1.2108700	1.4328002
C	0.9625759	-0.7036690	2.6123413
C	0.0923737	-3.0259262	1.1820800
C	1.2430950	2.3489223	-0.7297958
C	-1.3643246	0.7172255	-3.4994187
C	-0.1876052	1.4540805	-3.0479495
C	-2.0749011	-2.6041551	-2.3182493
C	-0.6354310	-3.4803190	0.0011385
C	-1.3569271	-0.6902930	-3.4996634
C	2.1450001	0.0329798	0.7046155

C	1.6925959	-1.1497709	1.4327172
C	1.2689316	-2.2922399	0.7319999
C	1.6813682	1.2107338	-1.4317315
C	0.9537755	0.7558701	-2.6113190
C	-0.6157363	-2.5969745	-2.3200826
C	0.0917891	-3.0259834	-1.1801610
C	-0.1725044	-1.4146497	-3.0484946
C	2.1445938	0.0329285	-0.7037169
C	1.2685457	-2.2922715	-0.7306155
C	0.9612063	-0.7038306	-2.6108162
C	1.6918078	-1.1498385	-1.4315414
C	5.0455727	-0.1375505	-1.5431195
C	5.0470195	-0.1381819	1.5421638
H	5.0314578	-0.2503875	2.6364584
H	5.0286007	-0.2492961	-2.6374376
H	4.8925972	0.8788586	1.1493989
H	4.8921312	0.8793877	-1.1497133
C	5.2575203	-1.2045662	0.7316650
H	5.4112559	-2.1897059	1.2049513
C	5.2566091	-1.2043297	-0.7332855
H	5.4092966	-2.1893714	-1.2071257

$TS_{Butadiene}$

C	-1.4655496	1.8299215	-3.8984573
C	-2.6440629	1.3124616	-3.2120137
C	-0.7592587	2.9216101	-3.3577463
C	-0.7385535	0.6976533	-4.4616547

C	-3.0760597	1.9055282	-2.0105680
C	-2.6444948	-0.1407330	-3.3503515
C	-1.2049954	3.5348809	-2.1130106
C	0.7008734	2.9211206	-3.3639392
C	-1.4673531	-0.5203818	-4.1220247
C	0.6693234	0.6971599	-4.4676084
C	-2.3434468	3.0375428	-1.4497655
C	-3.5227433	1.0665621	-0.9040694
C	-3.0770516	-0.9493240	-2.2828520
C	-0.0203622	3.9095975	-1.3471234
C	1.1575184	3.5341043	-2.1229825
C	1.4018404	1.8289373	-3.9106184
C	-0.7631653	-1.6956024	-3.7992005
C	1.4000970	-0.5213800	-4.1341216
C	-2.3408643	2.8994536	0.0014265
C	-3.0630170	1.6835357	0.3370913
C	-3.5234906	-0.3342419	-1.0377336
C	-2.3468130	-2.1677414	-1.9473536
C	-0.0144995	3.7703551	0.0537836
C	2.3012404	3.0359788	-1.4693561
C	2.5857862	1.3106419	-3.2341404
C	0.6978381	-1.6960923	-3.8053631
C	-1.2094874	-2.5325604	-2.6930339
C	2.5839930	-0.1425416	-3.3724406
C	-1.1940800	3.2557216	0.7423595
C	-2.6075746	0.8716895	1.3949179
C	-3.0649048	-1.1751312	0.0645229
C	-2.3433107	-2.3070384	-0.4960760

C	1.1704852	3.2548883	0.7323721
C	3.0283046	1.9034026	-2.0363342
C	2.3107503	2.8978362	-0.0181851
C	1.1528925	-2.5334012	-2.7030246
C	-0.0255863	-3.0482279	-2.0124399
C	3.0249870	-0.9514559	-2.3086185
C	-0.7432887	2.4215877	1.8459141
C	-1.4351909	1.2474910	2.1630907
C	-2.6096063	-0.5785525	1.2572736
C	-1.1981446	-2.8007351	0.1630995
C	0.7284301	2.4210891	1.8397246
C	3.4836278	1.0641227	-0.9336311
C	3.0347964	1.6813924	0.3113621
C	2.2967013	-2.1693551	-1.9669397
C	-0.0197182	-3.1777557	-0.6106242
C	3.4823229	-0.3366811	-1.0672976
C	-0.7324268	0.0221161	2.6074677
C	-1.4360808	-1.0955475	1.9409669
C	-0.7448696	-2.1903255	1.4047632
C	1.4221582	1.2464918	2.1510882
C	2.5877209	0.8698831	1.3729961
C	2.3052911	-2.3086067	-0.5156820
C	1.1654429	-2.8015158	0.1531254
C	3.0323653	-1.1772469	0.0387969
C	0.7222580	0.0215840	2.6013041
C	0.7230732	-2.1908148	1.3985378
C	2.5875241	-0.5803554	1.2352917
C	1.4195021	-1.0965213	1.9288455

C	-0.7030193	0.8008050	5.3834631
H	-1.2154573	1.7305628	5.6875285
C	0.7169265	0.7997276	5.3775114
H	1.2333338	1.7286710	5.6773042
C	1.4561181	-0.2054232	4.7633387
H	2.5484742	-0.1042341	4.6473163
C	-1.4488667	-0.2032383	4.7755946
H	-1.0632763	-1.2316031	4.6914797
H	1.0681117	-1.2331188	4.6821758
H	-2.5419636	-0.1002786	4.6686144

$INT_{Benzene}$

C	-4.4202773	1.1806268	1.4354641
C	-3.6907272	0.7297685	2.6154034
C	-3.9853183	2.3191174	0.7316325
C	-4.8716502	0.0000130	0.7058128
C	-2.5520951	1.4335413	3.0501830
C	-3.6907420	-0.7297659	2.6154032
C	-2.8052563	3.0486006	1.1821707
C	-3.9856548	2.3191182	-0.7279995
C	-4.4203008	-1.1806100	1.4354642
C	-4.8719752	0.0000129	-0.7017740
C	-2.1009701	2.6137428	2.3205332
C	-1.3718386	0.7037736	3.5016543
C	-2.5521235	-1.4335617	3.0501830
C	-2.0755922	3.4993938	0.0013763
C	-2.8057989	3.0486009	-1.1790854

C	-4.4209398	1.1806246	-1.4316331
C	-3.9853649	-2.3191090	0.7316328
C	-4.4209635	-1.1806077	-1.4316330
C	-0.6416536	2.6145215	2.3210733
C	-0.1913060	1.4343077	3.0501646
C	-1.3718527	-0.7038173	3.5016542
C	-2.1010227	-2.6137722	2.3205333
C	-0.6678332	3.4996730	0.0010509
C	-2.1020388	2.6137443	-2.3177678
C	-3.6919316	0.7297673	-2.6119075
C	-3.9857012	-2.3191103	-0.7279993
C	-2.8053174	-3.0486161	1.1821710
C	-3.6919458	-0.7297656	-2.6119076
C	0.0625937	3.0489338	1.1817255
C	0.9463672	0.7300734	2.6135814
C	-0.1913352	-1.4343754	3.0501648
C	-0.6417061	-2.6145800	2.3210734
C	0.0620463	3.0489281	-1.1799561
C	-2.5534998	1.4335388	-3.0472116
C	-0.6427248	2.6145151	-2.3189805
C	-2.8058601	-3.0486165	-1.1790849
C	-2.0756624	-3.4994241	0.0013766
C	-2.5535288	-1.4335596	-3.0472112
C	1.2437417	2.3215389	0.7309267
C	1.6742825	1.1804446	1.4325193
C	0.9463529	-0.7301634	2.6135813
C	0.0625325	-3.0490069	1.1817255
C	1.2434015	2.3215332	-0.7297066

C	-1.3734529	0.7037710	-3.4992206
C	-0.1927153	1.4343055	-3.0482727
C	-2.1020910	-2.6137741	-2.3177678
C	-0.6679034	-3.4997314	0.0010511
C	-1.3734670	-0.7038158	-3.4992206
C	2.1231043	-0.0000571	0.7030174
C	1.6742591	-1.1805505	1.4325192
C	1.2436955	-2.3216352	0.7309269
C	1.6736096	1.1804448	-1.4314918
C	0.9451531	0.7300720	-2.6122161
C	-0.6427771	-2.6145745	-2.3189801
C	0.0619853	-3.0490015	-1.1799561
C	-0.1927434	-1.4343737	-3.0482727
C	2.1227664	-0.0000575	-0.7022011
C	1.2433551	-2.3216308	-0.7297063
C	0.9451385	-0.7301635	-2.6122164
C	1.6735869	-1.1805500	-1.4314922
C	5.1755125	-0.0002970	-1.4048867
C	5.1764747	0.0002917	1.4032567
H	5.1623655	0.0005215	2.5037730
H	5.1606338	-0.0005270	-2.5053921
C	5.1797383	1.2190211	0.7012211
C	5.1792564	1.2187239	-0.7033647
H	5.1693570	2.1713455	1.2527979
H	5.1685046	2.1708133	-1.2553399
C	5.1797841	-1.2187299	0.7017316
H	5.1694398	-2.1708229	1.2537083
C	5.1793066	-1.2190250	-0.7028544

H	5.1685944	-2.1713465	-1.2544299

$TS_{Benzene}$

C	0.0000000	-0.7492753	-2.6831924
C	0.0000000	0.7492755	-2.6831932
C	-1.1743207	1.4278231	-2.0504060
C	-2.3108751	0.7370035	-1.6267301
C	-2.3108751	-0.7370035	-1.6267302
C	-1.1743207	-1.4278230	-2.0504060
C	-0.7281068	-2.5912684	-1.3127324
C	0.7281068	-2.5912684	-1.3127324
C	1.1743207	-1.4278230	-2.0504060
C	2.3108751	-0.7370035	-1.6267302
C	2.3108751	0.7370035	-1.6267301
C	1.1743207	1.4278231	-2.0504060
C	0.7281068	2.5912683	-1.3127324
C	-0.7281068	2.5912683	-1.3127324
C	-1.4364692	3.0494815	-0.1834850
C	-2.6143664	2.3267983	0.2619860
C	-3.0369924	1.1824168	-0.4480435
C	-3.4845336	0.0000000	0.2811787
C	-3.0369924	-1.1824168	-0.4480435
C	-2.6143665	-2.3267983	0.2619860
C	-1.4364692	-3.0494814	-0.1834850
C	-0.7035365	-3.5052996	0.9951676
C	0.7035365	-3.5052996	0.9951676
C	1.4364692	-3.0494814	-0.1834850

C	2.6143665	-2.3267983	0.2619860
C	3.0369924	-1.1824168	-0.4480435
C	3.4845336	0.0000000	0.2811787
C	3.0369924	1.1824168	-0.4480435
C	2.6143664	2.3267983	0.2619860
C	1.4364692	3.0494815	-0.1834850
C	0.7035365	3.5052996	0.9951675
C	-0.7035365	3.5052996	0.9951675
C	-1.4342813	3.0533530	2.1739044
C	-2.6146373	2.3233813	1.7195665
C	-3.0466325	1.1814946	2.4216314
C	-3.4927289	0.0000000	1.6890365
C	-3.0466326	-1.1814946	2.4216314
C	-2.6146373	-2.3233812	1.7195665
C	-1.4342813	-3.0533530	2.1739044
C	-0.7301157	-2.6155730	3.3115259
C	0.7301157	-2.6155730	3.3115259
C	1.4342813	-3.0533530	2.1739044
C	2.6146373	-2.3233812	1.7195665
C	3.0466326	-1.1814946	2.4216314
C	3.4927289	0.0000000	1.6890365
C	3.0466325	1.1814946	2.4216314
C	2.6146373	2.3233813	1.7195665
C	1.4342813	3.0533530	2.1739044
C	0.7301157	2.6155731	3.3115259
C	-0.7301157	2.6155731	3.3115259
C	-1.1805111	1.4341760	4.0375871
C	-2.3189892	0.7306486	3.5999123

C	-2.3189892	-0.7306485	3.5999123
C	-1.1805111	-1.4341759	4.0375871
C	-0.0000000	-0.7039516	4.4874546
C	1.1805111	-1.4341759	4.0375871
C	2.3189892	-0.7306485	3.5999123
C	2.3189892	0.7306486	3.5999123
C	1.1805111	1.4341760	4.0375871
C	-0.0000000	0.7039517	4.4874546
C	-0.0000000	-1.3280310	-4.6118869
H	-0.0000000	-2.4263294	-4.5295105
C	1.2398299	-0.6837146	-5.0266889
C	1.2398299	0.6837144	-5.0266882
C	0.0000000	1.3280303	-4.6118848
H	0.0000000	2.4263287	-4.5295084
C	-1.2398299	0.6837144	-5.0266882
C	-1.2398299	-0.6837145	-5.0266889
H	2.1509086	1.2785143	-5.1823188
H	2.1509087	-1.2785143	-5.1823202
H	-2.1509086	1.2785143	-5.1823188
H	-2.1509087	-1.2785143	-5.1823202

C_{60}:benzene Monoadduct

C	0.0299105	-0.8012691	-2.7282771
C	0.0299112	0.7983350	-2.7286663
C	-1.1510315	1.4344299	-1.9866374
C	-2.2765859	0.7395256	-1.5621116
C	-2.2765923	-0.7418242	-1.5617056

C	-1.1510328	-1.4369814	-1.9858903
C	-0.7072166	-2.5878092	-1.2370058
C	0.7497960	-2.5878473	-1.2286793
C	1.2020798	-1.4368255	-1.9721601
C	2.3229132	-0.7417775	-1.5355126
C	2.3229051	0.7394829	-1.5359223
C	1.2020906	1.4342718	-1.9729042
C	0.7497955	2.5857275	-1.2300865
C	-0.7072059	2.5856896	-1.2384112
C	-1.4206465	3.0498011	-0.1130692
C	-2.5987522	2.3282277	0.3249648
C	-3.0095420	1.1811295	-0.3879432
C	-3.4608176	-0.0006095	0.3383503
C	-3.0095419	-1.1827627	-0.3872901
C	-2.5987530	-2.3294473	0.3262545
C	-1.4206469	-3.0512715	-0.1113841
C	-0.6951098	-3.5077587	1.0711923
C	0.7115848	-3.5077860	1.0791980
C	1.4505256	-3.0513649	-0.0950397
C	2.6235893	-2.3294702	0.3559123
C	3.0424573	-1.1827508	-0.3528787
C	3.4854349	-0.0006083	0.3778086
C	3.0424656	1.1811179	-0.3535311
C	2.6236000	2.3282558	0.3546213
C	1.4505433	3.0498966	-0.0967222
C	0.7115919	3.5069944	1.0772521
C	-0.6950992	3.5069664	1.0692475
C	-1.4328954	3.0558721	2.2439330

C	-2.6101254	2.3255001	1.7820612
C	-3.0448440	1.1821620	2.4808953
C	-3.4849568	-0.0002075	1.7453368
C	-3.0448426	-1.1821537	2.4815525
C	-2.6101216	-2.3258915	1.7833479
C	-1.4328908	-3.0559931	2.2456253
C	-0.7351602	-2.6168897	3.3869929
C	0.7252685	-2.6168691	3.3952631
C	1.4359471	-3.0559488	2.2619513
C	2.6183695	-2.3259225	1.8130603
C	3.0451527	-1.1822024	2.5161678
C	3.4936320	-0.0002069	1.7849598
C	3.0451606	1.1822140	2.5155104
C	2.6183869	2.3255335	1.8117746
C	1.4359673	3.0558301	2.2602588
C	0.7252813	2.6174027	3.3938268
C	-0.7351599	2.6174228	3.3855558
C	-1.1892595	1.4353533	4.1076619
C	-2.3249187	0.7314494	3.6623767
C	-2.3249175	-0.7307733	3.6627798
C	-1.1892575	-1.4344191	4.1084430
C	-0.0116481	-0.7034284	4.5638579
C	1.1711172	-1.4344361	4.1218314
C	2.3117998	-0.7308322	3.6891213
C	2.3118054	0.7315092	3.6887183
C	1.1711260	1.4353717	4.1210508
C	-0.0116464	0.7046129	4.5634803
C	0.0399075	-1.2845660	-4.2757571

H	0.0401221	-2.3894669	-4.2904596
C	1.2889686	-0.6753740	-4.8792563
C	1.2889660	0.6715445	-4.8795755
C	0.0399127	1.2809879	-4.2763441
H	0.0401304	2.3858893	-4.2914518
C	-1.2010047	0.6715673	-4.8960235
C	-1.2010118	-0.6753940	-4.8957036
H	2.1253257	1.2992806	-5.2172107
H	2.1253391	-1.3032546	-5.2165865
H	-2.0326011	1.2993274	-5.2452784
H	-2.0326269	-1.3032964	-5.2446551

$INT_{Naphthalene}$

C	-4.4731488	0.9689125	1.4356990
C	-3.7045377	0.5884875	2.6153849
C	-4.1471455	2.1431002	0.7320438
C	-4.8122809	-0.2488122	0.7061274
C	-2.6368293	1.3955305	3.0499097
C	-3.5681226	-0.8643988	2.6157655
C	-3.0405886	2.9800051	1.1823408
C	-4.1476465	2.1431425	-0.7277973
C	-4.2524854	-1.3818016	1.4354278
C	-4.8127679	-0.2487700	-0.7015521
C	-2.2986235	2.6129371	2.3205763
C	-1.3933975	0.7799292	3.5016643
C	-2.3683827	-1.4587374	3.0507534
C	-2.3566707	3.4971652	0.0015386

C	-3.0414029	2.9800825	-1.1788197
C	-4.4741272	0.9690160	-1.4312913
C	-3.7124106	-2.4746656	0.7314109
C	-4.2534718	-1.3817242	-1.4313284
C	-0.8460613	2.7509810	2.3211768
C	-0.2866458	1.6179311	3.0506539
C	-1.2615006	-0.6216884	3.5017268
C	-1.8086030	-2.5917909	2.3207540
C	-0.9551117	3.6291093	0.0010472
C	-2.3002265	2.6131033	-2.3176124
C	-3.7063285	0.5886569	-2.6115567
C	-3.7129129	-2.4746254	-0.7277648
C	-2.4691602	-3.0908307	1.1821067
C	-3.5699152	-0.8642458	-2.6121364
C	-0.1857019	3.2493224	1.1815320
C	0.9122993	1.0237686	2.6138599
C	-0.0181472	-1.2383601	3.0502592
C	-0.3557060	-2.4557498	2.3214173
C	-0.1865103	3.2494159	-1.1800064
C	-2.6389344	1.3957334	-3.0467994
C	-0.8476481	2.7511586	-2.3192351
C	-2.4699765	-3.0907696	-1.1793802
C	-1.7006977	-3.4710687	0.0010841
C	-2.3704902	-1.4585648	-3.0480298
C	1.0589681	2.6358670	0.7303330
C	1.5970216	1.5409225	1.4327954
C	1.0474231	-0.4298364	2.6119452
C	0.3857980	-2.8216682	1.1814526

C	1.0584822	2.6359343	-0.7297195
C	-1.3958058	0.7801574	-3.4995008
C	-0.2887303	1.6181676	-3.0492209
C	-1.8101981	-2.5916853	-2.3184870
C	-0.2992164	-3.3396805	0.0005879
C	-1.2639059	-0.6214769	-3.4997489
C	2.1554838	0.4076504	0.7035317
C	1.8105824	-0.8085851	1.4301174
C	1.4915416	-1.9855307	0.7302011
C	1.5961207	1.5410633	-1.4326728
C	0.9105818	1.0239700	-2.6133383
C	-0.3572781	-2.4556515	-2.3201792
C	0.3850031	-2.8216248	-1.1807316
C	-0.0202124	-1.2382068	-3.0492161
C	2.1550918	0.4077000	-0.7038426
C	1.4910747	-1.9855193	-0.7301991
C	1.0457094	-0.4296872	-2.6116161
C	1.8097051	-0.8085214	-1.4303083
C	5.2257330	-0.2474438	-1.4107554
C	5.2261701	-0.2466914	1.4099128
H	5.2107916	-0.2451536	2.5109254
H	5.2101217	-0.2465546	-2.5117859
C	5.4690521	0.9284743	0.7097285
C	5.4689889	0.9280687	-0.7112741
H	5.6492150	1.8669042	1.2552759
H	5.6493224	1.8661486	-1.2573938
C	4.9782356	-1.4730575	0.7226222
C	4.6949330	-2.6899914	1.4115780

C	4.9777692	-1.4734023	-0.7227050
C	4.4149900	-3.8558260	0.7119167
H	4.6837119	-2.6847009	2.5125837
C	4.6935725	-2.6905335	-1.4109422
C	4.4141397	-3.8560698	-0.7105729
H	4.1855835	-4.7837064	1.2572069
H	4.6811842	-2.6856008	-2.5119560
H	4.1838320	-4.7840714	-1.2552800

$TS_{Naphthalene}$

C	-0.4586420	-0.8823129	-2.1644746
C	1.0211496	-0.8941551	-1.9728425
C	1.6624093	0.4004208	-1.5952573
C	0.9705753	1.6134749	-1.5899840
C	-0.4880551	1.6225320	-1.7917833
C	-1.1643861	0.4152204	-1.9827701
C	-2.4349043	0.1901316	-1.3231379
C	-2.4969591	-1.2126720	-0.9368800
C	-1.2646296	-1.8467769	-1.3624617
C	-0.6824848	-2.8322170	-0.5615119
C	0.7782119	-2.8394832	-0.3604300
C	1.5669166	-1.8633923	-0.9731663
C	2.6430912	-1.2406705	-0.2292725
C	2.7028320	0.1620474	-0.6161751
C	3.0392761	1.1465474	0.3354098
C	2.3135982	2.4051713	0.3482951
C	1.2897314	2.6282104	-0.5976695

C	0.0425210	3.2622512	-0.1824946
C	-1.0527784	2.6414954	-0.9205156
C	-2.2959676	2.4305557	-0.2864765
C	-3.0044905	1.1795303	-0.4965708
C	-3.6394455	0.7937860	0.7608830
C	-3.6982652	-0.5615863	1.1354539
C	-3.1251902	-1.5874853	0.2678406
C	-2.5158397	-2.6061933	1.1052558
C	-1.3069995	-3.2105961	0.6962861
C	-0.2488246	-3.4504306	1.6724664
C	1.0357610	-3.2227339	1.0193656
C	2.0956683	-2.6310797	1.7403010
C	2.9196610	-1.6204421	1.0999588
C	3.2476931	-0.5994255	2.0916734
C	3.3062448	0.7558451	1.7171135
C	2.7359158	1.7792230	2.5857478
C	2.1210614	2.7976449	1.7385622
C	0.9166289	3.4091898	2.1375980
C	-0.1399798	3.6479825	1.1588288
C	-1.4238391	3.4222145	1.8151065
C	-2.4819980	2.8228711	1.1044033
C	-3.3141233	1.8122552	1.7527594
C	-3.0572225	1.4380194	3.0855204
C	-3.1186455	0.0324862	3.4742929
C	-3.4341685	-0.9499125	2.5161027
C	-2.7008987	-2.2133006	2.4961118
C	-1.6787320	-2.4463792	3.4369382
C	-0.4319677	-3.0789827	3.0177672

C	0.6618218	-2.4588386	3.7587123
C	1.9022758	-2.2382018	3.1299693
C	2.6160352	-0.9828528	3.3490599
C	2.0640779	0.0040821	4.1878836
C	2.1251062	1.4100896	3.7992846
C	0.8788951	2.0456953	4.2109636
C	0.2866216	3.0279800	3.3942734
C	-1.1606951	3.0362497	3.1952920
C	-1.9621746	2.0611970	3.8198928
C	-1.3468788	1.0416072	4.6626507
C	-2.0610083	-0.2120723	4.4485474
C	-1.3546089	-1.4303017	4.4292559
C	0.0924734	-1.4382936	4.6284880
C	0.7800923	-0.2275077	4.8394852
C	0.0479288	1.0340997	4.8548503
C	-0.7942877	-1.3882026	-4.1713767
H	-1.8942111	-1.3626286	-4.2349197
C	-0.1378577	-2.6727575	-4.1641434
C	1.2235040	-2.6775915	-3.9638894
C	1.8595907	-1.3949134	-3.7676806
H	2.9356769	-1.3813937	-3.5298047
C	1.3404121	-0.2618971	-4.5356887
C	2.1124015	0.8495691	-4.9366278
H	3.1967287	0.8540523	-4.7474373
C	1.4954780	1.9341022	-5.5693807
H	2.1001966	2.7929871	-5.8974198
C	0.0979210	1.9402635	-5.7745666
H	-0.3793424	2.8038464	-6.2619153

C	-0.6837112	0.8614805	-5.3481868
H	-1.7763722	0.8740157	-5.4814737
C	-0.0684278	-0.2564722	-4.7428481
H	1.7834396	-3.6075221	-3.7891144
H	-0.7306106	-3.5987496	-4.1583031

C_{60}:naphthalene Monoadduct

C	-0.5219998	-0.8436159	-2.1886688
C	1.0673297	-0.8531088	-1.9724293
C	1.6443846	0.4713697	-1.4593517
C	0.9446285	1.6708581	-1.4214356
C	-0.5226477	1.6792997	-1.6209533
C	-1.1997587	0.4876128	-1.8457829
C	-2.4549682	0.2480791	-1.1760625
C	-2.5129820	-1.1620358	-0.8134686
C	-1.2935746	-1.7909050	-1.2616568
C	-0.7041103	-2.7724000	-0.4749287
C	0.7639758	-2.7809458	-0.2752374
C	1.5530300	-1.8070131	-0.8740950
C	2.6152387	-1.1908531	-0.1152319
C	2.6720188	0.2188808	-0.4781932
C	3.0138188	1.1860175	0.4915501
C	2.2869153	2.4398462	0.5274421
C	1.2582585	2.6684310	-0.4124359
C	0.0107594	3.2911200	0.0150881
C	-1.0837218	2.6816769	-0.7310729
C	-2.3283157	2.4658484	-0.1011694
C	-3.0328998	1.2202099	-0.3319079

C	-3.6661674	0.8111436	0.9188177
C	-3.7213819	-0.5501021	1.2695506
C	-3.1459795	-1.5584681	0.3837601
C	-2.5341476	-2.5879723	1.2006294
C	-1.3218818	-3.1752137	0.7772527
C	-0.2623959	-3.4299693	1.7465058
C	1.0201678	-3.1882876	1.0963884
C	2.0814393	-2.6140378	1.8293673
C	2.9009441	-1.5925945	1.2071611
C	3.2295434	-0.5892899	2.2161682
C	3.2845195	0.7719407	1.8654137
C	2.7137105	1.7788711	2.7526257
C	2.0954922	2.8100313	1.9232860
C	0.8886842	3.4105750	2.3336765
C	-0.1703978	3.6615862	1.3601938
C	-1.4536944	3.4237074	2.0143534
C	-2.5133628	2.8361639	1.2953463
C	-3.3424936	1.8131214	1.9278265
C	-3.0819903	1.4161233	3.2535266
C	-3.1397428	0.0036307	3.6177000
C	-3.4553049	-0.9624664	2.6427266
C	-2.7190890	-2.2233593	2.5987211
C	-1.6932003	-2.4697747	3.5326094
C	-0.4447980	-3.0907634	3.0996423
C	0.6490547	-2.4828065	3.8513235
C	1.8895611	-2.2492231	3.2263921
C	2.6008282	-0.9966070	3.4675404
C	2.0467413	-0.0258090	4.3239512

C	2.1043021	1.3871606	3.9600055
C	0.8567097	2.0120160	4.3829308
C	0.2611178	3.0065985	3.5830109
C	-1.1875111	3.0150662	3.3859653
C	-1.9863782	2.0280465	3.9958074
C	-1.3668921	0.9952615	4.8189126
C	-2.0792047	-0.2557645	4.5843330
C	-1.3698554	-1.4720879	4.5417037
C	0.0785703	-1.4802839	4.7387952
C	0.7636991	-0.2717790	4.9711317
C	0.0283149	0.9874394	5.0089495
C	-0.8092397	-1.2233587	-3.7288627
H	-1.9030451	-1.2235655	-3.8892568
C	-0.1637806	-2.5724001	-3.9632977
C	1.1721954	-2.5812638	-3.7814790
C	1.7494846	-1.2398738	-3.3815231
H	2.8463022	-1.2546115	-3.2450996
C	1.2976680	-0.1731119	-4.3560882
C	2.1038661	0.7892551	-4.9768055
H	3.1922714	0.7908010	-4.8100078
C	1.5048717	1.7535150	-5.8095447
H	2.1308189	2.5079102	-6.3099994
C	0.1120225	1.7615625	-5.9998771
H	-0.3481990	2.5219030	-6.6490010
C	-0.6995163	0.8058275	-5.3596481
H	-1.7925813	0.8200993	-5.4913184
C	-0.1005769	-0.1643529	-4.5463751
H	1.8057494	-3.4754530	-3.8631056

H	-0.7644644	-3.4579400	-4.2134915

INT$_{\text{Monoadduct}}$

C	-4.3939383	1.1804217	1.4352006
C	-3.6642799	0.7295597	2.6154917
C	-3.9583234	2.3190492	0.7314317
C	-4.8450884	0.0000146	0.7058274
C	-2.5254585	1.4334077	3.0504985
C	-3.6642953	-0.7295533	2.6154924
C	-2.7781611	3.0488081	1.1820350
C	-3.9586527	2.3190497	-0.7278518
C	-4.3939627	-1.1804012	1.4352014
C	-4.8454085	0.0000135	-0.7018543
C	-2.0738333	2.6139198	2.3206371
C	-1.3456105	0.7039315	3.5022734
C	-2.5254889	-1.4334248	3.0504998
C	-2.0484109	3.4990538	0.0013674
C	-2.7786909	3.0488099	-1.1789767
C	-4.3945873	1.1804227	-1.4314295
C	-3.9583720	-2.3190384	0.7314334
C	-4.3946126	-1.1804061	-1.4314288
C	-0.6149646	2.6156502	2.3220973
C	-0.1653641	1.4350055	3.0515283
C	-1.3456253	-0.7039732	3.5022741
C	-2.0738888	-2.6139469	2.3206392
C	-0.6406106	3.4999002	0.0010582
C	-2.0748732	2.6139176	-2.3178908

C	-3.6654585	0.7295581	-2.6120480
C	-3.9587017	-2.3190414	-0.7278502
C	-2.7782251	-3.0488214	1.1820373
C	-3.6654741	-0.7295584	-2.6120478
C	0.0899978	3.0497687	1.1819968
C	0.9717415	0.7301950	2.6136524
C	-0.1653944	-1.4350727	3.0515298
C	-0.6150201	-2.6157077	2.3220990
C	0.0894660	3.0497623	-1.1802028
C	-2.5268269	1.4334065	-3.0475545
C	-0.6160060	2.6156434	-2.3199893
C	-2.7787556	-3.0488275	-1.1789747
C	-2.0484849	-3.4990845	0.0013699
C	-2.5268573	-1.4334314	-3.0475543
C	1.2720556	2.3235648	0.7312627
C	1.6974847	1.1801310	1.4314924
C	0.9717265	-0.7302874	2.6136531
C	0.0899324	-3.0498420	1.1819986
C	1.2717221	2.3235605	-0.7299893
C	-1.3471788	0.7039273	-3.4998451
C	-0.1667336	1.4349988	-3.0496171
C	-2.0749284	-2.6139516	-2.3178896
C	-0.6406847	-3.4999602	0.0010607
C	-1.3471937	-0.7039772	-3.4998448
C	2.1476948	-0.0000588	0.7041454
C	1.6974611	-1.1802401	1.4314939
C	1.2720042	-2.3236623	0.7312636
C	1.6968268	1.1801256	-1.4304027

C	0.9705637	0.7301913	-2.6122414
C	-0.6160611	-2.6157082	-2.3199880
C	0.0894018	-3.0498402	-1.1802009
C	-0.1667636	-1.4350726	-3.0496161
C	2.1473567	-0.0000605	-0.7032558
C	1.2716746	-2.3236636	-0.7299882
C	0.9705483	-0.7302881	-2.6122412
C	1.6968032	-1.1802367	-1.4304022
C	5.0660641	-0.0002882	-1.4110951
C	5.0671941	0.0002897	1.4095026
H	5.0433007	0.0005166	2.5110123
H	5.0411174	-0.0005158	-2.5125779
C	5.0652831	1.2349294	0.7257151
C	5.0647617	1.2346144	-0.7278296
C	5.0013937	2.4901003	1.4140171
C	5.0006028	2.4894266	-1.4167329
C	4.9307805	3.6804324	0.7131120
H	4.9907045	2.4880250	2.5150013
C	4.9304599	3.6801058	-0.7163946
H	4.9893973	2.4867432	-2.5177102
H	4.8687109	4.6362265	1.2550931
H	4.8682787	4.6356375	-1.2588257
C	5.0653345	-1.2346312	0.7262221
C	5.0014996	-2.4895236	1.4150383
C	5.0648105	-1.2349097	-0.7273227
C	4.9309429	-3.6801453	0.7146190
H	4.9908010	-2.4869990	2.5160215
C	5.0007075	-2.4900064	-1.4157126

C	4.9306270	-3.6804026	-0.7148876
H	4.8689121	-4.6357217	1.2569882
H	4.9895030	-2.4877751	-2.5166910
H	4.8685009	-4.6361589	-1.2569292

$TS_{Monoadduct}$

C	-4.3474471	1.1804955	1.4341543
C	-3.6208180	0.7301920	2.6154804
C	-3.9095551	2.3188361	0.7305416
C	-4.7975675	0.0000252	0.7041964
C	-2.4831816	1.4343942	3.0528943
C	-3.6208176	-0.7299195	2.6155653
C	-2.7313071	3.0469671	1.1813277
C	-3.9095907	2.3187518	-0.7306295
C	-4.3474471	-1.1803604	1.4342912
C	-4.7976015	-0.0000565	-0.7039738
C	-2.0288134	2.6146553	2.3227704
C	-1.3044434	0.7039574	3.5056123
C	-2.4831803	-1.4340704	3.0530605
C	-1.9988626	3.4934614	-0.0001577
C	-2.7313631	3.0468303	-1.1815565
C	-4.3475166	1.1803294	-1.4340900
C	-3.9095542	-2.3187825	0.7308099
C	-4.3475152	-1.1805266	-1.4339531
C	-0.5711411	2.6155163	2.3267878
C	-0.1255702	1.4370709	3.0511108
C	-1.3044426	-0.7035804	3.5056934

C	-2.0288112	-2.6144161	2.3230734
C	-0.5910204	3.4869893	-0.0001910
C	-2.0289238	2.6143860	-2.3229827
C	-3.6209432	0.7298887	-2.6153990
C	-3.9095889	-2.3188670	-0.7303612
C	-2.7313050	-3.0468607	1.1816806
C	-3.6209427	-0.7302225	-2.6153141
C	0.1386784	3.0393246	1.1825416
C	1.0045802	0.7287901	2.5967141
C	-0.1255687	-1.4367457	3.0512773
C	-0.5711394	-2.6152752	2.3270908
C	0.1386212	3.0391859	-1.1829060
C	-2.4833268	1.4340400	-3.0529478
C	-0.5712524	2.6152450	-2.3270688
C	-2.7313616	-3.0469970	-1.1812035
C	-1.9988605	-3.4934910	0.0002471
C	-2.4833263	-1.4344238	-3.0527816
C	1.3180560	2.3141444	0.7366320
C	1.7382320	1.1745881	1.4280947
C	1.0045820	-0.7285172	2.5967988
C	0.1386805	-3.0392154	1.1828935
C	1.3180203	2.3140565	-0.7369687
C	-1.3046105	0.7035508	-3.5056357
C	-0.1257159	1.4367167	-3.0512757
C	-2.0289228	-2.6146846	-2.3226796
C	-0.5910182	-3.4870181	0.0002132
C	-1.3046104	-0.7039863	-3.5055545
C	2.3337321	0.0000311	0.7408565

C	1.7382378	-1.1744499	1.4282320
C	1.3180581	-2.3140854	0.7368998
C	1.7381688	1.1744233	-1.4283221
C	1.0044566	0.7284893	-2.5968506
C	-0.5712509	-2.6155436	-2.3267657
C	0.1386229	-3.0393518	-1.1825541
C	-0.1257155	-1.4370990	-3.0511091
C	2.3337118	-0.0000581	-0.7409773
C	1.3180212	-2.3141706	-0.7367007
C	1.0044560	-0.7288183	-2.5967659
C	1.7381660	-1.1746169	-1.4281852
C	4.3996674	-0.0001247	-1.3575015
C	4.3997772	0.0001078	1.3573054
H	4.2999790	0.0002025	2.4550974
H	4.2998166	-0.0002199	-2.4552893
C	4.7508105	1.2489725	0.7155549
C	4.7507704	1.2488484	-0.7159907
C	4.9330866	2.4684580	1.4128694
C	4.9330174	2.4682086	-1.4135295
C	5.1524362	3.6524953	0.7075311
H	4.9026476	2.4697229	2.5131553
C	5.1524048	3.6523699	-0.7084107
H	4.9025233	2.4692777	-2.5138139
H	5.3128542	4.5942733	1.2536039
H	5.3128009	4.5940508	-1.2546573
C	4.7508250	-1.2488631	0.7157692
C	4.9331260	-2.4682232	1.4132957
C	4.7507704	-1.2489873	-0.7157764

C	5.1524769	-3.6523818	0.7081622
H	4.9027042	-2.4692928	2.5135817
C	4.9330121	-2.4684698	-1.4131033
C	5.1524197	-3.6525058	-0.7077795
H	5.3129148	-4.5940620	1.2543976
H	4.9025005	-2.4697346	-2.5133875
H	5.3128128	-4.5942817	-1.2538636

C_{60}:anthracene Monoadduct

C	2.4784323	0.0000141	-0.8043082
C	2.4784313	0.0000013	0.8043153
C	1.7261880	1.1774635	1.4363040
C	1.2971297	2.3000891	0.7410018
C	1.2971323	2.3001022	-0.7409556
C	1.7261924	1.1774890	-1.4362773
C	0.9813630	0.7287676	-2.5874717
C	0.9813664	-0.7287131	-2.5874845
C	1.7261969	-1.1774504	-1.4362976
C	1.2971447	-2.3000795	-0.7409956
C	1.2971423	-2.3000909	0.7409617
C	1.7261931	-1.1774750	1.4362831
C	0.9813568	-0.7287579	2.5874752
C	0.9813530	0.7287224	2.5874881
C	-0.1481627	1.4358571	3.0511517
C	-0.5925397	2.6113334	2.3289655
C	0.1183489	3.0260205	1.1819963
C	-0.6101876	3.4731444	0.0000309

C	0.1183536	3.0260413	-1.1819392
C	-0.5925310	2.6113723	-2.3289163
C	-0.1481527	1.4359096	-3.0511213
C	-1.3264453	0.7034271	-3.5074943
C	-1.3264414	-0.7033695	-3.5075068
C	-0.1481445	-1.4358532	-3.0511466
C	-0.5925160	-2.6113315	-2.3289620
C	0.1183708	-3.0260169	-1.1819924
C	-0.6101674	-3.4731446	-0.0000298
C	0.1183662	-3.0260369	1.1819434
C	-0.5925245	-2.6113735	2.3289198
C	-0.1481546	-1.4359074	3.0511265
C	-1.3264547	-0.7034320	3.5075005
C	-1.3264588	0.7033668	3.5075129
C	-2.5051286	1.4344014	3.0557951
C	-2.0497124	2.6142492	2.3256412
C	-2.7506943	3.0451462	1.1821991
C	-2.0172690	3.4895677	0.0000292
C	-2.7506886	3.0451646	-1.1821504
C	-2.0497022	2.6142866	-2.3255945
C	-2.5051137	1.4344522	-3.0557683
C	-3.6425917	0.7302331	-2.6170710
C	-3.6425872	-0.7302046	-2.6170839
C	-2.5051054	-1.4344093	-3.0557934
C	-2.0496867	-2.6142538	-2.3256404
C	-2.7506704	-3.0451559	-1.1822036
C	-2.0172485	-3.4895753	-0.0000319
C	-2.7506760	-3.0451785	1.1821457

C	-2.0496968	-2.6142975	2.3255952
C	-2.5051201	-1.4344655	3.0557698
C	-3.6426010	-0.7302516	2.6170674
C	-3.6426055	0.7301884	2.6170804
C	-4.3670632	1.1802438	1.4348913
C	-3.9278752	2.3184338	0.7311564
C	-3.9278708	2.3184463	-0.7311245
C	-4.3670552	1.1802677	-1.4348802
C	-4.8161160	-0.0000060	-0.7040817
C	-4.3670481	-1.1802640	-1.4349008
C	-3.9278566	-2.3184523	-0.7311650
C	-3.9278607	-2.3184652	0.7311158
C	-4.3670557	-1.1802904	1.4348705
C	-4.8161199	-0.0000183	0.7040702
C	4.0050827	0.0000164	-1.2979829
H	4.0187594	0.0000238	-2.4042351
C	4.6447510	-1.2363670	-0.7063794
C	5.1473244	-2.3356036	-1.4142576
H	5.1318407	-2.3376302	-2.5150107
C	5.6659807	-3.4336541	-0.7030259
H	6.0695327	-4.2986433	-1.2511248
C	5.6659760	-3.4336678	0.7029750
H	6.0695223	-4.2986677	1.2510598
C	5.1473159	-2.3356289	1.4142238
H	5.1318255	-2.3376751	2.5149766
C	4.6447484	-1.2363796	0.7063635
C	4.0050832	-0.0000032	1.2979865
H	4.0187599	-0.0000125	2.4042384

C	4.6447504	1.2363808	0.7063809
C	5.1473224	2.3356199	1.4142560
H	5.1318511	2.3376428	2.5150086
C	5.6659605	3.4336773	0.7030206
H	6.0695083	4.2986698	1.2511175
C	5.6659394	3.4336964	-0.7029796
H	6.0694631	4.2987047	-1.2510683
C	5.1472902	2.3356507	-1.4142262
H	5.1317876	2.3376993	-2.5149787
C	4.6447439	1.2363938	-0.7063615

Bisadduct “e”

C	-0.4864361	3.5337053	3.2827683
C	-0.7152988	2.7553387	2.1303643
C	-1.2892448	1.4196793	2.2553873
C	-1.6252278	0.9154274	3.5244003
C	-1.3888285	1.7156037	4.7191448
C	-0.8212202	3.0034384	4.5985028
C	-1.3548909	4.0888053	5.3960803
C	-1.3485390	5.3015772	4.5847266
C	-0.8111289	4.9566993	3.2742648
C	-1.3516467	5.5495485	2.1157918
C	-1.5864439	4.7446246	0.9269877
C	-1.2720707	3.3695452	0.9319867
C	-2.1811799	2.4115381	0.3126654
C	-2.1920514	1.2134444	1.1246410
C	-3.4047039	0.5166424	1.3111248

C	-3.7461192	-0.0138162	2.6240078
C	-2.8675449	0.1745399	3.7165428
C	-3.4040596	0.5077858	5.0158600
C	-2.4813848	1.4730020	5.6491543
C	-2.9874889	2.5154267	6.4176234
C	-2.4343607	3.8364061	6.2714345
C	-3.5233923	4.8007386	6.3854761
C	-3.4998565	5.9883843	5.6213289
C	-2.3990247	6.2322362	4.6949941
C	-2.9540007	6.8546575	3.4993321
C	-2.4432172	6.5162676	2.2304640
C	-3.3495412	6.3057503	1.1123672
C	-2.8245462	5.2068429	0.3092275
C	-3.7084368	4.2780583	-0.2750228
C	-3.3843966	2.8575845	-0.2773907
C	-4.6172608	2.1090577	-0.0960797
C	-4.6252440	0.9545404	0.6750401
C	-5.8386056	0.4496757	1.4671576
C	-6.4237610	-0.8775333	0.7834394
C	-7.5429149	-1.3561690	1.6816779
C	-8.5982683	-0.4233640	1.7933614
C	-6.9895086	-0.4606150	-0.5553458
C	-8.0441586	0.4719520	-0.4435269
C	-5.1645112	0.0956374	2.7986033
C	-5.6580970	0.4474261	4.0537232
C	-4.7810347	0.6406090	5.1779919
C	-5.4394445	1.5531462	6.2177343
C	-4.4370138	2.6032065	6.9106630

C	-4.7464791	4.0733250	6.6020539
C	-5.9225069	4.5204052	6.0106304
C	-5.9164666	5.7250617	5.1947160
C	-4.7250087	6.4601981	5.0085923
C	-4.3940158	6.9940370	3.6933912
C	-5.2706500	6.7890255	2.6090667
C	-4.7414258	6.4413994	1.2966008
C	-5.6552283	5.4878395	0.6777809
C	-5.1471596	4.4183856	-0.0923306
C	-5.7239620	3.0885027	0.0202180
C	-6.7721389	2.8545772	0.9003867
C	-7.0389244	1.5119125	1.5935698
C	-8.3615935	0.8359354	0.9894752
C	-7.3083415	1.9947663	3.0241974
C	-6.7582889	1.4219145	4.1695500
C	-6.5366335	2.1950372	5.3628578
C	-6.8437889	3.5535860	5.3774185
C	-7.3855659	4.1753858	4.1914028
C	-6.8188379	5.5149375	4.0701488
C	-6.5080265	6.0413166	2.8037078
C	-6.7412197	5.2416482	1.6025071
C	-7.2687068	3.9377008	1.7168937
C	-7.5988656	3.3980644	3.0289937
C	-6.1021839	0.6657101	7.3796713
C	-6.8049104	1.6319488	8.3074934
C	-8.1836163	1.7118168	8.5426502
C	-8.6792079	2.7085840	9.4037336
C	-7.8018049	3.6247392	10.0096732

C	-6.4185766	3.5547225	9.7612594
C	-5.9239652	2.5536991	8.9156555
C	-4.4843293	2.3611235	8.4962884
C	-4.0798095	0.9217821	8.7211620
C	-2.9362061	0.4737651	9.3942876
C	-2.6793478	-0.9075951	9.4707238
C	-3.5539801	-1.8266857	8.8649089
C	-4.6954003	-1.3753778	8.1761065
C	-4.9596256	-0.0010928	8.1131454
C	-9.6862931	-0.6841832	2.6364101
C	-9.7238463	-1.8910336	3.3596386
C	-8.6727928	-2.8185828	3.2493966
C	-7.5724857	-2.5498341	2.4140075
C	-8.6394497	1.0086227	-1.5921742
C	-8.1846261	0.5987691	-2.8592804
C	-7.1347436	-0.3295836	-2.9707549
C	-6.5278829	-0.8586185	-1.8164825
H	-5.6057307	-1.6161626	0.6897643
H	-9.1953504	1.5580855	1.0727371
H	-6.7946301	-0.0620048	6.9156650
H	-8.8688773	1.0021100	8.0540172
H	-9.7601529	2.7736763	9.5999586
H	-8.1978766	4.4039339	10.6784329
H	-5.7289024	4.2785229	10.2222781
H	-3.7980644	3.0785211	8.9841838
H	-2.2473875	1.1986752	9.8547155
H	-1.7868825	-1.2689155	10.0037820
H	-3.3428135	-2.9050973	8.9254846

H	-5.3743341	-2.0909461	7.6875090
H	-10.5003303	0.0508710	2.7312234
H	-10.5800568	-2.1085825	4.0161033
H	-8.7088213	-3.7588567	3.8204056
H	-6.7399245	-3.2657276	2.3351710
H	-9.4516235	1.7460412	-1.4997673
H	-8.6501875	1.0115963	-3.7670744
H	-6.7813082	-0.6407244	-3.9654862
H	-5.6957213	-1.5747257	-1.9001279

Bisadduct “e” Intermediate

C	-0.5010689	3.4750558	3.3985622
C	-0.7237446	2.7000613	2.2440454
C	-1.2976660	1.3647003	2.3644917
C	-1.6252680	0.8491575	3.6321692
C	-1.3914257	1.6490875	4.8297092
C	-0.8387133	2.9406243	4.7143142
C	-1.3686253	4.0339326	5.5199834
C	-1.3575072	5.2441044	4.7051002
C	-0.8213470	4.8977704	3.3937351
C	-1.3550418	5.4955371	2.2350284
C	-1.5881129	4.6945236	1.0424326
C	-1.2773536	3.3201179	1.0432449
C	-2.1889413	2.3673008	0.4237122
C	-2.2039614	1.1672809	1.2366089
C	-3.4211612	0.4793965	1.4274993
C	-3.7606143	-0.0561534	2.7392407

C	-2.8730300	0.1145650	3.8244691
C	-3.4038066	0.4510967	5.1305865
C	-2.4929140	1.4028232	5.7563834
C	-3.0074369	2.4653350	6.5240761
C	-2.4344699	3.7977116	6.4104806
C	-3.5224341	4.7694642	6.5237489
C	-3.5045887	5.9419318	5.7430286
C	-2.4045469	6.1798018	4.8143842
C	-2.9547882	6.8038118	3.6165017
C	-2.4419625	6.4664911	2.3485526
C	-3.3460374	6.2645667	1.2261523
C	-2.8230967	5.1643087	0.4213258
C	-3.7089835	4.2410331	-0.1645024
C	-3.3906626	2.8181596	-0.1646684
C	-4.6266168	2.0766165	0.0202427
C	-4.6394997	0.9232798	0.7933043
C	-5.8557114	0.4223617	1.5818895
C	-6.4445936	-0.9004368	0.8913244
C	-7.5711384	-1.3774622	1.7813358
C	-8.6223264	-0.4402148	1.8919858
C	-7.0013217	-0.4739852	-0.4486534
C	-8.0520618	0.4630836	-0.3380228
C	-5.1881245	0.0594938	2.9140108
C	-5.6964525	0.3940824	4.1622377
C	-4.7977646	0.6065051	5.2830880
C	-5.3254115	1.7006398	6.0871085
C	-4.4475630	2.6115202	6.7029214
C	-4.7645971	4.0351418	6.7072663

C	-5.9572212	4.4973681	6.1183407
C	-5.9372297	5.7095206	5.3044296
C	-4.7335973	6.4194446	5.1210871
C	-4.3933833	6.9517676	3.8051987
C	-5.2685638	6.7592923	2.7188193
C	-4.7362675	6.4092718	1.4045839
C	-5.6523688	5.4607422	0.7855563
C	-5.1480871	4.3876798	0.0187281
C	-5.7286262	3.0603421	0.1353401
C	-6.7775341	2.8317528	1.0162806
C	-7.0523983	1.4904177	1.7070640
C	-8.3760380	0.8219790	1.0952550
C	-7.3267973	1.9701925	3.1375999
C	-6.7985899	1.3785532	4.2774929
C	-6.5547903	2.1757197	5.4667464
C	-6.8733525	3.5499148	5.4930577
C	-7.4124574	4.1690959	4.2987174
C	-6.8409140	5.5081896	4.1770214
C	-6.5125657	6.0228907	2.9092027
C	-6.7423928	5.2207529	1.7105409
C	-7.2712583	3.9176252	1.8293595
C	-7.6123367	3.3842389	3.1416746
C	-6.4837244	0.1396790	8.3744551
C	-6.9836913	1.3987837	8.7707607
C	-8.3314887	1.8054838	8.5014798
C	-8.7724107	3.0718354	8.8430136
C	-7.8890800	3.9985240	9.4802704
C	-6.5828265	3.6400174	9.7631389

C	-6.0858011	2.3406657	9.4183632
C	-4.7412397	1.9670749	9.6313510
C	-4.2410884	0.7079107	9.2347773
C	-2.8627722	0.3480338	9.3919700
C	-2.3897260	-0.8679459	8.9313701
C	-3.2736799	-1.7950247	8.2955640
C	-4.6127053	-1.4867387	8.1322797
C	-5.1393050	-0.2339866	8.5876895
C	-9.7160054	-0.6993960	2.7284312
C	-9.7627412	-1.9091003	3.4472157
C	-8.7154138	-2.8417515	3.3376043
C	-7.6101143	-2.5747027	2.5075890
C	-8.6386697	1.0083778	-1.4873505
C	-8.1792264	0.6020477	-2.7545095
C	-7.1327609	-0.3312696	-2.8648145
C	-6.5343889	-0.8683696	-1.7091949
H	-5.6288756	-1.6439666	0.7977982
H	-9.2085961	1.5481847	1.1768622
H	-7.1578275	-0.5635606	7.8569021
H	-9.0066583	1.0940483	7.9978041
H	-9.8077823	3.3753122	8.6179733
H	-8.2533337	5.0058447	9.7399710
H	-5.8968899	4.3576848	10.2430756
H	-4.0533473	2.6917431	10.0990155
H	-2.1799499	1.0687753	9.8717164
H	-1.3243009	-1.1253398	9.0471818
H	-2.8798577	-2.7569227	7.9287987
H	-5.2935872	-2.1943410	7.6308742

H	-10.5287503	0.0397912	2.8221725
H	-10.6239922	-2.1247407	4.1007843
H	-8.7579319	-3.7855236	3.9059449
H	-6.7801098	-3.2962816	2.4284915
H	-9.4487204	1.7508570	-1.3959170
H	-8.6390233	1.0221630	-3.6641425
H	-6.7747349	-0.6403618	-3.8605803
H	-5.7036072	-1.5888903	-1.7920127

Bisadduct “e” TS

C	-0.5061353	3.4677481	3.4298114
C	-0.7300121	2.6948664	2.2732809
C	-1.3079175	1.3605890	2.3905710
C	-1.6447435	0.8468693	3.6564843
C	-1.4114005	1.6431934	4.8561018
C	-0.8466327	2.9327009	4.7427454
C	-1.3798800	4.0208153	5.5438332
C	-1.3655547	5.2355863	4.7349082
C	-0.8249828	4.8919152	3.4252788
C	-1.3565319	5.4914991	2.2664111
C	-1.5881110	4.6923427	1.0726341
C	-1.2790203	3.3166505	1.0734904
C	-2.1893390	2.3650736	0.4479902
C	-2.2077070	1.1635651	1.2565406
C	-3.4248914	0.4731140	1.4384397
C	-3.7710692	-0.0650200	2.7467437
C	-2.8919364	0.1095773	3.8413827

C	-3.4288643	0.4425150	5.1422335
C	-2.5120815	1.3984816	5.7786393
C	-3.0295903	2.4523294	6.5409585
C	-2.4594650	3.7767986	6.4181807
C	-3.5445995	4.7458822	6.5301156
C	-3.5182064	5.9306104	5.7652660
C	-2.4125038	6.1710772	4.8433123
C	-2.9594431	6.7985536	3.6464439
C	-2.4438971	6.4626996	2.3791159
C	-3.3454081	6.2615842	1.2548980
C	-2.8209426	5.1632190	0.4499561
C	-3.7061247	4.2406589	-0.1410987
C	-3.3882667	2.8184079	-0.1449863
C	-4.6252070	2.0755575	0.0310344
C	-4.6409791	0.9191702	0.7992648
C	-5.8601148	0.4173917	1.5833066
C	-6.4482938	-0.9041945	0.8910622
C	-7.5749142	-1.3809378	1.7813935
C	-8.6261766	-0.4435223	1.8914473
C	-7.0049470	-0.4785674	-0.4490897
C	-8.0556817	0.4584556	-0.3390492
C	-5.1938816	0.0527656	2.9157660
C	-5.6976620	0.3996869	4.1649570
C	-4.8139501	0.6018690	5.2907008
C	-5.3975753	1.6097367	6.2079736
C	-4.4763423	2.5663882	6.8609825
C	-4.7782637	4.0143339	6.7210436
C	-5.9615981	4.4793405	6.1360530

C	-5.9421465	5.6896063	5.3256190
C	-4.7414755	6.4109379	5.1463652
C	-4.3995402	6.9449085	3.8334513
C	-5.2717649	6.7507813	2.7441312
C	-4.7369150	6.4044497	1.4319725
C	-5.6519128	5.4572890	0.8070018
C	-5.1451699	4.3872379	0.0369745
C	-5.7277671	3.0596691	0.1453462
C	-6.7806070	2.8289257	1.0208007
C	-7.0569344	1.4856373	1.7077095
C	-8.3794754	0.8181990	1.0938956
C	-7.3341120	1.9648239	3.1379731
C	-6.7952202	1.3797890	4.2790109
C	-6.5607028	2.1612275	5.4722362
C	-6.8817323	3.5259332	5.5002034
C	-7.4163980	4.1501673	4.3105545
C	-6.8415511	5.4883873	4.1952651
C	-6.5146887	6.0108645	2.9303281
C	-6.7443165	5.2148288	1.7266904
C	-7.2766098	3.9123269	1.8374538
C	-7.6209346	3.3732725	3.1460045
C	-6.2855613	0.4242893	7.7955734
C	-6.9027598	1.5385572	8.4806182
C	-8.2899136	1.8235810	8.4288045
C	-8.7896095	2.9832062	9.0234600
C	-7.9112334	3.9046347	9.6447033
C	-6.5368590	3.6619748	9.6685995
C	-6.0148985	2.4700179	9.1083682

C	-4.5999782	2.1923207	8.9835694
C	-4.1517491	0.8175824	8.9240334
C	-2.8545565	0.3950321	9.3063568
C	-2.4615150	-0.9296968	9.1075589
C	-3.3388246	-1.8499999	8.4828479
C	-4.6052167	-1.4417847	8.0610425
C	-5.0391383	-0.1129407	8.2945086
C	-9.7187056	-0.7010882	2.7299562
C	-9.7650320	-1.9098316	3.4505215
C	-8.7177038	-2.8426573	3.3415171
C	-7.6129474	-2.5767313	2.5102237
C	-8.6413854	1.0041247	-1.4886208
C	-8.1815027	0.5976526	-2.7555906
C	-7.1352088	-0.3358651	-2.8653415
C	-6.5372495	-0.8727318	-1.7093951
H	-5.6326677	-1.6479031	0.7981386
H	-9.2119763	1.5445239	1.1753067
H	-6.9409230	-0.2500166	7.2177331
H	-8.9661494	1.1191361	7.9175150
H	-9.8718070	3.1908935	8.9983106
H	-8.3146724	4.8240536	10.0993311
H	-5.8471251	4.3909264	10.1250017
H	-3.8942885	2.9436843	9.3780177
H	-2.1633633	1.1216601	9.7642313
H	-1.4587731	-1.2586885	9.4253154
H	-3.0136061	-2.8899137	8.3170584
H	-5.2797844	-2.1464200	7.5478092
H	-10.5307012	0.0389889	2.8239795

H	-10.6260883	-2.1247148	4.1046978
H	-8.7600405	-3.7859157	3.9108071
H	-6.7822984	-3.2977043	2.4323436
H	-9.4506537	1.7474961	-1.3973578
H	-8.6408788	1.0177907	-3.6654456
H	-6.7767811	-0.6451025	-3.8609386
H	-5.7057858	-1.5925445	-1.7916148

Bisadduct “t1”

C	-1.6045390	3.2725666	1.7818628
C	-2.5459297	2.7665152	0.8594738
C	-3.3848186	1.6304922	1.2201802
C	-3.2577366	1.0333520	2.4934474
C	-2.3050503	1.5763733	3.4556506
C	-1.4952805	2.6726981	3.1071992
C	-1.2742870	3.7541028	4.0618622
C	-1.2442623	5.0063986	3.3297832
C	-1.4483291	4.7083345	1.9188103
C	-2.2379856	5.5658175	1.1223067
C	-3.1753076	5.0223605	0.1557138
C	-3.3199555	3.6469176	0.0203431
C	-4.6125737	2.9509279	-0.4220200
C	-4.6750796	1.8116133	0.6022088
C	-5.8213592	1.4392808	1.2939767
C	-5.7169728	0.8548654	2.6196290
C	-4.4542338	0.6379715	3.2127357
C	-4.2503656	0.9357767	4.6238469
C	-2.9281405	1.5144929	4.7738125

C	-2.7389642	2.5739852	5.6884943
C	-1.9000135	3.7101048	5.3272635
C	-2.4664171	4.8938905	5.9242670
C	-2.4433374	6.0918988	5.2203407
C	-1.8359060	6.1532439	3.9027286
C	-2.6383274	7.0466730	3.0750286
C	-2.8354230	6.7585417	1.7114658
C	-4.1433037	6.9671686	1.1011627
C	-4.3694458	5.9002591	0.1418105
C	-5.6371619	5.3505711	-0.0070536
C	-5.9093362	3.9033479	-0.4370246
C	-6.9921440	3.5154189	0.5774760
C	-7.0153029	2.3173897	1.2814048
C	-7.6227594	2.2560717	2.5989784
C	-6.8203707	1.3625888	3.4266841
C	-6.6232583	1.6507427	4.7902177
C	-5.3153820	1.4420932	5.4004793
C	-5.0892304	2.5090122	6.3597539
C	-3.8215444	3.0587038	6.5084191
C	-3.5493103	4.5057649	6.9386534
C	-4.8461074	5.4582510	6.9238811
C	-4.7835806	6.5977525	5.8996891
C	-3.6373176	6.9700002	5.2077965
C	-3.7416866	7.5543898	3.8821142
C	-5.0044022	7.7712890	3.2889792
C	-5.2082607	7.4734961	1.8778390
C	-6.5304771	6.8947835	1.7278448
C	-6.7196899	5.8353350	0.8130409

C	-7.5586139	4.6992115	1.1743887
C	-8.1843257	4.6552230	2.4398157
C	-8.2143780	3.4029330	3.1719176
C	-8.0103207	3.7010109	4.5828853
C	-7.2206945	2.8434741	5.3793587
C	-6.2833704	3.3869321	6.3459120
C	-6.1387238	4.7623410	6.4813059
C	-6.9126834	5.6427894	5.6422180
C	-6.0737840	6.7788010	5.2815652
C	-6.2008751	7.3759058	4.0082881
C	-7.1535420	6.8329084	3.0460441
C	-7.9633369	5.7366211	3.3945071
C	-7.8540883	5.1367656	4.7198321
C	-4.4266185	2.3480890	-1.8971016
C	-4.2845880	3.5308734	-2.8287239
C	-5.4252520	4.3635484	-2.8428572
C	-6.5218536	3.8801601	-1.9199761
C	-6.8426695	2.4343431	-2.2280720
C	-5.7023628	1.6006066	-2.2169504
C	-5.4369970	5.5353629	-3.6104381
C	-4.3045842	5.8676734	-4.3780983
C	-3.1679702	5.0393689	-4.3625000
C	-3.1517034	3.8691225	-3.5801398
C	-5.8311087	0.2212793	-2.4249588
C	-7.1078254	-0.3236498	-2.6596897
C	-8.2435345	0.5061340	-2.6702011
C	-8.1151569	1.8901977	-2.4466856
C	-2.9371633	4.5277033	8.4217813

C	-4.0341304	4.0436844	9.3438746
C	-5.1744014	4.8768880	9.3304773
C	-5.0319792	6.0602423	8.3993484
C	-3.7560399	6.8073099	8.7196078
C	-2.6160406	5.9731301	8.7314299
C	-1.3436395	6.5165643	8.9521806
C	-1.2148397	7.9005436	9.1760125
C	-2.3500642	8.7309794	9.1633696
C	-3.6267721	8.1866407	8.9272968
C	-6.3071067	4.5385373	10.0822430
C	-6.2909813	3.3677174	10.8638265
C	-5.1549673	2.5385985	10.8780213
C	-4.0227841	2.8709656	10.1100811
H	-3.5342025	1.6918771	-1.9007649
H	-7.4173135	4.5309164	-1.9415450
H	-6.3247131	6.1893280	-3.6076471
H	-4.3083979	6.7842733	-4.9905734
H	-2.2831808	5.3094091	-4.9620397
H	-2.2573735	3.2246246	-3.5542863
H	-4.9399352	-0.4271059	-2.4004852
H	-7.2175652	-1.4070924	-2.8310406
H	-9.2403362	0.0708270	-2.8494914
H	-9.0045629	2.5418925	-2.4396740
H	-2.0419469	3.8766852	8.4430528
H	-5.9241607	6.7166687	8.4033966
H	-0.4545639	5.8643824	8.9467290
H	-0.2181154	8.3352663	9.3570835
H	-2.2399107	9.8144728	9.3341600

H	-4.5175364	8.8354973	8.9014738
H	-7.2011896	5.1833592	10.0574818
H	-7.1754948	3.0978040	11.4638475
H	-5.1513913	1.6214085	11.4896293
H	-3.1355709	2.2163502	10.1059385

Bisadduct “t1” Intermediate

C	-1.5978344	3.2930095	1.8684416
C	-2.5374033	2.7857538	0.9459341
C	-3.3763562	1.6507043	1.3073433
C	-3.2507188	1.0561668	2.5811604
C	-2.2954511	1.5967570	3.5437144
C	-1.4852612	2.6928105	3.1944617
C	-1.2601145	3.7714439	4.1508175
C	-1.2331618	5.0306376	3.4117905
C	-1.4397318	4.7279858	2.0017928
C	-2.2247476	5.5857362	1.2010986
C	-3.1641092	5.0404713	0.2359608
C	-3.3106584	3.6657159	0.1036440
C	-4.6037480	2.9692541	-0.3380001
C	-4.6670569	1.8304567	0.6872771
C	-5.8129087	1.4568641	1.3774689
C	-5.7096205	0.8709648	2.7036868
C	-4.4468522	0.6595573	3.2985666
C	-4.2455440	0.9550103	4.7108583
C	-2.9135725	1.5342668	4.8637936
C	-2.7028213	2.5778618	5.7862102
C	-1.8614201	3.7162207	5.4233961

C	-2.4547319	4.9155827	6.0006631
C	-2.4219708	6.1327784	5.2938744
C	-1.8082512	6.1880992	3.9756520
C	-2.6088089	7.0843239	3.1450808
C	-2.8168924	6.7829806	1.7863764
C	-4.1278725	6.9871705	1.1814788
C	-4.3571766	5.9187055	0.2231265
C	-5.6243314	5.3688223	0.0788475
C	-5.8988973	3.9220535	-0.3515479
C	-6.9806163	3.5337539	0.6644604
C	-7.0058261	2.3352570	1.3658498
C	-7.6132225	2.2722056	2.6845248
C	-6.8155357	1.3731970	3.5106574
C	-6.6270594	1.6481237	4.8777727
C	-5.3163691	1.4423505	5.4884101
C	-5.0962121	2.5149298	6.4472779
C	-3.8134629	3.0775006	6.5866775
C	-3.6578395	4.5200457	6.7213022
C	-4.7914894	5.3546944	6.7097943
C	-4.7619820	6.6145364	5.9776662
C	-3.6004723	7.0005647	5.2821233
C	-3.7130253	7.5902383	3.9563505
C	-4.9814888	7.7900646	3.3739161
C	-5.1905557	7.4896414	1.9637919
C	-6.5122771	6.9109667	1.8183969
C	-6.7050572	5.8536680	0.9031270
C	-7.5440033	4.7185437	1.2650324
C	-8.1657274	4.6737777	2.5315550

C	-8.1978522	3.4209680	3.2607833
C	-7.9936664	3.7147734	4.6730308
C	-7.2206027	2.8447346	5.4688381
C	-6.2747247	3.3824795	6.4347256
C	-6.1207949	4.7759338	6.5627418
C	-6.9171547	5.6802059	5.7431598
C	-6.0758536	6.8184299	5.3806063
C	-6.1853654	7.3965271	4.1009652
C	-7.1356193	6.8520560	3.1377168
C	-7.9457589	5.7559981	3.4870848
C	-7.8381603	5.1597477	4.8138567
C	-4.4196513	2.3656763	-1.8128901
C	-4.2772507	3.5477039	-2.7460205
C	-5.4163090	4.3827087	-2.7581478
C	-6.5127127	3.9011137	-1.8336478
C	-6.8359722	2.4559385	-2.1433839
C	-5.6970097	1.6202502	-2.1326816
C	-5.4287149	5.5523677	-3.5289595
C	-4.2989861	5.8798241	-4.3026817
C	-3.1645135	5.0486382	-4.2901811
C	-3.1472455	3.8807897	-3.5041363
C	-5.8278058	0.2418106	-2.3453891
C	-7.1050320	-0.3001159	-2.5844955
C	-8.2391939	0.5317179	-2.5952582
C	-8.1088241	1.9148352	-2.3670007
C	-2.6729270	4.7097801	9.5732852
C	-3.9294393	4.1394986	9.8693378
C	-5.1086339	4.9896952	9.8583121

C	-4.9613923	6.3593812	9.5521704
C	-3.7058188	6.9283967	9.2500909
C	-2.5266514	6.0781732	9.2605953
C	-1.2636017	6.6477361	8.8934507
C	-1.1649282	7.9781396	8.5265993
C	-2.3251240	8.8143894	8.5160300
C	-3.5603772	8.3034469	8.8728479
C	-6.3896922	4.3937058	10.0994121
C	-6.5078844	3.0345244	10.3294092
C	-5.3476861	2.1983663	10.3405297
C	-4.0928537	2.7381937	10.1213687
H	-3.5283881	1.7079302	-1.8178739
H	-7.4071931	4.5532858	-1.8546968
H	-6.3151884	6.2080339	-3.5248914
H	-4.3037576	6.7942901	-4.9183574
H	-2.2823896	5.3140624	-4.8957719
H	-2.2547560	3.2335996	-3.4818037
H	-4.9378268	-0.4082342	-2.3222616
H	-7.2162040	-1.3827594	-2.7600318
H	-9.2362740	0.0989828	-2.7793791
H	-8.9970408	2.5682842	-2.3612676
H	-1.7814047	4.0602662	9.5570147
H	-5.8598690	6.9985372	9.5199767
H	-0.3720995	5.9987621	8.8907352
H	-0.1893353	8.3994911	8.2342917
H	-2.2300819	9.8705133	8.2153319
H	-4.4580611	8.9431437	8.8536577
H	-7.2844612	5.0379052	10.0796404

H	-7.5007643	2.5874193	10.5000233
H	-5.4602577	1.1166006	10.5195758
H	-3.1985140	2.0934205	10.1180580

Bisadduct “t1” TS

C	-1.5874284	3.3016437	1.9092408
C	-2.5283904	2.7945362	0.9870563
C	-3.3665773	1.6584861	1.3487028
C	-3.2397241	1.0623922	2.6222002
C	-2.2857001	1.6047048	3.5842842
C	-1.4762396	2.7015757	3.2349585
C	-1.2540683	3.7828211	4.1895301
C	-1.2244273	5.0384057	3.4553579
C	-1.4316122	4.7376780	2.0454100
C	-2.2200476	5.5946098	1.2472026
C	-3.1583597	5.0491850	0.2814864
C	-3.3027650	3.6740790	0.1462095
C	-4.5958378	2.9771870	-0.2947774
C	-4.6573512	1.8383700	0.7306226
C	-5.8029819	1.4652876	1.4222584
C	-5.6988315	0.8801262	2.7479962
C	-4.4358435	0.6662920	3.3415349
C	-4.2329012	0.9612697	4.7533297
C	-2.9075089	1.5419722	4.9030546
C	-2.7104434	2.5968881	5.8177790
C	-1.8722200	3.7327729	5.4559456
C	-2.4564528	4.9220166	6.0428115
C	-2.4191674	6.1325665	5.3430882

C	-1.8091395	6.1904729	4.0256259
C	-2.6126474	7.0845256	3.1968117
C	-2.8158905	6.7886739	1.8354919
C	-4.1254858	6.9944026	1.2276918
C	-4.3524665	5.9263860	0.2692719
C	-5.6195373	5.3760640	0.1227461
C	-5.8921765	3.9298110	-0.3081009
C	-6.9741124	3.5404757	0.7066974
C	-6.9970079	2.3426185	1.4099605
C	-7.6042375	2.2799511	2.7283502
C	-6.8032356	1.3849839	3.5555767
C	-6.6112441	1.6655534	4.9217503
C	-5.3010502	1.4582800	5.5321087
C	-5.0794500	2.5276063	6.4905354
C	-3.8066389	3.0919381	6.6262916
C	-3.6024379	4.5366175	6.9053002
C	-4.7980913	5.4140766	6.8938989
C	-4.7608397	6.6153313	6.0203547
C	-3.6076098	7.0050846	5.3310383
C	-3.7170506	7.5917290	4.0061632
C	-4.9833721	7.7996137	3.4169218
C	-5.1895242	7.4982979	2.0069688
C	-6.5112964	6.9186875	1.8588925
C	-6.7015224	5.8602569	0.9443933
C	-7.5397315	4.7243238	1.3058580
C	-8.1634348	4.6796558	2.5715069
C	-8.1936348	3.4269947	3.3028458
C	-7.9918685	3.7226117	4.7145986

C	-7.2089567	2.8596465	5.5123342
C	-6.2679257	3.4001424	6.4783717
C	-6.1113893	4.7846241	6.6014428
C	-6.9005337	5.6749790	5.7743778
C	-6.0622075	6.8111112	5.4131851
C	-6.1823590	7.4033477	4.1390610
C	-7.1347632	6.8583751	3.1768759
C	-7.9442114	5.7615304	3.5259171
C	-7.8359127	5.1623277	4.8521796
C	-4.4128419	2.3719904	-1.7695949
C	-4.2676030	3.5544970	-2.7016667
C	-5.4054524	4.3915034	-2.7136618
C	-6.5038062	3.9103203	-1.7915722
C	-6.8288426	2.4658843	-2.1008845
C	-5.6911219	1.6287954	-2.0887562
C	-5.4124969	5.5656801	-3.4778802
C	-4.2793528	5.8949760	-4.2456899
C	-3.1463568	5.0616377	-4.2336033
C	-3.1341617	3.8895945	-3.4537911
C	-5.8249348	0.2495378	-2.2950221
C	-7.1033379	-0.2913707	-2.5300194
C	-8.2360799	0.5422894	-2.5425933
C	-8.1028799	1.9260530	-2.3201194
C	-2.8113640	4.6022279	8.9066885
C	-3.9907562	4.0700678	9.5556423
C	-5.1516152	4.9072391	9.5450321
C	-5.0111499	6.1894900	8.8879746
C	-3.7325548	6.8670514	8.9289599

C	-2.5720770	6.0294053	8.9369699
C	-1.2876587	6.6156203	8.8192804
C	-1.1555265	8.0028415	8.7387182
C	-2.3041839	8.8318141	8.7314805
C	-3.5798364	8.2699488	8.8050332
C	-6.3846311	4.3963075	10.0202218
C	-6.4546736	3.1001208	10.5333864
C	-5.3054527	2.2720326	10.5448384
C	-4.0913248	2.7436797	10.0430821
H	-3.5227456	1.7128411	-1.7730691
H	-7.3977227	4.5639740	-1.8138557
H	-6.2967916	6.2242599	-3.4721895
H	-4.2792132	6.8137748	-4.8549020
H	-2.2610035	5.3291772	-4.8335152
H	-2.2423783	3.2415058	-3.4292188
H	-4.9361667	-0.4026191	-2.2691670
H	-7.2164436	-1.3747434	-2.6998516
H	-9.2343239	0.1104086	-2.7222614
H	-8.9899012	2.5810102	-2.3133597
H	-1.9342132	3.9382892	8.8155590
H	-5.9166207	6.8123337	8.7836756
H	-0.3976753	5.9655291	8.7957896
H	-0.1533351	8.4559396	8.6670109
H	-2.1892779	9.9253245	8.6546650
H	-4.4769494	8.9096465	8.7698510
H	-7.2833989	5.0335021	9.9825024
H	-7.4116987	2.7132844	10.9197456
H	-5.3745490	1.2456058	10.9404717

H	-3.2021941	2.0922976	10.0231261

Bisadduct “t2”

C	-0.5336244	2.7802489	3.7428461
C	-0.7016876	1.9085978	2.6755062
C	-1.3793799	0.6522140	2.8844126
C	-1.8426013	0.2734327	4.1631653
C	-1.6635029	1.1774676	5.2800676
C	-1.0199461	2.4180361	5.0644387
C	-1.5565983	3.6082138	5.6917836
C	-1.4044632	4.7294420	4.7718015
C	-0.7744320	4.2320049	3.5599716
C	-1.1670867	4.7218271	2.3210018
C	-1.1104209	3.9208263	1.0152348
C	0.0516095	4.5006910	0.0732019
C	1.3584841	4.2011037	0.7731451
C	1.5892088	2.8182639	0.9453496
C	-0.0195821	3.7230438	-1.2216585
C	0.2098323	2.3400209	-1.0492045
C	-0.8489910	2.3459324	1.2133017
C	0.4743818	1.9589238	0.3910008
C	-2.0138185	1.4508066	0.7722585
C	-2.1840043	0.3642792	1.7034440
C	-3.4214454	-0.3022404	1.8369096
C	-3.9030180	-0.6842032	3.1596710
C	-3.1320077	-0.3933719	4.3046997
C	-3.7630188	0.1047704	5.5157658
C	-2.8413450	1.0915483	6.1283318

C	-3.3494249	2.2333974	6.7324285
C	-2.7120064	3.5062542	6.4963323
C	-3.7474190	4.5290269	6.4173778
C	-3.5905474	5.6272848	5.5441774
C	-2.4006863	5.7261110	4.7066350
C	-2.8122224	6.2354654	3.4148863
C	-2.2122653	5.7147542	2.2476728
C	-3.0255796	5.4292656	1.0741614
C	-2.4819295	4.2638643	0.4218405
C	-3.3429557	3.3376624	-0.1538410
C	-3.1013175	1.8876678	0.0234666
C	-4.3924326	1.2386614	0.1658393
C	-4.5547550	0.1483854	1.0499440
C	-5.7428127	0.0580071	1.8845224
C	-5.3329631	-0.4571389	3.1904226
C	-5.9221516	0.0590835	4.3652288
C	-5.1350254	0.3196355	5.5471610
C	-5.8271774	1.3752776	6.4168967
C	-4.8275327	2.4451048	7.0817412
C	-5.0248242	3.8852048	6.5909757
C	-6.1166726	4.3193752	5.8466048
C	-5.9732462	5.4272373	4.9190186
C	-4.7318350	6.0863373	4.7737477
C	-4.2565282	6.4618337	3.4510064
C	-5.0398319	6.1823411	2.3144884
C	-4.4167450	5.6732713	1.1010784
C	-5.3160492	4.7083241	0.4938095
C	-4.7796867	3.5530116	-0.1161793

C	-5.4280807	2.2626718	0.0818729
C	-6.5856796	2.1670949	0.8769682
C	-6.7400571	1.0487647	1.8016356
C	-7.3685322	1.5598414	3.0114347
C	-6.9539378	1.0823910	4.2745145
C	-6.8062069	1.9720906	5.3996846
C	-7.0323808	3.3324215	5.2314426
C	-7.4343335	3.8515274	3.9349192
C	-6.7826426	5.1401238	3.7394320
C	-6.3310036	5.5180422	2.4607273
C	-6.5019927	4.6093834	1.3291136
C	-7.1304452	3.3620265	1.5186382
C	-7.6108618	2.9810328	2.8368908
C	-6.6420259	0.6592279	7.5985154
C	-7.3621579	1.7564874	8.3498650
C	-8.7489367	1.9296039	8.4462727
C	-9.2573969	3.0397264	9.1469440
C	-8.3819324	3.9730713	9.7305891
C	-6.9882746	3.8069649	9.6197559
C	-6.4827913	2.6937963	8.9354392
C	-5.0256183	2.3814453	8.6736767
C	-4.7308812	0.9558757	9.0856616
C	-3.6780691	0.5231101	9.9024157
C	-3.5155695	-0.8541496	10.1451659
C	-4.3920088	-1.7868257	9.5620694
C	-5.4411798	-1.3524666	8.7300862
C	-5.6111754	0.0189857	8.5009287
C	-0.4123622	3.3617233	-3.5860772

C	-0.3384997	4.2365049	-2.4855422
C	0.1215946	1.4670510	-2.1415729
C	-0.1830842	1.9846738	-3.4149971
C	3.4157628	4.6899489	1.9582793
C	2.2644873	5.1395664	1.2842017
C	2.7281951	2.3708611	1.6275603
C	3.6466157	3.3131535	2.1283513
H	-0.1176210	5.5858088	-0.0701456
H	0.6654825	0.8753939	0.5180058
H	-7.3369695	-0.0796187	7.1524518
H	-9.4313664	1.2035506	7.9743019
H	-10.3474080	3.1794499	9.2343208
H	-8.7883681	4.8416169	10.2744322
H	-6.2988855	4.5444244	10.0633209
H	-4.3406797	3.1130014	9.1456970
H	-2.9842635	1.2561370	10.3462800
H	-2.6942407	-1.2027722	10.7926150
H	-4.2549208	-2.8638272	9.7530712
H	-6.1218024	-2.0808337	8.2588990
H	-0.6553553	3.7585182	-4.5854454
H	-0.5313966	5.3148173	-2.6120340
H	0.2866705	0.3859366	-2.0009939
H	-0.2463286	1.3058707	-4.2812327
H	4.1363608	5.4218120	2.3585571
H	2.0723451	6.2183480	1.1608509
H	2.8986998	1.2909787	1.7717959
H	4.5485915	2.9690532	2.6604989

Bisadduct “t2” Intermediate

C	-0.5511992	2.7719831	3.8315414
C	-0.7350804	1.8961517	2.7446482
C	-1.3966046	0.6103556	2.9400818
C	-1.8738036	0.2535026	4.2150603
C	-1.6954657	1.1606044	5.3424979
C	-1.0386119	2.3969586	5.1520389
C	-1.5710797	3.5867485	5.7885525
C	-1.4137846	4.7101639	4.8684039
C	-0.7815146	4.2054777	3.6552722
C	-1.1848854	4.7015514	2.4015258
C	-1.3621843	3.7929912	1.2767730
C	0.9205998	4.6643012	-0.4890715
C	1.7149244	4.2149588	0.5874517
C	1.9378894	2.7878096	0.7504337
C	0.3327546	3.7710041	-1.4098049
C	0.5553686	2.3437201	-1.2465761
C	-1.1401081	2.4127320	1.4470089
C	1.3532997	1.8946045	-0.1725388
C	-2.0493323	1.4476172	0.8356035
C	-2.2039371	0.3302164	1.7544099
C	-3.4532628	-0.3078131	1.8861133
C	-3.9407831	-0.6861172	3.2061468
C	-3.1687408	-0.4033241	4.3541400
C	-3.8001125	0.0941040	5.5647406
C	-2.8773523	1.0741096	6.1837875
C	-3.3824367	2.2118770	6.7991006
C	-2.7369009	3.4833148	6.5774934

C	-3.7693062	4.5078627	6.4936653
C	-3.6059984	5.6052578	5.6215367
C	-2.4113450	5.7002706	4.7879454
C	-2.8193282	6.2221951	3.4892157
C	-2.2165213	5.7300271	2.3152275
C	-3.0314406	5.4528379	1.1364742
C	-2.5028908	4.2545769	0.4956594
C	-3.3750843	3.3253943	-0.1013736
C	-3.1425508	1.8933719	0.0685148
C	-4.4381567	1.2401082	0.2090684
C	-4.5918574	0.1576451	1.0984990
C	-5.7810263	0.0688435	1.9366276
C	-5.3706701	-0.4515284	3.2383255
C	-5.9588314	0.0591804	4.4151504
C	-5.1712166	0.3118867	5.5975229
C	-5.8618072	1.3629991	6.4738965
C	-4.8612368	2.4257353	7.1470180
C	-5.0519697	3.8684987	6.6624701
C	-6.1380114	4.3093612	5.9169644
C	-5.9861151	5.4183851	4.9901672
C	-4.7416896	6.0704325	4.8488753
C	-4.2622084	6.4497677	3.5271864
C	-5.0464473	6.1785616	2.3883392
C	-4.4220957	5.6758680	1.1729074
C	-5.3307918	4.7082431	0.5613043
C	-4.8147585	3.5554689	-0.0651988
C	-5.4727017	2.2673358	0.1252271
C	-6.6226219	2.1765546	0.9330839

C	-6.7780396	1.0577264	1.8550732
C	-7.4051122	1.5679041	3.0709000
C	-6.9911393	1.0839614	4.3301489
C	-6.8399535	1.9680048	5.4603193
C	-7.0597141	3.3293044	5.2972353
C	-7.4571512	3.8542896	4.0017259
C	-6.7957505	5.1393856	3.8097935
C	-6.3396289	5.5170345	2.5331356
C	-6.5166164	4.6132937	1.3996702
C	-7.1563713	3.3714492	1.5823646
C	-7.6404832	2.9884033	2.9016544
C	-6.6776839	0.6379592	7.6485698
C	-7.3984041	1.7289909	8.4084658
C	-8.7851729	1.8985057	8.5096929
C	-9.2939763	3.0012502	9.2216959
C	-8.4187596	3.9311991	9.8110215
C	-7.0250427	3.7683114	9.6960717
C	-6.5192730	2.6621607	9.0010260
C	-5.0618410	2.3521545	8.7375699
C	-4.7684249	0.9234189	9.1404826
C	-3.7182156	0.4847079	9.9573339
C	-3.5589240	-0.8940646	10.1937449
C	-4.4358406	-1.8222564	9.6042798
C	-5.4815522	-1.3819236	8.7710454
C	-5.6485114	-0.0090778	8.5482494
C	-1.1427685	3.3116086	-3.3107763
C	-0.5266979	4.2177879	-2.4660913
C	-0.0930569	1.4380426	-2.1483071

C	-0.9238601	1.9075719	-3.1500975
C	2.9787539	4.6352416	2.6438736
C	2.2603464	5.1129340	1.5620315
C	2.6943948	2.3335046	1.8797715
C	3.1977268	3.2311839	2.8045509
H	0.7308148	5.7457897	-0.5985028
H	1.5024098	0.8100956	-0.0345644
H	-7.3720091	-0.0973251	7.1955745
H	-9.4673736	1.1753160	8.0329989
H	-10.3840227	3.1377106	9.3132752
H	-8.8250869	4.7945924	10.3629389
H	-6.3357916	4.5022871	10.1456148
H	-4.3769490	3.0801046	9.2153317
H	-3.0245115	1.2144412	10.4068886
H	-2.7401204	-1.2469513	10.8420977
H	-4.3023656	-2.9003983	9.7916328
H	-6.1623223	-2.1066489	8.2944894
H	-1.8122500	3.6688111	-4.1103295
H	-0.7029137	5.3002620	-2.5818165
H	0.0688707	0.3552298	-2.0168364
H	-1.4270939	1.1985413	-3.8275915
H	3.3809222	5.3370435	3.3926712
H	2.0794570	6.1942184	1.4434332
H	2.8520594	1.2496493	2.0083995
H	3.7659438	2.8661177	3.6756343

Bisadduct “t2” TS

C	-0.5172295	2.7655993	3.7985948

C	-0.7043340	1.8996804	2.7170178
C	-1.3729792	0.6281963	2.9172977
C	-1.8416084	0.2550645	4.1929987
C	-1.6610210	1.1562911	5.3174576
C	-1.0071970	2.3945928	5.1168451
C	-1.5408123	3.5851516	5.7498838
C	-1.3813699	4.7105901	4.8339104
C	-0.7491787	4.2110807	3.6223876
C	-1.1521800	4.7001294	2.3761340
C	-1.2108868	3.8422618	1.1649736
C	0.3757447	4.5672561	-0.0871797
C	1.4623361	4.1863172	0.7911987
C	1.6835534	2.7814437	0.9520316
C	0.0667998	3.7339064	-1.2298097
C	0.2838857	2.3286917	-1.0663980
C	-0.9813109	2.3882263	1.3443776
C	0.7957510	1.9043360	0.2190846
C	-2.0103688	1.4559749	0.8151368
C	-2.1765202	0.3489594	1.7333847
C	-3.4197200	-0.3046088	1.8590478
C	-3.9059976	-0.6875517	3.1796920
C	-3.1355603	-0.4048426	4.3283193
C	-3.7671864	0.0918927	5.5392774
C	-2.8430518	1.0717961	6.1589459
C	-3.3481744	2.2119486	6.7693092
C	-2.7038354	3.4829115	6.5437261
C	-3.7353407	4.5093333	6.4646650
C	-3.5712767	5.6093222	5.5954515

C	-2.3770569	5.7073855	4.7634650
C	-2.7846698	6.2252150	3.4694145
C	-2.1856660	5.7155872	2.2990394
C	-2.9972729	5.4394772	1.1222662
C	-2.4610502	4.2576801	0.4765989
C	-3.3283210	3.3384250	-0.1226944
C	-3.0950254	1.8943906	0.0471884
C	-4.3886997	1.2458569	0.1851904
C	-4.5523644	0.1563566	1.0696571
C	-5.7411673	0.0693885	1.9047708
C	-5.3349607	-0.4526306	3.2089283
C	-5.9240595	0.0598271	4.3849625
C	-5.1382218	0.3117558	5.5693508
C	-5.8286074	1.3643715	6.4442196
C	-4.8266277	2.4273418	7.1157909
C	-5.0170290	3.8703055	6.6320162
C	-6.1043706	4.3117954	5.8868546
C	-5.9529653	5.4225054	4.9629609
C	-4.7084069	6.0760508	4.8234513
C	-4.2283965	6.4559794	3.5032207
C	-5.0108238	6.1850405	2.3633000
C	-4.3871024	5.6797777	1.1481468
C	-5.2915430	4.7185105	0.5335835
C	-4.7651344	3.5645231	-0.0876163
C	-5.4208861	2.2752410	0.1031410
C	-6.5756421	2.1828705	0.9039668
C	-6.7357258	1.0621447	1.8238358
C	-7.3643619	1.5707943	3.0367583

C	-6.9538864	1.0861229	4.2979454
C	-6.8047877	1.9694036	5.4284647
C	-7.0233872	3.3315235	5.2651313
C	-7.4197396	3.8575780	3.9697850
C	-6.7608790	5.1438913	3.7806274
C	-6.3043266	5.5242474	2.5046656
C	-6.4779197	4.6210960	1.3689971
C	-7.1142562	3.3770289	1.5512311
C	-7.5995412	2.9927235	2.8680700
C	-6.6448848	0.6429791	7.6214134
C	-7.3632714	1.7361686	8.3805818
C	-8.7496196	1.9066111	8.4854604
C	-9.2560068	3.0091059	9.1995685
C	-8.3790165	3.9389235	9.7865149
C	-6.9858640	3.7755156	9.6675100
C	-6.4824796	2.6688619	8.9714710
C	-5.0261747	2.3564181	8.7068416
C	-4.7338667	0.9282889	9.1112525
C	-3.6807958	0.4903508	9.9247993
C	-3.5182397	-0.8884132	10.1587200
C	-4.3953624	-1.8170074	9.5701052
C	-5.4447290	-1.3771641	8.7410582
C	-5.6149235	-0.0042450	8.5206411
C	-0.9437468	3.3177817	-3.4085930
C	-0.5681421	4.2103375	-2.4031278
C	-0.1432072	1.4348655	-2.0795223
C	-0.7313287	1.9269086	-3.2460562
C	3.1407288	4.6377240	2.4994498

C	2.1880586	5.1025745	1.5910551
C	2.6248293	2.3277671	1.9082002
C	3.3595689	3.2475291	2.6583862
H	0.1263813	5.6403650	-0.1554144
H	0.8818795	0.8191382	0.4025900
H	-7.3409815	-0.0923244	7.1711260
H	-9.4334483	1.1833906	8.0111275
H	-10.3456281	3.1448046	9.2955852
H	-8.7834882	4.8023080	10.3398812
H	-6.2948577	4.5091670	10.1148749
H	-4.3399428	3.0841999	9.1829492
H	-2.9865139	1.2208573	10.3721499
H	-2.6960115	-1.2409893	10.8029813
H	-4.2584235	-2.8953194	9.7539068
H	-6.1249907	-2.1025692	8.2647931
H	-1.4199556	3.6952257	-4.3281412
H	-0.7588960	5.2906697	-2.5131120
H	-0.0026177	0.3508614	-1.9369526
H	-1.0445951	1.2289248	-4.0394325
H	3.7171076	5.3550347	3.1062833
H	1.9947788	6.1827860	1.4856307
H	2.7713527	1.2443992	2.0495975
H	4.1049580	2.8910669	3.3880423

Bisadduct “t3”

C	-0.6393644	2.8896284	3.9270453
C	-0.8232092	2.1290516	2.7789954
C	-1.4663294	0.8268282	2.8603137

C	-1.8942940	0.3164356	4.1074950
C	-1.7048348	1.1108466	5.3007488
C	-1.1052442	2.3851122	5.1950447
C	-1.6310694	3.5050481	5.9636176
C	-1.4909669	4.7001681	5.1687542
C	-0.5961467	4.4223765	3.9557378
C	0.8993915	4.9164629	4.2615487
C	-1.0854260	5.1257499	2.5946279
C	0.1110297	6.0545035	2.0649674
C	1.3030971	5.1434678	1.8662393
C	1.7315905	4.5241445	3.0613996
C	0.4097801	7.0435098	3.1711109
C	0.8415637	6.4240810	4.3649403
C	-1.5154388	4.1435011	1.4971189
C	-1.2763026	2.7764156	1.5275376
C	-2.1930751	1.8562919	0.8718119
C	-2.3077169	0.6620458	1.6844942
C	-3.5552613	0.0095853	1.7870916
C	-3.9989851	-0.5024564	3.0801117
C	-3.1816009	-0.3576040	4.2178315
C	-3.7802581	0.0126083	5.4995112
C	-2.8674966	0.9251945	6.1697434
C	-3.3707797	2.0074199	6.9165279
C	-2.7375530	3.3197129	6.8208306
C	-3.7733241	4.3309678	6.8682263
C	-3.6530972	5.4817281	6.0562752
C	-2.4882766	5.6654860	5.2036674
C	-2.9410437	6.3114019	3.9534018

C	-2.3681867	5.9576462	2.7376232
C	-3.2132574	5.7630634	1.5861823
C	-2.6921583	4.6442494	0.8280702
C	-3.5938493	3.7686055	0.1772926
C	-3.3393641	2.3427507	0.2004667
C	-4.6067527	1.6614087	0.2884842
C	-4.7157487	0.5216262	1.0761242
C	-5.8919709	0.3325088	1.9507160
C	-5.4359113	-0.3012432	3.1791349
C	-6.0152183	0.0429280	4.4218844
C	-5.1724497	0.2096455	5.5974414
C	-5.6955511	1.3329745	6.3723088
C	-4.8091671	2.2156252	7.0203944
C	-5.0575587	3.6554087	6.9891792
C	-6.1842755	4.1583274	6.3082810
C	-6.0646281	5.3569937	5.4796013
C	-4.8171123	5.9982087	5.3533910
C	-4.3784519	6.5037064	4.0561705
C	-5.2060392	6.3356773	2.9250087
C	-4.6127635	5.9581190	1.6578716
C	-5.5198996	5.0490595	0.9742492
C	-5.0198761	3.9820157	0.2401399
C	-5.7534889	2.6500310	0.0330449
C	-6.2520542	2.5277365	-1.4876292
C	-6.8775690	1.1559062	-1.6234814
C	-7.9994521	0.9745262	-0.7840309
C	-7.3141503	3.5887027	-1.6780508
C	-8.4350904	3.4060224	-0.8386374

C	-7.0310825	2.4442885	0.9876286
C	-8.3126887	2.1929092	0.0558762
C	-6.8914166	1.2954606	1.9927918
C	-7.4551721	1.6792802	3.2638731
C	-7.0494690	1.0563811	4.4645894
C	-6.8594336	1.8579163	5.6701622
C	-7.0980871	3.2452084	5.6401845
C	-7.5433187	3.8863757	4.4025611
C	-6.9160245	5.1858553	4.3093615
C	-6.4892972	5.6607310	3.0478601
C	-6.6978370	4.8607142	1.8511226
C	-7.3034757	3.6133671	1.9422527
C	-7.7085128	3.1130329	3.2326896
C	-8.3033946	5.6237091	-2.5471903
C	-7.2415311	4.6996158	-2.5281901
C	-9.4851474	4.3327830	-0.8459781
C	-9.4190948	5.4414760	-1.7106681
C	-7.0946056	-1.1309341	-2.3989901
C	-6.4174399	0.1033830	-2.4256636
C	-8.6642404	-0.2581010	-0.7453745
C	-8.2122492	-1.3106002	-1.5638935
C	2.9984678	3.9256771	0.6338452
C	1.9293253	4.8416440	0.6500027
C	2.7856586	3.6017542	3.0439092
C	3.4244090	3.3092079	1.8241381
C	0.5349829	9.2085334	4.2554473
C	0.2462143	8.4338340	3.1156252
C	1.1143756	7.1927371	5.5040889

C	0.9674368	8.5915566	5.4430331
H	1.2459090	4.4368116	5.1976033
H	-0.2118594	6.5478531	1.1273520
H	-5.3817990	2.6681785	-2.1581623
H	-9.1982102	2.0478494	0.7050353
H	-8.2570557	6.4972628	-3.2182262
H	-6.3586255	4.8470827	-3.1722345
H	-10.3509984	4.1934135	-0.1773967
H	-10.2447177	6.1718081	-1.7274800
H	-6.7429377	-1.9618436	-3.0323074
H	-5.5323891	0.2432437	-3.0677360
H	-9.5298099	-0.3989911	-0.0772012
H	-8.7347783	-2.2811508	-1.5458496
H	3.5001038	3.6868484	-0.3182961
H	1.5828139	5.3158323	-0.2830503
H	3.1056414	3.1093713	3.9772502
H	4.2590578	2.5892987	1.8024071
H	0.4169164	10.3039091	4.2167783
H	-0.1074009	8.9127706	2.1876032
H	1.4387048	6.7033171	6.4374928
H	1.1887209	9.2043943	6.3323242

Bisadduct “t3” Intermediate

C	-0.7037542	2.8652887	3.8718406
C	-0.8903397	2.1049005	2.7250428
C	-1.5336057	0.8041414	2.8075846
C	-1.9586553	0.2921135	4.0532513
C	-1.7688734	1.0889131	5.2489120

C	-1.1692219	2.3618758	5.1410956
C	-1.6933943	3.4839206	5.9091275
C	-1.5507969	4.6787419	5.1133473
C	-0.6580950	4.3976333	3.8984167
C	0.8395805	4.8896925	4.1972631
C	-1.1488120	5.0998485	2.5376211
C	0.0459188	6.0272353	2.0022839
C	1.2367621	5.1163533	1.8000307
C	1.6681680	4.4969378	2.9941811
C	0.3473109	7.0164660	3.1064238
C	0.7808638	6.3975519	4.2998549
C	-1.5793376	4.1194769	1.4400713
C	-1.3412630	2.7513931	1.4708835
C	-2.2538143	1.8344788	0.8075849
C	-2.3743516	0.6353438	1.6285924
C	-3.6102877	-0.0323036	1.7302152
C	-4.0550911	-0.5470187	3.0228517
C	-3.2426434	-0.3868241	4.1629993
C	-3.8449197	-0.0096944	5.4393921
C	-2.9315035	0.9050436	6.1136122
C	-3.4372311	1.9879764	6.8557652
C	-2.8017990	3.2997723	6.7630333
C	-3.8373371	4.3126887	6.8060078
C	-3.7116243	5.4635047	5.9975709
C	-2.5462591	5.6459628	5.1490065
C	-2.9987120	6.2939464	3.8960962
C	-2.4293494	5.9327721	2.6816091
C	-3.2753014	5.7440792	1.5280798

C	-2.7497577	4.6220653	0.7613389
C	-3.6340530	3.7528298	0.0875614
C	-3.3816659	2.3239998	0.1135075
C	-4.6632640	1.6428982	0.2337250
C	-4.7781523	0.4805916	1.0200159
C	-5.9407910	0.2949644	1.8783444
C	-5.4932677	-0.3399787	3.1162408
C	-6.0749747	0.0241324	4.3481350
C	-5.2357085	0.1938708	5.5282118
C	-5.7609229	1.3180669	6.2984202
C	-4.8769422	2.1986606	6.9514136
C	-5.1235452	3.6379159	6.9197915
C	-6.2463581	4.1422615	6.2341190
C	-6.1218513	5.3412669	5.4092756
C	-4.8757516	5.9841850	5.2902242
C	-4.4344842	6.4950602	3.9975518
C	-5.2630637	6.3458734	2.8637447
C	-4.6691674	5.9633794	1.5968149
C	-5.5846622	5.0528565	0.9158488
C	-5.0745698	3.9661467	0.1840474
C	-5.7100662	2.6579950	0.2732470
C	-6.8320700	2.4185304	-2.5099458
C	-7.1545957	1.1116069	-2.0857885
C	-8.3127045	0.9147579	-1.2301246
C	-7.5981813	3.5402639	-2.1276168
C	-8.7558435	3.3435526	-1.2712282
C	-6.8320575	2.4787505	1.1042537
C	-9.0792862	2.0363537	-0.8483361

C	-6.9455569	1.2793873	1.9225840
C	-7.5456831	1.6585267	3.1960348
C	-7.1179632	1.0426188	4.3882166
C	-6.9238479	1.8429181	5.5931861
C	-7.1613299	3.2314447	5.5630602
C	-7.6087462	3.8704402	4.3260429
C	-6.9714422	5.1751166	4.2339746
C	-6.5476700	5.6682938	2.9822025
C	-6.7498190	4.8691803	1.7769888
C	-7.3562653	3.6028932	1.8722889
C	-7.7984333	3.0961172	3.1647071
C	-7.9747514	5.9601352	-2.0604178
C	-7.2405673	4.8752733	-2.5057446
C	-9.4951588	4.4921247	-0.8379223
C	-9.1136486	5.7666164	-1.2177291
C	-6.6507027	-1.2811298	-1.9344176
C	-6.3447247	-0.0222541	-2.4202008
C	-8.6010132	-0.4058938	-0.7545863
C	-7.7908172	-1.4749778	-1.0935580
C	2.9351883	3.9075964	0.5634975
C	1.8621211	4.8187576	0.5822275
C	2.7257839	3.5785918	2.9736362
C	3.3646720	3.2911042	1.7525609
C	0.4582511	9.1806027	4.1926751
C	0.1772675	8.4058840	3.0511365
C	1.0474623	7.1664451	5.4401210
C	0.8910572	8.5643567	5.3806031
H	1.1893776	4.4105343	5.1323838

H	-0.2804199	6.5194879	1.0651317
H	-5.9388073	2.5708253	-3.1393825
H	-9.9431008	1.8902382	-0.1777959
H	-7.6803787	6.9822584	-2.3494869
H	-6.3554652	5.0231842	-3.1465945
H	-10.3665255	4.3413613	-0.1792272
H	-9.6843775	6.6415955	-0.8663051
H	-6.0108110	-2.1416450	-2.1891717
H	-5.4593968	0.1314619	-3.0592461
H	-9.4734632	-0.5511143	-0.0963149
H	-8.0178431	-2.4831255	-0.7101949
H	3.4377183	3.6730583	-0.3892498
H	1.5127124	5.2936036	-0.3494968
H	3.0497239	3.0867171	3.9058907
H	4.2029750	2.5755634	1.7286601
H	0.3328483	10.2751358	4.1555792
H	-0.1767248	8.8830288	2.1222607
H	1.3726920	6.6774946	6.3734655
H	1.1040318	9.1771971	6.2717850

Bisadduct “t3” TS

C	-0.7273291	2.8586893	3.8382035
C	-0.9110976	2.0994364	2.6896996
C	-1.5566203	0.7982769	2.7682361
C	-1.9869688	0.2865950	4.0134228
C	-1.7989376	1.0807291	5.2087614
C	-1.1971910	2.3538864	5.1051287
C	-1.7223442	3.4745991	5.8733857

C	-1.5779595	4.6704516	5.0798476
C	-0.6815798	4.3916722	3.8672227
C	0.8148637	4.8854464	4.1708362
C	-1.1690310	5.0960413	2.5063364
C	0.0267214	6.0244031	1.9746216
C	1.2183461	5.1142278	1.7748212
C	1.6465624	4.4936503	2.9694713
C	0.3243014	7.0130329	3.0802657
C	0.7543428	6.3934092	4.2746322
C	-1.5970025	4.1162910	1.4073163
C	-1.3592879	2.7485159	1.4367155
C	-2.2736057	1.8304992	0.7750812
C	-2.3938323	0.6325170	1.5886068
C	-3.6383474	-0.0261602	1.6863465
C	-4.0870434	-0.5394656	2.9785118
C	-3.2742131	-0.3877432	4.1195072
C	-3.8764554	-0.0155164	5.3982176
C	-2.9637695	0.8962888	6.0730067
C	-3.4681223	1.9787208	6.8179474
C	-2.8321430	3.2900786	6.7265718
C	-3.8666214	4.3032585	6.7710092
C	-3.7412110	5.4548230	5.9620712
C	-2.5740841	5.6372948	5.1136128
C	-3.0234457	6.2865610	3.8625822
C	-2.4502145	5.9300081	2.6478958
C	-3.2920640	5.7426014	1.4928990
C	-2.7685717	4.6214975	0.7323071
C	-3.6613646	3.7487350	0.0714806

C	-3.4100006	2.3227039	0.0948426
C	-4.6869619	1.6463426	0.1985591
C	-4.7998324	0.4877811	0.9747805
C	-5.9728278	0.3006976	1.8396952
C	-5.5253709	-0.3351369	3.0724315
C	-6.1076561	0.0182478	4.3108398
C	-5.2681157	0.1856921	5.4893030
C	-5.7922012	1.3095488	6.2626267
C	-4.9071179	2.1895551	6.9154130
C	-5.1529167	3.6294770	6.8852556
C	-6.2759114	4.1351923	6.2006166
C	-6.1512101	5.3350945	5.3749241
C	-4.9030662	5.9755168	5.2555004
C	-4.4601213	6.4839799	3.9615410
C	-5.2864682	6.3288123	2.8268954
C	-4.6900697	5.9508649	1.5597124
C	-5.6006423	5.0438093	0.8754621
C	-5.0944621	3.9602028	0.1527939
C	-5.7818945	2.6460138	0.1029737
C	-6.4874009	2.4888990	-1.9413656
C	-6.9772160	1.1330147	-1.8219038
C	-8.1171984	0.9409565	-0.9770708
C	-7.4223707	3.5898427	-1.8646226
C	-8.5626087	3.3977193	-1.0207079
C	-6.9643211	2.4563349	0.9732805
C	-8.6488395	2.1250886	-0.3372350
C	-6.9660196	1.2836439	1.8833853
C	-7.5523782	1.6605746	3.1547593

C	-7.1431968	1.0361893	4.3512759
C	-6.9536610	1.8366657	5.5578060
C	-7.1900603	3.2249746	5.5287890
C	-7.6325744	3.8684794	4.2912395
C	-7.0006701	5.1701186	4.2014749
C	-6.5724151	5.6546274	2.9444484
C	-6.7754976	4.8575808	1.7426512
C	-7.3740617	3.5965434	1.8343699
C	-7.8036881	3.0947733	3.1244993
C	-8.0911859	5.9055651	-2.2278075
C	-7.1905797	4.8616477	-2.4444263
C	-9.4425463	4.4814803	-0.7796589
C	-9.2199533	5.7150501	-1.3937186
C	-6.7860916	-1.2810192	-2.1002542
C	-6.3094456	0.0050317	-2.3596693
C	-8.5601823	-0.3742383	-0.6920053
C	-7.9141230	-1.4710380	-1.2648931
C	2.9146938	3.9007018	0.5399654
C	1.8446508	4.8153633	0.5578318
C	2.7014430	3.5720442	2.9497479
C	3.3406684	3.2824657	1.7293372
C	0.4293678	9.1766766	4.1682809
C	0.1531328	8.4023546	3.0253431
C	1.0151704	7.1620017	5.4166034
C	0.8578275	8.5598613	5.3574681
H	1.1629627	4.4060882	5.1064617
H	-0.2978367	6.5171253	1.0370995
H	-5.5528588	2.6473505	-2.5073058

H	-9.4667756	1.9892397	0.3914167
H	-7.9171890	6.8876138	-2.6969670
H	-6.2954544	5.0144775	-3.0696318
H	-10.3041440	4.3378299	-0.1069493
H	-9.9187476	6.5493953	-1.2188524
H	-6.2749132	-2.1547165	-2.5364818
H	-5.4149119	0.1555303	-2.9858870
H	-9.4200144	-0.5198076	-0.0178172
H	-8.2744936	-2.4914370	-1.0559045
H	3.4173135	3.6645753	-0.4123533
H	1.4974277	5.2912908	-0.3741630
H	3.0223405	3.0779866	3.8818695
H	4.1759624	2.5633639	1.7059491
H	0.3035392	10.2712134	4.1313457
H	-0.1986056	8.8798155	2.0957490
H	1.3362239	6.6730624	6.3513999
H	1.0666167	9.1723663	6.2499249

Bisadduct “t4”

C	-0.5676416	2.8927991	3.1991791
C	-0.7428080	2.0136164	2.1404459
C	-1.2985354	0.6902196	2.3756001
C	-1.6416237	0.2765584	3.6808370
C	-1.4602267	1.1961085	4.7870382
C	-0.9525983	2.4881692	4.5316490
C	-1.5234565	3.6425724	5.2079609
C	-1.4951555	4.7600622	4.2934716

C	-0.6243767	4.4192254	3.0779070
C	0.8450172	5.0332717	3.2728713
C	0.6889086	6.5370989	3.2312778
C	0.1809087	7.0061709	1.9994873
C	1.6604616	4.5757626	2.0839513
C	1.1530242	5.0453449	0.8522268
C	-1.2031101	4.9534602	1.6752759
C	-0.0889232	5.8949444	1.0088483
C	-1.6056172	3.8431248	0.6944373
C	-1.2778643	2.5019284	0.8475720
C	-2.1525386	1.4702082	0.3147992
C	-2.1677615	0.3565463	1.2547417
C	-3.3540435	-0.3712139	1.4733524
C	-3.7155931	-0.7851257	2.8278165
C	-2.8717575	-0.4685448	3.9114482
C	-3.4478168	-0.0097735	5.1717988
C	-2.5720431	1.0224168	5.7158856
C	-3.1217618	2.1385918	6.3741581
C	-2.5809395	3.4738141	6.1276411
C	-3.6816360	4.4154616	6.1153065
C	-3.6764290	5.4821452	5.1871890
C	-2.5583438	5.6526535	4.2743056
C	-3.0960038	6.1431956	2.9877308
C	-2.5312157	5.7134969	1.7893602
C	-3.3988580	5.3532742	0.7097551
C	-2.8320695	4.1991268	0.0217399
C	-3.6790202	3.2167312	-0.5303232
C	-3.3343877	1.8185811	-0.3781665

C	-4.5674627	1.0767191	-0.1398696
C	-4.5749464	0.0014052	0.7719838
C	-5.6884246	-0.1666407	1.6950335
C	-5.1571584	-0.6588689	2.9646998
C	-5.7165476	-0.2193861	4.1814215
C	-4.8450953	0.1125994	5.3043301
C	-5.4135614	1.2709536	5.9853201
C	-4.5671913	2.2651986	6.5113861
C	-4.9063467	3.6773769	6.3484351
C	-6.0719875	4.0403776	5.6395042
C	-6.0778438	5.1607905	4.7279452
C	-4.8994499	5.8577410	4.4965291
C	-4.5353271	6.2690073	3.1244291
C	-5.3792668	5.9628769	2.0597487
C	-4.8035406	5.4762077	0.8431594
C	-5.6783735	4.4479588	0.2919538
C	-5.1309836	3.3439097	-0.3924364
C	-5.6765292	2.0236176	-0.1555447
C	-6.7500063	1.8724679	0.7513605
C	-6.7512277	0.7577865	1.6897476
C	-7.3259042	1.2171872	2.9473053
C	-6.8216884	0.7294203	4.1720190
C	-6.6325427	1.6482747	5.2775692
C	-6.9487566	3.0125450	5.1005441
C	-7.5004870	3.4992365	3.8569781
C	-7.2054103	4.9952000	3.7022467
C	-8.4838669	5.8503034	4.1590462
C	-8.0806613	7.3051235	4.0647316

C	-7.7385075	7.6995527	2.7520965
C	-9.5741968	5.5604845	3.1520297
C	-9.2329883	5.9549853	1.8394675
C	-6.8154471	5.4443695	2.2078843
C	-7.8557651	6.5744943	1.7466789
C	-6.8004747	4.2972345	1.1873901
C	-7.3193485	3.0301823	1.4211218
C	-7.6797021	2.6202462	2.7986678
C	-11.6758101	4.6712461	2.3363148
C	-10.7898926	4.9117218	3.4034384
C	-10.1081935	5.7035158	0.7750807
C	-11.3369833	5.0651707	1.0292819
C	-7.5306234	9.5229008	4.8729178
C	-7.9710989	8.2104416	5.1281556
C	-7.2860577	9.0012352	2.5001237
C	-7.1900159	9.9159518	3.5661647
C	3.3862249	3.3503070	0.9032496
C	2.7708301	3.7223761	2.1135316
C	1.7568513	4.6642745	-0.3530723
C	2.8821015	3.8188361	-0.3232386
C	0.6946140	8.8036327	4.0904528
C	0.9393372	7.4303973	4.2810043
C	-0.0761958	8.3708552	1.8145050
C	0.1898353	9.2711736	2.8637891
H	1.2538254	4.6713943	4.2367349
H	-0.4769731	6.2692695	0.0416729
H	-8.7598514	5.5485022	5.1883389
H	-7.5975650	6.8920147	0.7174811

H	-12.6375750	4.1671252	2.5264746
H	-11.0447572	4.5913288	4.4272587
H	-9.8322758	6.0004616	-0.2503496
H	-12.0339831	4.8685845	0.1980371
H	-7.4487802	10.2438022	5.7030326
H	-8.2249648	7.8933001	6.1532719
H	-7.0061953	9.3016192	1.4768323
H	-6.8412971	10.9443099	3.3752744
H	4.2646227	2.6843339	0.9181937
H	3.1532170	3.3448639	3.0764659
H	1.3493776	5.0219383	-1.3132094
H	3.3659658	3.5183404	-1.2671106
H	0.8962777	9.5140827	4.9089559
H	1.3211047	7.0570369	5.2456448
H	-0.4850246	8.7321367	0.8562616
H	-0.0032170	10.3475572	2.7235495

Bisadduct “t4” Intermediate

C	-0.4617627	2.9578705	3.1606394
C	-0.6257113	2.0631971	2.0864930
C	-1.1714941	0.7331050	2.3312200
C	-1.5152487	0.3376773	3.6395909
C	-1.3301325	1.2603815	4.7535762
C	-0.8140429	2.5497221	4.5184973
C	-1.3877817	3.7018954	5.2010297
C	-1.3964814	4.8198412	4.2627875
C	-0.8154958	4.3599549	3.0066419
C	1.9161604	5.6464190	3.1591369

C	1.1661362	6.8415641	3.1322074
C	0.6356653	7.3116093	1.8631837
C	2.1600316	4.8894353	1.9935906
C	1.6281885	5.3587261	0.7247506
C	-1.3287437	4.8266625	1.7812479
C	0.8847778	6.5579184	0.6967296
C	-1.5076154	3.8993890	0.6693978
C	-1.1597022	2.5434998	0.8152980
C	-2.0366183	1.5087610	0.2757037
C	-2.0428001	0.3899905	1.2118894
C	-3.2317838	-0.3301137	1.4408816
C	-3.5884224	-0.7394588	2.7981362
C	-2.7433155	-0.4123204	3.8766518
C	-3.3154157	0.0443087	5.1380628
C	-2.4414233	1.0796580	5.6807402
C	-2.9950042	2.1926966	6.3430764
C	-2.4577674	3.5300027	6.1012355
C	-3.5706628	4.4697141	6.0943032
C	-3.5836036	5.5451972	5.1782447
C	-2.4722122	5.7249693	4.2521268
C	-3.0081171	6.2090833	2.9831203
C	-2.4394121	5.7672251	1.7699496
C	-3.3040645	5.4258113	0.6590782
C	-2.7316833	4.2706700	-0.0298438
C	-3.5731702	3.2729532	-0.5548498
C	-3.2206384	1.8665528	-0.4005472
C	-4.4529650	1.1204866	-0.1600025
C	-4.4556292	0.0413506	0.7455930

C	-5.5687258	-0.1300338	1.6742805
C	-5.0319133	-0.6195713	2.9408537
C	-5.5879261	-0.1809357	4.1589037
C	-4.7122035	0.1576327	5.2775860
C	-5.2840257	1.3119454	5.9610373
C	-4.4415310	2.3105553	6.4832386
C	-4.7899526	3.7202688	6.3247608
C	-5.9623187	4.0780803	5.6253348
C	-5.9800625	5.2001717	4.7182333
C	-4.8111447	5.9147956	4.4916381
C	-4.4501603	6.3300608	3.1158412
C	-5.2814814	6.0060527	2.0503906
C	-4.7027240	5.5269541	0.8191799
C	-5.5742875	4.4916102	0.2780563
C	-5.0223196	3.3887072	-0.4084026
C	-5.5624496	2.0648143	-0.1703545
C	-6.6329998	1.9089241	0.7369839
C	-6.6327245	0.7906509	1.6725051
C	-7.2092128	1.2476723	2.9314187
C	-6.6984634	0.7618369	4.1546134
C	-6.5099539	1.6816170	5.2591103
C	-6.8348550	3.0438340	5.0847764
C	-7.3916754	3.5286893	3.8448551
C	-7.1048515	5.0272816	3.6905345
C	-8.3884112	5.8766896	4.1442707
C	-7.9910663	7.3333130	4.0502327
C	-7.6478452	7.7285706	2.7381579
C	-9.4756402	5.5823077	3.1349586

C	-9.1328613	5.9765097	1.8227233
C	-6.7140301	5.4777834	2.1970899
C	-7.7588399	6.6031930	1.7326344
C	-6.6921257	4.3323357	1.1765909
C	-7.2058120	3.0631602	1.4090209
C	-7.5665092	2.6488948	2.7847401
C	-11.5737992	4.6881315	2.3156627
C	-10.6909619	4.9320235	3.3846001
C	-10.0039910	5.7198360	0.7562738
C	-11.2319856	5.0792937	1.0086210
C	-7.4480714	9.5528487	4.8584276
C	-7.8858469	8.2394039	5.1134564
C	-7.1973083	9.0308883	2.4865276
C	-7.1054241	9.9461808	3.5523194
C	3.0279475	2.8893854	0.8757993
C	2.8636494	3.6411608	2.0256508
C	1.8272815	4.5554384	-0.4450869
C	2.5044325	3.3512583	-0.3721103
C	0.0604383	8.7069864	4.2719650
C	0.8568767	7.5769333	4.3226476
C	-0.1758578	8.4926934	1.8512096
C	-0.4608105	9.1698723	3.0235114
H	2.2994366	5.2774189	4.1257178
H	0.4611626	6.9022845	-0.2622242
H	-8.6658503	5.5745057	5.1729800
H	-7.5007985	6.9220949	0.7037794
H	-12.5355688	4.1833882	2.5042866
H	-10.9481314	4.6135811	4.4084343

H	-9.7256334	6.0149807	-0.2690056
H	-11.9266973	4.8797037	0.1762156
H	-7.3697811	10.2745219	5.6881722
H	-8.1410808	7.9221518	6.1381966
H	-6.9160778	9.3310368	1.4635549
H	-6.7592434	10.9754485	3.3617553
H	3.5602603	1.9250249	0.9177763
H	3.2575590	3.2808353	2.9905971
H	1.4134723	4.9076745	-1.4045567
H	2.6389202	2.7377855	-1.2779187
H	-0.1816233	9.2538328	5.1978619
H	1.2508575	7.2126371	5.2859267
H	-0.5865113	8.8422611	0.8892102
H	-1.0982750	10.0689184	3.0011026

Bisadduct “t4” TS

C	-0.4546488	2.9687287	3.1693233
C	-0.6091176	2.0790866	2.1026844
C	-1.1556962	0.7511760	2.3403675
C	-1.4997609	0.3414533	3.6467863
C	-1.3223981	1.2616758	4.7578630
C	-0.8193097	2.5557704	4.5134969
C	-1.3948698	3.7045113	5.1936551
C	-1.3885481	4.8211205	4.2652673
C	-0.6719617	4.4279189	3.0264108
C	1.3056379	5.2939673	3.2473053
C	0.8664331	6.6718138	3.2075993
C	0.3437023	7.1354183	1.9584694

C	1.8625001	4.6926602	2.0554064
C	1.3379473	5.1552135	0.8066354
C	-1.2034285	4.9232935	1.7332513
C	0.3043844	6.1674336	0.8816238
C	-1.4937450	3.9109981	0.6815005
C	-1.1455352	2.5640335	0.8194986
C	-2.0172050	1.5303034	0.2811106
C	-2.0251042	0.4130559	1.2186395
C	-3.2113549	-0.3144047	1.4408612
C	-3.5702514	-0.7306503	2.7952014
C	-2.7273941	-0.4085683	3.8776794
C	-3.3046868	0.0448026	5.1394020
C	-2.4337518	1.0800953	5.6859698
C	-2.9895406	2.1921385	6.3477763
C	-2.4555981	3.5312914	6.1059614
C	-3.5642779	4.4692607	6.0976909
C	-3.5692336	5.5427453	5.1767055
C	-2.4552501	5.7237705	4.2590571
C	-2.9935818	6.2106489	2.9798693
C	-2.4253360	5.7695403	1.7770593
C	-3.2903421	5.4212401	0.6813190
C	-2.7176794	4.2705886	-0.0073535
C	-3.5561239	3.2799874	-0.5539076
C	-3.2024551	1.8798063	-0.4044467
C	-4.4326191	1.1324093	-0.1652842
C	-4.4347867	0.0538697	0.7419681
C	-5.5481672	-0.1211511	1.6663575
C	-5.0132749	-0.6122035	2.9341087

C	-5.5737379	-0.1774347	4.1518430
C	-4.7022081	0.1584877	5.2740312
C	-5.2766126	1.3120500	5.9577873
C	-4.4359184	2.3101385	6.4847974
C	-4.7836818	3.7207844	6.3256021
C	-5.9532835	4.0787023	5.6208904
C	-5.9671093	5.2013021	4.7130607
C	-4.7956270	5.9119988	4.4864140
C	-4.4342069	6.3293645	3.1131918
C	-5.2717468	6.0133573	2.0467868
C	-4.6926106	5.5331181	0.8241670
C	-5.5612999	4.4988503	0.2740596
C	-5.0078580	3.3981749	-0.4130470
C	-5.5459162	2.0741602	-0.1777387
C	-6.6179713	1.9155036	0.7286631
C	-6.6150175	0.7977392	1.6638363
C	-7.1929068	1.2520261	2.9222932
C	-6.6844065	0.7650260	4.1457675
C	-6.4995258	1.6831155	5.2525008
C	-6.8241887	3.0457818	5.0789851
C	-7.3797693	3.5317036	3.8376810
C	-7.0928174	5.0301821	3.6856546
C	-8.3764902	5.8784900	4.1415148
C	-7.9804972	7.3355218	4.0474070
C	-7.6406496	7.7319020	2.7347412
C	-9.4646291	5.5828011	3.1334969
C	-9.1242541	5.9784733	1.8210805
C	-6.7038783	5.4833336	2.1926482

C	-7.7510716	6.6064062	1.7295963
C	-6.6809853	4.3385609	1.1703430
C	-7.1933535	3.0684097	1.4010355
C	-7.5531051	2.6533548	2.7770145
C	-11.5612868	4.6833881	2.3156407
C	-10.6777421	4.9285827	3.3837358
C	-9.9963961	5.7212395	0.7555160
C	-11.2225209	5.0774750	1.0086622
C	-7.4360115	9.5548531	4.8555366
C	-7.8725276	8.2410481	5.1108551
C	-7.1921842	9.0348510	2.4826162
C	-7.0978188	9.9495123	3.5486676
C	3.1545511	2.9958634	0.8752130
C	2.7572724	3.5940592	2.0720527
C	1.7221016	4.5090886	-0.3936729
C	2.6364984	3.4547104	-0.3604561
C	0.2412753	8.7872322	4.2452435
C	0.7881895	7.5071605	4.3495133
C	-0.2427035	8.4223630	1.8820355
C	-0.2750128	9.2461355	3.0087613
H	1.6185391	4.8831507	4.2229138
H	-0.1770018	6.4760532	-0.0628472
H	-8.6520097	5.5756222	5.1705485
H	-7.4940667	6.9251743	0.7004592
H	-12.5211738	4.1752498	2.5047876
H	-10.9326719	4.6079156	4.4074474
H	-9.7200473	6.0182133	-0.2698178
H	-11.9179096	4.8772162	0.1769242

H	-7.3550798	10.2757931	5.6856434
H	-8.1243681	7.9229423	6.1361487
H	-6.9139862	9.3356779	1.4589888
H	-6.7528211	10.9791362	3.3578081
H	3.8651638	2.1535041	0.8917067
H	3.1369782	3.2215465	3.0377225
H	1.2935140	4.8492496	-1.3507527
H	2.9468429	2.9669410	-1.2988721
H	0.1998017	9.4403969	5.1320477
H	1.1658697	7.1361758	5.3163939
H	-0.6697588	8.7649714	0.9251102
H	-0.7161737	10.2538630	2.9401278

C_{60}:anthracene Monoadduct BP86/def2-TZVP/D3

C	2.4684299	0.0000141	-0.8015586
C	2.4684343	0.0000015	0.8015778
C	1.7181243	1.1750329	1.4320452
C	1.2892786	2.2876836	0.7386867
C	1.2892783	2.2876974	-0.7386303
C	1.7181321	1.1750549	-1.4320034
C	0.9750118	0.7259623	-2.5767410
C	0.9750167	-0.7259077	-2.5767534
C	1.7181338	-1.1750194	-1.4320228
C	1.2892922	-2.2876715	-0.7386704
C	1.2892882	-2.2876864	0.7386469
C	1.7181312	-1.1750413	1.4320244
C	0.9750048	-0.7259522	2.5767562

C	0.9750022	0.7259180	2.5767684
C	-0.1487564	1.4281505	3.0363601
C	-0.5918822	2.5986644	2.3169906
C	0.1147636	3.0107774	1.1772589
C	-0.6109183	3.4564869	0.0000332
C	0.1147712	3.0107983	-1.1771955
C	-0.5918716	2.5987066	-2.3169403
C	-0.1487400	1.4282029	-3.0363279
C	-1.3226535	0.6989142	-3.4912094
C	-1.3226493	-0.6988571	-3.4912205
C	-0.1487337	-1.4281469	-3.0363516
C	-0.5918565	-2.5986637	-2.3169844
C	0.1147856	-3.0107739	-1.1772475
C	-0.6108994	-3.4564863	-0.0000269
C	0.1147824	-3.0107927	1.1772069
C	-0.5918682	-2.5987047	2.3169469
C	-0.1487471	-1.4281989	3.0363365
C	-1.3226666	-0.6989146	3.4912108
C	-1.3226704	0.6988518	3.4912218
C	-2.4970637	1.4270501	3.0414964
C	-2.0432996	2.6024692	2.3140545
C	-2.7399747	3.0306233	1.1777073
C	-2.0091697	3.4732644	0.0000300
C	-2.7399701	3.0306441	-1.1776590
C	-2.0432874	2.6025112	-2.3140123
C	-2.4970494	1.4271032	-3.0414776
C	-3.6275423	0.7275152	-2.6056308
C	-3.6275371	-0.7274865	-2.6056433

C	-2.4970409	-1.4270594	-3.0415016
C	-2.0432723	-2.6024774	-2.3140558
C	-2.7399514	-3.0306340	-1.1777121
C	-2.0091492	-3.4732716	-0.0000300
C	-2.7399577	-3.0306550	1.1776542
C	-2.0432840	-2.6025166	2.3140108
C	-2.4970557	-1.4271127	3.0414724
C	-3.6275495	-0.7275297	2.6056190
C	-3.6275534	0.7274689	2.6056316
C	-4.3490257	1.1758028	1.4277656
C	-3.9127972	2.3071012	0.7285317
C	-3.9127930	2.3071154	-0.7285026
C	-4.3490201	1.1758273	-1.4277599
C	-4.7962231	-0.0000054	-0.6997241
C	-4.3490126	-1.1758231	-1.4277801
C	-3.9127787	-2.3071202	-0.7285424
C	-3.9127829	-2.3071314	0.7284917
C	-4.3490184	-1.1758475	1.4277451
C	-4.7962256	-0.0000176	0.6997085
C	3.9917071	0.0000167	-1.2947715
H	4.0065152	0.0000152	-2.3924833
C	4.6315923	-1.2303138	-0.7021503
C	5.1370181	-2.3204068	-1.4063711
H	5.1211600	-2.3235027	-2.4976961
C	5.6590149	-3.4096840	-0.6991215
H	6.0635070	-4.2647899	-1.2420796
C	5.6589962	-3.4097195	0.6990543
H	6.0634566	-4.2648458	1.2419899

C	5.1369930	-2.3204547	1.4063464
H	5.1211096	-2.3235926	2.4976659
C	4.6315770	-1.2303098	0.7021398
C	3.9917258	-0.0000065	1.2947925
H	4.0065303	-0.0000070	2.3924971
C	4.6315875	1.2303121	0.7021437
C	5.1370128	2.3204361	1.4063662
H	5.1211568	2.3235406	2.4976949
C	5.6589860	3.4097216	0.6991016
H	6.0634573	4.2648370	1.2420463
C	5.6589616	3.4097285	-0.6990753
H	6.0634138	4.2648643	-1.2420233
C	5.1369728	2.3204590	-1.4063489
H	5.1210865	2.3235862	-2.4976711
C	4.6315809	1.2303326	-0.7021293

C_{60} BP86/def2-TZVP/D3

C	-4.5586361	1.2512936	3.8527378
C	-3.1052739	1.2513272	3.8526907
C	-2.4059299	2.4628734	3.8526961
C	-3.1326990	3.7215928	3.8525375
C	-4.5313409	3.7215580	3.8525836
C	-5.2580414	2.4628032	3.8527893
C	-5.0079917	0.1522383	3.0136965
C	-3.8319588	-0.5266857	2.4948345
C	-2.6559204	0.1522931	3.0136165
C	-1.5240930	0.3066190	2.2058056

C	-1.2297942	2.6232031	3.0130119
C	-2.4058688	4.6599238	3.0132257
C	-3.1053191	5.5628170	2.2055653
C	-4.5589367	5.5627810	2.2056168
C	-5.2582798	4.6598512	3.0133251
C	-6.4341412	3.9807952	2.4944722
C	-6.4342425	2.6230754	3.0131916
C	-6.8665505	1.5657933	2.2057328
C	-6.1398847	0.3065089	2.2059662
C	-3.8319939	-1.0258436	1.1878797
C	-5.0080576	-0.8653584	0.3486463
C	-6.1398993	-0.2121504	0.8478263
C	-6.8664685	0.7264559	0.0086032
C	-7.3150824	1.8251784	0.8477957
C	-7.3151311	3.1316364	0.3488695
C	-6.8665106	4.2303728	1.1880284
C	-6.1400574	5.1690102	0.3487551
C	-5.0082184	5.8222828	0.8478549
C	-1.2300067	3.9809262	2.4942881
C	-2.6562131	4.8047433	-1.8172755
C	-1.5243273	4.6504664	-1.0095414
C	-0.7976667	3.3911894	-1.0093095
C	-1.2299648	2.3339118	-1.8167719
C	-2.4061644	2.4941777	-2.6563760
C	-4.5589381	3.7056536	-2.6562696
C	-5.0082921	4.8046851	-1.8171933
C	-3.8322518	5.4836706	-1.2984208
C	-3.8322179	5.9828296	0.0085392

C	-2.6561484	5.8223381	0.8477700
C	-1.5243139	5.1691214	0.3485907
C	-0.3491337	3.1318077	0.3486215
C	-0.3490753	1.8253522	0.8475481
C	-0.7976928	0.7266049	0.0083876
C	-1.2300642	0.9761839	-1.2980601
C	-2.4059339	0.2971269	-1.8169067
C	-3.1328706	1.2354223	-2.6561663
C	-4.5315128	1.2353887	-2.6561140
C	-5.2582816	2.4941061	-2.6562705
C	-6.1401144	4.6503537	-1.0093780
C	-6.8667079	3.3910381	-1.0090933
C	-6.4344095	2.3337808	-1.8165840
C	-6.4342030	0.9760569	-1.2978741
C	-5.2583385	0.2970589	-1.8168016
C	-4.5588904	-0.6058320	-1.0091445
C	-3.1052779	-0.6057985	-1.0091969
C	-2.6559973	-0.8653017	0.3485627
C	-1.5241524	-0.2120391	0.8476634
C	-0.7977499	4.2305229	1.1878115
C	-0.7974912	1.5659417	2.2055206
C	-3.1055720	3.7056904	-2.6563225

Anthracene BP86/def2-TZVP/D3

C	3.6637068	0.7122681	-0.0000189
C	2.4791155	1.4079083	0.0000313
C	1.2251157	0.7241847	0.0000368
C	1.2251261	-0.7242014	0.0000218
C	2.4790962	-1.4079260	-0.0000251
C	3.6637305	-0.7122621	-0.0000551
C	0.0000001	1.4057984	0.0000360
C	-0.0000013	-1.4058148	0.0000378
C	-1.2251264	-0.7242014	0.0000345
C	-1.2251177	0.7241848	0.0000174
C	-2.4791161	1.4079087	-0.0000307
H	-2.4779666	2.4999270	-0.0000596
C	-3.6637079	0.7122687	-0.0000514
C	-3.6637317	-0.7122615	-0.0000123
C	-2.4790979	-1.4079256	0.0000308
H	-0.0000004	2.4989075	0.0000367
H	4.6134274	1.2491234	-0.0000344
H	2.4779659	2.4999265	0.0000605
H	2.4779844	-2.4999197	-0.0000470
H	4.6134312	-1.2490934	-0.0001076
H	-0.0000008	-2.4989148	0.0000395
H	-4.6134284	1.2491242	-0.0000992
H	-4.6134326	-1.2490926	-0.0000201
H	-2.4779860	-2.4999192	0.0000575

Total Electronic Energies and Thermodynamic Corrections

Table S10. Total electronic energies as well as zero-point energy corrections (ZPE), entropic and enthalpic corrections, S_{corr} and $H_{corr,}$ provided by the Turbomole calculations, at 0.1 MPa and 298.15 K using a scaling factor of 0.9914. Imaginary frequencies are available for transition states, as minima only have positive frequencies. The electronic energies are for single point calculations with BP86/def2-TZVP/D3//BP86/def2-SVP/D3, while corrections are provided from the BP86/def2-SVP/D3 harmonic frequency calculations.

Structure	Electronic Energy / a.u.	ZPE / kJ mol^{-1}	S_{corr} / kJ mol^{-1} K^{-1}	H_{corr} / kJ mol^{-1}	Imaginary Freqency/ cm^{-1}
1	-5114.282119	2409.0	1.21346	2562.58	n/a
TS(1-INT_{Mono})	-5114.251892	2400.0	1.24397	2555.14	-326.32
INT_{Mono}	-5114.273818	2402.0	1.27484	2559.83	n/a
TS(INT_{Mono}-1')	-5114.282119	2409.0	1.21346	2562.58	-326.32
1'	-5114.282119	2409.0	1.21346	2562.58	n/a
2	-5654.061335	2911.0	1.42117	3091.89	n/a
TS(2-INT_{Bis})	-5654.032103	2902.0	1.43693	3084.33	-324.97
INT_{Bis}	-5654.054073	2904.0	1.46680	3089.25	n/a
TS(INT_{Bis}-3)	-5654.029084	2901.0	1.43700	3083.91	-343.60
3	-5654.058341	2910.0	1.42158	3091.38	n/a
Naphthalene Transfer Intermediate	-4955.498886	n/a	n/a	n/a	n/a
Benzene Transfer Intermediate	-4801.940272	n/a	n/a	n/a	n/a
Anthracene	-539.755753	492.4	0.40299	520.56	n/a
C_{60}	-2287.239624	952.3	0.59274	1013.45	n/a

$INT_{Butadiene}$	-2443.297400	1167.0	0.73146	1244.42	n/a
$TS_{Butadiene}$	-2443.285788	1171.0	0.68765	1245.32	-320.06
$INT_{Benzene}$	-2519.592300	1207.0	0.75847	1285.94	n/a
$TS_{Benzene}$	-2519.543430	1205.0	0.69919	1280.82	-492.90
C_{60}:benzene Monoadduct	-2519.558521	1212.0	0.67358	1285.66	n/a
$INT_{Naphthalene}$	-2673.306730	1328.0	0.76776	1411.02	n/a
$TS_{Naphthalene}$	-2673.268293	1326.0	0.75034	1408.70	-450.00
C_{60}:naphthalene Monoadduct	-2673.289803	1334.0	0.72709	1415.02	n/a
$INT_{Monoadduct}$	-2827.013263	1447.0	0.81889	1537.21	n/a
$TS_{Monoadduct}$	-2826.989507	1444.0	0.80496	1534.27	-347.64
C_{60}:anthracene Monoadduct	-2827.019600	1453.0	0.78409	1541.90	n/a
Bisadduct “e”	-3366.800898	1958.0	0.97029	2073.94	n/a
Bisadduct “e” Intermediate	-3366.794662	1949.0	1.00712	2066.84	n/a
Bisadduct “e” TS	-3366.771171	1947.0	0.98948	2065.02	-341.17
Bisadduct “t1”	-3366.797394	1959.0	0.96821	2074.31	n/a
Bisadduct “t1” Intermediate	-3366.793586	1949.0	1.00758	2066.82	n/a
Bisadduct “t1” TS	-3366.767988	1948.0	0.98868	2065.26	-354.45
Bisadduct “t2”	-3366.798658	1958.0	0.96973	2073.99	n/a
Bisadduct “t2” Intermediate	-3366.793946	1949.0	1.00413	2066.88	n/a
Bisadduct “t2” TS	-3366.769130	1947.0	0.98878	2065.02	-352.81
Bisadduct “t3”	-3366.800352	1958.0	0.96986	2074.22	n/a
Bisadduct “t3” Intermediate	-3366.794302	1950.	1.04758	2069.93	n/a

Bisadduct "t3" TS	-3366.770331	1948.0	0.98941	2065.24	-340.62
Bisadduct "t4"	-3366.797586	1958.0	0.97080	2073.73	n/a
Bisadduct "t4" Intermediate	-3366.793671	1949.0	1.00809	2067.09	n/a
Bisadduct "t4" TS	-3366.768105	1947.0	0.98865	2064.88	-357.00
C_{60}:anthracene Monoadduct BP86/def2-TZVP/D3	-2287.239624	1418.0	0.83009	1511.50	n/a
C_{60} BP86/def2-TZVP/D3	-2827.019600	924.7	0.39793	513.62	n/a
Anthracene BP86/def2-TZVP/D3	-539.755753	485.9	0.59906	987.25	n/a

In Table S10, the zero point energy corrections, S_{corr}, and H_{corr} values for **Naphthalene Transfer Intermediate** and **Benzene Transfer Intermediate** are not available. This is due to the fact that a reduced version of harmonic frequency calculations was performed, that returned only the 5 lowest frequencies using the keywords $les all 5, $h0hessian, $nomw as implemented in Turbomole. This reduced the computational time significantly, at the expense of providing a full harmonic frequency output, thus, not allowing the calculation of ZPE and thermal corrections. However, the lowest 5 frequencies are all positive, indicating energy minima.

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