Supporting Information

Transition State Distortion Energies Correlate with Activation Energies of 1,4-Dihydrogenations and Diels-Alder Cycloadditions of Aromatic Molecules

*Amy E. Hayden and K. N. Houk**

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Comparison of Two DFT Methods

In a previous study on these reactions,[S1] a higher level of theory was employed to compute the reaction energetics than was utilized in our paper. Thus, before using the lower level method, it was verified that this method was sufficient for the examination of these reactions. There is a linear correlation of both the activation (Figure S1a) and the reaction energies (Figure S1b) using the higher level method (MPWB1K/6-311+G(3df,2p)//B3LYP/6-31G(d)) and the lower level method (B3LYP/6-31G(d)). B3LYP transition state and reaction energies were slightly higher (1 – 3 kcal/mol) than MPWB1K energies, but this was a systematic occurrence.

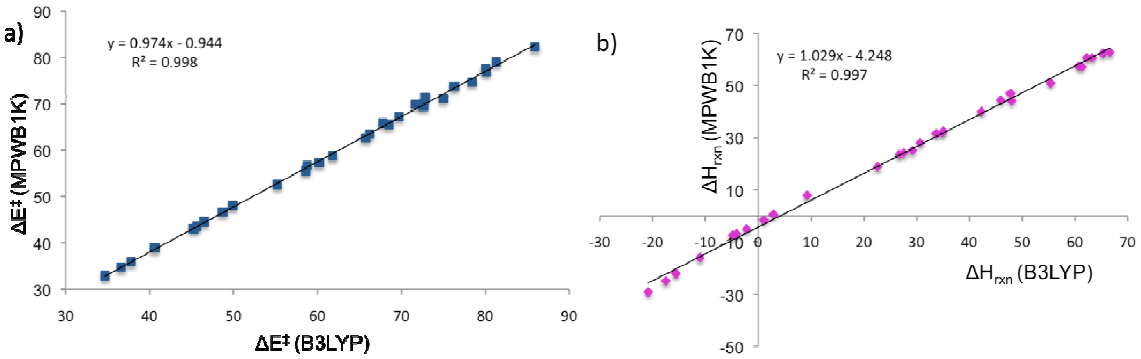

Figure S1. Demonstration of the applicability of B3LYP/6-31G(d) to a subset of reactions in this paper by examining a) activation and b) reaction energies (kcal/mol).

Linear Equations for Graphs in the Manuscript

Below is a list of the linear equations and R^2 values for several plots shown in this paper, which are ordered according to figure number.

Figure 6. Transition state energy versus distortion energy in the transition state for:

All four sets of reactions: $\Delta E^{\ddagger}_{d} = 0.90\ \Delta E^{\ddagger} + 8.2$, $R^2 = 0.987$.

Reactions of PAHs with H_2: $\Delta E^{\ddagger}_{d} = 0.92\ \Delta E^{\ddagger} + 7.8$, $R^2 = 0.994$.

Reactions of PAHs with C_2H_4: $\Delta E^{\ddagger}_{d} = 0.93\ \Delta E^{\ddagger} + 5.7$, $R^2 = 0.996$.

Reactions of heterocycles with H_2: $\Delta E^{\ddagger}_{d} = 0.79\ \Delta E^{\ddagger} + 14.2$, $R^2 = 0.977$.

Reactions of heterocycles with C_2H_4: $\Delta E^{\ddagger}_{d} = 0.70\ \Delta E^{\ddagger} + 15.3$, $R^2 = 0.907$.

Figure 7. Transition state energy versus distortion energy in the transition state for:

a) PAH fragment in the reactions of PAHs with H_2: $\Delta E^{\ddagger}_d = 2.56\ \Delta E^{\ddagger} - 46.3$, $R^2 = 0.938$; H_2 fragment in the reactions of PAHs with H_2: $\Delta E^{\ddagger}_d = 1.80\ \Delta E^{\ddagger} + 21.3$, $R^2 = 0.982$.

b) PAH fragment in the reactions of PAHs with C_2H_4: $\Delta E^{\ddagger}_d = 1.91\ \Delta E^{\ddagger} - 13.8$, $R^2 = 0.994$; C_2H_4 fragment in the reactions of PAHs with C_2H_4: $\Delta E^{\ddagger}_d = 2.44\ \Delta E^{\ddagger} + 3.99$; $R^2 = 0.992$.

c) Heterocycle fragment in the reactions of heterocycles with H_2: $\Delta E^{\ddagger}_d = 1.80\ \Delta E^{\ddagger} - 21.5$, $R^2 = 0.984$; H_2 fragment in the reactions of heterocycles with H_2: $\Delta E^{\ddagger}_d = 3.91\ \Delta E^{\ddagger} - 4.42$, $R^2 = 0.934$.

d) Heterocycle fragment in the reactions of heterocycles with C_2H_4: $\Delta E^{\ddagger}_d = 1.78$ x $\Delta E^{\ddagger} - 15.0$, $R^2 = 0.970$; H_2 fragment in the reactions of heterocycles with H_2: $\Delta E^{\ddagger}_d = 3.91\ \Delta E^{\ddagger} - 11.7$, $R^2 = 0.958$.

Figure 9. Correlation between:

a) $\Delta E^{\ddagger}_d$ and the H-H bond distance in the transition state for hydrogenation reactions:

$\Delta E^{\ddagger}_d = 107$ (H-H distance) $- 89.2$, $R^2 = 0.998$.

b) $\Delta E^{\ddagger}_d$ and the HCCH dihedral angle in the ethylene fragment in the transition state for the Diels-Alder reactions: $\Delta E^{\ddagger}_d = -0.92$ (H-C-C-H dihedral angle) $- 150$, $R^2 = 0.968$.

Interaction Energy in the Transition State vs. Activation Energy

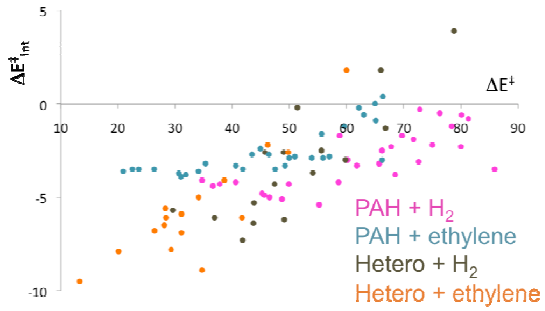

Figure S2. Interaction energy in the product versus activation energy for all reactions examined in this paper (ΔE, kcal/mol, B3LYP/6-31G(d)).

Figure S2. Interaction energy in the product versus activation energy for:

All four sets of reactions: $\Delta E^{\ddagger}_{int} = 0.10\ \Delta E^{\ddagger} - 8.2$, $R^2 = 0.481$.

Reactions of PAHs with H_2: $\Delta E^{\ddagger}_{int} = 0.08\ \Delta E^{\ddagger} - 7.8$, $R^2 = 0.570$.

Reactions of PAHs with C_2H_4: $\Delta E^{\ddagger}_{int} = 0.07\ \Delta E^{\ddagger} - 5.7$, $R^2 = 0.593$.

Reactions of heterocycles with H_2: $\Delta E^{\ddagger}_{int} = 0.21\ \Delta E^{\ddagger} - 14.6$, $R^2 = 0.710$.

Reactions of heterocycles with C_2H_4: $\Delta E^{\ddagger}_{int} = 0.22\ \Delta E^{\ddagger} - 12.9$, $R^2 = 0.778$.

Significance of Product Interaction Energy

The computed product interaction energies (ΔE_{int}) were found to be linearly related to ΔE (Figure S3a), $\Delta E^{\ddagger}$ (Figure S3b), and $\Delta E^{\ddagger}_d$ (Figure S3c).

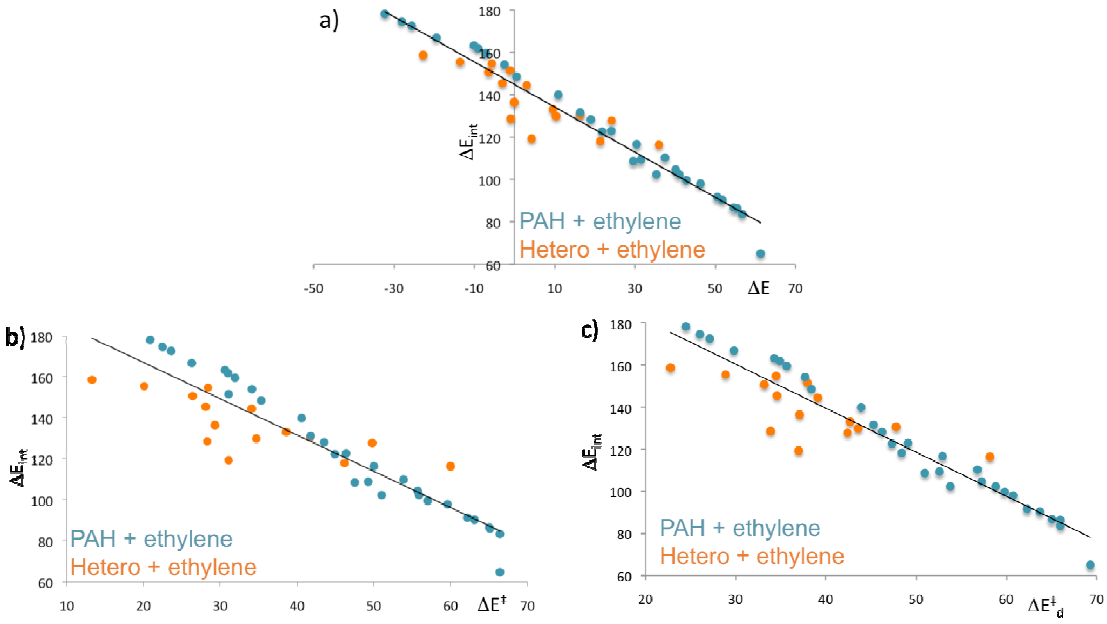

Figure S3. Product interaction energy was found to have correlations with a number of quantities including a) product energy, b) activation energy, and c) distortion energy in the transition state. All energies are in kcal/mol (B3LYP/6-31G(d)).

Figure S3. Interaction energy in the product in the reactions of PAHs and C_2H_4 versus:

a) Reaction energy: $\Delta E_{int} = -1.06\ \Delta E + 145$, $R^2 = 0.946$.

b) Activation energy: $\Delta E_{int} = -1.77\ \Delta E^{\ddagger} + 203$, $R^2 = 0.851$.

c) Distortion energy in the transition state: $\Delta E_{int} = -2.09\ \Delta E^{\ddagger}_d + 22$, $R^2 = 0.903$.

The interaction energy of the product was also found to decrease with increasing activation energy and distortion energy in the transition state. However, these two relationships are a result of the fact that these two sets of reactions adhere to the BEP principle. This claim is evidenced by the near doubling of the slope when comparing the reaction of ΔE_{int} versus ΔE and $\Delta E^{\ddagger}$ (the slope of $\Delta E^{\ddagger}$ versus ΔE is roughly 0.5). In addition, the loose correlation could be the result of the fact that the

BEP/Hammond Leffler plots of these two data sets have differing slopes. Further support is gained by examining the product interaction energies of 18 1,3-dipolar cycloadditions that were previously shown to follow the distortion/interaction model, but not the BEP principle.[S2] The product interaction energy is inversely related to ΔE (Figure S4a), but no correlation is observed with $\Delta E^{\ddagger}$ (Figure S4b) or $\Delta E^{\ddagger}_{d}$ (Figure S4c).

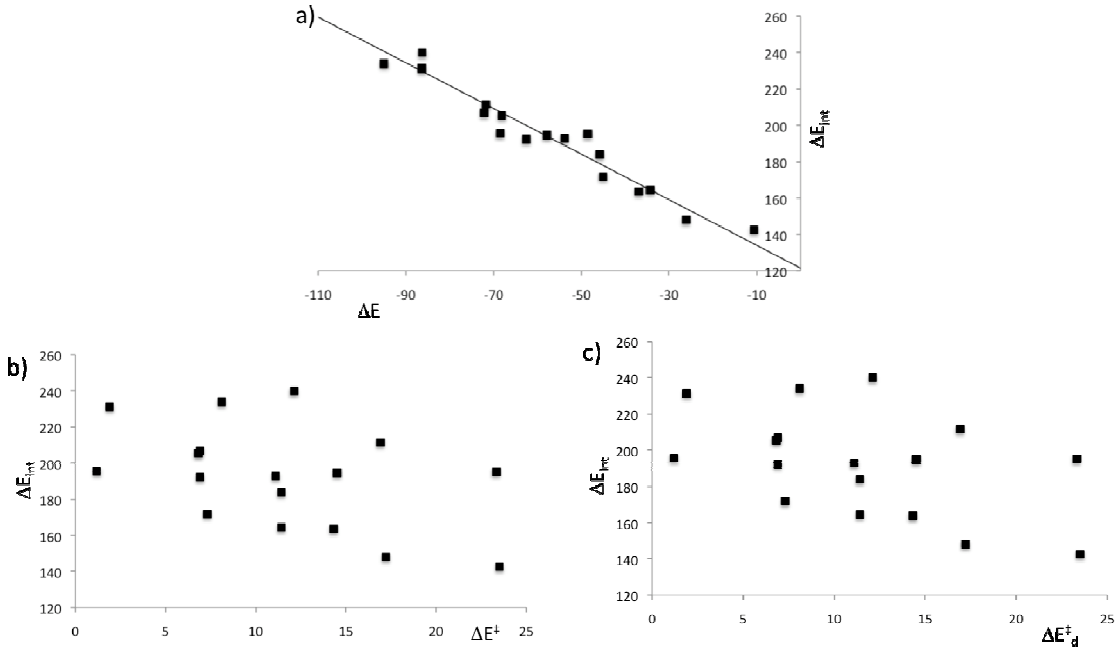

Figure S4. Product interaction energy for 18 1,3-dipolar cycloadditions was found to have a correlation with a) product energy, but not with b) activation energy or c) distortion energy in the transition state. All energies are in kcal/mol (B3LYP/6-31G(d)).

Figure S4. Interaction energy in the product for 1,3-dipolar cycloadditions versus:

a) Reaction energy: $\Delta E_{int} = -1.25\ \Delta E + 122$, $R^2 = 0.956$.

Structures of the Endpoints of the IRCs

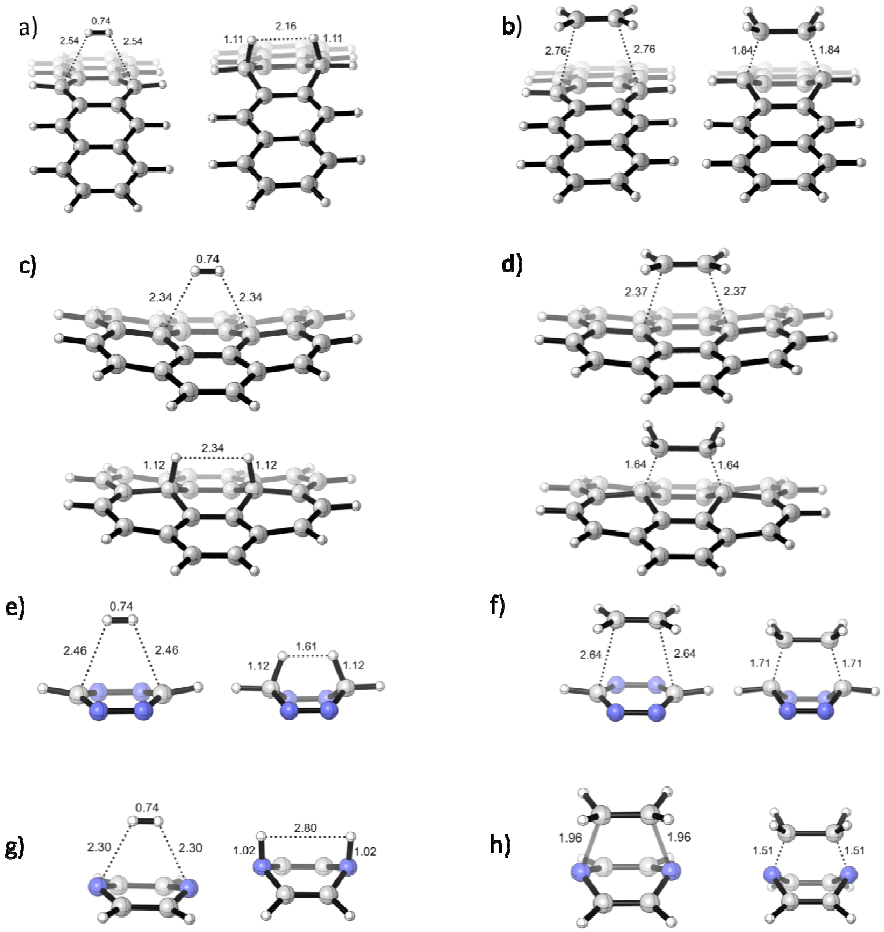

Figure S5. Structures of the endpoints of the IRCs of the reactions of a) pentacene and H_2, b) pentacene and C_2H_4, c) coronene and H_2, d) coronene and C_2H_4, e) tetrazine and H_2, f) tetrazine and C_2H_4, g) pyrazine and H_2, and h) pyrazine and C_2H_4 (B3LYP/6-31G(d)).

Reference 27

Gaussian 03, revision C.02; Frisch, M.J.; Trucks, G.W.; Schlegel, H.B.; Scuseria, G.E.; Robb, M.A.; Cheeseman, J.R.; Montgomery, J.A., Jr.; Vreven, T.; Kudin, K.; Burant, J.C.; Millam, J.M.; Iyengay, S.S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G.A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J.E.; Hratchian, H.P.; Cross, J.B.; Adamo, C.; Jaramillo, J.; Comperts, R.; Startmann, R.E.; Yazyev, O.; Austin, A.J.; Cammi, R.; Pomelli, C.; Ochterski, J.W.; Ayala, P.Y.; Morokuma, K.; Voth, G.A.; Salvador, P.; Dannenbuerg, J.J.; Zakrzewski, V.G.; Dapprich, S.; Daniels, A.D.; Strain, M.C.; Farkas, O.; Malick, D.K.; Rabuck, A.D.; Raghavachari,

K.; Foresman, J.B.; Ortiz, J.V.; Cui, Q.; Baboul, A.G.; Clifford, S.; Cioslowski, J.; Stefanov, B.B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R.L.; Fox, D.J.; Keith, T.; Al-Laham, M.A.; Peng, C.Y.; Nanayakkara, A.; Challacombe, M.; Gill, P.M.W.; Johnson, B.; Chem, W.; Wong, M.W., Gonzalez, C.; Pople, J.A.; Gaussian, Inc.: Wallingford CT, 2004.

Energetics and Pertinent Bond Lengths and Angles

On the next pages, are tables that include computed values of transition state and reaction energies and enthalpies as well as distortion and interaction energies for all reactions. In addition, forming bond lengths in transition states and the distance between the two hydrogens in the H_2 fragment for the hydrogenation reactions or the distance between the two carbons in the C_2H_4 fragment and the H-C-C-H dihedral angle in the C_2H_4 fragment for the Diels-Alder reactions are included. In Figure S6, the reactants are numbered such that the reacting positions can be identified in these tables.

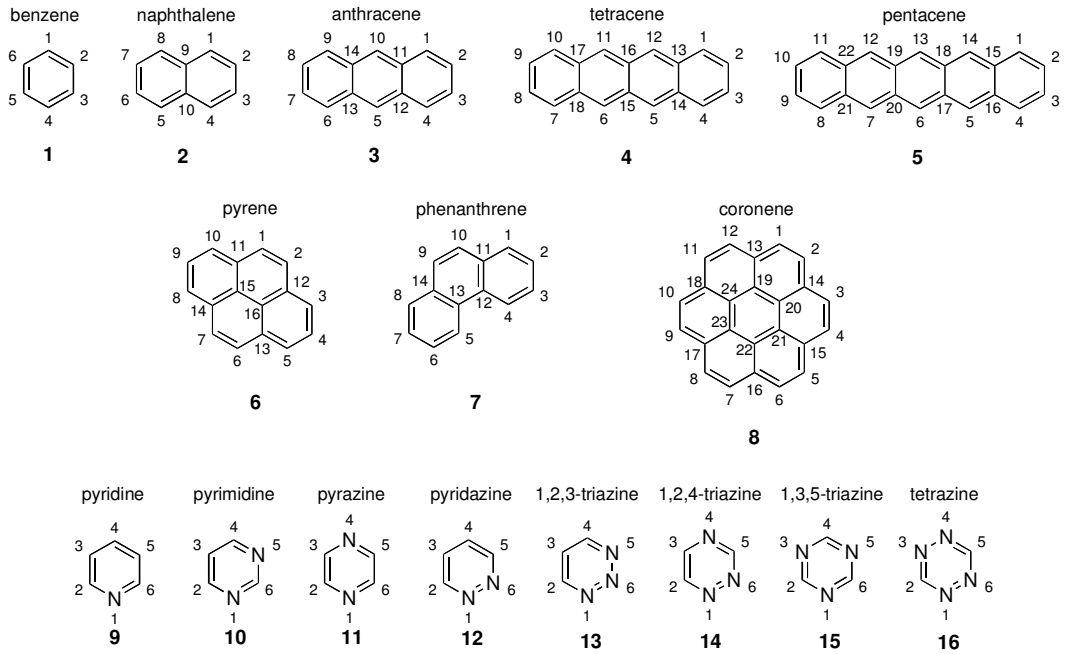

Figure S6. PAHs and heterocycles used in this study.

Table S1. Reactions of PAHs and H_2.

PAH	*Reaction Position*	*Mode of Reaction*	$\Delta E^{\ddagger}$	ΔE	$\Delta H^{\ddagger}$	ΔH	*Distortion Energy (TS)*	*Distortion Energy PAH (TS)*
benzene (**1**)	1,4	[1,1]	55.2	3.5	55.5	9.3	60.6	43.1
naphthalene (**2**)	1,4	[1,1]	48.7	-5.0	49.1	1.1	53.8	38.9
naphthalene (**2**)	2,10	[1,2]	65.7	29.6	65.8	34.9	68.9	45.6
anthracene (**3**)	5,10	[1,1]	40.6	-16.7	41.1	-11	44.8	33.6
anthracene (**3**)	1,4	[1,1]	46.5	-8.3	47	-2.2	51.5	37.5
anthracene (**3**)	12,14	[2,2]	75	50.5	75	55.4	77.2	48.2
anthracene (**3**)	2,12	[1,2]	69.7	37.2	69.8	42.3	71.4	45.5
tetracene (**4**)	5,12	[1,1]	37.8	-21.4	38.3	-15.6	42.1	31.9
tetracene (**4**)	1,4	[1,1]	45.6	-9.7	46.1	-4.1	50.5	36.9
tetracene (**4**)	14,16	[2,2]	78.4	40.9	78.4	61.3	79.6	48.3
tetracene (**4**)	2,14	[1,2]	71.7	56.6	71.7	45.9	73.6	45.3
pentacene (**5**)	6,13	[1,1]	34.7	-26.8	35.3	-20.8	38.8	29.9
pentacene (**5**)	5,14	[1,1]	36.6	-23.5	37.2	-17.5	41.0	31.1
pentacene (**5**)	2,16	[1,2]	72.8	42.9	72.7	47.8	73.1	45.1
pentacene (**5**)	1,4	[1,1]	45.2	-10.4	45.7	-4.8	50.0	36.6
pentacene (**5**)	16,18	[2,2]	80.1	59.6	80	64.2	80.7	48.2
pentacene (**5**)	17,19	[2,2]	81.3	61.9	81.3	66.6	82.1	48.5
pyrene (**6**)	3,13	[1,2]	58.6	17.1	58.8	22.6	62.8	42.3
pyrene (**6**)	4,16	[1,3]	68.5	29.6	68.8	35.1	72.3	44.4
pyrene (**6**)	11,12	[2,2]	80	58.7	79.9	63.3	82.3	47.5
pyrene (**6**)	6,15	[1,3]	67.8	28.2	68	33.7	70.1	43.2
phenanthrene (**7**)	1,4	[1,1]	49.9	-3.1	50.3	2.9	54.2	39.0
phenanthrene (**7**)	9,13	[1,2]	58.8	23.6	59	29.2	60.5	40.3
phenanthrene (**7**)	3,11	[1,2]	61.8	22.1	62	27.6	65.1	44.2
phenanthrene (**7**)	2,12	[1,2]	60.2	21.0	60.4	26.7	63.2	43.3
phenanthrene (**7**)	11,14	[2,2]	76.3	56.1	76.2	60.7	76.8	46.8
coronene (**8**)	1,20	[1,3]	66.2	25.0	66.6	30.7	69.5	42.5
coronene (**8**)	5,14	[2,2]	72.6	43.0	72.7	50	75.7	46.0
coronene (**8**)	20,23	[3,3]	85.9	57.6	85.8	65.3	89.4	43.4

Table S1. (con.)

PAH	*Reaction Position*	*Distortion Energy H_2 (TS)*	*Interaction Energy (TS)*	*Distortion Energy PAH (Prod)*	*Forming C-H Distances*	*Breaking H-H Distance*
benzene (**1**)	1,4	17.5	5.4	68.7	1.50, 1.50	1.004
naphthalene (**2**)	1,4	15.0	5.1	67.5	1.54, 1.54	0.979
naphthalene (**2**)	2,10	23.3	3.2	61.6	1.43, 1.47	1.058
anthracene (**3**)	5,10	11.2	4.2	64.4	1.59, 1.59	0.941
anthracene (**3**)	1,4	14.0	5.0	67.2	1.55, 1.55	0.969
anthracene (**3**)	12,14	29.0	2.2	62.3	1.40, 1.45	1.082
anthracene (**3**)	2,12	25.9	1.7	62.0	1.40, 1.44	1.110
tetracene (**4**)	5,12	10.2	4.3	63.4	1.60, 1.61	0.930
tetracene (**4**)	1,4	13.6	4.9	67.2	1.55, 1.55	0.965
tetracene (**4**)	14,16	31.3	1.2	62.1	1.38, 1.39	1.130
tetracene (**4**)	2,14	28.2	1.9	62.3	1.39, 1.44	1.095
pentacene (**5**)	6,13	9.0	4.1	62.0	1.63, 1.63	0.916
pentacene (**5**)	5,14	9.8	4.4	63.0	1.62, 1.62	0.925
pentacene (**5**)	2,16	28.0	0.3	62.3	1.39, 1.43	1.101
pentacene (**5**)	1,4	13.4	4.8	67.2	1.56, 1.56	0.963
pentacene (**5**)	16,18	32.6	0.6	62.2	1.38, 1.38	1.142
pentacene (**5**)	17,19	33.6	0.8	62.1	1.37, 1.37	1.151
pyrene (**6**)	3,13	30.0	0.5	68.3	1.45, 1.53	1.032
pyrene (**6**)	4,16	27.0	2.5	57.8	1.43, 1.45	1.100
pyrene (**6**)	11,12	29.7	3.1	65.3	1.38, 1.38	1.161
pyrene (**6**)	6,15	46.0	3.5	56.4	1.42, 1.48	1.092
phenanthrene (**7**)	1,4	20.5	4.2	58.4	1.53, 1.53	0.981
phenanthrene (**7**)	9,13	27.8	3.8	59.7	1.45, 1.49	1.030
phenanthrene (**7**)	3,11	34.7	2.3	65.1	1.44, 1.48	1.036
phenanthrene (**7**)	2,12	27.0	2.3	59.3	1.46, 1.48	1.027
phenanthrene (**7**)	11,14	15.2	4.3	66.6	1.38, 1.38	1.119
coronene (**8**)	1,20	20.2	1.7	62.3	1.42, 1.49	1.092
coronene (**8**)	5,14	20.9	3.3	64.4	1.43, 1.43	1.117
coronene (**8**)	20,23	19.9	3.0	64.3	1.39, 1.39	1.261

Table S2. Reactions of PAHs and C_2H_4.

PAH	*Reaction Position*	*Mode of Reaction*	$\Delta E^{\ddagger}$	ΔE	$\Delta H^{\ddagger}$	ΔH	*Distortion Energy (TS)*	*Distortion Energy PAH (TS)*
benzene (**1**)	1,4	[1,1]	40.6	10.9	41.1	13.7	43.9	29.5
naphthalene (**2**)	1,4	[1,1]	34.1	-2.5	34.7	0.8	37.7	25.6
naphthalene (**2**)	2,10	[1,2]	50.0	30.5	50.4	32.7	52.9	34.2
anthracene (**3**)	5,10	[1,1]	26.3	-19.5	26.9	-15.7	29.8	20.6
anthracene (**3**)	1,4	[1,1]	31.9	-7.1	32.6	-3.7	35.7	24.4
anthracene (**3**)	12,14	[2,2]	59.6	46.3	59.9	48.2	60.8	38.6
anthracene (**3**)	2,12	[1,2]	53.9	37.5	54.2	39.6	56.8	36.0
tetracene (**4**)	5,12	[1,1]	23.6	-25.5	24.4	-21.6	27.1	18.9
tetracene (**4**)	1,4	[1,1]	31.0	-9.1	31.7	-5.6	34.9	23.9
tetracene (**4**)	14,16	[2,2]	63.1	51.8	63.4	53.7	63.7	39.9
tetracene (**4**)	2,14	[1,2]	55.9	40.9	56.1	43.0	58.8	36.9
pentacene (**5**)	6,13	[1,1]	20.9	-32.2	21.6	-28.1	24.5	17.2
pentacene (**5**)	5,14	[1,1]	22.5	-28.1	23.3	-24.1	26.0	18.2
pentacene (**5**)	2,16	[1,2]	57.0	42.7	57.2	44.7	59.8	37.3
pentacene (**5**)	1,4	[1,1]	30.6	-10.0	31.3	-6.5	34.3	23.5
pentacene (**5**)	16,18	[2,2]	65.0	54.5	65.2	56.3	65.0	40.3
pentacene (**5**)	17,19	[2,2]	66.4	56.7	66.6	58.4	66.0	40.9
pyrene (**6**)	3,13	[2,2]	41.8	16.3	42.3	19.0	45.3	29.4
pyrene (**6**)	4,16	[1,3]	51.0	35.3	51.6	37.8	53.8	34.1
pyrene (**6**)	11,12	[2,2]	65.1	55.4	65.3	57.1	66.0	41.2
pyrene (**6**)	6,15	[3,3]	49.3	31.4	49.9	34.0	52.6	33.4
phenanthrene (**7**)	1,4	[1,2]	35.3	0.5	35.9	3.7	38.4	26.0
phenanthrene (**7**)	9,13	[1,3]	43.5	19.0	44.1	21.8	46.2	29.8
phenanthrene (**7**)	3,11	[2,2]	46.4	24.0	46.8	26.5	49.1	32.1
phenanthrene (**7**)	2,12	[1,3]	44.9	21.8	45.4	24.3	47.3	31.1
phenanthrene (**7**)	11,14	[1,1]	62.2	50.5	62.4	52.3	62.3	39.3
coronene (**8**)	1,20	[1,2]	47.5	29.6	48.2	32.3	51.0	32.3
coronene (**8**)	5,14	[1,2]	55.7	40.1	56.0	42.1	57.3	36.8
coronene (**8**)	20,23	[1,2]	66.3	61.3	66.6	63.0	69.3	41.3

Table S2. (con.)

PAH	*Reaction Position*	*Distortion Energy C_2H_4 (TS)*	*Interaction Energy (TS)*	*Distortion Energy (Product)*	*Distortion Energy PAH (Product)*	*Distortion Energy C_2H_4 (Product)*
benzene (**1**)	1,4	14.4	3.3	150.7	92.1	58.6
naphthalene (**2**)	1,4	12.0	3.6	151.6	92.2	59.4
naphthalene (**2**)	2,10	18.7	2.9	146.8	89.4	57.4
anthracene (**3**)	5,10	9.2	3.5	147.5	87.6	60.0
anthracene (**3**)	1,4	11.3	3.8	152.4	92.9	59.5
anthracene (**3**)	12,14	22.3	1.2	144.0	87.6	56.4
anthracene (**3**)	2,12	20.8	2.9	144.4	87.3	57.2
tetracene (**4**)	5,12	8.2	3.5	147.0	86.9	60.2
tetracene (**4**)	1,4	11.0	3.9	152.8	93.3	59.5
tetracene (**4**)	14,16	23.8	0.6	142.0	85.8	56.1
tetracene (**4**)	2,14	21.9	2.9	143.1	86.1	57.1
pentacene (**5**)	6,13	7.3	3.6	145.8	85.5	60.3
pentacene (**5**)	5,14	7.8	3.5	146.5	86.4	60.1
pentacene (**5**)	2,16	22.5	2.8	142.3	85.3	57.0
pentacene (**5**)	1,4	10.8	3.7	153.2	93.6	59.6
pentacene (**5**)	16,18	24.6	0.0	140.8	84.8	56.0
pentacene (**5**)	17,19	25.1	0.4	140.1	84.3	55.8
pyrene (**6**)	3,13	12.4	3.2	149.1	90.3	58.8
pyrene (**6**)	4,16	16.4	2.7	147.3	89.2	58.1
pyrene (**6**)	11,12	17.0	2.7	146.8	89.4	57.4
pyrene (**6**)	6,15	16.2	2.4	144.2	86.5	55.7
phenanthrene (**7**)	1,4	23.1	0.2	141.8	86.1	55.7
phenanthrene (**7**)	9,13	18.8	3.5	138.0	80.0	58.1
phenanthrene (**7**)	3,11	21.0	1.6	144.6	86.9	57.8
phenanthrene (**7**)	2,12	28.0	3.0	126.1	80.8	55.2
phenanthrene (**7**)	11,14	16.0	3.5	147.7	89.1	58.6
coronene (**8**)	1,20	19.7	2.8	137.6	80.5	57.1
coronene (**8**)	5,14	24.7	0.9	141.6	85.5	56.1
coronene (**8**)	20,23	19.3	3.3	140.4	82.4	58.0

Table S2. (con.)

PAH	*Reaction Position*	*Interaction Energy (Product)*	*Forming C-C Distances*	*C_2H_4 TS C-C Lengths*	*C_2H_4 TS H-C-C-H Dihedrals*	*C_2H_4 Prod. C-C Lengths*	*C_2H_4 Prod. H-C-C-H Dihedrals*
benzene (**1**)	1,4	139.8	2.12, 2.12	1.410	146.0	1.551	119.6
naphthalene (**2**)	1,4	154.1	2.17, 2.17	1.404	149.0	1.555	119.4
naphthalene (**2**)	2,10	116.4	1.93, 2.15	1.426	142.6	1.547	120.9
anthracene (**3**)	5,10	166.9	2.24, 2.24	1.395	153.0	1.557	119.3
anthracene (**3**)	1,4	159.5	2.19, 2.19	1.402	150.0	1.555	119.4
anthracene (**3**)	12,14	97.7	1.97, 1.97	1.437	139.6	1.543	122.1
anthracene (**3**)	2,12	110.0	1.87, 2.15	1.433	140.8	1.546	121.2
tetracene (**4**)	5,12	172.5	2.27, 2.27	1.391	154.5	1.558	119.2
tetracene (**4**)	1,4	161.9	2.20, 2.20	1.401	150.4	1.555	119.4
tetracene (**4**)	14,16	90.2	1.93, 1.97	1.442	136.9	1.542	118.4
tetracene (**4**)	2,14	102.2	1.85, 2.14	1.436	139.8	1.545	118.9
pentacene (**5**)	6,13	178.1	2.31, 2.31	1.389	156.1	1.558	119.2
pentacene (**5**)	5,14	174.6	2.29, 2.29	1.390	155.2	1.558	119.3
pentacene (**5**)	2,16	99.6	1.83, 2.13	1.438	139.5	1.545	121.5
pentacene (**5**)	1,4	163.2	2.20, 2.20	1.400	150.6	1.555	119.4
pentacene (**5**)	16,18	86.3	1.91, 1.96	1.445	138.0	1.542	122.4
pentacene (**5**)	17,19	83.4	1.93, 1.93	1.446	137.6	1.541	118.5
pyrene (**6**)	3,13	148.6	1.96, 2.26	1.419	145.7	1.552	120.1
pyrene (**6**)	4,16	128.3	1.96, 2.09	1.430	141.4	1.549	120.4
pyrene (**6**)	11,12	122.8	1.94, 1.94	1.445	137.0	1.542	120.5
pyrene (**6**)	6,15	122.4	1.91, 2.16	1.430	142.3	1.553	121.2
phenanthrene (**7**)	1,4	91.3	2.15, 2.16	1.405	148.5	1.552	119.8
phenanthrene (**7**)	9,13	108.4	1.95, 2.21	1.419	145.2	1.549	120.3
phenanthrene (**7**)	3,11	104.5	1.97, 2.17	1.420	144.1	1.546	120.7
phenanthrene (**7**)	2,12	64.8	2.00, 2.16	1.418	144.8	1.547	121.1
phenanthrene (**7**)	11,14	131.4	1.95, 1.95	1.439	138.2	1.540	121.5
coronene (**8**)	1,20	102.3	1.93, 2.16	1.429	142.6	1.553	119.5
coronene (**8**)	5,14	86.2	2.00, 2.00	1.434	140.1	1.549	120.0
coronene (**8**)	20,23	109.0	1.90, 1.90	1.460	135.2	1.547	121.6

Table S3. Reactions of heterocycles and H_2.

Heterocycle	*Reaction Position*	*Mode of Reaction*	$\Delta E^{\ddagger}$	ΔE	$\Delta H^{\ddagger}$	ΔH	*Distortion Energy (TS)*	*Distortion Energy Hetero (TS)*
pyridine (**9**)	1,4	[C,N]	66.8	3.2	66.9	8.7	68.1	49.5
pyridine (**9**)	2,5	[C,C]	49.1	1.8	49.7	7.6	55.3	40.1
pyrimidine (**10**)	1,4	[C,N]	59.8	-0.2	60.3	4.0	62.8	46.0
pyrimidine (**10**)	3,6	[C,C]	43.7	-0.7	44.6	5.2	50.1	36.7
pyrazine (**11**)	1,4	[N,N]	78.8	17.8	78.6	22.0	74.9	54.9
pyrazine (**11**)	2,5	[C,C]	41.8	-2.2	42.7	3.2	49.1	36.2
pyridazine (**12**)	1,4	[C,N]	55.6	-8.4	56.0	-3.6	58.1	43.0
pyridazine (**12**)	2,5	[C,C]	43.8	1.2	44.6	6.9	49.1	37.0
1,2,3-triazine (**13**)	1,4	[C,N]	49.0	-10.2	49.7	-4.1	51.6	39.4
1,2,3-triazine (**13**)	2,5	[C,N]	45.7	-21.3	46.5	-14.1	48.3	35.9
1,2,4-triazine (**14**)	1,4	[N,N]	66.0	2.3	66.1	6.8	64.2	47.0
1,2,4-triazine (**14**)	3,6	[C,N]	47.4	-15.8	48.1	-9.6	51.7	38.6
1,2,4-triazine (**14**)	2,5	[C,C]	36.9	-1.5	37.9	3.9	43.0	32.6
1,3,5-triazine (**15**)	1,4	[C,N]	54.1	-7.0	54.9	-1.2	57.8	42.5
1,2,4,5-tetrazine (**16**)	1,4	[N,N]	51.4	-18.9	51.8	-13.1	51.6	37.9
1,2,4,5-tetrazine (**16**)	2,5	[C,C]	29.6	-2.6	30.8	3.1	35.3	27.1

Heterocycle	*Reaction Position*	*Distortion Energy H_2 (TS)*	*Interaction Energy (TS)*	*Forming X-H Distances*	*Breaking H-H Distance*
pyridine (**9**)	1,4	18.5	1.3	1.42, 1.48	1.014
pyridine (**9**)	2,5	15.3	6.2	1.49, 1.52	0.982
pyrimidine (**10**)	1,4	16.8	3.0	1.44, 1.46	0.997
pyrimidine (**10**)	3,6	13.4	6.4	1.48, 1.53	0.963
pyrazine (**11**)	1,4	20.1	3.9	1.41, 1.41	1.029
pyrazine (**11**)	2,5	12.9	7.3	1.52, 1.52	0.950
pyridazine (**12**)	1,4	15.2	2.5	1.42, 1.52	0.982
pyridazine (**12**)	2,5	12.1	5.3	1.51, 1.51	0.958
1,2,3-triazine (**13**)	1,4	12.3	2.6	1.45, 1.49	0.952
1,2,3-triazine (**13**)	2,5	12.5	2.6	1.42, 1.53	0.954
1,2,4-triazine (**14**)	1,4	17.2	1.8	1.33, 1.45	1.001
1,2,4-triazine (**14**)	3,6	13.1	4.3	1.44, 1.50	0.960
1,2,4-triazine (**14**)	2,5	10.4	6.1	1.50, 1.52	0.932
1,3,5-triazine (**15**)	1,4	15.3	3.7	1.44, 1.44	0.983
1,2,4,5-tetrazine (**16**)	1,4	13.7	0.2	1.43, 1.43	0.966
1,2,4,5-tetrazine (**16**)	2,5	8.2	5.7	1.52, 1.52	0.907

Table S4. Reactions of heterocycles and C_2H_4.

Heterocycle	*Reaction Position*	*Mode of Reaction*	*$\Delta E^{\ddagger}$*	*ΔE*	*$\Delta H^{\ddagger}$*	*ΔH*	*Distortion Energy (TS)*	*Distortion Energy Hetero (TS)*
pyridine (**9**)	1,4	[C,N]	49.8	24.2	50.1	26.7	42.4	36.2
pyridine (**9**)	2,5	[C,C]	34.1	3.1	34.7	6.1	39.1	26.8
pyrimidine (**10**)	1,4	[C,N]	41.7	16.4	42.3	19.2	47.8	33.5
pyrimidine (**10**)	3,6	[C,C]	28.1	-3.0	29.0	0.2	34.6	24.3
pyrazine (**11**)	1,4	[N,N]	60.0	36.0	70.2	38.4	58.2	41.0
pyrazine (**11**)	2,5	[C,C]	26.4	-6.4	27.3	-3.0	33.2	23.3
pyridazine (**12**)	1,4	[C,N]	38.6	9.6	39.2	12.5	42.7	30.0
pyridazine (**12**)	2,5	[C,C]	28.4	-5.6	29.2	-2.5	34.5	24.6
1,2,3-triazine (**13**)	1,4	[C,N]	31.1	-1.1	31.9	1.8	38.0	27.5
1,2,3-triazine (**13**)	2,5	[C,N]	28.3	-0.9	29.2	2.3	33.9	23.8
1,2,4-triazine (**14**)	1,4	[N,N]	46.2	21.4	46.8	24.2	48.4	37.8
1,2,4-triazine (**14**)	3,6	[C,N]	29.3	0.0	30.2	3.3	37.1	26.3
1,2,4-triazine (**14**)	2,5	[C,C]	20.1	-13.5	22.0	-10.1	28.9	20.9
1,3,5-triazine (**15**)	1,4	[C,N]	34.7	10.4	35.6	13.4	43.6	31.1
1,2,4,5-tetrazine (**16**)	1,4	[N,N]	31.1	4.3	31.9	7.5	37.0	25.9
1,2,4,5-tetrazine (**16**)	2,5	[C,C]	13.3	-22.7	14.4	-19.0	22.8	16.8

Heterocycle	*Reaction Position*	*Distortion Energy C_2H_4 (TS)*	*Interaction Energy (TS)*	*Distortion Energy (Product)*	*Distortion Energy Hetero (Product)*	*Distortion Energy C_2H_4 (Product)*
pyridine (**9**)	1,4	16.1	2.6	152.0	94.4	57.6
pyridine (**9**)	2,5	12.2	5.0	147.6	90.4	57.2
pyrimidine (**10**)	1,4	14.2	6.1	147.0	91.0	56.1
pyrimidine (**10**)	3,6	10.3	6.5	142.5	86.7	55.8
pyrazine (**11**)	1,4	17.2	1.8	152.4	95.1	57.3
pyrazine (**11**)	2,5	10.0	6.8	144.3	88.4	55.8
pyridazine (**12**)	1,4	12.8	4.1	142.7	86.1	56.6
pyridazine (**12**)	2,5	9.9	6.1	149.2	93.3	55.9
1,2,3-triazine (**13**)	1,4	10.5	6.9	150.4	93.9	56.5
1,2,3-triazine (**13**)	2,5	10.1	5.6	127.7	72.9	54.9
1,2,4-triazine (**14**)	1,4	14.6	2.2	139.4	83.9	55.5
1,2,4-triazine (**14**)	3,6	10.7	7.8	136.4	81.5	54.9
1,2,4-triazine (**14**)	2,5	8.0	7.9	142.0	87.7	54.3
1,3,5-triazine (**15**)	1,4	12.5	8.9	140.3	85.9	54.4
1,2,4,5-tetrazine (**16**)	1,4	11.2	5.9	123.6	69.9	53.6
1,2,4,5-tetrazine (**16**)	2,5	6.0	9.5	136.0	83.6	52.4

Table S4. (con)

Heterocycle	*Reaction Position*	*Interaction Energy (Prod)*	*Forming X-C Distances*	*C_2H_4 TS C-C Lengths*	*C_2H_4 TS H-C-C-H Dihedrals*	*C_2H_4 Prod C-C Lengths*	*C_2H_4 Prod H-C-C-H Dihedrals*
pyridine (**9**)	1,4	127.8	1.97, 2.11	1.419	145.3	1.555	120.6
pyridine (**9**)	2,5	144.5	2.09, 2.18	1.404	149.4	1.548	117.5
pyrimidine (**10**)	1,4	130.6	1.94, 2.15	1.414	148.4	1.552	120.2
pyrimidine (**10**)	3,6	145.5	2.07, 2.21	1.397	151.3	1.546	121.0
pyrazine (**11**)	1,4	116.4	1.96, 1.96	1.428	144.3	1.562	121.6
pyrazine (**11**)	2,5	150.7	2.15, 2.15	1.396	152.9	1.545	115.2
pyridazine (**12**)	1,4	133.1	2.06, 2.08	1.409	147.5	1.554	119.0
pyridazine (**12**)	2,5	154.8	2.14, 2.14	1.396	151.8	1.545	120.9
1,2,3-triazine (**13**)	1,4	151.5	2.03, 2.14	1.401	155.5	1.553	122.5
1,2,3-triazine (**13**)	2,5	128.6	2.06, 2.13	1.400	152.1	1.550	122.1
1,2,4-triazine (**14**)	1,4	118.0	1.88, 2.09	1.421	148.9	1.557	118.4
1,2,4-triazine (**14**)	3,6	136.4	2.04, 2.14	1.401	153.6	1.549	116.6
1,2,4-triazine (**14**)	2,5	155.5	2.14, 2.19	1.389	155.1	1.542	118.3
1,3,5-triazine (**15**)	1,4	129.9	1.92, 2.18	1.408	150.0	1.548	122.0
1,2,4,5-tetrazine (**16**)	1,4	119.3	2.02, 2.02	1.409	149.0	1.552	118.2
1,2,4,5-tetrazine (**16**)	2,5	158.7	2.19, 2.19	1.381	148.0	1.537	123.9

Table S5. 1,3-Dipolar cycloaddition product distortion and interaction energies. Other data can be found in previous publications from our group.[S2] Numbering corresponds to the numbering scheme used in the original paper.

Dipole	*Dipolarophile*	*Distortion Energy (Product)*	*Interaction Energy (Product)*
1	ethylene	132.0	142.8
2	ethylene	122.0	148.2
3	ethylene	126.7	163.8
4	ethylene	138.2	184.0
5	ethylene	129.9	192.4
6	ethylene	134.7	206.9
7	ethylene	130.3	164.7
8	ethylene	126.9	172.1
9	ethylene	127.2	195.8
1	acetylene	146.7	195.3
2	acetylene	139.8	211.6
3	acetylene	136.7	194.7
4	acetylene	153.7	240.0
5	acetylene	156.6	266.7
6	acetylene	138.9	234.0
7	acetylene	139.1	193.1
8	acetylene	137.2	205.5
9	acetylene	144.9	231.3

Cartesian Coordinates and Energies of Computed Structures

Hydrogen (H_2)

H	0.000000	0.000000	0.371394
H	0.000000	0.000000	-0.371394

Energy = -1.17548238770
Number of Imaginary Frequencies = 0

Ethylene (C_2H_4)

C	0.000000	0.000000	0.665430
C	0.000000	0.000000	-0.665430
H	0.000000	0.923674	1.239556
H	0.000000	-0.923674	1.239556
H	0.000000	-0.923674	-1.239556
H	0.000000	0.923674	-1.239556

Energy = -78.5874582768
Number of Imaginary Frequencies = 0

Benzene (**1**)

C	1.062892	-0.905825	-0.000005
C	-0.253162	-1.373268	-0.000069
C	-1.315957	-0.467552	0.000055
C	-1.062815	0.905913	-0.000008
C	0.253047	1.373287	-0.000062
C	1.315997	0.467446	0.000057
H	1.889825	-1.610868	0.000066
H	-0.449965	-2.442016	-0.000078
H	-2.339973	-0.831256	0.000154
H	-1.889920	1.610743	-0.000006
H	0.450096	2.441982	-0.000019
H	2.339931	0.831405	0.000064

Energy = -232.248651906
Number of Imaginary Frequencies = 0

Benzene + H_2 [1,4] TS

C	-1.232308	-0.679366	-0.218501
C	-0.000003	-1.292677	0.244596
C	1.232306	-0.679371	-0.218501
C	1.232308	0.679366	-0.218501
C	0.000003	1.292677	0.244596
C	-1.232306	0.679371	-0.218501
H	-2.120315	-1.277715	-0.397443
H	-0.000005	-2.366035	0.424834
H	2.120310	-1.277723	-0.397449
H	2.120315	1.277715	-0.397443
H	0.000005	2.366035	0.424835
H	-2.120310	1.277722	-0.397449
H	0.000005	0.501947	1.524492
H	-0.000005	-0.501949	1.524490

Energy = -233.334933752
Number of Imaginary Frequencies = 1

Benzene + H_2 [1,4] Adduct

C	-0.667403	1.255266	-0.000025
C	-1.500617	0.000000	0.000041
C	-0.667404	-1.255264	-0.000025
C	0.667403	-1.255265	-0.000023
C	1.500617	-0.000002	0.000040
C	0.667404	1.255265	-0.000023
H	-1.207240	2.201175	-0.000076
H	-2.178070	0.000001	-0.870752
H	-1.207240	-2.201174	-0.000076
H	1.207238	-2.201175	-0.000072
H	2.178062	-0.000001	-0.870760
H	1.207242	2.201174	-0.000072
H	2.177928	-0.000001	0.870946
H	-2.177920	0.000002	0.870954

Energy = -233.418498886
Number of Imaginary Frequencies = 0

Benzene + C_2H_4 [1,4] TS

C	0.381892	1.328445	0.000003
C	0.771678	0.680341	-1.227422
C	0.771683	-0.680334	-1.227423
C	0.381902	-1.328442	0.000001
C	0.771664	-0.680336	1.227433
C	0.771659	0.680339	1.227434
C	-1.644067	-0.705129	-0.000012
C	-1.644072	0.705118	-0.000011
H	0.314741	2.414598	0.000004
H	0.921692	1.263542	-2.132085
H	0.921701	-1.263532	-2.132087
H	0.314758	-2.414596	0.000000
H	0.921667	-1.263536	2.132098
H	0.921658	1.263539	2.132100
H	-1.922552	-1.227036	-0.910639
H	-1.922563	-1.227037	0.910612
H	-1.922561	1.227024	-0.910638
H	-1.922572	1.227023	0.910613

Energy = -310.771363828
Number of Imaginary Frequencies = 1

Benzene + C_2H_4 [1,4] Adduct

C	1.281965	-0.000088	-0.114127
C	0.667818	1.238545	-0.749258
C	-0.667624	1.238597	-0.749351
C	-1.281964	0.000093	-0.114140
C	-0.667810	-1.238487	-0.749350
C	0.667632	-1.238543	-0.749437
C	-0.775446	0.000035	1.380036
C	0.775432	-0.000136	1.380048
H	2.374310	-0.000163	-0.154803
H	1.287858	2.050763	-1.118206
H	-1.287529	2.050879	-1.118385
H	-2.374307	0.000180	-0.154824
H	-1.287847	-2.050675	-1.118375
H	1.287539	-2.050803	-1.118514
H	-1.169653	0.882969	1.894156
H	-1.169834	-0.882832	1.894129
H	1.169812	0.882699	1.894198
H	1.169631	-0.883111	1.894098

Energy = -310.818763282
Number of Imaginary Frequencies = 0

Naphthalene (**2**)

C	2.433641	0.708448	0.000001
C	1.244796	1.402476	-0.000003
C	0.000014	0.716887	0.000000
C	-0.000016	-0.716882	0.000000
C	1.244773	-1.402480	-0.000002
C	2.433625	-0.708470	0.000002
H	-1.242018	2.490170	-0.000006
H	3.378349	1.245568	0.000004
H	1.242058	2.490157	-0.000001
C	-1.244777	1.402487	0.000000
C	-1.244798	-1.402482	0.000001
H	1.242024	-2.490163	0.000000
H	3.378328	-1.245598	0.000005
C	-2.433637	-0.708451	-0.000001
C	-2.433621	0.708467	0.000003

H	-1.242047	-2.490162	-0.000004
H	-3.378356	-1.245555	0.000001
H	-3.378328	1.245588	0.000002

Energy = -385.892729656
Number of Imaginary Frequencies = 0

Naphthalene + H_2 [1,4] TS

C	-2.355163	0.684481	-0.395550
C	-1.251822	1.307442	0.282041
C	0.066695	0.706584	0.079237
C	0.066694	-0.706585	0.079237
C	-1.251823	-1.307441	0.282041
C	-2.355162	-0.684479	-0.395553
H	1.280687	2.493370	0.001056
H	-3.215147	1.268218	-0.709806
H	-1.464125	0.489677	1.567435
C	1.281028	1.405942	-0.011503
C	1.281029	-1.405942	-0.011503
H	-1.464113	-0.489696	1.567418
H	-3.215150	-1.268212	-0.709806
C	2.472154	-0.702851	-0.136218
C	2.472153	0.702852	-0.136219
H	1.280689	-2.493370	0.001056
H	3.411228	-1.241834	-0.230056
H	3.411227	1.241835	-0.230057
H	-1.289998	2.380288	0.463355
H	-1.289998	-2.380288	0.463347

Energy = -386.990572141
Number of Imaginary Frequencies = 1

Naphthalene + H_2 [1,4] Adduct

C	-2.466703	0.666731	-0.000001
C	-1.218275	1.502466	0.000001
C	0.070557	0.701369	0.000001
C	0.070557	-0.701369	0.000001
C	-1.218275	-1.502466	0.000001
C	-2.466703	-0.666731	-0.000001
H	1.292731	2.472286	0.000000
H	-3.412110	1.206949	-0.000003
H	-1.230029	2.177119	0.871304
C	1.296279	1.383705	0.000000
C	1.296279	-1.383705	0.000000
H	-1.230029	-2.177119	0.871304
H	-3.412110	-1.206949	-0.000003
C	2.507262	-0.698813	-0.000001
C	2.507262	0.698813	-0.000001
H	1.292731	-2.472286	0.000000
H	3.444722	-1.248756	-0.000001
H	3.444722	1.248756	-0.000001
H	-1.230027	2.177123	-0.871298
H	-1.230027	-2.177123	-0.871298

Energy = -387.076129658
Number of Imaginary Frequencies = 0

Naphthalene + C_2H_4 [1,4] TS

C	0.916901	-1.341755	-0.389133
C	1.898864	-0.686023	-1.187181
C	1.898863	0.686025	-1.187180
C	0.916901	1.341756	-0.389132
C	-0.384106	0.707547	-0.268155
C	-0.384105	-0.707547	-0.268156
C	1.643144	0.701870	1.553608
C	1.643143	-0.701873	1.553606
C	1.593435	-1.402025	-0.079698
C	-2.781694	-0.703295	0.078525
C	-2.781695	0.703294	0.078526
C	-1.593435	1.402026	-0.079696
H	0.944902	-2.427995	-0.322018
H	2.705449	-1.256927	-1.639481
H	2.705449	1.256929	-1.639480
H	0.944901	2.427996	-0.322015
H	0.871051	1.230051	2.104265
H	0.871050	-1.230054	2.104263
H	-1.590622	-2.489913	-0.073500
H	-3.716304	-1.243722	0.203717
H	-3.716304	1.243721	0.203719
H	-1.590623	2.489913	-0.073498
H	2.587487	1.231923	1.479215
H	2.587486	-1.231926	1.479213

Energy = -464.425901367
Number of Imaginary Frequencies = 1

Naphthalene + C_2H_4 [1,4] Adduct

C	1.006926	-1.290379	-0.090400
C	1.769079	-0.668331	-1.250579
C	1.769175	0.668394	-1.250472
C	1.006964	1.290373	-0.090331
C	-0.393869	0.702798	-0.072351
C	-0.393873	-0.702789	-0.072330
C	1.709774	0.777233	1.217565
C	1.709782	-0.777316	1.217509
C	-1.595072	-1.403145	-0.024303
C	-2.804501	-0.697670	0.011598
C	-2.804475	0.697689	0.011593
C	-1.595058	1.403173	-0.024321
H	0.995248	-2.383713	-0.125907
H	2.282393	-1.284276	-1.983728
H	2.282496	1.284390	-1.983567
H	0.995289	2.383709	-0.125746
H	1.177139	1.169306	2.090531
H	1.177139	-1.169472	2.090440
H	-1.595152	-2.491395	-0.020564
H	-3.746027	-1.240441	0.037598
H	-3.746026	1.240432	0.037613
H	-1.595154	2.491410	-0.020536
H	2.731773	1.168675	1.252434
H	2.731768	-1.168800	1.252371

Energy = -464.484140027
Number of Imaginary Frequencies = 0

Naphthalene + H_2 [2,10] TS

C	-2.276932	0.639902	0.377090
C	-1.153021	1.454624	-0.014513
C	0.039441	0.778370	-0.124603
C	-0.054558	-0.677803	0.145554
C	-1.240661	-1.337537	-0.432063
C	-2.394772	-0.651296	-0.317278
H	1.384978	2.457419	-0.426788
H	-3.200219	1.147196	0.651634
H	-1.207282	2.539383	-0.004416
C	1.333491	1.385844	-0.247217
C	1.204364	-1.408734	0.234417
H	-1.165587	-2.344784	-0.830146
H	-3.365456	-1.042336	-0.605036

C	2.399854	-0.769463	0.134956
C	2.470709	0.645871	-0.111551
H	1.161899	-2.486297	0.375119
H	3.325444	-1.333959	0.216482
H	3.445069	1.120300	-0.190065
H	-1.623374	0.068152	1.507312
H	-0.722963	-0.483754	1.437161

Energy = -386.963539822
Number of Imaginary Frequencies = 1

Naphthalene + H_2 [2,10] Adduct

C	2.479856	-0.724188	-0.108416
C	1.142447	-1.406470	-0.039251
C	-0.020629	-0.757318	0.157363
C	-0.050629	0.737347	0.466143
C	1.226119	1.429653	0.041339
C	2.362049	0.775342	-0.202153
H	-1.318012	-2.522749	0.107820
H	3.047285	-1.111096	-0.969744
H	1.127921	-2.485136	-0.192457
C	-1.310658	-1.434743	0.089814
C	-1.309394	1.410992	-0.043797
H	1.191943	2.516024	-0.031161
H	3.258953	1.326680	-0.479126
C	-2.436904	0.710874	-0.249676
C	-2.457380	-0.740663	-0.089772
H	-1.287412	2.492042	-0.167104
H	-3.352178	1.212991	-0.554137
H	-3.405688	-1.263488	-0.183709
H	3.096471	-0.995089	0.767731
H	-0.108539	0.824872	1.572321

Energy = -386.933309550
Number of Imaginary Frequencies = 0

Naphthalene + C_2H_4 [2,10] TS

C	0.849721	1.528404	-0.424455
C	2.056540	0.741529	-0.368223
C	2.015701	-0.513717	-1.124471
C	0.866154	-1.215027	-1.053059
C	-0.234030	-0.629346	-0.290651
C	-0.336136	0.838962	-0.333666
C	-1.618648	1.451309	-0.117360
C	-2.732295	0.696131	0.103325
C	-2.655413	-0.740089	0.089695
C	-1.470934	-1.372551	-0.129035
C	0.787961	-0.707698	1.603565
C	1.976628	0.061244	1.434428
H	0.885715	2.610535	-0.325928
H	2.996122	1.291683	-0.400849
H	2.911888	-0.893879	-1.606496
H	0.750085	-2.208289	-1.479462
H	-1.676271	2.537705	-0.119229
H	-3.692778	1.173593	0.277998
H	-3.565208	-1.318193	0.230802
H	-1.425867	-2.458629	-0.178925
H	-0.032941	-0.292289	2.179199
H	0.865236	-1.788959	1.650068
H	2.036187	0.999632	1.981374
H	2.916334	-0.487821	1.450900

Energy = -464.400566756
Number of Imaginary Frequencies = 1

Naphthalene + C_2H_4 [2,10] Adduct

C	0.013331	0.048701	0.022494
C	0.033551	-0.005879	1.532779
C	1.479586	-0.010034	2.004401
C	2.238424	-0.944044	1.429061
C	1.507546	-1.811353	0.403019
C	0.773784	-0.887137	-0.582759
C	0.898427	-1.106705	-2.006471
C	1.681769	-2.096359	-2.496842
C	2.438186	-2.966682	-1.605252
C	2.378009	-2.832750	-0.267646
C	0.341964	-2.510935	1.239123
C	-0.529857	-1.428449	1.917360
H	-0.612797	0.755680	-0.515249
H	-0.560602	0.786401	1.994482
H	1.824671	0.677259	2.771456
H	3.284326	-1.125563	1.659645
H	0.346423	-0.449299	-2.675207
H	1.766146	-2.250202	-3.569348
H	3.070358	-3.732814	-2.048239
H	2.959576	-3.486544	0.380688
H	-0.246172	-3.127694	0.552898
H	0.795927	-3.179590	1.977957
H	-1.573491	-1.501270	1.595227
H	-0.510819	-1.537781	3.006776

Energy = -464.431700630
Number of Imaginary Frequencies = 0

Anthracene (**3**)

C	3.660679	-0.713146	0.000016
C	2.479530	-1.407037	-0.000045
C	1.223922	-0.722624	-0.000027
C	1.223924	0.722625	-0.000020
C	2.479532	1.407036	0.000024
C	3.660681	0.713142	0.000058
C	0.000000	-1.403377	-0.000022
C	0.000001	1.403379	-0.000026
C	-1.223922	0.722626	-0.000023
C	-1.223923	-0.722623	-0.000006
C	-2.479531	-1.407037	0.000025
H	-2.476863	-2.494580	0.000063
C	-3.660680	-0.713145	0.000052
C	-3.660679	0.713143	0.000006
C	-2.479531	1.407037	-0.000028
H	-0.000006	-2.491747	-0.000044
H	4.607361	-1.246655	0.000042
H	2.476860	-2.494580	-0.000093
H	2.476864	2.494579	0.000026
H	4.607357	1.246660	0.000113
H	-0.000004	2.491749	-0.000045
H	-4.607358	-1.246660	0.000086
H	-4.607358	1.246658	0.000021
H	2.476867	2.494580	-0.000070

Energy = -539.530523542
Number of Imaginary Frequencies = 0

Anthracene + H_2 [5,10] TS

C	-3.580969	-0.705165	-0.437335
C	-2.430605	-1.406361	-0.120040
C	-1.237449	-0.710307	0.163145
C	-1.237449	0.710307	0.163145
C	-2.430605	1.406361	-0.120040

C	-3.580969	0.705165	-0.437335
C	0.000000	-1.322692	0.597660
C	0.000000	1.322692	0.597660
C	1.237449	0.710307	0.163145
C	1.237449	-0.710307	0.163145
C	2.430605	-1.406361	-0.120040
H	2.432769	-2.493620	-0.104992
C	3.580969	-0.705165	-0.437335
C	3.580969	0.705165	-0.437335
C	2.430605	1.406361	-0.120040
H	0.000000	-2.396057	0.782244
H	-4.492731	-1.242719	-0.683665
H	-2.432769	-2.493620	-0.104990
H	-2.432769	2.493620	-0.104991
H	-4.492731	1.242719	-0.683666
H	0.000000	0.470410	1.939872
H	4.492731	-1.242719	-0.683665
H	4.492731	1.242719	-0.683665
H	2.432769	2.493620	-0.104991
H	0.000000	2.396058	0.782243
H	0.000000	-0.470409	1.939873

Energy = -540.641345482
Number of Imaginary Frequencies = 1

Anthracene + H_2 [5,10] Adduct

C	3.720320	0.699239	-0.000002
C	2.510175	1.383370	-0.000001
C	1.283639	0.700005	0.000002
C	1.283639	-0.700005	0.000002
C	2.510175	-1.383370	-0.000002
C	3.720320	-0.699239	-0.000005
C	0.000000	1.502353	0.000005
C	0.000000	-1.502353	0.000007
C	-1.283639	-0.700005	0.000002
C	-1.283639	0.700005	0.000002
C	-2.510175	1.383370	-0.000001
H	-2.505819	2.471870	-0.000001
C	-3.720320	0.699239	-0.000004
C	-3.720320	-0.699239	-0.000004
C	-2.510175	-1.383370	-0.000002
H	0.000000	2.174923	-0.871492
H	4.657759	1.249057	-0.000003
H	2.505819	2.471870	-0.000001
H	2.505819	-2.471870	-0.000002
H	4.657759	-1.249057	-0.000008
H	0.000000	-2.174914	0.871511
H	-4.657759	1.249057	-0.000006
H	-4.657759	-1.249057	-0.000007
H	-2.505819	-2.471870	-0.000002
H	0.000000	-2.174927	-0.871487
H	0.000000	2.174918	0.871505

Energy = -540.684319542
Number of Imaginary Frequencies = 0

Anthracene + C_2H_4 [5,10] TS

C	0.000000	1.354781	0.121016
C	-1.235738	0.711329	-0.224157
C	-1.235738	-0.711327	-0.224159
C	0.000000	-1.354781	0.121012
C	1.235738	-0.711327	-0.224160
C	1.235738	0.711329	-0.224157
C	0.000001	-0.697476	2.266641
C	-0.000002	0.697465	2.266646
C	2.446153	1.403198	-0.458107
C	3.611993	0.706082	-0.714483
C	3.611993	-0.706079	-0.714486
C	2.446153	-1.403196	-0.458112
C	-2.446153	-1.403196	-0.458112
C	-3.611992	-0.706079	-0.714486
C	-3.611992	0.706082	-0.714484
C	-2.446153	1.403198	-0.458108
H	0.000000	2.441470	0.194298
H	0.000000	-2.441471	0.194290
H	0.916457	-1.235202	2.486720
H	0.916453	1.235194	2.486727
H	2.445695	2.490951	-0.449711
H	4.534017	1.244674	-0.916607
H	4.534017	-1.244670	-0.916612
H	2.445695	-2.490949	-0.449720
H	-0.916453	-1.235205	2.486723
H	-0.916458	1.235190	2.486727
H	-2.445694	-2.490949	-0.449719
H	-4.534017	-1.244670	-0.916611
H	-4.534017	1.244674	-0.916607
H	-2.445694	2.490951	-0.449711

Energy = -618.076133427
Number of Imaginary Frequencies = 1

Anthracene + C_2H_4 [5,10] Adduct

C	0.000003	-1.299047	0.690056
C	1.227970	-0.703287	0.023871
C	1.227954	0.703285	0.024067
C	-0.000002	1.298828	0.690461
C	-1.227962	0.703283	0.024077
C	-1.227961	-0.703290	0.023859
C	0.000000	0.778042	2.168376
C	-0.000002	-0.778746	2.168132
C	-2.297582	-1.402665	-0.527296
C	-3.369740	-0.697560	-1.086870
C	-3.369740	0.697901	-1.086652
C	-2.297583	1.402831	-0.526856
C	2.297569	1.402836	-0.526877
C	3.369734	0.697909	-1.086659
C	3.369746	-0.697553	-1.086862
C	2.297598	-1.402660	-0.527273
H	0.000006	-2.393113	0.656803
H	-0.000004	2.392904	0.657556
H	-0.882911	1.168272	2.685305
H	-0.882917	-1.169144	2.684927
H	-2.298432	-2.490612	-0.526188
H	-4.203520	-1.240406	-1.524435
H	-4.203521	1.240885	-1.524049
H	-2.298432	2.490778	-0.525407
H	0.882913	1.168271	2.685301
H	0.882908	-1.169144	2.684936
H	2.298409	2.490782	-0.525437
H	4.203510	1.240895	-1.524060
H	4.203529	-1.240397	-1.524425
H	2.298454	-2.490607	-0.526157

Energy = -618.143289010
Number of Imaginary Frequencies = 0

Anthracene + H_2 [1,4] TS

C	3.538954	-0.686594	-0.484603
C	2.481571	-1.312404	0.249718
C	1.146833	-0.715032	0.125348
C	1.146833	0.715032	0.125347
C	2.481571	1.312404	0.249718
C	3.538954	0.686594	-0.484603
C	-0.049810	-1.409953	0.089691
C	-0.049811	1.409953	0.089691
C	-1.280834	0.719899	0.017599
C	-1.280834	-0.719899	0.017599
C	-2.529208	-1.403538	-0.051391
H	-2.526529	-2.491217	-0.052619
C	-3.713449	-0.710247	-0.114716
C	-3.713449	0.710247	-0.114716
C	-2.529209	1.403538	-0.051390
H	-0.051490	-2.497966	0.101675
H	4.388032	-1.264944	-0.836539
H	2.750726	-0.484617	1.531071
H	2.750724	0.484608	1.531080
H	4.388031	1.264945	-0.836539
H	-0.051491	2.497966	0.101674
H	-4.657236	-1.246535	-0.165812
H	-4.657236	1.246535	-0.165811
H	-2.526529	2.491217	-0.052618
H	2.532160	2.384200	0.432338
H	2.532160	-2.384200	0.432336

Energy = -540.631877269
Number of Imaginary Frequencies = 1

Anthracene + H_2 [1,4] Adduct

C	3.687673	-0.666614	-0.000002
C	2.441477	-1.504912	-0.000002
C	1.145842	-0.712605	0.000001
C	1.145842	0.712605	0.000001
C	2.441477	1.504912	0.000005
C	3.687673	0.666614	-0.000002
C	-0.059439	-1.388872	0.000002
C	-0.059439	1.388872	-0.000001
C	-1.304817	0.716058	-0.000001
C	-1.304817	-0.716058	0.000001
C	-2.549634	-1.403760	0.000002
C	-2.546470	-2.491494	0.000003
C	-3.737356	-0.709218	0.000000
C	-3.737356	0.709218	-0.000002
C	-2.549634	1.403760	-0.000002
H	-0.060061	-2.478164	0.000002
H	4.633272	-1.206370	-0.000005
H	2.456665	-2.178784	0.871383
H	2.456665	2.178775	0.871397
H	4.633272	1.206370	-0.000004
H	-0.060061	2.478164	-0.000001
H	-4.682546	-1.245579	0.000001
H	-4.682546	1.245579	-0.000003
H	-2.546470	2.491494	-0.000004
H	2.456663	2.178789	-0.871377
H	2.456663	-2.178779	-0.871391

Energy = -540.719269954
Number of Imaginary Frequencies = 0

Anthracene + C_2H_4 [1,4] TS

C	2.068903	-1.347021	-0.374476
C	3.079510	-0.688453	-1.122337
C	3.079510	0.688452	-1.122337
C	2.068903	1.347021	-0.374477
C	0.757999	0.715944	-0.302246
C	0.757999	-0.715944	-0.302246
C	2.693527	0.700752	1.620781
C	2.693527	-0.700752	1.620782
C	-0.439727	-1.405811	-0.181675
C	-1.669523	-0.720026	-0.083957
C	-1.669523	0.720026	-0.083957
C	-0.439727	1.405811	-0.181675
C	-2.916184	-1.403796	0.015310
C	-4.098063	-0.710533	0.111691
C	-4.098063	0.710533	0.111691
C	-2.916184	1.403796	0.015310
H	2.096371	-2.432752	-0.303089
H	3.912407	-1.254597	-1.530933
H	3.912407	1.254597	-1.530933
H	2.096371	2.432752	-0.303089
H	1.888044	1.231218	2.118606
H	1.888042	-1.231217	2.118606
H	-0.440228	-2.494311	-0.176533
H	-0.440228	2.494311	-0.176533
H	3.638799	1.233346	1.592225
H	3.638798	-1.233347	1.592227
H	-2.913741	-2.491575	0.013290
H	-5.040305	-1.246677	0.187888
H	-5.040305	1.246677	0.187888
H	-2.913741	2.491575	0.013290

Energy = -618.067097047
Number of Imaginary Frequencies = 1

Anthracene + C_2H_4 [1,4] Adduct

C	2.145544	-1.293030	-0.082950
C	2.900422	-0.668589	-1.246116
C	2.900431	0.668596	-1.246114
C	2.145543	1.293030	-0.082940
C	0.741633	0.713607	-0.073390
C	0.741634	-0.713604	-0.073388
C	2.841995	0.777469	1.225586
C	2.842004	-0.777477	1.225577
C	-0.440061	-1.409440	-0.040631
C	-1.685585	-0.717170	-0.018187
C	-1.685584	0.717172	-0.018188
C	-0.440063	1.409443	-0.040632
C	-2.929570	-1.400734	0.002552
C	-4.120330	-0.707616	0.023306
C	-4.120331	0.707612	0.023305
C	-2.929572	1.400732	0.002552
H	2.137202	-2.386081	-0.118552
H	3.402738	-1.282699	-1.988298
H	3.402762	1.282704	-1.988284
H	2.137209	2.386082	-0.118536
H	2.306390	1.169427	2.096846
H	2.306427	-1.169455	2.096844
H	-0.443626	-2.498156	-0.036705
H	-0.443620	2.498159	-0.036712
H	3.863634	1.169275	1.264165
H	3.863649	-1.169272	1.264131
H	-2.926564	-2.488617	0.001742

H	-5.064143	-1.246154	0.039786
H	-5.064140	1.246154	0.039782
H	-2.926568	2.488616	0.001738

Energy = -618.129312828
Number of Imaginary Frequencies = 0

Anthracene + H_2 [12,14] TS

C	0.713016	3.588714	0.258991
C	1.338232	2.407589	0.485267
C	0.652162	1.127651	0.274447
C	-0.753334	1.206877	-0.232281
C	-1.338232	2.497550	-0.481652
C	-0.642445	3.640437	-0.236623
C	1.414366	-0.013627	-0.235296
C	-1.414366	0.013627	-0.235296
C	-0.652162	-1.127651	0.274447
C	0.753334	-1.206877	-0.232281
C	1.338232	-2.497550	-0.481652
C	2.362975	-2.535413	-0.844342
C	0.642445	-3.640437	-0.236623
C	-0.713016	-3.588714	0.258991
C	-1.338232	-2.407589	0.485267
H	2.475929	0.077217	-0.446418
H	1.242291	4.523383	0.427338
H	2.373541	2.381299	0.816942
H	-2.362975	2.535413	-0.844342
H	-1.101882	4.609519	-0.410752
H	-2.475929	-0.077217	-0.446418
H	1.101882	-4.609519	-0.410752
H	-1.242291	-4.523383	0.427338
H	-2.373541	-2.381299	0.816942
H	-0.286877	-0.475077	1.460118
H	0.286877	0.475077	1.460118

Energy = -540.586480565
Number of Imaginary Frequencies = 1

Anthracene + H_2 [12,14] Adduct

C	-3.576629	0.710406	-0.388252
C	-2.510837	1.394415	0.057853
C	-1.272816	0.698939	0.579255
C	-1.198594	-0.780460	0.190771
C	-2.433193	-1.444719	-0.199945
C	-3.560699	-0.747068	-0.463882
C	0.012493	1.415068	0.228365
C	-0.012493	-1.415068	0.228365
C	1.272816	-0.698939	0.579255
C	1.198594	0.780460	0.190771
C	2.433193	1.444719	-0.199945
H	2.407143	2.524784	-0.328894
C	3.560699	0.747068	-0.463882
C	3.576629	-0.710406	-0.388252
C	2.510838	-1.394415	0.057853
H	-0.046518	2.478969	0.004389
H	-4.471089	1.236704	-0.712821
H	-2.524689	2.481470	0.107988
H	-2.407143	-2.524784	-0.328894
H	-4.462236	-1.263065	-0.783402
H	0.046518	-2.478969	0.004389
H	4.462236	1.263065	-0.783402
H	4.471089	-1.236704	-0.712821
H	2.524689	-2.481470	0.107988
H	1.361751	-0.723450	1.687756
H	-1.361751	0.723450	1.687756

Energy = -540.625467422
Number of Imaginary Frequencies = 0

Anthracene + C_2H_4 [12,14] TS

C	0.003164	1.408196	-0.439567
C	1.169555	0.656673	0.004927
C	1.198642	-0.764436	-0.438207
C	-0.003164	-1.408196	-0.439566
C	-1.169555	-0.656672	0.004927
C	-1.198642	0.764436	-0.438206
C	-2.470592	1.397717	-0.677601
C	-3.636018	0.709867	-0.545215
C	-3.627158	-0.692470	-0.194064
C	-2.464921	-1.348202	0.036568
C	-0.625998	-0.352962	1.877443
C	0.625998	0.352962	1.877444
C	2.470592	-1.397717	-0.677601
C	3.636018	-0.709868	-0.545214
C	3.627158	0.692469	-0.194065
C	2.464921	1.348202	0.036568
H	0.085101	2.476506	-0.625586
H	-0.085103	-2.476504	-0.625593
H	-2.473831	2.449137	-0.957070
H	-4.588155	1.203854	-0.718916
H	-4.573666	-1.225015	-0.142867
H	-2.464376	-2.412103	0.265002
H	2.473831	-2.449138	-0.957070
H	4.588155	-1.203855	-0.718916
H	4.573667	1.225014	-0.142865
H	2.464376	2.412104	0.264997
H	-1.503984	0.194597	2.211168
H	-0.614750	-1.383332	2.222555
H	1.503984	-0.194596	2.211169
H	0.614749	1.383332	2.222555

Energy = -618.023035711
Number of Imaginary Frequencies = 1

Anthracene + C_2H_4 [12,14] Adduct

C	0.049354	1.405064	-0.347368
C	1.167598	0.588271	0.276323
C	1.160320	-0.811014	-0.360134
C	-0.049356	-1.405061	-0.347371
C	-1.167597	-0.588270	0.276324
C	-1.160321	0.811016	-0.360130
C	-2.392605	1.383870	-0.855288
C	-3.558245	0.697900	-0.793740
C	-3.609460	-0.649725	-0.240371
C	-2.509909	-1.258220	0.239823
C	-0.692738	-0.339612	1.779131
C	0.692740	0.339609	1.779131
C	2.392603	-1.383868	-0.855289
C	3.558245	-0.697902	-0.793739
C	3.609460	0.649724	-0.240371
C	2.509909	1.258220	0.239822
H	0.233134	2.410678	-0.716071
H	-0.233134	-2.410675	-0.716075
H	-2.355669	2.383573	-1.283138
H	-4.476609	1.141793	-1.168658
H	-4.565972	-1.167140	-0.232559
H	-2.565165	-2.270180	0.637903
H	2.355665	-2.383571	-1.283143

H	4.476608	-1.141797	-1.168655
H	4.565973	1.167139	-0.232560
H	2.565165	2.270181	0.637898
H	-1.442202	0.286312	2.272668
H	-0.667472	-1.302144	2.299603
H	1.442205	-0.286316	2.272666
H	0.667474	1.302140	2.299606

Energy = -618.044223797
Number of Imaginary Frequencies = 0

Anthracene + H_2 [2,12] TS

C	-3.553677	0.777043	-0.303087
C	-2.444612	1.423366	0.056818
C	-1.200479	0.715285	0.548912
C	-1.196946	-0.765155	0.178619
C	-2.343529	-1.409715	-0.129136
C	-3.671840	-0.725157	-0.278146
C	0.083537	1.411781	0.170437
C	0.086933	-1.430986	0.187886
C	1.267780	-0.741308	0.129654
C	1.253018	0.737749	0.033662
C	2.519309	1.413400	-0.197152
H	2.506427	2.496802	-0.291751
C	3.683893	0.723712	-0.265373
C	3.700546	-0.718009	-0.125012
C	2.548812	-1.411556	0.061598
H	0.066997	2.497920	0.097288
H	-4.428488	1.337367	-0.628270
H	-2.409430	2.511658	0.032253
H	-2.314007	-2.483064	-0.312831
H	-4.169003	-1.078734	-1.195601
H	0.100386	-2.518610	0.137546
H	4.623165	1.247197	-0.422571
H	4.651803	-1.240403	-0.180499
H	2.561477	-2.495495	0.150552
H	-1.229934	0.751798	1.660550
H	-4.355863	-1.029136	0.535260

Energy = -540.646686042
Number of Imaginary Frequencies = 1

Anthracene + H_2 [2,12] Adduct

C	3.585463	-0.678812	-0.350006
C	2.420904	-1.332050	-0.506856
C	1.243028	-0.678551	0.110907
C	1.184813	0.798517	-0.085861
C	2.399941	1.440152	0.064615
C	3.492315	0.575515	0.425044
C	-0.022020	-1.377392	0.147585
C	-0.077680	1.438942	-0.177429
C	-1.264124	0.734826	-0.083075
C	-1.229833	-0.718114	0.091102
C	-2.488496	-1.420708	0.162468
H	-2.465266	-2.501048	0.284612
C	-3.673943	-0.755252	0.085130
C	-3.705004	0.673524	-0.073337
C	-2.545849	1.385482	-0.153462
H	-0.008556	-2.463405	0.214862
H	4.548321	-1.060108	-0.674616
H	2.320157	-2.304198	-0.978886
H	2.476997	2.520506	0.144294
H	4.427098	1.040932	0.733217
H	-0.104565	2.520010	-0.301124
H	-4.611705	-1.301197	0.145116
H	-4.664589	1.179942	-0.130858
H	-2.565953	2.466006	-0.275744
H	1.900551	-0.578906	1.396387
H	2.830428	-0.035013	1.501789

Energy = -540.594917634
Number of Imaginary Frequencies = 0

Anthracene + C_2H_4 [2,12] TS

C	2.017883	1.521917	-0.404772
C	3.196897	0.706761	-0.235168
C	3.186453	-0.547519	-1.011656
C	2.026692	-1.228894	-1.019811
C	0.881881	-0.621960	-0.330971
C	0.810209	0.854616	-0.389233
C	-0.458162	1.487348	-0.266583
C	-1.627234	0.766473	-0.112540
C	-1.575605	-0.696201	-0.110578
C	-0.363459	-1.336437	-0.256594
C	1.784936	-0.705675	1.617174
C	2.993201	0.056532	1.506832
C	-2.909951	1.404507	0.031498
C	-4.052873	0.672902	0.154970
C	-4.005004	-0.764423	0.143779
C	-2.817291	-1.418641	0.015059
H	2.067385	2.603580	-0.309189
H	4.146957	1.240229	-0.215929
H	4.103850	-0.928848	-1.450743
H	1.915893	-2.211595	-1.470790
H	-0.498280	2.575069	-0.282867
H	-0.338349	-2.423742	-0.306961
H	0.940968	-0.279827	2.150158
H	1.852093	-1.786884	1.675008
H	3.028922	0.985013	2.073911
H	3.917701	-0.511656	1.603750
H	-2.944265	2.491647	0.035299
H	-5.013259	1.170336	0.259937
H	-4.930618	-1.325509	0.241185
H	-2.780446	-2.505644	0.008798

Energy = -618.032128451
Number of Imaginary Frequencies = 1

Anthracene + C_2H_4 [2,12] Adduct

C	2.015574	1.568751	-0.149718
C	3.220505	0.662155	-0.112154
C	3.077532	-0.388226	-1.203350
C	1.919411	-1.049068	-1.179147
C	0.959903	-0.606862	-0.071875
C	0.824604	0.923077	-0.124433
C	-0.473262	1.528780	-0.086033
C	-1.625830	0.787927	-0.035430
C	-1.553386	-0.690262	-0.034431
C	-0.350327	-1.322912	-0.072852
C	1.766846	-0.891057	1.280496
C	3.115872	-0.137691	1.244913
C	-2.932397	1.404490	0.006369
C	-4.067473	0.659476	0.041238
C	-4.001567	-0.786107	0.036021
C	-2.806753	-1.425702	-0.001354
H	2.111666	2.650900	-0.134889
H	4.165344	1.207668	-0.170454
H	3.882013	-0.581594	-1.906962

H	1.647114	-1.855317	-1.853900
H	-0.533465	2.615815	-0.103754
H	-0.317909	-2.411923	-0.085941
H	1.146025	-0.564172	2.119764
H	1.912717	-1.971673	1.376772
H	3.202529	0.562144	2.081889
H	3.954499	-0.838782	1.309388
H	-2.981685	2.491090	0.007829
H	-5.040400	1.142378	0.071699
H	-4.927195	-1.354975	0.063110
H	-2.756779	-2.512174	-0.004109

Energy = -618.034015523
Number of Imaginary Frequencies = 0

Tetracene (**4**)

C	-4.889407	0.715178	0.000000
C	-3.711400	1.409179	0.000000
C	-2.450868	0.725814	0.000000
C	-2.450868	-0.725813	0.000000
C	-3.711400	-1.409179	0.000000
C	-4.889407	-0.715177	0.000000
C	-1.235382	1.406223	0.000000
C	-1.235382	-1.406223	0.000000
C	-0.000290	-0.726256	0.000000
C	-0.000289	0.726256	0.000000
C	1.235395	1.406381	0.000000
H	1.234924	2.494684	0.000000
C	2.450712	0.726344	0.000000
C	2.450712	-0.726345	0.000000
C	1.235394	-1.406381	0.000000
H	-1.235842	2.494519	0.000000
H	-5.836708	1.247753	0.000000
H	-3.709444	2.496765	0.000000
H	-3.709444	-2.496765	0.000000
H	-5.836708	-1.247753	0.000000
H	-1.235842	-2.494519	0.000000
H	1.234924	-2.494684	0.000000
C	3.711682	-1.409174	0.000000
H	3.709812	-2.496833	0.000000
C	3.711682	1.409174	0.000000
H	3.709812	2.496833	0.000000
C	4.889623	-0.715319	0.000000
C	4.889624	0.715318	0.000000
H	5.836872	-1.248129	0.000000
H	5.836872	1.248129	0.000000

Energy = -693.165810903
Number of Imaginary Frequencies = 0

Tetracene + H_2 [5,12] TS

C	4.834145	-0.711520	-0.430949
C	3.668118	-1.404945	-0.226767
C	2.434519	-0.721294	-0.007705
C	2.434519	0.721294	-0.007705
C	3.668118	1.404945	-0.226767
C	4.834145	0.711520	-0.430949
C	1.225882	-1.409322	0.211014
C	1.225882	1.409323	0.211014
C	0.032184	0.717831	0.383982
C	0.032184	-0.717831	0.383982
C	-1.250923	-1.328205	0.684261
H	-1.370747	-0.464976	2.034998
C	-2.431948	-0.711979	0.133438
C	-2.431948	0.711979	0.133438
C	-1.250923	1.328205	0.684261
H	1.229175	-2.497230	0.225342
H	5.765660	-1.246673	-0.594548
H	3.665311	-2.492559	-0.227939
H	3.665311	2.492559	-0.227939
H	5.765660	1.246673	-0.594548
H	1.229175	2.497230	0.225342
H	-1.270818	2.401008	0.869502
C	-3.599311	1.406745	-0.253833
H	-3.603082	2.493957	-0.238376
C	-3.599311	-1.406745	-0.253833
H	-3.603082	-2.493957	-0.238376
C	-4.714995	0.706228	-0.671851
C	-4.714995	-0.706228	-0.671851
H	-5.601529	1.243104	-0.998518
H	-5.601529	-1.243103	-0.998518
H	-1.270818	-2.401008	0.869501
H	-1.370747	0.464976	2.034998

Energy = -694.281077462
Number of Imaginary Frequencies = 1

Tetracene + H_2 [5,12] Adduct

C	0.000000	0.709509	4.952270
C	0.000000	1.404143	3.765121
C	0.000000	0.716244	2.519859
C	0.000000	-0.716244	2.519859
C	0.000000	-1.404143	3.765121
C	0.000000	-0.709509	4.952270
C	0.000000	1.388340	1.275349
C	0.000000	-1.388340	1.275349
C	0.000000	-0.711004	0.069362
C	0.000000	0.711004	0.069362
C	0.000000	1.504606	-1.221638
H	0.871605	2.176349	-1.224818
C	0.000000	0.699792	-2.503379
C	0.000000	-0.699792	-2.503379
C	0.000000	-1.504606	-1.221638
H	0.000000	2.477569	1.275174
H	0.000000	1.245437	5.897680
H	0.000000	2.491852	3.761759
H	0.000000	-2.491852	3.761759
H	0.000000	-1.245437	5.897680
H	0.000000	-2.477569	1.275174
H	-0.871605	-2.176349	-1.224818
C	0.000000	-1.383183	-3.730286
H	0.000000	-2.471664	-3.725827
C	0.000000	1.383183	-3.730286
H	0.000000	2.471664	-3.725827
C	0.000000	-0.699317	-4.940244
C	0.000000	0.699317	-4.940244
H	0.000000	-1.249178	-5.877625
H	0.000000	1.249178	-5.877625
H	-0.871605	2.176349	-1.224818
H	0.871605	-2.176349	-1.224818

Energy = -694.375462733
Number of Imaginary Frequencies = 0

Tetracene + C_2H_4 [5,12] TS

C	1.102850	1.360078	0.195301
C	-0.174037	0.718686	0.016585
C	-0.174037	-0.718685	0.016582

C	1.102851	-1.360077	0.195297
C	2.281127	-0.713318	-0.288604
C	2.281127	0.713320	-0.288601
C	1.346343	-0.695736	2.356076
C	1.346348	0.695718	2.356082
C	3.462875	1.404045	-0.653680
C	4.591287	0.707459	-1.035649
C	4.591288	-0.707453	-1.035652
C	3.462875	-1.404041	-0.653685
C	-1.384028	-1.405880	-0.073373
C	-2.605919	-0.721830	-0.193795
C	-2.605919	0.721831	-0.193792
C	-1.384028	1.405882	-0.073366
C	-3.853795	1.405430	-0.315181
C	-5.031852	0.712042	-0.426350
C	-5.031851	-0.712040	-0.426354
C	-3.853794	-1.405428	-0.315187
H	1.112927	2.446406	0.269928
H	1.112927	-2.446406	0.269916
H	2.280797	-1.236929	2.461237
H	2.280805	1.236905	2.461242
H	3.463598	2.491751	-0.645044
H	5.486066	1.245097	-1.337816
H	5.486066	-1.245089	-1.337821
H	3.463599	-2.491747	-0.645053
H	0.457410	-1.236896	2.662878
H	0.457418	1.236882	2.662890
H	-1.385270	-2.494262	-0.065856
H	-1.385270	2.494263	-0.065845
H	-3.851124	2.493128	-0.316967
H	-5.973548	1.246900	-0.516315
H	-5.973547	-1.246898	-0.516321
H	-3.851123	-2.493126	-0.316979

Energy = -771.715614652
Number of Imaginary Frequencies = 1

Tetracene + C_2H_4 [5,12] Adduct

C	1.213941	1.301124	0.827940
C	-0.139648	0.714166	0.469304
C	-0.139645	-0.714212	0.469235
C	1.213944	-1.301212	0.827804
C	2.240596	-0.703435	-0.118026
C	2.240581	0.703447	-0.117958
C	1.563542	-0.779011	2.260940
C	1.563533	0.778766	2.261025
C	3.137924	1.402972	-0.919958
C	4.036756	0.697943	-1.728587
C	4.036766	-0.697751	-1.728657
C	3.137946	-1.402871	-0.920098
C	-1.288136	-1.409068	0.184134
C	-2.494756	-0.717075	-0.122898
C	-2.494767	0.717087	-0.122824
C	-1.288136	1.409048	0.184277
C	-3.699990	1.401177	-0.431692
C	-4.853352	0.707717	-0.726842
C	-4.853344	-0.707646	-0.726908
C	-3.699994	-1.401134	-0.431829
H	1.209104	2.395173	0.796537
H	1.209108	-2.395258	0.796284
H	2.543869	-1.169273	2.553875
H	2.543865	1.168999	2.553993
H	3.137794	2.490888	-0.920297
H	4.735341	1.240542	-2.360149
H	4.735358	-1.240282	-2.360270
H	3.137808	-2.490787	-0.920533
H	0.828947	-1.169139	2.973307
H	0.828948	1.168811	2.973440
H	-1.291505	-2.497661	0.184668
H	-1.291520	2.497643	0.184920
H	-3.697030	2.488953	-0.431806
H	-5.767808	1.246185	-0.961050
H	-5.767817	-1.246076	-0.961154
H	-3.697025	-2.488911	-0.432054

Energy = -771.793945795
Number of Imaginary Frequencies = 0

Tetracene + H_2 [1,4] TS

C	0.099083	4.949880	0.714067
C	0.059006	3.770699	1.407820
C	0.016208	2.513742	0.723794
C	0.016208	2.513742	-0.723794
C	0.059006	3.770699	-1.407820
C	0.099083	4.949880	-0.714067
C	-0.024564	1.294049	1.403886
C	-0.024564	1.294049	-1.403886
C	-0.068195	0.065104	-0.724798
C	-0.068195	0.065104	0.724798
C	-0.115791	-1.178257	1.413927
H	-0.127522	-1.176909	2.501790
C	-0.128098	-2.367362	0.719236
C	-0.128098	-2.367362	-0.719236
C	-0.115791	-1.178257	-1.413927
H	-0.022863	1.294170	2.492220
H	0.131582	5.896310	1.247075
H	0.059118	3.768154	2.495410
H	0.059118	3.768154	-2.495410
H	0.131582	5.896310	-1.247075
H	-0.022863	1.294170	-2.492220
H	-0.127522	-1.176909	-2.501790
C	-0.218391	-3.707894	-1.314616
H	-1.497394	-4.000784	-0.482688
C	-0.218391	-3.707894	1.314616
H	0.401375	-3.764212	2.385972
C	0.539304	-4.744644	-0.687578
C	0.539304	-4.744644	0.687578
H	0.907082	-5.588636	-1.263602
H	0.907082	-5.588636	1.263602
H	-1.497394	-4.000784	0.482688
H	-0.401375	-3.764212	-2.385972

Energy = -694.268625348
Number of Imaginary Frequencies = 1

Tetracene + H_2 [1,4] Adduct

C	0.000000	0.713374	4.969307
C	0.000000	1.407041	3.788342
C	0.000000	0.723190	2.531883
C	0.000000	-0.723190	2.531883
C	0.000000	-1.407041	3.788342
C	0.000000	-0.713374	4.969307
C	0.000000	1.404496	1.309157
C	0.000000	-1.404496	1.309157
C	0.000000	-0.721343	0.085264
C	0.000000	0.721343	0.085264
C	0.000000	1.392968	-1.170955

H	0.000000	2.482136	-1.169832
C	0.000000	0.717894	-2.368734
C	0.000000	-0.717894	-2.368734
C	0.000000	-1.392968	-1.170955
H	0.000000	2.492886	1.308706
H	0.000000	1.246928	5.916011
H	0.000000	2.494657	3.785754
H	0.000000	-2.494657	3.785754
H	0.000000	-1.246928	5.916011
H	0.000000	-2.492886	1.308706
H	0.000000	-2.482136	-1.169832
C	0.000000	-1.505918	-3.667345
H	0.871378	-2.179586	-3.684059
C	0.000000	1.505918	-3.667345
H	-0.871378	2.179586	-3.684059
C	0.000000	-0.666564	-4.912626
C	0.000000	0.666564	-4.912626
H	0.000000	-1.206166	-5.858276
H	0.000000	1.206166	-5.858276
H	0.871378	2.179586	-3.684059
H	-0.871378	-2.179586	-3.684059

Energy = -694.356777811
Number of Imaginary Frequencies = 0

Tetracene + C_2H_4 [1,4] TS

C	-3.246773	1.349349	-0.350651
C	-4.271820	0.689565	-1.072510
C	-4.271820	-0.689564	-1.072510
C	-3.246773	-1.349348	-0.350651
C	-1.931697	-0.720133	-0.304552
C	-1.931697	0.720134	-0.304552
C	-3.817221	-0.700311	1.667942
C	-3.817220	0.700309	1.667943
C	-0.739041	1.409636	-0.216010
C	0.503778	0.724824	-0.148051
C	0.503778	-0.724824	-0.148051
C	-0.739041	-1.409636	-0.216010
C	1.732066	1.404118	-0.081022
C	2.950260	0.724055	-0.011929
C	2.950260	-0.724055	-0.011929
C	1.732066	-1.404118	-0.081022
C	4.206314	1.407730	0.058296
C	5.384421	0.714143	0.124073
C	5.384421	-0.714143	0.124073
C	4.206313	-1.407731	0.058295
H	-3.273944	2.434871	-0.277211
H	-5.116902	1.253629	-1.458388
H	-5.116902	-1.253627	-1.458389
H	-3.273944	-2.434870	-0.277212
H	-0.738351	2.497975	-0.211760
H	-0.738351	-2.497974	-0.211760
H	-2.996451	-1.231643	2.139018
H	-2.996448	1.231639	2.139019
H	1.732372	2.492545	-0.083105
H	1.732372	-2.492545	-0.083106
H	4.203855	2.495387	0.057875
H	6.329945	1.247237	0.176797
H	6.329944	-1.247238	0.176796
H	4.203855	-2.495387	0.057874
H	-4.762254	-1.233949	1.663257
H	-4.762252	1.233949	1.663261

Energy = -771.703821586
Number of Imaginary Frequencies = 1

Tetracene + C_2H_4 [1,4] Adduct

C	3.318058	-1.294134	-0.076090
C	4.069662	-0.668732	-1.240592
C	4.069682	0.668729	-1.240579
C	3.318060	1.294133	-0.076090
C	1.912757	0.718538	-0.071288
C	1.912755	-0.718540	-0.071281
C	4.011476	0.777518	1.232740
C	4.011484	-0.777514	1.232735
C	0.738085	-1.414158	-0.045539
C	-0.518141	-0.723223	-0.029878
C	-0.518139	0.723221	-0.029880
C	0.738085	1.414156	-0.045548
C	-1.741217	-1.402240	-0.016301
C	-2.967078	-0.721919	-0.002071
C	-2.967081	0.721920	-0.002071
C	-1.741215	1.402243	-0.016302
C	-4.221621	-1.406311	0.012256
C	-5.403730	-0.712669	0.025498
C	-5.403731	0.712669	0.025497
C	-4.221622	1.406313	0.012255
H	3.311469	-2.387149	-0.111648
H	4.566973	-1.282303	-1.986601
H	4.567004	1.282301	-1.986579
H	3.311471	2.387148	-0.111652
H	0.734942	-2.502668	-0.041625
H	0.734946	2.502666	-0.041641
H	3.474435	1.169428	2.103177
H	3.474453	-1.169429	2.103177
H	-1.741526	-2.490693	-0.017042
H	-1.741522	2.490697	-0.017038
H	-4.218900	-2.493967	0.012050
H	-6.350073	-1.246826	0.035942
H	-6.350074	1.246824	0.035940
H	-4.218903	2.493968	0.012049
H	5.033065	1.169289	1.273340
H	5.033075	-1.169278	1.273328

Energy = -771.767723272
Number of Imaginary Frequencies = 0

Tetracene + H_2 [14,16] TS

C	-4.859713	-0.739430	0.182542
C	-3.676396	-1.385658	0.360415
C	-2.414298	-0.699287	0.197166
C	-2.448855	0.719098	-0.181213
C	-3.733351	1.350148	-0.350927
C	-4.890768	0.655005	-0.177581
C	-1.212555	-1.343305	0.354057
C	-1.267132	1.406295	-0.362908
C	0.001347	0.790170	-0.169488
C	0.064544	-0.658483	0.216019
C	1.206076	-1.384403	-0.361076
H	1.101391	-2.415852	-0.683946
C	2.401318	-0.737065	-0.294765
C	2.331079	0.621132	0.341321
C	1.208599	1.437553	-0.111555
H	-1.200024	-2.407847	0.578798
H	-5.798066	-1.271755	0.313530
H	-3.653563	-2.437745	0.634546
H	-3.753595	2.402454	-0.624925

H	-5.850805	1.145848	-0.311434
H	-1.294662	2.460296	-0.633152
H	1.308086	2.513831	-0.217088
C	3.619881	1.272699	0.616856
H	3.602126	2.270293	1.049297
C	3.689436	-1.300170	-0.607115
H	3.720216	-2.285664	-1.066361
C	4.794539	0.665194	0.325124
C	4.836004	-0.637353	-0.301662
H	5.733605	1.168990	0.540498
H	5.801912	-1.082411	-0.523997
H	0.706505	-0.414231	1.420530
H	1.678330	0.160961	1.472441

Energy = -694.216427967
Number of Imaginary Frequencies = 1

Tetracene + H_2 [14,16] Adduct

C	-4.818659	-0.713654	-0.462114
C	-3.687779	-1.405705	-0.182644
C	-2.432480	-0.724723	0.092095
C	-2.420616	0.754696	0.016858
C	-3.666024	1.428954	-0.279589
C	-4.809748	0.734315	-0.506828
C	-1.299870	-1.398878	0.411230
C	-1.242920	1.435003	0.165934
C	0.014299	0.773364	0.417500
C	-0.017035	-0.709975	0.795528
C	1.224139	-1.421635	0.301044
H	1.140247	-2.481073	0.065588
C	2.400046	-0.784322	0.154144
C	2.512667	0.688335	0.560271
C	1.203050	1.410267	0.345060
H	-1.311973	-2.486509	0.460245
H	-5.750041	-1.239519	-0.654360
H	-3.694593	-2.492504	-0.142704
H	-3.658114	2.515646	-0.323834
H	-5.734322	1.259001	-0.731758
H	-1.228457	2.514531	0.025214
H	1.239673	2.477498	0.134082
C	3.698185	1.393749	-0.060714
H	3.719861	2.479356	0.011944
C	3.588605	-1.439425	-0.371228
H	3.547725	-2.516395	-0.520399
C	4.714134	0.718924	-0.621937
C	4.686582	-0.736380	-0.728553
H	5.574878	1.251634	-1.019031
H	5.551275	-1.245577	-1.145810
H	0.019349	-0.743635	1.908006
H	2.705035	0.690091	1.656477

Energy = -694.251130316
Number of Imaginary Frequencies = 0

Tetracene + C_2H_4 [14,16] TS

C	1.060361	-1.369423	-0.524547
C	-0.089160	-0.663898	0.041337
C	-0.134002	0.795410	-0.269565
C	1.075148	1.438061	-0.267323
C	2.249622	0.648014	0.072709
C	2.258447	-0.725459	-0.516427
C	3.517841	-1.321154	-0.889058
C	4.686692	-0.642543	-0.751404
C	4.696275	0.718344	-0.257609
C	3.550422	1.339490	0.103814
C	1.800770	0.181465	1.892299
C	0.546215	-0.529514	1.898736
C	-1.399014	1.443651	-0.387012
C	-2.588853	0.760102	-0.263030
C	-2.569499	-0.692361	-0.040420
C	-1.372717	-1.353086	0.060666
C	-3.838944	-1.381690	0.035785
C	-5.015151	-0.708665	-0.073589
C	-5.031450	0.718829	-0.274613
C	-3.867534	1.418195	-0.365346
H	0.963322	-2.410609	-0.822058
H	1.151364	2.519457	-0.350385
H	3.507056	-2.338724	-1.273786
H	5.628475	-1.109282	-1.026883
H	5.644169	1.248315	-0.205474
H	3.562434	2.373976	0.441075
H	-1.413239	2.516345	-0.571932
H	-1.367039	-2.435367	0.179015
H	2.687027	-0.396308	2.145319
H	1.806096	1.169105	2.346870
H	0.309207	-0.017145	2.332178
H	0.576877	-1.585827	2.151449
H	-3.826911	-2.458190	0.190129
H	-5.959173	-1.243120	-0.008313
H	-5.986529	1.230384	-0.357027
H	-3.877546	2.494386	-0.522602

Energy = -771.652609250
Number of Imaginary Frequencies = 1

Tetracene + C_2H_4 [14,16] Adduct

C	0.992419	-1.318591	-0.553067
C	-0.064696	-0.662157	0.319230
C	-0.106685	0.837247	-0.011920
C	1.108077	1.433368	0.016917
C	2.269391	0.521476	0.359364
C	2.198087	-0.716740	-0.548635
C	3.377671	-1.155436	-1.261802
C	4.547174	-0.480471	-1.164007
C	4.655440	0.722176	-0.347519
C	3.607122	1.201490	0.346043
C	1.927241	-0.039213	1.814873
C	0.544151	-0.721145	1.797586
C	-1.362825	1.480038	-0.262603
C	-2.551563	0.797668	-0.241024
C	-2.562915	-0.657247	0.031087
C	-1.402385	-1.324565	0.267332
C	-3.849585	-1.333881	0.023530
C	-5.001209	-0.660406	-0.217048
C	-4.985802	0.762940	-0.478265
C	-3.815936	1.452641	-0.489180
H	0.771869	-2.227959	-1.105144
H	1.261713	2.496160	-0.148207
H	3.296960	-2.044512	-1.883731
H	5.425131	-0.823083	-1.705088
H	5.611553	1.239433	-0.316867
H	3.703142	2.108586	0.940556
H	-1.359138	2.546571	-0.481518
H	-1.428199	-2.398379	0.449236
H	2.713232	-0.746027	2.096987
H	1.956429	0.793728	2.524106
H	-0.156118	-0.217877	2.470509

H	0.608120	-1.769517	2.104399
H	-3.860806	-2.403352	0.220986
H	-5.953093	-1.184805	-0.215886
H	-5.925798	1.273922	-0.667924
H	-3.804021	2.521955	-0.687770

Energy = -771.670730745
Number of Imaginary Frequencies = 0

Tetracene + H_2 [2,14] TS

C	4.940860	0.684505	-0.058687
C	3.775283	1.389091	-0.115173
C	2.500706	0.724191	-0.057805
C	2.482282	-0.732349	0.063429
C	3.743210	-1.426180	0.119272
C	4.923675	-0.747836	0.060936
C	1.303975	1.414470	-0.116043
C	1.272336	-1.395651	0.123315
C	0.023203	-0.706736	0.072459
C	0.045619	0.754371	-0.063009
C	-1.155767	1.451761	-0.138955
H	-1.136809	2.535675	-0.234799
C	-2.405963	0.799566	-0.063536
C	-2.453080	-0.686969	0.095086
C	-1.187450	-1.376729	0.107996
H	1.316592	2.498693	-0.208939
H	5.895745	1.201058	-0.103564
H	3.785651	2.472837	-0.205532
H	3.729406	-2.509795	0.209859
H	5.866397	-1.286582	0.104508
H	1.260794	-2.479716	0.216480
H	-1.192176	-2.464303	0.137278
C	-3.628553	-1.329431	-0.545731
H	3.519492	-2.282048	-1.054084
C	-3.629836	1.428028	0.105669
H	3.713584	2.504617	0.221008
C	-4.795567	-0.688259	-0.370173
C	-4.710526	0.543825	0.446289
H	-5.755664	-1.058537	-0.715032
H	-4.048410	-0.089193	1.496904
H	-5.649076	0.991068	0.769694
H	-3.105807	-0.631792	1.374190

Energy = -694.226969838
Number of Imaginary Frequencies = 1

Tetracene + H_2 [2,14] Adduct

C	-4.939758	-0.713568	-0.129755
C	-3.777225	-1.407123	0.003181
C	-2.502667	-0.731828	0.043007
C	-2.492428	0.735441	-0.065417
C	-3.760007	1.415779	-0.204154
C	-4.930645	0.725594	-0.235775
C	-1.314707	-1.413652	0.167551
C	-1.298873	1.410893	-0.026210
C	-0.036131	0.734974	0.135733
C	-0.047015	-0.747218	0.200356
C	1.142916	-1.437494	0.194158
H	1.126841	-2.522594	0.107339
C	2.420119	-0.770404	0.152800
C	2.436449	0.701455	0.558533
C	1.143361	1.407339	0.239527
H	-1.325007	-2.500191	0.228533
H	-5.890632	-1.238746	-0.157884
H	-3.783738	-2.491806	0.082428
H	-3.751549	2.500461	-0.282832
H	-5.874913	1.252891	-0.341275
H	-1.292301	2.497071	-0.092536
H	1.158061	2.494330	0.185695
C	3.664012	1.422708	0.044216
H	3.628540	2.511197	0.050750
C	3.558579	-1.406135	-0.209271
H	3.525166	-2.476202	-0.410211
C	4.759064	0.786981	-0.372761
C	4.878469	-0.715084	-0.391792
H	5.621767	1.356505	-0.713830
H	5.593762	-1.038444	0.386710
H	5.341019	-1.044293	-1.336189
H	2.501904	0.707861	1.669747

Energy = -694.276093546
Number of Imaginary Frequencies = 0

Tetracene + C_2H_4 [2,14] TS

C	3.203410	1.512905	-0.364327
C	4.363634	0.682519	-0.140721
C	4.369931	-0.567944	-0.931180
C	3.206608	-1.238374	-0.984774
C	2.041001	-0.623539	-0.332535
C	1.986029	0.858157	-0.392839
C	0.726689	1.503242	-0.316390
C	-0.462656	0.793649	-0.200316
C	-0.425869	-0.673425	-0.197178
C	0.791954	-1.325287	-0.306936
C	2.872866	-0.719509	1.636836
C	4.091069	0.038447	1.568176
C	-1.725638	1.441849	-0.099199
C	-2.910575	0.735422	-0.010580
C	-2.877098	-0.726248	-0.020429
C	-1.662655	-1.378387	-0.112528
C	-4.126672	-1.436176	0.070580
C	-5.311490	-0.769129	0.162823
C	-5.343959	0.668063	0.171957
C	-4.189514	1.387919	0.088679
H	3.260631	2.593844	-0.265670
H	5.318046	1.206356	-0.089194
H	5.297670	-0.948622	-1.348477
H	3.100541	-2.213957	-1.451862
H	0.697197	2.591050	-0.336881
H	0.807319	-2.412246	-0.363599
H	2.016338	-0.290587	2.146898
H	2.934255	-1.800899	1.697054
H	4.111431	0.959571	2.148425
H	5.004298	-0.540412	1.705243
H	-1.750740	2.529889	-0.096430
H	-1.639119	-2.466416	-0.116150
H	-4.100981	-2.523421	0.063745
H	-6.245595	-1.320273	0.230610
H	-6.301727	1.175919	0.246367
H	-4.211948	2.475274	0.095195

Energy = -771.664184661
Number of Imaginary Frequencies = 1

Tetracene + C_2H_4 [2,14] Adduct

C	3.198799	1.554652	-0.136678
C	4.388629	0.631771	-0.083436
C	4.244939	-0.414617	-1.178647

C	3.078064	-1.060150	-1.171334
C	2.109217	-0.607546	-0.076267
C	1.995398	0.925025	-0.127479
C	0.711543	1.548564	-0.103102
C	-0.459706	0.823009	-0.062802
C	-0.407795	-0.657558	-0.062567
C	0.792251	-1.306826	-0.093147
C	2.895666	-0.904817	1.287489
C	4.254518	-0.169868	1.270671
C	-1.741891	1.455165	-0.031896
C	-2.917828	0.739978	-0.005222
C	-2.872557	-0.729071	-0.010176
C	-1.659627	-1.371119	-0.039597
C	-4.125940	-1.447467	0.018186
C	-5.315106	-0.788851	0.048332
C	-5.358256	0.652876	0.052553
C	-4.209052	1.381096	0.026756
H	3.308945	2.635292	-0.117018
H	5.342083	1.163278	-0.127856
H	5.054838	-0.615148	-1.873929
H	2.803787	-1.860314	-1.852365
H	0.665737	2.636082	-0.122892
H	0.809969	-2.395859	-0.109989
H	2.267708	-0.570263	2.118209
H	3.025010	-1.987402	1.383507
H	4.341063	0.526720	2.110233
H	5.082165	-0.883096	1.342719
H	-1.777419	2.542952	-0.030494
H	-1.627169	-2.458875	-0.041533
H	-4.092203	-2.534510	0.015163
H	-6.248558	-1.344848	0.069766
H	-6.323013	1.152252	0.076789
H	-4.240536	2.468257	0.029876

Energy = -771.688105830
Number of Imaginary Frequencies = 0

Pentacene (**5**)

C	0.000000	0.716434	-6.117782
C	0.000000	1.410437	-4.941595
C	0.000000	0.727636	-3.678693
C	0.000000	-0.727636	-3.678693
C	0.000000	-1.410437	-4.941595
C	0.000000	-0.716434	-6.117782
C	0.000000	1.407867	-2.467490
C	0.000000	-1.407867	-2.467490
C	0.000000	-0.728657	-1.226573
C	0.000000	0.728657	-1.226573
C	0.000000	1.408564	0.000063
H	0.000000	2.496667	-0.000139
C	0.000000	0.728805	1.226382
C	0.000000	-0.728805	1.226382
C	0.000000	-1.408564	0.000063
C	0.000000	2.496080	-2.467795
H	0.000000	1.247767	-7.065637
H	0.000000	2.497934	-4.939615
H	0.000000	-2.497934	-4.939615
H	0.000000	-1.247767	-7.065637
H	0.000000	-2.496080	-2.467795
H	0.000000	-2.496667	-0.000139
C	0.000000	-1.407912	2.467636
H	0.000000	-2.496156	2.467661
C	0.000000	1.407912	2.467636
H	0.000000	2.496156	2.467661
C	0.000000	-0.727834	3.678573
C	0.000000	0.727834	3.678573
C	0.000000	-1.410491	4.941737
C	0.000000	1.410491	4.941737
C	0.000000	-0.716549	6.117772
C	0.000000	0.716549	6.117772
H	0.000000	-2.498009	4.939691
H	0.000000	-1.247828	7.065643
H	0.000000	1.247828	7.065643
H	0.000000	2.498009	4.939691

Energy = -846.799943083
Number of Imaginary Frequencies = 0

Pentacene + H_2 [6,13] TS

C	0.740568	5.950422	0.712143
C	0.432310	4.808582	1.405658
C	0.102300	3.598584	0.722030
C	0.102300	3.598584	-0.722030
C	0.432310	4.808582	-1.405658
C	0.740568	5.950422	-0.712143
C	-0.223996	2.416933	1.409352
C	-0.223996	2.416933	-1.409352
C	-0.502371	1.239097	-0.719275
C	-0.502371	1.239097	0.719275
C	-0.923537	0.000000	1.334534
H	-2.298633	0.000001	0.457925
C	-0.502373	-1.239097	0.719275
C	-0.502373	-1.239097	-0.719275
C	-0.923537	0.000000	-1.334534
H	-0.238294	2.421572	2.497223
H	0.987551	6.863678	1.246747
H	0.433322	4.805716	2.493242
H	0.433322	4.805716	-2.493242
H	0.987551	6.863678	-1.246747
H	-0.238294	2.421572	-2.497223
H	-1.111021	0.000000	-2.406882
C	-0.223998	-2.416934	-1.409352
H	-0.238295	-2.421572	-2.497223
C	-0.223998	-2.416934	1.409352
H	-0.238295	-2.421572	2.497223
C	0.102300	-3.598584	-0.722030
C	0.102300	-3.598584	0.722030
C	0.432311	-4.808582	-1.405658
C	0.432311	-4.808582	1.405658
C	0.740568	-5.950422	-0.712143
C	0.740568	-5.950422	0.712143
H	0.433321	-4.805716	-2.493242
H	0.987552	-6.863678	-1.246746
H	0.987552	-6.863678	1.246746
H	0.433321	-4.805716	2.493242
H	-1.111021	0.000000	2.406882
H	-2.298633	0.000001	-0.457925

Energy = -847.920094876
Number of Imaginary Frequencies = 1

Pentacene + H_2 [6,13] Adduct

C	0.000000	0.709578	6.172111
C	0.000000	1.404258	4.985124
C	0.000000	0.716282	3.739760
C	0.000000	-0.716282	3.739760
C	0.000000	-1.404258	4.985124

C	0.000000	-0.709578	6.172111
C	0.000000	1.388126	2.495488
C	0.000000	-1.388126	2.495488
C	0.000000	-0.710756	1.289177
C	0.000000	0.710756	1.289177
C	0.000000	1.506961	-0.000005
H	0.871724	2.177852	0.000001
C	0.000000	0.710755	-1.289174
C	0.000000	-0.710755	-1.289174
C	0.000000	-1.506961	-0.000005
H	0.000000	2.477343	2.495165
H	0.000000	1.245382	7.117580
H	0.000000	2.491952	4.981751
H	0.000000	-2.491952	4.981751
H	0.000000	-1.245382	7.117580
H	0.000000	-2.477343	2.495165
H	-0.871724	-2.177852	0.000001
C	0.000000	-1.388124	-2.495490
H	0.000000	-2.477341	-2.495161
C	0.000000	1.388124	-2.495490
H	0.000000	2.477341	-2.495161
C	0.000000	-0.716283	-3.739758
C	0.000000	0.716283	-3.739758
C	0.000000	-1.404259	-4.985125
C	0.000000	1.404259	-4.985125
C	0.000000	-0.709580	-6.172109
C	0.000000	0.709580	-6.172109
H	0.000000	-2.491952	-4.981749
H	0.000000	-1.245378	-7.117581
H	0.000000	1.245378	-7.117581
H	0.000000	2.491952	-4.981749
H	-0.871724	2.177852	0.000001
H	0.871724	-2.177852	0.000001

Energy = -848.018209591
Number of Imaginary Frequencies = 0

Pentacene + C_2H_4 [6,13] TS

C	0.000000	1.365739	0.453093
C	-1.238089	0.720104	0.129875
C	-1.238091	-0.720088	0.129765
C	0.000000	-1.365771	0.452952
C	1.238091	-0.720088	0.129765
C	1.238089	0.720104	0.129875
C	0.000000	-0.694628	2.658754
C	-0.000001	0.693930	2.659016
C	2.435073	1.406207	-0.093990
C	3.632947	0.722854	-0.350490
C	3.632946	-0.722768	-0.350607
C	2.435068	-1.406157	-0.094210
C	-2.435068	-1.406157	-0.094210
C	-3.632946	-0.722768	-0.350607
C	-3.632947	0.722854	-0.350491
C	-2.435073	1.406207	-0.093990
C	-4.860621	1.406329	-0.612465
C	-6.017343	0.712872	-0.856020
C	-6.017341	-0.712715	-0.856133
C	-4.860615	-1.406205	-0.612689
C	4.860621	1.406329	-0.612464
C	6.017343	0.712872	-0.856020
C	6.017341	-0.712715	-0.856133
C	4.860615	-1.406205	-0.612689
H	0.000000	2.451732	0.529741
H	0.000000	-2.451788	0.529324
H	0.918191	-1.238764	2.853129
H	0.918190	1.238028	2.853475
H	2.437083	2.494549	-0.086572
H	2.437077	-2.494501	-0.086954
H	-0.918190	-1.238765	2.853131
H	-0.918191	1.238027	2.853476
H	-2.437077	-2.494501	-0.086954
H	-2.437082	2.494549	-0.086573
H	-4.857835	2.493999	-0.614002
H	-6.943185	1.247093	-1.051835
H	-6.943181	-1.246908	-1.052032
H	-4.857825	-2.493875	-0.614398
H	4.857835	2.493999	-0.614001
H	6.943185	1.247093	-1.051835
H	6.943181	-1.246908	-1.052033
H	4.857825	-2.493875	-0.614399

Energy = -925.354156000
Number of Imaginary Frequencies = 1

Pentacene + C_2H_4 [6,13] Adduct

C	0.000002	1.363726	-1.303153
C	-1.224924	0.687403	-0.714285
C	-1.224933	0.687419	0.714278
C	0.000004	1.363754	1.303131
C	1.224927	0.687418	0.714275
C	1.224926	0.687400	-0.714282
C	0.000004	2.837009	0.779160
C	0.000002	2.836993	-0.779202
C	2.270376	0.132167	-1.408830
C	3.368375	-0.454505	-0.717224
C	3.368372	-0.454497	0.717230
C	2.270380	0.132193	1.408826
C	-2.270376	0.132194	1.408832
C	-3.368376	-0.454498	0.717234
C	-3.368372	-0.454511	-0.717227
C	-2.270373	0.132163	-1.408827
C	-4.465691	-1.041274	-1.401151
C	-5.515807	-1.601776	-0.707785
C	-5.515810	-1.601763	0.707805
C	-4.465694	-1.041248	1.401163
C	4.465694	-1.041274	-1.401153
C	5.515804	-1.601777	-0.707782
C	5.515803	-1.601767	0.707807
C	4.465692	-1.041254	1.401168
H	-0.000006	1.333398	-2.397194
H	0.000004	1.333449	2.397176
H	0.882773	3.354757	1.168779
H	0.882759	3.354747	-1.168840
H	2.273473	0.131245	-2.497433
H	2.273471	0.131290	2.497432
H	-0.882755	3.354767	1.168785
H	-0.882761	3.354743	-1.168837
H	-2.273483	0.131279	2.497436
H	-2.273471	0.131236	-2.497433
H	-4.462727	-1.040637	-2.488955
H	-6.348495	-2.046662	-1.246001
H	-6.348500	-2.046640	1.246024
H	-4.462740	-1.040592	2.488967
H	4.462730	-1.040633	-2.488954
H	6.348490	-2.046671	-1.245996
H	6.348494	-2.046651	1.246021

H	4.462734	-1.040598	2.488970

Energy = -925.438760437
Number of Imaginary Frequencies = 0

Pentacene + H_2 [5,14] TS

C	0.842771	-5.876668	0.706761
C	0.369673	-4.784203	1.406944
C	-0.075341	-3.635765	0.712776
C	-0.075341	-3.635765	-0.712776
C	0.369673	-4.784203	-1.406944
C	0.842771	-5.876668	-0.706761
C	-0.688053	-2.490022	1.330668
C	-0.688053	-2.490022	-1.330668
C	-0.462976	-1.188375	-0.721672
C	-0.462976	-1.188375	0.721672
C	-0.351932	0.004516	1.412925
H	-0.366336	0.007053	2.500688
C	-0.194976	1.233934	0.725655
C	-0.194976	1.233934	-0.725655
C	-0.351932	0.004516	-1.412925
H	-0.872842	-2.521161	2.403179
H	1.213500	-6.745882	1.243303
H	0.354115	-4.788852	2.494132
H	0.354115	-4.788852	-2.494132
H	1.213500	-6.745882	-1.243303
H	-2.037427	-2.677349	-0.462689
H	-0.366336	0.007053	-2.500688
C	-0.042191	2.457119	-1.404809
H	-0.040070	2.456963	-2.493092
C	-0.042191	2.457119	1.404809
H	-0.040070	2.456963	2.493092
C	0.105222	3.666067	-0.724751
C	0.105222	3.666067	0.724751
C	0.258384	4.915804	-1.408525
C	0.258384	4.915804	1.408525
C	0.401678	6.085889	-0.714714
C	0.401678	6.085889	0.714714
H	0.258308	4.913368	-2.496081
H	0.517197	7.026084	-1.247179
H	0.517197	7.026084	1.247179
H	0.258308	4.913368	2.496081
H	-2.037427	-2.677349	0.462689
H	-0.872842	-2.521161	-2.403179

Energy = -847.917123831
Number of Imaginary Frequencies = 1

Pentacene + H_2 [5,14] Adduct

C	0.000000	0.699354	-6.163790
C	0.000000	1.383124	-4.953918
C	0.000000	0.699702	-3.726853
C	0.000000	-0.699702	-3.726853
C	0.000000	-1.383124	-4.953918
C	0.000000	-0.699354	-6.163790
C	0.000000	1.505525	-2.445867
C	0.000000	-1.505525	-2.445867
C	0.000000	-0.716188	-1.151626
C	0.000000	0.716188	-1.151626
C	0.000000	1.392342	0.046784
H	0.000000	2.481452	0.047115
C	0.000000	0.721391	1.302162
C	0.000000	-0.721391	1.302162
C	0.000000	-1.392342	0.046784
H	-0.871617	2.177038	-2.450436
H	0.000000	1.249220	-7.101150
H	0.000000	2.471594	-4.949423
H	0.000000	-2.471594	-4.949423
H	0.000000	-1.249220	-7.101150
H	0.871617	-2.177038	-2.450436
H	0.000000	-2.481452	0.047115
C	0.000000	-1.404746	2.526595
H	0.000000	-2.493117	2.525868
C	0.000000	1.404746	2.526595
H	0.000000	2.493117	2.525868
C	0.000000	-0.723400	3.748651
C	0.000000	0.723400	3.748651
C	0.000000	-1.407224	5.005504
C	0.000000	1.407224	5.005504
C	0.000000	-0.713559	6.186141
C	0.000000	0.713559	6.186141
H	0.000000	-2.494828	5.002782
H	0.000000	-1.246841	7.132983
H	0.000000	1.246841	7.132983
H	0.000000	2.494828	5.002782
H	0.871617	2.177038	-2.450436
H	-0.871617	-2.177038	-2.450436

Energy = -848.012839622
Number of Imaginary Frequencies = 0

Pentacene + C_2H_4 [5,14] TS

C	2.244368	1.362512	0.191271
C	0.957222	0.722446	0.073678
C	0.957222	-0.722443	0.073674
C	2.244369	-1.362510	0.191267
C	3.398156	-0.714259	-0.338345
C	3.398156	0.714265	-0.338340
C	2.569840	-0.695103	2.353530
C	2.569842	0.695073	2.353544
C	4.567508	1.404473	-0.747150
C	5.679792	0.708149	-1.170609
C	5.679792	-0.708138	-1.170614
C	4.567508	-1.404465	-0.747159
C	-0.247524	-1.409288	0.032948
C	-1.484350	-0.726004	-0.035905
C	-1.484350	0.726006	-0.035900
C	-0.247525	1.409290	0.032957
C	-2.716258	1.405234	-0.102419
C	-3.931948	0.725185	-0.163273
C	-3.931948	-0.725183	-0.163278
C	-2.716257	-1.405232	-0.102428
C	-5.190015	1.408582	-0.226334
C	-6.367274	0.714914	-0.284868
C	-6.367274	-0.714913	-0.284872
C	-5.190014	-1.408581	-0.226342
H	2.258564	2.448712	0.266120
H	2.258564	-2.448711	0.266102
H	3.507109	-1.237524	2.419775
H	3.507110	1.237492	2.419791
H	4.568637	2.492157	-0.738343
H	6.562902	1.245316	-1.506033
H	6.562902	-1.245303	-1.506041
H	4.568638	-2.492149	-0.738358
H	1.691543	-1.237659	2.687136
H	1.691544	1.237625	2.687153
H	-0.248522	-2.497511	0.039788

H	-0.248523	2.497513	0.039803
H	-2.716307	2.493586	-0.104650
H	-2.716305	-2.493584	-0.104665
H	-5.187645	2.496187	-0.226527
H	-7.313390	1.247363	-0.332353
H	-7.313389	-1.247362	-0.332360
H	-5.187643	-2.496185	-0.226541

Energy = -925.351523033
Number of Imaginary Frequencies = 1

Pentacene + C_2H_4 [5,14] Adduct

C	2.389293	1.302151	0.804444
C	1.008128	0.719162	0.565075
C	1.008126	-0.719172	0.565070
C	2.389293	-1.302166	0.804423
C	3.326973	-0.703464	-0.228849
C	3.326976	0.703468	-0.228835
C	2.860912	-0.778945	2.201502
C	2.860932	0.778904	2.201509
C	4.150013	1.402958	-1.107274
C	4.974368	0.697921	-1.991463
C	4.974368	-0.697886	-1.991474
C	4.150013	-1.402938	-1.107299
C	-0.154453	-1.413617	0.386412
C	-1.394986	-0.723235	0.191322
C	-1.394986	0.723231	0.191334
C	-0.154451	1.413609	0.386428
C	-2.603706	1.402384	0.003276
C	-3.815095	0.722055	-0.183049
C	-3.815096	-0.722052	-0.183060
C	-2.603707	-1.402385	0.003253
C	-5.055420	1.406469	-0.372569
C	-6.223913	0.712770	-0.550808
C	-6.223915	-0.712758	-0.550819
C	-5.055423	-1.406460	-0.372590
H	2.383262	2.396137	0.773800
H	2.383261	-2.396152	0.773757
H	3.862807	-1.169267	2.408584
H	3.862847	1.169196	2.408560
H	4.149835	2.490837	-1.107738
H	5.614954	1.240486	-2.681773
H	5.614956	-1.240440	-2.681793
H	4.149840	-2.490817	-1.107781
H	2.190223	-1.168742	2.974432
H	2.190282	1.168714	2.974464
H	-0.157797	-2.502072	0.388079
H	-0.157797	2.502064	0.388114
H	-2.603892	2.490832	0.002790
H	-2.603894	-2.490832	0.002752
H	-5.052631	2.494105	-0.372278
H	-7.159542	1.246722	-0.693696
H	-7.159543	-1.246706	-0.693716
H	-5.052636	-2.494096	-0.372316

Energy = -925.432207648
Number of Imaginary Frequencies = 0

Pentacene + H_2 [2,16] TS

C	-5.932575	0.525248	0.455116
C	-4.857089	1.419355	0.128436
C	-3.628719	0.797320	-0.050404
C	-3.671227	-0.694064	0.085072
C	-4.845139	-1.328094	-0.570378
C	-6.013155	-0.692946	-0.385280
C	-2.384479	1.454667	-0.114434
C	-2.405597	-1.379677	0.084994
C	-1.192939	-0.705739	0.063455
C	-1.175604	0.760312	-0.048330
C	0.072020	1.426329	-0.089970
H	0.080632	2.511801	-0.165084
C	1.281481	0.739800	-0.043129
C	1.268739	-0.722017	0.053907
C	0.051897	-1.390468	0.103348
H	-2.368952	2.539912	-0.193913
H	-6.873208	0.962742	0.785784
H	-4.943479	2.493218	0.265052
H	-4.731919	-2.268928	-1.099242
H	-6.971606	-1.055426	-0.742745
H	-2.406911	-2.467565	0.091514
H	0.044732	-2.475764	0.178809
C	2.515630	-1.407317	0.097170
H	2.508564	-2.493025	0.169502
C	2.535250	1.407442	-0.089722
H	2.543032	2.493241	-0.161868
C	3.724460	-0.737257	0.050100
C	3.735597	0.720562	-0.047124
C	4.987174	-1.426523	0.092809
C	5.006954	1.391798	-0.095187
C	6.165330	-0.742401	0.044039
C	6.175843	0.691212	-0.051783
H	4.977966	-2.511564	0.165128
H	7.110289	-1.277880	0.077300
H	7.128291	1.212847	-0.089361
H	5.012658	2.476900	-0.167529
H	-4.321907	-0.663851	1.358913
H	-5.271291	-0.121899	1.491510

Energy = -847.859364489
Number of Imaginary Frequencies = 1

Pentacene + H_2 [2,16] Adduct

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.500535
C	1.125982	0.000000	2.253809
C	2.501480	-0.162125	1.610072
C	2.486953	0.179127	0.135220
C	1.367072	0.243976	-0.585007
C	1.095212	0.130263	3.686438
C	3.590827	0.538262	2.379810
C	3.482772	0.784668	3.716924
C	2.207838	0.488683	4.418907
C	2.154369	0.685272	5.830844
H	1.224332	0.458397	6.348079
C	3.229322	1.169802	6.553881
C	4.482190	1.504535	5.854375
C	4.570185	1.316509	4.491459
C	0.133030	0.052414	4.189667
H	-0.709356	0.757650	-0.370346
H	-0.968380	0.027352	1.998462
H	3.454187	0.351191	-0.334774
H	1.416611	0.475179	-1.647546
H	4.519305	0.761836	1.857949
H	5.500455	1.549197	3.977434
C	5.573986	2.010737	6.627702
H	6.500614	2.255854	6.112475
C	3.168744	1.370534	7.965202

H	2.243161	1.125043	8.482220
C	5.485706	2.193817	7.990493
C	4.237952	1.861748	8.685182
C	6.584757	2.704461	8.771797
C	4.177667	2.064262	10.110378
C	6.472818	2.876076	10.117643
C	5.247050	2.550045	10.799525
H	7.509807	2.950115	8.255399
H	7.310643	3.262206	10.691861
H	5.184771	2.696841	11.874377
H	3.251414	1.817911	10.624318
H	2.743751	-1.246052	1.687676
H	-0.400541	-0.955883	-0.385163

Energy = -847.907086202
Number of Imaginary Frequencies = 0

Pentacene + C_2H_4 [2,16] TS

C	4.398865	1.503629	-0.324295
C	5.546964	0.664569	-0.070259
C	5.563994	-0.583274	-0.868639
C	4.399433	-1.247381	-0.949646
C	3.222282	-0.628360	-0.319001
C	3.176847	0.856109	-0.379983
C	1.923060	1.508173	-0.331028
C	0.722893	0.805480	-0.239037
C	0.751149	-0.664752	-0.236196
C	1.971312	-1.322801	-0.323503
C	4.009255	-0.732405	1.660841
C	5.233303	0.021789	1.619376
C	-0.530177	1.461554	-0.162946
C	-1.730594	0.762205	-0.096995
C	-1.705766	-0.703109	-0.107105
C	-0.484315	-1.362149	-0.176471
C	-2.944313	-1.401065	-0.040985
C	-4.157426	-0.740956	0.030693
C	-4.181327	0.720096	0.039821
C	-2.989408	1.419354	-0.022857
C	-5.457144	1.380948	0.114534
C	-6.617795	0.668252	0.175568
C	-6.594522	-0.768517	0.166806
C	-5.411916	-1.443113	0.097275
H	4.460339	2.584054	-0.222977
H	6.503295	1.182623	0.001906
H	6.497862	-0.963478	-1.272425
H	4.297042	-2.218766	-1.426106
H	1.900019	2.596034	-0.353474
H	1.981690	-2.409520	-0.384297
H	3.145461	-0.301301	2.156700
H	4.066286	-1.813960	1.722424
H	5.244676	0.938423	2.207246
H	6.138668	-0.563997	1.779062
H	-0.548934	2.549543	-0.160206
H	-0.467473	-2.450115	-0.179776
H	-2.927467	-2.489136	-0.047515
H	-3.007197	2.507448	-0.016142
H	-5.472749	2.468377	0.120967
H	-7.573431	1.182417	0.231672
H	-7.533140	-1.313817	0.216553
H	-5.392874	-2.530465	0.090585

Energy = -925.296560364
Number of Imaginary Frequencies = 1

Pentacene + C_2H_4 [2,16] Adduct

C	4.393876	1.541058	-0.121030
C	5.574804	0.609000	-0.058191
C	5.432393	-0.433919	-1.157043
C	4.260900	-1.070994	-1.161551
C	3.285207	-0.613376	-0.074517
C	3.183520	0.920436	-0.123907
C	1.907704	1.553943	-0.109213
C	0.725902	0.837412	-0.077384
C	0.766414	-0.645157	-0.078519
C	1.964453	-1.303115	-0.103095
C	4.057648	-0.919350	1.296240
C	5.421836	-0.194726	1.293087
C	-0.543987	1.480261	-0.054299
C	-1.735092	0.774295	-0.034618
C	-1.701633	-0.697298	-0.040041
C	-0.486020	-1.348964	-0.063477
C	-2.946118	-1.401305	-0.018082
C	-4.159230	-0.747222	0.007335
C	-4.190539	0.717902	0.011254
C	-3.004120	1.423021	-0.009564
C	-5.473546	1.371749	0.037628
C	-6.630879	0.653744	0.059124
C	-6.600707	-0.785504	0.055889
C	-5.415160	-1.454703	0.030948
H	4.511920	2.620721	-0.097313
H	6.533036	1.132533	-0.092707
H	6.246378	-0.637545	-1.846592
H	3.986479	-1.867184	-1.847081
H	1.870414	2.641715	-0.129325
H	1.974376	-2.392095	-0.122583
H	3.424551	-0.581687	2.121716
H	4.177749	-2.003043	1.390867
H	5.506697	0.499352	2.134816
H	6.243120	-0.914717	1.370241
H	-0.570981	2.568107	-0.052460
H	-0.462557	-2.436736	-0.065630
H	-2.923454	-2.489263	-0.020902
H	-3.028397	2.511018	-0.006388
H	-5.494883	2.459106	0.040104
H	-7.590719	1.162699	0.079115
H	-7.538541	-1.334136	0.073754
H	-5.390968	-2.541973	0.028519

Energy = -925.319336567
Number of Imaginary Frequencies = 0

Pentacene + H_2 [1,4] TS

C	0.577024	-5.959997	0.688056
C	-0.192806	-4.934171	1.315711
C	-0.120391	-3.591093	0.721328
C	-0.120391	-3.591093	-0.721328
C	-0.192806	-4.934171	-1.315711
C	0.577024	-5.959997	-0.688056
C	-0.120506	-2.405550	1.415946
C	-0.120506	-2.405550	-1.415946
C	-0.086367	-1.156393	-0.727762
C	-0.086367	-1.156393	0.727762
C	-0.056034	0.064159	1.406501
H	-0.054165	0.064497	2.494680
C	-0.027967	1.295631	0.726981
C	-0.027967	1.295631	-0.726981
C	-0.056034	0.064159	-1.406501

H	-0.132009	-2.404643	2.503767
H	0.953328	-6.801020	1.262954
H	-0.375918	-4.993518	2.386841
H	-0.375918	-4.993518	-2.386841
H	0.953328	-6.801020	-1.262954
H	-0.132009	-2.404643	-2.503767
H	-0.054165	0.064497	-2.494680
C	0.001164	2.533108	-1.406862
H	0.001327	2.533017	-2.495116
C	0.001164	2.533108	1.406862
H	0.001327	2.533017	2.495116
C	0.029782	3.746255	-0.726624
C	0.029782	3.746255	0.726624
C	0.059735	5.007611	-1.409665
C	0.059735	5.007611	1.409665
C	0.087628	6.184456	-0.715863
C	0.087628	6.184456	0.715863
H	0.059759	5.005386	-2.497211
H	0.110236	7.131904	-1.247515
H	0.110236	7.131904	1.247515
H	0.059759	5.005386	2.497211
H	-1.470135	-5.239711	0.481763
H	-1.470135	-5.239711	-0.481763

Energy = -847.903444154
Number of Imaginary Frequencies = 1

Pentacene + H_2 [1,4] Adduct

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.501672
C	1.378558	0.000000	2.139766
C	2.573077	0.000000	1.333867
C	2.497540	0.000000	-0.183327
C	1.105094	0.000000	-0.745567
C	1.487430	0.000000	3.507235
C	3.800318	0.000000	1.946813
C	3.949838	0.000000	3.367407
C	2.748713	0.000000	4.177761
C	2.862241	0.000000	5.566937
H	1.959923	0.000000	6.175279
C	4.116766	0.000000	6.209446
C	5.321533	0.000000	5.396633
C	5.195464	0.000000	3.992796
H	0.585168	0.000000	4.117275
H	-0.976156	0.000000	-0.482183
H	-0.568152	-0.871361	1.863961
H	3.046199	-0.871361	-0.574510
H	1.023465	0.000000	-1.831254
H	4.703801	0.000000	1.338583
H	6.097393	0.000000	3.383878
C	6.576407	0.000000	6.041445
H	7.478528	0.000000	5.432734
C	4.244841	0.000000	7.614468
H	3.342643	0.000000	8.223065
C	6.691942	0.000000	7.428934
C	5.488151	0.000000	8.241087
C	7.963527	0.000000	8.092135
C	5.627021	0.000000	9.668490
C	8.047097	0.000000	9.456450
C	6.860811	0.000000	10.256794
H	8.863783	0.000000	7.481944
H	9.018004	0.000000	9.944495
H	6.949842	0.000000	11.339809
H	4.724149	0.000000	10.274805
H	-0.568152	0.871361	1.863961
H	3.046199	0.871361	-0.574510

Energy = -847.991978391
Number of Imaginary Frequencies = 0

Pentacene + C_2H_4 [1,4] TS

C	-4.439760	1.350499	-0.325303
C	-5.474153	0.690120	-1.030691
C	-5.474153	-0.690120	-1.030691
C	-4.439760	-1.350499	-0.325303
C	-3.122740	-0.722223	-0.296588
C	-3.122740	0.722223	-0.296588
C	-4.975970	-0.700110	1.706034
C	-4.975969	0.700109	1.706035
C	-1.932371	1.411583	-0.227197
C	-0.683411	0.727743	-0.177291
C	-0.683411	-0.727743	-0.177290
C	-1.932371	-1.411583	-0.227197
C	0.536958	1.406713	-0.128431
C	1.767379	0.727226	-0.076128
C	1.767379	-0.727226	-0.076128
C	0.536958	-1.406713	-0.128431
C	3.004473	1.406793	-0.024383
C	4.216921	0.726696	0.026155
C	4.216921	-0.726697	0.026155
C	3.004473	-1.406793	-0.024383
C	5.477673	1.409584	0.078407
C	6.653934	0.715889	0.127048
C	6.653934	-0.715889	0.127047
C	5.477673	-1.409584	0.078405
H	-4.466521	2.435916	-0.250699
H	-6.326310	1.253169	-1.402246
H	-6.326310	-1.253168	-1.402244
H	-4.466521	-2.435916	-0.250699
H	-1.931858	2.499874	-0.223446
H	-1.931858	-2.499873	-0.223445
H	-4.146481	-1.231860	2.161017
H	-4.146477	1.231857	2.161016
H	0.537430	2.494978	-0.130638
H	0.537430	-2.494978	-0.130638
H	3.004478	2.495110	-0.024653
H	3.004477	-2.495110	-0.024653
H	-5.920651	-1.234221	1.716337
H	-5.920649	1.234222	1.716342
H	5.475471	2.497180	0.078240
H	7.600839	1.247619	0.166294
H	7.600839	-1.247620	0.166289
H	5.475471	-2.497180	0.078238

Energy = -925.338645708
Number of Imaginary Frequencies = 1

Pentacene + C_2H_4 [1,4] Adduct

C	-4.508788	1.294586	-0.070551
C	-5.257960	0.668805	-1.236452
C	-5.257963	-0.668794	-1.236456
C	-4.508792	-1.294587	-0.070562
C	-3.102868	-0.720920	-0.067613
C	-3.102867	0.720917	-0.067604
C	-5.201381	-0.777648	1.237827
C	-5.201399	0.777635	1.237823
C	-1.931153	1.416527	-0.045721

C	-0.670081	0.726910	-0.033698
C	-0.670079	-0.726907	-0.033703
C	-1.931154	-1.416528	-0.045734
C	0.544482	1.405168	-0.023727
C	1.781941	0.725890	-0.013282
C	1.781944	-0.725888	-0.013283
C	0.544480	-1.405164	-0.023731
C	3.016286	1.405833	-0.003339
C	4.232510	0.725714	0.005923
C	4.232513	-0.725716	0.005927
C	3.016284	-1.405833	-0.003337
C	5.492710	1.408819	0.015122
C	6.671093	0.715155	0.023629
C	6.671091	-0.715157	0.023635
C	5.492707	-1.408820	0.015129
H	-4.502893	2.387591	-0.106153
H	-5.751989	1.282076	-1.984872
H	-5.752005	-1.282050	-1.984877
H	-4.502903	-2.387592	-0.106178
H	-1.928255	2.505018	-0.041975
H	-1.928261	-2.505018	-0.042002
H	-4.664242	-1.169378	2.108311
H	-4.664312	1.169386	2.108330
H	0.545021	2.493562	-0.024507
H	0.545024	-2.493558	-0.024520
H	3.016098	2.494227	-0.003512
H	3.016102	-2.494227	-0.003508
H	-6.222952	-1.169390	1.278671
H	-6.222982	1.169356	1.278623
H	5.490218	2.496438	0.014992
H	7.618391	1.247514	0.030425
H	7.618388	-1.247517	0.030420
H	5.490213	-2.496438	0.015011

Energy = -925.403346189
Number of Imaginary Frequencies = 0

Pentacene + H_2 [16,18] TS

C	2.186005	-1.349073	-0.578417
C	1.039934	-0.668577	0.030393
C	0.993116	0.805330	-0.220061
C	2.206392	1.446821	-0.203361
C	3.379719	0.641270	0.099322
C	3.382587	-0.705393	-0.555775
C	4.637687	-1.278844	-0.976740
C	5.806922	-0.604892	-0.825065
C	5.822502	0.731441	-0.265837
C	4.682854	1.332282	0.143467
C	2.954168	0.101299	1.883963
C	1.697308	-0.610825	1.880088
C	-0.265819	1.458601	-0.297460
C	-1.463656	0.771382	-0.185458
C	-1.443896	-0.691798	-0.022244
C	-0.239500	-1.357434	0.032428
C	-2.699269	-1.377240	0.043767
C	-3.904694	-0.712360	-0.020590
C	-3.920242	0.745379	-0.166110
C	-2.725430	1.431996	-0.243430
C	-5.169183	-1.401402	0.054169
C	-6.347146	-0.721362	-0.008313
C	-6.361451	0.710815	-0.151710
C	-5.195688	1.411377	-0.226948
H	2.083680	-2.373704	-0.926941
H	2.282403	2.530764	-0.238275
H	4.622430	-2.276715	-1.409862
H	6.745041	-1.055352	-1.137596
H	6.770625	1.259935	-0.203745
H	4.699352	2.349236	0.530219
H	-0.281321	2.537407	-0.441041
H	-0.233947	-2.443872	0.099595
H	3.840200	-0.490140	2.105100
H	2.966132	1.064856	2.387882
H	0.849851	-0.115862	2.347959
H	1.731872	-1.676109	2.090706
H	-2.689768	-2.459649	0.155624
H	-2.736996	2.514282	-0.357319
H	-5.157583	-2.483468	0.162478
H	-7.291277	-1.256295	0.049625
H	-7.315652	1.228418	-0.199432
H	-5.204368	2.493510	-0.335452

Energy = -925.283782606
Number of Imaginary Frequencies = 1

Pentacene + H_2 [16,18] Adduct

C	2.107200	-1.279134	-0.639266
C	1.075102	-0.691296	0.308721
C	1.016468	0.827987	0.084304
C	2.232792	1.427999	0.114482
C	3.405879	0.502259	0.357185
C	3.309926	-0.671538	-0.631045
C	4.467372	-1.052660	-1.410548
C	5.637286	-0.380082	-1.302878
C	5.767813	0.763578	-0.408534
C	4.740576	1.188583	0.348888
C	3.111512	-0.158918	1.781448
C	1.733127	-0.849056	1.760670
C	-0.244076	1.479823	-0.074504
C	-1.437644	0.791287	-0.053877
C	-1.434847	-0.680739	0.115526
C	-0.258619	-1.357480	0.257540
C	-2.707246	-1.357516	0.112402
C	-3.896614	-0.687767	-0.031908
C	-3.893759	0.773102	-0.194936
C	-2.696746	1.452837	-0.202360
C	-5.171189	-1.368503	-0.028490
C	-6.336489	-0.682716	-0.171458
C	-6.332350	0.750766	-0.332043
C	-5.161547	1.444054	-0.342897
H	1.872883	-2.149208	-1.246171
H	2.376230	2.500868	0.021855
H	4.369477	-1.896829	-2.089912
H	6.498595	-0.679679	-1.893916
H	6.722911	1.282295	-0.371979
H	4.852857	2.052756	1.001608
H	-0.251729	2.558618	-0.219962
H	-0.274165	-2.441620	0.360822
H	3.909585	-0.877535	1.990211
H	3.158494	0.624594	2.543854
H	1.051343	-0.400354	2.488742
H	1.812967	-1.915973	1.989212
H	-2.710641	-2.438882	0.234236
H	-2.696446	2.534206	-0.325248
H	-5.173190	-2.449280	0.092688
H	-7.286470	-1.210337	-0.166165
H	-7.278964	1.272241	-0.444621

H	-5.157304	2.524896	-0.463786

Energy = -925.300498660
Number of Imaginary Frequencies = 0

Pentacene + C_2H_4 [16,18] TS

C	2.186005	-1.349073	-0.578417
C	1.039934	-0.668577	0.030393
C	0.993116	0.805330	-0.220061
C	2.206392	1.446821	-0.203361
C	3.379719	0.641270	0.099322
C	3.382587	-0.705393	-0.555775
C	4.637687	-1.278844	-0.976740
C	5.806922	-0.604892	-0.825065
C	5.822502	0.731441	-0.265837
C	4.682854	1.332282	0.143467
C	2.954168	0.101299	1.883963
C	1.697308	-0.610825	1.880088
C	-0.265819	1.458601	-0.297460
C	-1.463656	0.771382	-0.185458
C	-1.443896	-0.691798	-0.022244
C	-0.239500	-1.357434	0.032428
C	-2.699269	-1.377240	0.043767
C	-3.904694	-0.712360	-0.020590
C	-3.920242	0.745379	-0.166110
C	-2.725430	1.431996	-0.243430
C	-5.169183	-1.401402	0.054169
C	-6.347146	-0.721362	-0.008313
C	-6.361451	0.710815	-0.151710
C	-5.195688	1.411377	-0.226948
H	2.083680	-2.373704	-0.926941
H	2.282403	2.530764	-0.238275
H	4.622430	-2.276715	-1.409862
H	6.745041	-1.055352	-1.137596
H	6.770625	1.259935	-0.203745
H	4.699352	2.349236	0.530219
H	-0.281321	2.537407	-0.441041
H	-0.233947	-2.443872	0.099595
H	3.840200	-0.490140	2.105100
H	2.966132	1.064856	2.387882
H	0.849851	-0.115862	2.347959
H	1.731872	-1.676109	2.090706
H	-2.689768	-2.459649	0.155624
H	-2.736996	2.514282	-0.357319
H	-5.157583	-2.483468	0.162478
H	-7.291277	-1.256295	0.049625
H	-7.315652	1.228418	-0.199432
H	-5.204368	2.493510	-0.335452

Energy = -925.283782589
Number of Imaginary Frequencies = 1

Pentacene + C_2H_4 [16,18] Adduct

C	2.107200	-1.279134	-0.639266
C	1.075102	-0.691296	0.308721
C	1.016468	0.827987	0.084304
C	2.232792	1.427999	0.114482
C	3.405879	0.502259	0.357185
C	3.309926	-0.671538	-0.631045
C	4.467372	-1.052660	-1.410548
C	5.637286	-0.380082	-1.302878
C	5.767813	0.763578	-0.408534
C	4.740576	1.188583	0.348888
C	3.111512	-0.158918	1.781448
C	1.733127	-0.849056	1.760670
C	-0.244076	1.479823	-0.074504
C	-1.437644	0.791287	-0.053877
C	-1.434847	-0.680739	0.115526
C	-0.258619	-1.357480	0.257540
C	-2.707246	-1.357516	0.112402
C	-3.896614	-0.687767	-0.031908
C	-3.893759	0.773102	-0.194936
C	-2.696746	1.452837	-0.202360
C	-5.171189	-1.368503	-0.028490
C	-6.336489	-0.682716	-0.171458
C	-6.332350	0.750766	-0.332043
C	-5.161547	1.444054	-0.342897
H	1.872883	-2.149208	-1.246171
H	2.376230	2.500868	0.021855
H	4.369477	-1.896829	-2.089912
H	6.498595	-0.679679	-1.893916
H	6.722911	1.282295	-0.371979
H	4.852857	2.052756	1.001608
H	-0.251729	2.558618	-0.219962
H	-0.274165	-2.441620	0.360822
H	3.909585	-0.877535	1.990211
H	3.158494	0.624594	2.543854
H	1.051343	-0.400354	2.488742
H	1.812967	-1.915973	1.989212
H	-2.710641	-2.438882	0.234236
H	-2.696446	2.534206	-0.325248
H	-5.173190	-2.449280	0.092688
H	-7.286470	-1.210337	-0.166165
H	-7.278964	1.272241	-0.444621
H	-5.157304	2.524896	-0.463786

Energy = -925.300498660
Number of Imaginary Frequencies = 0

Pentacene + H_2 [17,19] TS

C	6.089562	0.643155	-0.253929
C	4.930290	1.315904	-0.488391
C	3.647149	0.703038	-0.249713
C	3.617627	-0.672301	0.267968
C	4.883174	-1.336596	0.491786
C	6.063472	-0.709277	0.243820
C	2.464687	1.368029	-0.489639
C	2.420023	-1.300441	0.493602
C	1.136668	-0.637713	0.289229
C	1.196087	0.773325	-0.228908
C	-0.010159	1.418054	-0.233646
H	-0.119398	2.475473	-0.454142
C	-1.136668	0.637714	0.289231
C	-1.196086	-0.773318	-0.228913
C	0.010159	-1.418049	-0.233652
H	2.488894	2.391737	-0.858627
H	7.047925	1.119524	-0.441232
H	4.946950	2.336141	-0.864736
H	4.864323	-2.356575	0.868410
H	7.003806	-1.224264	0.421511
H	2.411583	-2.337176	0.823704
H	0.119395	-2.475470	-0.454146
C	-2.464685	-1.368026	-0.489642
H	-2.488889	-2.391735	-0.858629
C	-2.420024	1.300441	0.493602
H	-2.411585	2.337176	0.823702
C	-3.647148	-0.703038	-0.249713

C	-3.617628	0.672301	0.267967
C	-4.930288	-1.315908	-0.488388
C	-4.883176	1.336595	0.491783
C	-6.089561	-0.643159	-0.253926
C	-6.063473	0.709273	0.243819
H	-4.946947	-2.336145	-0.864731
H	-7.047923	-1.119531	-0.441227
H	-7.003807	1.224260	0.421510
H	-4.864326	2.356574	0.868405
H	0.495601	-0.292985	1.452083
H	-0.495609	0.292983	1.452068

Energy = -847.845881710
Number of Imaginary Frequencies = 1

Pentacene + H_2 [17,19] Adduct

C	-5.905779	-0.727776	-0.861729
C	-4.784982	-1.425670	-0.547102
C	-3.579599	-0.757514	-0.106359
C	-3.609052	0.718400	0.016799
C	-4.836749	1.403784	-0.354882
C	-5.929762	0.717642	-0.767659
C	-2.418833	-1.439227	0.138115
C	-2.517149	1.385758	0.465520
C	-1.269515	0.691155	0.943053
C	-1.196933	-0.783795	0.535855
C	-0.004964	-1.417184	0.574646
H	0.061592	-2.478542	0.343986
C	1.269515	-0.691152	0.943053
C	1.196933	0.783797	0.535850
C	0.004964	1.417186	0.574639
H	-2.384918	-2.513875	-0.033143
H	-6.799888	-1.247773	-1.194717
H	-4.765071	-2.510104	-0.627770
H	-4.855221	2.488476	-0.278479
H	-6.841655	1.246325	-1.032010
H	-2.541314	2.471080	0.548982
H	-0.061592	2.478544	0.343978
C	2.418833	1.439228	0.138110
H	2.384920	2.513875	-0.033150
C	2.517147	-1.385756	0.465519
H	2.541310	-2.471079	0.548977
C	3.579599	0.757513	-0.106360
C	3.609051	-0.718400	0.016799
C	4.784984	1.425668	-0.547101
C	4.836747	-1.403785	-0.354882
C	5.905780	0.727774	-0.861727
C	5.929761	-0.717645	-0.767659
H	4.765075	2.510103	-0.627767
H	6.799891	1.247769	-1.194713
H	6.841653	-1.246329	-1.032009
H	4.855218	-2.488478	-0.278481
H	-1.328886	0.696594	2.055664
H	1.328891	-0.696584	2.055664

Energy = -847.876803477
Number of Imaginary Frequencies = 0

Pentacene + C_2H_4 [17,19] TS

C	-2.465183	1.333145	0.214496
C	-1.172301	0.650906	0.194589
C	-1.194753	-0.773744	-0.266853
C	-2.449827	-1.403817	-0.523921
C	-3.646683	-0.735233	-0.400384
C	-3.647968	0.687515	-0.026237
C	-4.924805	1.365921	0.046746
C	-6.088054	0.708955	-0.201968
C	-6.084822	-0.690511	-0.552060
C	-4.914485	-1.377553	-0.646385
C	0.013747	-1.411168	-0.268314
C	1.172301	-0.650906	0.194589
C	1.194753	0.773745	-0.266851
C	0.013746	1.411169	-0.268312
C	2.449827	1.403817	-0.523920
C	3.646683	0.735234	-0.400383
C	3.647968	-0.687514	-0.026236
C	2.465183	-1.333145	0.214495
C	4.914485	1.377553	-0.646385
C	6.084822	0.690511	-0.552060
C	6.088054	-0.708954	-0.201968
C	4.924805	-1.365921	0.046746
C	0.631300	-0.352602	2.022929
C	-0.631302	0.352598	2.022929
H	-2.472930	2.396605	0.447698
H	-2.448419	-2.451785	-0.818666
H	-4.927667	2.420228	0.313641
H	-7.037346	1.234043	-0.137174
H	-7.030846	-1.189421	-0.743718
H	-4.909607	-2.431353	-0.915594
H	0.105417	-2.476253	-0.465004
H	-0.105417	2.476254	-0.465000
H	2.448419	2.451786	-0.818664
H	2.472931	-2.396605	0.447696
H	4.909608	2.431353	-0.915594
H	7.030847	1.189421	-0.743719
H	7.037346	-1.234042	-0.137175
H	4.927667	-2.420228	0.313641
H	0.619518	-1.376417	2.387660
H	1.496564	0.204369	2.375313
H	-1.496566	-0.204373	2.375310
H	-0.619520	1.376412	2.387662

Energy = -925.286462570
Number of Imaginary Frequencies = 1

Pentacene + C_2H_4 [17,19] Adduct

C	2.516872	-1.234422	0.526130
C	1.174362	-0.580318	0.558215
C	1.155001	0.818841	-0.076585
C	2.370658	1.398318	-0.567187
C	3.570767	0.738333	-0.512862
C	3.637412	-0.628073	0.052304
C	4.932213	-1.288781	0.067028
C	6.043190	-0.677677	-0.412383
C	5.974298	0.660398	-0.959530
C	4.793912	1.330367	-1.005666
C	-0.064204	1.405626	-0.063277
C	-1.174362	0.580320	0.558213
C	-1.155000	-0.818840	-0.076587
C	0.064204	-1.405625	-0.063276
C	-2.370657	-1.398316	-0.567192
C	-3.570766	-0.738333	-0.512865
C	-3.637411	0.628074	0.052301
C	-2.516872	1.234424	0.526125
C	-4.793911	-1.330370	-1.005664
C	-5.974298	-0.660402	-0.959527
C	-6.043190	0.677674	-0.412382

C	-4.932213	1.288780	0.067028
C	-0.694926	0.333062	2.065837
C	0.694924	-0.333061	2.065838
H	2.581105	-2.246827	0.923135
H	2.325034	2.396091	-1.000424
H	4.983346	-2.294001	0.478943
H	7.002180	-1.188457	-0.390880
H	6.882584	1.122867	-1.336108
H	4.741755	2.334975	-1.419239
H	-0.254066	2.410955	-0.428293
H	0.254066	-2.410954	-0.428291
H	-2.325032	-2.396091	-1.000425
H	-2.581105	2.246831	0.923126
H	-4.741754	-2.334977	-1.419236
H	-6.882584	-1.122871	-1.336103
H	-7.002180	1.188455	-0.390881
H	-4.983347	2.294001	0.478941
H	-0.681547	1.295400	2.586014
H	-1.439077	-0.302306	2.554745
H	1.439074	0.302307	2.554748
H	0.681543	-1.295400	2.586014

Energy = -925.258111561
Number of Imaginary Frequencies = 0

Pyrene (**6**)

C	3.523942	0.000000	0.000004
C	2.832984	-1.210622	0.000003
C	1.429098	-1.236257	-0.000001
C	0.713303	0.000000	-0.000001
C	1.429098	1.236258	0.000000
C	2.832982	1.210624	0.000002
C	0.680796	-2.463863	-0.000002
C	-0.713303	0.000000	-0.000001
C	-1.429096	-1.236258	-0.000001
C	-0.680793	-2.463864	-0.000003
C	-2.832983	-1.210624	0.000000
H	-3.379808	-2.150502	0.000001
C	-3.523941	-0.000002	0.000004
C	-2.832983	1.210622	0.000004
C	-1.429100	1.236258	0.000000
C	0.680795	2.463864	-0.000003
C	0.680792	2.463864	-0.000005
H	1.230409	3.402217	-0.000011
H	-1.230413	3.402216	0.000000
H	1.230411	-3.402216	-0.000005
H	4.610646	0.000002	0.000007
H	3.379811	-2.150500	0.000004
H	3.379812	2.150500	0.000001
H	-1.230410	-3.402215	-0.000006
H	-4.610646	-0.000001	0.000005
H	-3.379812	2.150498	0.000005

Energy = -615.773134321
Number of Imaginary Frequencies = 0

Pyrene + H_2 [3,13] TS

C	-3.429599	0.062444	-0.439872
C	-2.764374	1.099123	0.337939
C	-1.335777	1.261125	0.090042
C	-0.650706	0.047795	0.005524
C	-1.462205	-1.167366	0.134176
C	-2.761596	-1.113865	-0.533530
C	-0.601667	2.478889	0.085418
C	0.761610	0.005052	-0.024463
C	1.493478	1.229676	-0.077429
C	0.767551	2.460060	-0.030154
C	2.904873	1.162228	-0.138398
H	3.477168	2.085330	-0.192325
C	3.555638	-0.061115	-0.114572
C	2.832405	-1.262849	-0.019503
C	1.440034	-1.251286	0.028295
C	0.638657	-2.453967	0.154672
C	-0.714690	-2.425632	0.205917
H	-1.279031	-3.352358	0.276567
H	1.161908	-3.406872	0.198432
H	-1.133418	3.424589	0.157066
H	-4.453355	0.191655	-0.777103
H	-2.558903	0.236342	1.479414
H	-3.187988	-2.011995	-0.970301
H	1.324963	3.393143	-0.062974
H	4.641048	-0.094465	-0.156023
H	3.363100	-2.211051	0.024461
H	-2.062623	-0.668950	1.450061
H	-3.334662	1.992765	0.588357

Energy = -616.855301494
Number of Imaginary Frequencies = 1

Pyrene + H_2 [3,13] Adduct

C	3.453597	0.054037	-0.383165
C	2.866683	-1.250134	0.100616
C	1.350082	-1.236694	0.102825
C	0.662567	-0.035895	0.180757
C	1.431496	1.259376	0.407668
C	2.794718	1.205956	-0.257832
C	0.625920	-2.450907	0.004304
C	-0.757359	-0.016269	0.082279
C	-1.480594	-1.245990	0.001830
C	-0.749405	-2.461790	-0.020181
C	-2.900543	-1.209187	-0.070183
H	-3.447318	-2.148193	-0.112398
C	-3.570614	-0.006873	-0.097425
C	-2.854330	1.210809	-0.075588
C	-1.471984	1.225122	0.008322
C	-0.706530	2.467337	-0.051203
C	0.627232	2.492197	0.080147
H	1.170534	3.433317	0.018139
H	-1.259080	3.387752	-0.229384
H	1.176055	-3.388013	-0.050081
H	4.445435	0.027917	-0.829469
H	3.243634	-1.463280	1.116519
H	3.229907	2.143809	-0.597822
H	-1.291916	-3.402316	-0.080443
H	-4.655638	0.012011	-0.155368
H	-3.394194	2.152821	-0.139118
H	1.630949	1.320718	1.498142
H	3.226015	-2.083115	-0.517745

Energy = -616.921413891
Number of Imaginary Frequencies = 0

Pyrene + C_2H_4 [3,13] TS

C	0.955487	-2.446856	-0.079809
C	-0.391245	-2.419038	-0.238400
C	-1.126518	-1.167194	-0.335506
C	-0.338033	0.055403	-0.302152
C	1.071201	0.018483	-0.137171

C	1.748227	-1.235888	-0.027374
C	3.134649	-1.243480	0.126914
C	3.857206	-0.040217	0.171497
C	3.208731	1.180912	0.076655
C	1.803439	1.243147	-0.069638
C	-1.022275	1.275628	-0.330819
C	-2.473213	1.169869	-0.290843
C	-3.048567	0.083495	-1.063469
C	-2.386674	-1.101275	-1.044075
C	-2.063363	-0.756772	1.678656
C	-2.718525	0.492413	1.528570
C	1.081076	2.473999	-0.131370
C	-0.288757	2.489074	-0.234605
H	1.476715	-3.398999	-0.007329
H	-0.952352	-3.348548	-0.306783
H	3.657716	-2.192991	0.213584
H	4.937385	-0.069750	0.287651
H	3.776444	2.107362	0.121478
H	-3.020718	2.112324	-0.287487
H	-4.039146	0.186180	-1.497492
H	-2.802002	-2.007891	-1.477435
H	-1.115912	-0.810710	2.203586
H	-2.295222	1.338685	2.065543
H	1.636993	3.407111	-0.079382
H	-0.824560	3.435609	-0.253972
H	-2.646038	-1.671498	1.687448
H	-3.806368	0.482899	1.548226

Energy = -694.294057796
Number of Imaginary Frequencies = 1

Pyrene + C_2H_4 [3,13] Adduct

C	0.881141	-2.443680	-0.038583
C	-0.462885	-2.395339	-0.072464
C	-1.239095	-1.109858	-0.057836
C	-0.332146	0.106964	-0.073374
C	1.072202	0.027847	-0.029374
C	1.721977	-1.248008	-0.010183
C	3.104703	-1.292156	0.025422
C	3.866726	-0.098845	0.041791
C	3.253071	1.134838	0.021718
C	1.834150	1.237287	-0.014594
C	-0.987319	1.324833	-0.095641
C	-2.496191	1.171227	-0.101502
C	-2.880048	0.221646	-1.226756
C	-2.244424	-0.952776	-1.202143
C	-2.111899	-0.949374	1.260970
C	-2.857372	0.411371	1.228617
C	1.139848	2.476389	-0.033961
C	-0.241969	2.522327	-0.069301
H	1.388205	-3.406946	-0.038546
H	-1.038399	-3.319416	-0.099012
H	3.613492	-2.253429	0.038727
H	4.951253	-0.163519	0.069307
H	3.847101	2.045752	0.034419
H	-3.016790	2.131308	-0.157676
H	-3.639759	0.490554	-1.955084
H	-2.411599	-1.763204	-1.906049
H	-1.444538	-1.017135	2.125681
H	-2.575717	1.031746	2.085849
H	1.715995	3.398745	-0.021943
H	-0.755670	3.481127	-0.082306
H	-2.815157	-1.786883	1.319751
H	-3.941238	0.263132	1.270041

Energy = -694.334685876
Number of Imaginary Frequencies = 0

Pyrene + H_2 [4,16] TS

C	-0.486562	-3.305676	0.000000
C	0.063554	-2.777266	-1.236911
C	0.216806	-1.420239	-1.263151
C	-0.147898	-0.737001	0.000000
C	0.216806	-1.420239	1.263151
C	0.063554	-2.777266	1.236911
C	0.373270	-0.634005	-2.462539
C	-0.104022	0.729578	0.000000
C	-0.052306	1.439371	-1.226270
C	0.176791	0.707295	-2.456347
C	-0.118312	2.842856	-1.207791
H	-0.095592	3.386910	-2.148958
C	-0.179146	3.534910	0.000000
C	-0.118312	2.842856	1.207791
C	-0.052306	1.439371	1.226270
C	0.176791	0.707295	2.456347
C	0.373270	-0.634005	2.462539
H	0.588314	-1.157010	3.391425
H	0.240164	1.275435	3.381373
H	0.588314	-1.157010	-3.391425
H	-0.805136	-4.346630	0.000000
H	0.114991	-3.388865	-2.132992
H	0.114991	-3.388865	2.132992
H	0.240164	1.275435	-3.381373
H	-0.233714	4.620248	0.000000
H	-0.095592	3.386910	2.148958
H	-1.470774	-1.320555	0.000000
H	-1.598005	-2.413023	0.000000

Energy = -616.839449029
Number of Imaginary Frequencies = 1

Pyrene + H_2 [4,16] Adduct

C	-0.221015	-3.565877	0.000000
C	-0.192504	-2.736396	1.253181
C	0.085206	-1.420087	1.268889
C	0.501097	-0.691543	0.000000
C	0.085206	-1.420087	-1.268889
C	-0.192504	-2.736396	-1.253181
C	0.064967	-0.629025	2.491805
C	0.145662	0.788069	0.000000
C	0.041799	1.477662	1.219938
C	0.079785	0.721481	2.470083
C	-0.141461	2.871201	1.206954
H	-0.223684	3.405531	2.150589
C	-0.225200	3.562760	0.000000
C	-0.141461	2.871201	-1.206954
C	0.041799	1.477662	-1.219938
C	0.079785	0.721481	-2.470083
C	0.064967	-0.629025	-2.491805
H	-0.006786	-1.160661	-3.438471
H	0.043372	1.283742	-3.400510
H	-0.006786	-1.160661	3.438471
H	-1.114637	-4.210570	0.000000
H	-0.420389	-3.244087	2.189620
H	-0.420389	-3.244087	-2.189620
H	0.043372	1.283742	3.400510
H	-0.363157	4.640631	0.000000

H	-0.223684	3.405531	-2.150589
H	1.611114	-0.699332	0.000000
H	0.624887	-4.278256	0.000000

Energy = -616.901413840
Number of Imaginary Frequencies = 0

Pyrene + C_2H_4 [4,16] TS

C	0.978934	-2.460828	-0.291259
C	-0.338459	-2.464921	-0.611357
C	-1.126406	-1.255361	-0.579398
C	-0.477367	0.000000	-0.172584
C	0.982683	0.000000	-0.070481
C	1.693499	-1.226504	-0.029290
C	3.083117	-1.207846	0.177443
C	3.766841	-0.000002	0.301558
C	3.083118	1.207843	0.177444
C	1.693500	1.226503	-0.029288
C	-1.126404	1.255364	-0.579396
C	-2.489745	1.229128	-0.667853
C	-3.140840	0.000003	-0.261123
C	-2.489746	-1.229123	-0.667855
C	-1.253960	0.000001	1.765412
C	-2.678316	-0.000007	1.638384
C	0.978937	2.460828	-0.291256
C	-0.338456	2.464923	-0.611354
H	1.544346	-3.389732	-0.276027
H	-0.844726	-3.397007	-0.852350
H	3.625067	-2.149669	0.219846
H	4.841358	-0.000003	0.464136
H	3.625069	2.149665	0.219847
H	-3.069364	2.136111	-0.820223
H	-4.229690	0.000004	-0.273472
H	-3.069367	-2.136105	-0.820224
H	-0.764013	-0.910720	2.096965
H	-0.764022	0.910729	2.096962
H	-3.199924	-0.904736	1.943214
H	-3.199936	0.904713	1.943216
H	1.544350	3.389731	-0.276025
H	-0.844722	3.397010	-0.852346

Energy = -694.279321503
Number of Imaginary Frequencies = 1

Pyrene + C_2H_4 [4,16] Adduct

C	-0.972470	2.450508	-0.318943
C	0.331332	2.451551	-0.677151
C	1.153415	1.268511	-0.545129
C	0.539542	-0.000002	0.048928
C	-0.971395	0.000001	0.034502
C	-1.680985	1.218128	0.012647
C	-3.078800	1.205277	0.166027
C	-3.768089	-0.000002	0.278283
C	-3.078798	-1.205282	0.166029
C	-1.680984	-1.218128	0.012651
C	1.153412	-1.268500	-0.545131
C	2.498019	-1.237535	-0.635471
C	3.133328	-0.000002	-0.054987
C	2.498024	1.237541	-0.635452
C	1.131435	0.000005	1.542895
C	2.678281	-0.000012	1.470325
C	-0.972467	-2.450509	-0.318939
C	0.331334	-2.451547	-0.677154
H	-1.553405	3.368998	-0.361329
H	0.812190	3.370158	-1.006557
H	-3.620470	2.148241	0.167231
H	-4.847401	0.000000	0.404997
H	-3.620464	-2.148249	0.167233
H	3.096453	-2.095334	-0.931442
H	4.222695	-0.000002	-0.136143
H	3.096461	2.095343	-0.931405
H	0.750548	0.884610	2.062147
H	0.750535	-0.884588	2.062159
H	3.094648	0.884384	1.963718
H	3.094630	-0.884424	1.963704
H	-1.553400	-3.369000	-0.361324
H	0.812196	-3.370147	-1.006566

Energy = -694.304318173
Number of Imaginary Frequencies = 0

Pyrene + H_2 [11,12] TS

C	0.030422	0.315570	-3.446609
C	1.215763	0.332435	-2.755757
C	1.246288	0.157206	-1.312504
C	-0.064205	-0.106420	-0.688764
C	-1.284352	-0.107184	-1.436287
C	-1.219864	0.090340	-2.809056
C	2.373665	-0.585085	-0.670138
C	-0.064205	-0.106420	0.688764
C	1.246288	0.157206	1.312504
C	2.373665	-0.585085	0.670138
C	1.215763	0.332435	2.755757
H	2.155869	0.464977	3.285600
C	0.030422	0.315570	3.446609
C	-1.219864	0.090340	2.809056
C	-1.284352	-0.107184	1.436287
C	-2.507730	-0.255870	0.681674
C	-2.507730	-0.255870	-0.681674
H	-3.446013	-0.322486	-1.227542
H	-3.446013	-0.322486	1.227542
H	3.146595	-1.037161	-1.283298
H	0.043106	0.458842	-4.524494
H	2.155869	0.464977	-3.285600
H	-2.131463	0.089602	-3.401226
H	3.146595	-1.037161	1.283298
H	0.043106	0.458842	4.524494
H	-2.131463	0.089602	3.401226
H	1.491985	1.300274	0.580604
H	1.491985	1.300274	-0.580604

Energy = -616.821129420
Number of Imaginary Frequencies = 1

Pyrene + H_2 [11,12] Adduct

C	-0.011280	-0.155811	3.512128
C	-1.192754	0.020934	2.884032
C	-1.272123	0.372465	1.422530
C	0.046680	0.187834	0.681121
C	1.281103	0.032875	1.432040
C	1.241467	-0.104210	2.799507
C	-2.403237	-0.312230	0.665616
C	0.046680	0.187834	-0.681121
C	-1.272123	0.372465	-1.422530
C	-2.403237	-0.312230	-0.665616
C	-1.192754	0.020934	-2.884032
H	-2.129582	-0.032216	-3.434659
H	-0.011280	-0.155811	-3.512128

C	1.241467	-0.104210	-2.799507
C	1.281103	0.032875	-1.432040
C	2.512458	-0.032744	-0.678301
C	2.512458	-0.032744	0.678301
H	3.446391	-0.111255	1.230201
H	3.446391	-0.111255	-1.230201
H	-3.201313	-0.775262	1.240924
H	0.010902	-0.358598	4.580350
H	-2.129582	-0.032216	3.434659
H	2.168787	-0.237507	3.351013
H	-3.201313	-0.775262	-1.240924
H	0.010902	-0.358598	-4.580350
H	2.168787	-0.237507	-3.351013
H	-1.509063	1.460159	-1.377893
H	-1.509063	1.460159	1.377893

Energy = -616.855094794
Number of Imaginary Frequencies = 0

Pyrene + C_2H_4 [11,12] TS

C	-0.680429	2.724216	0.015433
C	0.680430	2.724216	0.015433
C	1.435387	1.495194	-0.072536
C	0.688852	0.279364	-0.244901
C	-0.688852	0.279364	-0.244901
C	-1.435387	1.495194	-0.072536
C	-2.815923	1.427486	0.021156
C	-3.487159	0.172752	-0.063878
C	-2.804662	-1.001795	-0.215248
C	-1.345806	-1.039414	-0.221642
C	1.345806	-1.039415	-0.221641
C	2.804662	-1.001795	-0.215247
C	3.487159	0.172752	-0.063878
C	2.815923	1.427486	0.021155
C	-0.670236	-2.061311	-1.060341
C	0.670237	-2.061311	-1.060340
C	-0.722414	-1.645715	1.507990
C	0.722413	-1.645716	1.507990
H	-1.228678	3.658972	0.108620
H	1.228678	3.658972	0.108621
H	-3.395514	2.338777	0.145428
H	-4.574084	0.161032	-0.031546
H	-3.345151	-1.940834	-0.313937
H	3.345151	-1.940834	-0.313932
H	4.574083	0.161032	-0.031546
H	3.395514	2.338777	0.145424
H	-1.268206	-2.795182	-1.593397
H	1.268206	-2.795184	-1.593393
H	-1.212836	-0.908645	2.139126
H	-1.206286	-2.618771	1.549501
H	1.212836	-0.908647	2.139127
H	1.206284	-2.618772	1.549500

Energy = -694.256871416
Number of Imaginary Frequencies = 1

Pyrene + C_2H_4 [11,12] Adduct

C	-0.680153	2.748068	0.020277
C	0.680165	2.748066	0.020287
C	1.441977	1.515853	-0.018018
C	0.678831	0.294253	-0.074762
C	-0.678827	0.294254	-0.074782
C	-1.441971	1.515855	-0.018048
C	-2.815086	1.439780	-0.008343
C	-3.482192	0.159460	-0.065177
C	-2.810804	-1.015270	-0.111326
C	-1.315463	-1.081105	-0.069152
C	1.315460	-1.081107	-0.069162
C	2.810797	-1.015277	-0.111350
C	3.482191	0.159445	-0.065180
C	2.815089	1.439773	-0.008312
C	-0.666488	-1.914760	-1.179277
C	0.666472	-1.914713	-1.179319
C	-0.771140	-1.772059	1.272266
C	0.771139	-1.772091	1.272240
H	-1.226479	3.688111	0.051823
H	1.226493	3.688108	0.051830
H	-3.413570	2.346411	0.029485
H	-4.569829	0.153824	-0.079827
H	-3.354590	-1.956774	-0.163988
H	3.354576	-1.956786	-0.164035
H	4.569831	0.153815	-0.079836
H	3.413578	2.346403	0.029522
H	-1.283478	-2.470181	-1.879209
H	1.283459	-2.470108	-1.879279
H	-1.171228	-1.216295	2.124892
H	-1.169614	-2.790336	1.318315
H	1.171270	-1.216374	2.124880
H	1.169574	-2.790383	1.318248

Energy = -694.272372350
Number of Imaginary Frequencies = 0

Pyrene + H_2 [6,15] TS

C	3.487397	0.051852	-0.266092
C	2.822628	-1.133178	-0.463832
C	1.420204	-1.233256	-0.221646
C	0.695019	-0.040006	0.266133
C	1.415955	1.238012	0.255817
C	2.784506	1.238141	0.076915
C	0.716941	-2.419061	-0.125447
C	-0.746949	0.019760	-0.009680
C	-1.431990	-1.198133	0.084253
C	-0.564344	-2.316583	0.513930
C	-2.822904	-1.225964	-0.065091
H	-3.364438	-2.165359	0.012291
C	-3.508150	-0.031171	-0.302694
C	-2.834074	1.191852	-0.308558
C	-1.442401	1.242020	-0.122131
C	-0.694689	2.471676	0.047581
C	0.645397	2.461554	0.272334
H	1.186962	3.399415	0.374122
H	-1.234324	3.414460	-0.002392
H	1.208877	-3.380943	-0.240662
H	4.561600	0.102546	-0.422239
H	3.360155	-2.023414	-0.781225
H	3.323325	2.182801	0.103782
H	-0.087538	-1.610581	1.645296
H	-4.585920	-0.049292	-0.440936
H	-3.390604	2.118677	-0.425899
H	0.433569	-0.652573	1.590353
H	-1.066945	-3.240830	0.796753

Energy = -616.840638862
Number of Imaginary Frequencies = 1

Pyrene + H_2 [6,15] Adduct

C	-3.513604	0.005287	-0.240057
C	-2.865231	1.196857	-0.163121
C	-1.433278	1.268998	0.054946
C	-0.735011	-0.013223	0.489602
C	-1.460468	-1.288441	0.074289
C	-2.797720	-1.246642	-0.173297
C	-0.738509	2.419235	-0.054380
C	0.751188	-0.014317	0.166835
C	1.457959	1.184617	0.051757
C	0.742985	2.516698	0.160263
C	2.843313	1.150107	-0.161966
H	3.390662	2.085604	-0.255268
C	3.521606	-0.064445	-0.251837
C	2.816930	-1.260447	-0.145393
C	1.427792	-1.251789	0.054742
C	0.665491	-2.490819	0.088637
C	-0.690853	-2.505371	0.060048
H	-1.226336	-3.448962	-0.022971
H	1.221341	-3.424881	0.050043
H	1.269188	3.341710	-0.285488
H	-4.584499	-0.018091	-0.424696
H	-3.403819	2.129152	-0.318415
H	-3.338677	-2.171488	-0.362349
H	0.944684	2.960302	1.152257
H	4.596515	-0.077284	-0.411346
H	3.335597	-2.212536	-0.230793
H	-0.802322	-0.028470	1.598332
H	1.180501	3.227098	-0.555713

Energy = -616.903661581
Number of Imaginary Frequencies = 0

Pyrene + C_2H_4 [6,15] TS

C	-0.699250	2.624904	0.213643
C	0.651468	2.590059	0.363470
C	1.411709	1.385116	0.128554
C	0.684468	0.128387	-0.030765
C	-0.758396	0.208082	-0.223349
C	-1.454648	1.435627	-0.116649
C	-2.849999	1.428960	-0.283092
C	-3.533448	0.232154	-0.496874
C	-2.848113	-0.986543	-0.506091
C	-1.456913	-1.001837	-0.364204
C	1.389505	-1.000381	-0.647135
C	2.798102	-0.889382	-0.859775
C	3.475527	0.255949	-0.520409
C	2.783171	1.399608	-0.040346
C	0.491846	-0.810389	1.910513
C	-0.628705	-2.210825	-0.185750
C	0.672196	-2.172147	-0.792277
C	-0.202529	-2.037402	1.669454
H	-1.239676	3.560746	0.336351
H	1.199603	3.503062	0.585646
H	-3.397644	2.366788	-0.225426
H	-4.612715	0.243917	-0.623950
H	-3.393821	-1.921182	-0.612661
H	3.328268	-1.741426	-1.278695
H	4.551604	0.311372	-0.662825
H	3.331168	2.325009	0.122199
H	-0.038004	0.013555	2.376929
H	1.558138	-0.834575	2.112273
H	-1.168539	-3.155765	-0.249887
H	1.166721	-3.092921	-1.091914
H	0.366514	-2.953160	1.815658
H	-1.207566	-2.105054	2.082791

Energy = -694.282082344
Number of Imaginary Frequencies = 1

Pyrene + C_2H_4 [6,15] Adduct

C	-0.669510	2.611778	0.243568
C	0.671141	2.558587	0.450961
C	1.428770	1.343469	0.241057
C	0.683919	0.025961	0.244471
C	-0.779587	0.185172	-0.118074
C	-1.434111	1.427109	-0.115465
C	-2.812129	1.446628	-0.402698
C	-3.505183	0.258597	-0.629220
C	-2.856408	-0.978623	-0.524210
C	-1.487987	-1.007740	-0.253385
C	1.352270	-1.056467	-0.611937
C	2.722613	-0.882121	-1.022705
C	3.411842	0.244872	-0.697166
C	2.750729	1.376398	-0.093393
C	0.615685	-0.654719	1.692204
C	-0.641700	-2.217382	0.085729
C	0.633234	-2.197118	-0.715359
C	-0.184922	-1.980685	1.586255
H	-1.196661	3.560116	0.318307
H	1.224723	3.472545	0.657130
H	-3.338259	2.398108	-0.431131
H	-4.568586	0.291160	-0.851827
H	-3.417121	-1.904242	-0.631018
H	3.202319	-1.690417	-1.569977
H	4.458536	0.342302	-0.973201
H	3.290489	2.319945	-0.038152
H	0.140479	0.046385	2.385004
H	1.639965	-0.825943	2.037333
H	-1.194450	-3.155744	-0.009330
H	1.017795	-3.097352	-1.188030
H	0.423103	-2.832245	1.906911
H	-1.074340	-1.946919	2.224189

Energy = -694.310574723
Number of Imaginary Frequencies = 0

Phenanthrene (**7**)

C	3.561749	-0.296289	0.000037
C	2.837357	0.879087	0.000110
C	1.422927	0.865935	0.000061
C	0.728914	-0.380857	-0.000017
C	1.500350	-1.566897	-0.000137
C	2.882889	-1.529311	-0.000110
C	0.679768	2.093903	0.000048
C	-0.728915	-0.380854	0.000009
C	-1.422926	0.865934	-0.000067
C	-0.679768	2.093903	-0.000057
C	-2.837359	0.879086	-0.000099
H	-3.347931	1.839423	-0.000175
C	-3.561748	-0.296288	-0.000025
C	-2.882887	-1.529313	0.000111
C	-1.500351	-1.566899	0.000132
H	1.232801	3.030199	0.000111
H	4.648016	-0.271906	0.000078
H	3.347931	1.839422	0.000189
H	1.006855	-2.532895	-0.000308

H	3.446802	-2.458243	-0.000224
H	-1.232800	3.030199	-0.000119
H	-4.648016	-0.271911	-0.000049
H	-3.446806	-2.458241	0.000221
H	-1.006847	-2.532892	0.000291

Energy = -539.538656243
Number of Imaginary Frequencies = 0

Phenanthrene + H_2 [1,4] TS

C	3.451295	-0.274515	-0.442915
C	2.785762	0.805698	0.238238
C	1.339356	0.895897	0.065695
C	0.665889	-0.330188	0.092840
C	1.545141	-1.478941	0.301882
C	2.798775	-1.473093	-0.409694
C	0.615864	2.118267	0.004373
C	-0.769026	-0.369806	0.040827
C	-1.477884	0.872187	-0.047894
C	-0.751565	2.101343	-0.063011
C	-2.894653	0.855472	-0.111707
H	-3.422548	1.803914	-0.181819
C	-3.595234	-0.330937	-0.084001
C	-2.898270	-1.556218	0.000385
C	-1.519821	-1.573331	0.055381
H	1.159398	3.059873	0.000275
H	4.474076	-0.169108	-0.791421
H	3.328383	1.736974	0.391597
H	2.154726	-0.852532	1.555190
H	3.260608	-2.403523	-0.725837
H	-1.310411	3.032022	-0.126211
H	-4.680771	-0.327076	-0.132044
H	-3.451244	-2.491665	0.014494
H	-1.002068	-2.526483	0.099983
H	1.091068	-2.441992	0.520156
H	2.625008	0.008579	1.533235

Energy = -540.634571172
Number of Imaginary Frequencies = 1

Phenanthrene + H_2 [1,4] Adduct

C	3.554829	-0.339931	0.000000
C	2.846956	0.982674	0.000000
C	1.334065	0.884626	0.000000
C	0.664996	-0.327074	0.000000
C	1.418932	-1.643667	0.000000
C	2.915234	-1.508803	0.000000
C	0.597733	2.102131	0.000000
C	-0.771818	-0.346031	0.000000
C	-1.497484	0.889513	0.000000
C	-0.772163	2.111203	0.000000
C	-2.916298	0.867968	0.000000
H	-3.449767	1.815956	0.000000
C	-3.608658	-0.322309	0.000000
C	-2.899943	-1.544845	0.000000
C	-1.520989	-1.555194	0.000000
H	1.147030	3.041527	0.000000
H	4.643175	-0.313970	0.000000
H	3.171456	1.575569	-0.871000
H	1.112847	-2.245745	0.870977
H	3.482324	-2.438275	0.000000
H	-1.320657	3.050295	0.000000
H	-4.695296	-0.325261	0.000000
H	-3.446666	-2.484219	0.000000
H	-1.001062	-2.507237	0.000000
H	1.112840	-2.245745	-0.870975
H	3.171427	1.575548	0.871025

Energy = -540.719079071
Number of Imaginary Frequencies = 0

Phenanthrene + C_2H_4 [1,4] TS

C	-2.405876	1.006914	-0.360958
C	-3.038343	-0.024145	-1.120789
C	-2.431108	-1.249152	-1.121153
C	-1.224526	-1.383887	-0.364857
C	-0.328687	-0.244380	-0.312846
C	-0.958038	1.008346	-0.306675
C	-2.078390	-1.100515	1.597121
C	-2.702159	0.158364	1.597634
C	-0.193051	2.198016	-0.141531
C	1.167254	2.135670	-0.010546
C	1.850421	0.881649	-0.016915
C	1.101581	-0.331356	-0.161484
C	3.259402	0.815071	0.124461
C	3.919552	-0.395043	0.130594
C	3.186173	-1.592211	-0.013324
C	1.814066	-1.558454	-0.160209
H	-2.900599	1.974171	-0.291262
H	-4.028420	0.130503	-1.540885
H	-2.911442	-2.129774	-1.539227
H	-0.792396	-2.377578	-0.292165
H	-1.134405	-1.222748	2.119340
H	-2.227357	0.981741	2.122272
H	-0.704826	3.157671	-0.129938
H	1.752873	3.044979	0.102372
H	-2.693162	-1.994651	1.563972
H	-3.786043	0.210823	1.566266
H	3.814503	1.744529	0.230470
H	5.000020	-0.429827	0.240881
H	3.705789	-2.546781	-0.016084
H	1.275847	-2.492378	-0.287140

Energy = -618.070040213
Number of Imaginary Frequencies = 1

Phenanthrene + C_2H_4 [1,4] Adduct

C	-2.452675	0.937404	-0.092266
C	-2.881238	0.037008	-1.239654
C	-2.291393	-1.161489	-1.235539
C	-1.320800	-1.372220	-0.083354
C	-0.317591	-0.225681	-0.080213
C	-0.935655	1.015238	-0.081881
C	-2.165999	-1.209664	1.233645
C	-2.853393	0.181871	1.226922
C	-0.179148	2.204870	-0.038961
C	1.196782	2.139340	-0.006914
C	1.868151	0.888514	-0.007434
C	1.101208	-0.329364	-0.039429
C	3.287292	0.809993	0.023918
C	3.933197	-0.404239	0.026762
C	3.181394	-1.604057	-0.002693
C	1.805799	-1.566677	-0.035007
H	-2.914892	1.927853	-0.132131
H	-3.626365	0.356797	-1.962535
H	-2.491290	-1.950105	-1.955444
H	-0.849661	-2.355945	-0.114959
H	-1.505556	-1.318869	2.100325

H	-2.543790	0.778009	2.091884
H	-0.685258	3.167684	-0.036784
H	1.790742	3.050049	0.017646
H	-2.907355	-2.014030	1.281807
H	-3.943107	0.083536	1.268080
H	3.856960	1.736459	0.046415
H	5.018758	-0.447492	0.050681
H	3.696719	-2.561029	-0.001794
H	1.248515	-2.498001	-0.060603

Energy = -618.125366220
Number of Imaginary Frequencies = 0

Phenanthrene + H_2 [9,13] TS

C	-3.462313	-0.356359	-0.391013
C	-2.748843	0.785298	-0.620129
C	-1.370988	0.880800	-0.241193
C	-0.713802	-0.281541	0.389808
C	-1.525482	-1.469816	0.582404
C	-2.841217	-1.490490	0.228578
C	-0.649877	2.060693	-0.189851
C	0.741646	-0.401121	0.100153
C	1.445166	0.816678	0.166632
C	0.603111	1.984845	0.496739
C	2.832147	0.841049	-0.015964
H	3.370658	1.783665	0.047715
C	3.510382	-0.342438	-0.295650
C	2.810308	-1.553115	-0.378920
C	1.432748	-1.587405	-0.175460
H	-1.106873	3.016816	-0.429110
H	-4.511271	-0.411689	-0.668643
H	-3.220535	1.654620	-1.072747
H	-1.061986	-2.346598	1.026310
H	-3.433434	-2.385632	0.401263
H	0.073502	1.338047	1.676546
H	4.585426	-0.325856	-0.453830
H	3.343688	-2.471996	-0.607385
H	0.893967	-2.527426	-0.252703
H	-0.431794	0.440458	1.661886
H	1.120733	2.913132	0.733870

Energy = -540.620492151
Number of Imaginary Frequencies = 1

Phenanthrene + H_2 [9,13] Adduct

C	-3.545810	-0.352210	-0.166458
C	-2.912206	0.820196	0.056183
C	-1.456772	0.886407	0.155181
C	-0.736581	-0.416600	0.487373
C	-1.457453	-1.613458	-0.115936
C	-2.778099	-1.577691	-0.358458
C	-0.795838	2.045097	-0.009560
C	0.768210	-0.371609	0.211605
C	1.428456	0.844845	-0.026885
C	0.694978	2.170477	-0.000255
C	2.810735	0.844908	-0.261216
H	3.309601	1.792199	-0.457244
C	3.550803	-0.332741	-0.239854
C	2.903666	-1.539587	0.030310
C	1.529408	-1.550116	0.253225
H	-1.365386	2.960038	-0.169543
H	-4.626182	-0.382981	-0.280611
H	-3.467075	1.755493	0.090576
H	-0.895017	-2.524880	-0.290075
H	-3.292017	-2.461044	-0.730154
H	1.012120	2.740101	0.890974
H	4.621691	-0.309423	-0.423369
H	3.465315	-2.469252	0.067644
H	1.044930	-2.496301	0.476587
H	-0.846493	-0.541293	1.584642
H	1.017523	2.789843	-0.850952

Energy = -540.676477915
Number of Imaginary Frequencies = 0

Phenanthrene + C_2H_4 [9,13] TS

C	0.656867	1.845226	-0.384527
C	-0.624469	1.716748	-1.003561
C	-1.354077	0.579979	-0.705453
C	-0.699319	-0.434925	0.122093
C	0.760421	-0.572930	-0.058747
C	1.465383	0.615271	-0.340719
C	2.857090	0.589219	-0.497159
C	3.549420	-0.613642	-0.398187
C	2.852349	-1.799303	-0.132270
C	1.471403	-1.780374	0.038466
C	-1.502820	-1.559545	0.543819
C	-2.832781	-1.635487	0.249879
C	-3.468873	-0.625716	-0.543220
C	-2.749349	0.437141	-1.008653
C	0.196470	1.995739	1.502903
C	-0.502084	0.833588	1.922391
H	1.212308	2.761949	-0.581074
H	-1.096767	2.569894	-1.484282
H	3.390105	1.513918	-0.707809
H	4.627449	-0.633833	-0.534110
H	3.389572	-2.741931	-0.068349
H	0.941980	-2.710960	0.219537
H	-1.034684	-2.341096	1.135684
H	-3.420410	-2.477607	0.606443
H	-4.527937	-0.713826	-0.769952
H	-3.225726	1.210738	-1.607008
H	1.206367	2.125692	1.886804
H	-0.364309	2.926694	1.465385
H	0.020436	0.081687	2.503857
H	-1.572161	0.882740	2.092564

Energy = -618.056840184
Number of Imaginary Frequencies = 1

Phenanthrene + C_2H_4 [9,13] Adduct

C	0.720764	1.901666	-0.209444
C	-0.533722	1.716792	-1.031359
C	-1.296063	0.660089	-0.676703
C	-0.725323	-0.150919	0.499145
C	0.722632	-0.515495	0.145115
C	1.494391	0.595044	-0.232807
C	2.837235	0.438751	-0.562709
C	3.414025	-0.836295	-0.528231
C	2.645469	-1.941449	-0.163389
C	1.296240	-1.783497	0.176632
C	-1.586562	-1.314590	0.896347
C	-2.755595	-1.591087	0.290290
C	-3.252776	-0.789264	-0.820749
C	-2.556209	0.278625	-1.275194
C	0.256999	2.095788	1.277667
C	-0.603741	0.879796	1.701914
H	1.328892	2.746129	-0.545036

H	-0.802294	2.407417	-1.826354
H	3.432878	1.302406	-0.850955
H	4.460173	-0.964420	-0.793989
H	3.091493	-2.932574	-0.149140
H	0.698038	-2.649497	0.446477
H	-1.242432	-1.920627	1.732181
H	-3.358063	-2.430955	0.628613
H	-4.198632	-1.064728	-1.279323
H	-2.928378	0.876211	-2.104839
H	1.140379	2.189234	1.918082
H	-0.311176	3.027794	1.358331
H	-0.163372	0.361629	2.560440
H	-1.614089	1.188244	1.986359

Energy = -618.095908012
Number of Imaginary Frequencies = 0

Phenanthrene + H_2 [3,11] TS

C	-3.306617	-0.398548	0.453160
C	-2.770441	0.909605	0.158733
C	-1.415645	0.951846	-0.054520
C	-0.737172	-0.356826	0.038619
C	-1.465802	-1.458615	-0.606108
C	-2.798479	-1.484392	-0.384544
C	-0.629940	2.155197	-0.159578
C	0.742437	-0.361473	0.044509
C	1.450696	0.865742	-0.044590
C	0.724401	2.113967	-0.157965
C	2.859811	0.846241	-0.031577
H	3.397110	1.789379	-0.101246
C	3.558828	-0.347702	0.068123
C	2.858650	-1.558221	0.163530
C	1.468710	-1.558282	0.153531
H	-1.155495	3.105143	-0.224252
H	-4.336543	-0.462068	0.799281
H	-3.367116	1.808244	0.285242
H	-0.928567	-2.234799	-1.140353
H	-3.446600	-2.294756	-0.702857
H	1.302371	3.032239	-0.229835
H	4.645444	-0.343331	0.078452
H	3.399961	-2.496113	0.253030
H	0.930949	-2.497415	0.252681
H	-1.331320	-0.653352	1.363708
H	-2.346823	-0.664411	1.518211

Energy = -540.618248268
Number of Imaginary Frequencies = 1

Phenanthrene + H_2 [3,11] Adduct

C	-3.510688	-0.306384	-0.445948
C	-2.668619	0.930044	-0.329661
C	-1.392004	0.939355	0.093892
C	-0.696091	-0.310638	0.618682
C	1.503714	-1.561659	0.366491
C	-2.755021	-1.558390	-0.096200
C	-0.596586	2.160532	0.120635
C	0.779836	-0.372418	0.200238
C	1.482282	0.852248	0.083607
C	0.751810	2.115324	0.159625
C	2.862453	0.838144	-0.165468
H	3.391121	1.784761	-0.254371
C	3.551571	-0.363323	-0.317977
C	2.856599	-1.567720	-0.225654
C	1.481727	-1.565859	0.034945
H	-1.115221	3.114431	0.049960
H	-3.920657	-0.384495	-1.466966
H	-3.129098	1.870607	-0.631297
H	-1.044892	-2.509800	0.635047
H	-3.283307	-2.502268	-0.221152
H	1.333148	3.034717	0.148858
H	4.620519	-0.358034	-0.513416
H	3.378158	-2.512774	-0.351827
H	0.964774	-2.517203	0.105574
H	-0.652252	-0.175486	1.718530
H	-4.403619	-0.219999	0.197814

Energy = -540.680631308
Number of Imaginary Frequencies = 0

Phenanthrene + C_2H_4 [3,11] TS

C	-1.128874	2.168965	0.004947
C	0.211680	2.287948	-0.149897
C	1.055672	1.131669	-0.324916
C	0.456077	-0.207000	-0.318271
C	-1.011692	-0.303814	-0.183605
C	-1.782718	0.876992	-0.006003
C	-3.179697	0.773618	0.145004
C	-3.814209	-0.459788	0.126128
C	-3.055358	-1.626076	-0.039605
C	-1.675695	-1.543179	-0.188227
C	1.184631	-1.211787	-1.081411
C	2.534872	-1.135144	-1.094381
C	3.135099	-0.061048	-0.317332
C	2.426837	1.190166	-0.355223
C	1.243733	-0.771875	1.609023
C	2.655268	-0.674108	1.522415
H	-1.749076	3.051799	0.141150
H	0.685257	3.267108	-0.135088
H	-3.759784	1.684260	0.277139
H	-4.892679	-0.520956	0.244450
H	-3.542288	-2.597560	-0.045934
H	-1.098641	-2.457632	-0.293283
H	0.646736	-2.020966	-1.565059
H	3.159156	-1.888406	-1.566679
H	4.222541	-0.014849	-0.295302
H	2.954625	2.132205	-0.229089
H	0.693976	-0.017005	2.162439
H	0.780841	-1.753030	1.612742
H	3.142156	0.123225	2.078179
H	3.223415	-1.601423	1.522454

Energy = -618.054542816
Number of Imaginary Frequencies = 1

Phenanthrene + C_2H_4 [3,11] Adduct

C	-1.123252	2.179556	-0.011429
C	0.218197	2.319217	-0.084383
C	1.097529	1.174627	-0.132247
C	0.521048	-0.247463	-0.057335
C	-0.995599	-0.309489	-0.042102
C	-1.771211	0.872984	0.003039
C	-3.172708	0.774421	0.042430
C	-3.809036	-0.463146	0.034655
C	-3.044210	-1.629842	-0.014762
C	-1.651068	-1.544131	-0.052395
C	1.164546	-1.078932	-1.167604
C	2.496979	-1.022670	-1.206617
C	3.113928	-0.144788	-0.130905

C	2.444572	1.210284	-0.172653
C	1.129729	-0.836137	1.294865
C	2.674813	-0.787507	1.240159
H	-1.764867	3.056920	0.026110
H	0.669468	3.309014	-0.108051
H	-3.761577	1.688502	0.075332
H	-4.893904	-0.518254	0.065007
H	-3.527301	-2.603199	-0.023383
H	-1.063170	-2.458249	-0.089434
H	0.548401	-1.667264	-1.840497
H	3.114387	-1.566711	-1.915639
H	4.202431	-0.083845	-0.203755
H	3.020056	2.132088	-0.176026
H	0.739213	-0.245784	2.129636
H	0.768983	-1.860901	1.422415
H	3.080805	-0.191118	2.063625
H	3.101544	-1.793113	1.318360

Energy = -618.091363915
Number of Imaginary Frequencies = 0

Phenanthrene + H_2 [2,12] TS

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.332625
C	1.254811	0.000000	2.174146
C	2.514381	0.249739	1.356959
C	2.493486	0.251592	0.014270
C	1.261747	0.028468	-0.818241
C	1.169265	0.959914	3.347993
C	3.742105	0.536227	2.136192
C	3.608658	1.182154	3.392077
C	2.269723	1.485585	3.902513
C	4.758333	1.528427	4.114910
H	4.647444	2.033824	5.071820
C	6.029216	1.228931	3.628196
C	6.162155	0.573846	2.402180
C	5.026593	0.233265	1.666970
H	0.183467	1.168364	3.758883
H	-0.943196	-0.020440	-0.543434
H	-0.942773	-0.023095	1.878414
H	3.412397	0.458459	-0.531379
H	1.191236	0.813548	-1.588441
H	2.196352	2.132649	4.774403
H	6.910236	1.497194	4.204999
H	7.147924	0.320419	2.021327
H	5.136523	-0.294853	0.723858
H	1.345491	-1.011571	2.622283
H	1.357337	-0.909189	-1.393932

Energy = -540.678942314
Number of Imaginary Frequencies = 1

Phenanthrene + H_2 [2,12] Adduct

C	-3.525036	-0.215581	-0.109322
C	-2.843371	0.859103	0.285995
C	-1.358546	0.858053	0.565284
C	-0.673297	-0.423996	0.114213
C	-1.377335	-1.495039	-0.286353
C	-2.878269	-1.552138	-0.349408
C	-0.657443	2.078693	-0.004947
C	0.808400	-0.392660	0.100875
C	1.454781	0.845617	-0.146390
C	0.645363	2.054474	-0.316299
C	2.852792	0.887926	-0.235379
H	3.339936	1.839548	-0.436637
C	3.617870	-0.264006	-0.063798
C	2.984695	-1.480092	0.201058
C	1.593234	-1.538677	0.281276
H	-1.238126	2.993463	-0.105362
H	-4.599219	-0.147779	-0.273306
H	-3.360516	1.804441	0.447669
H	-0.847137	-2.383753	-0.623995
H	-3.190378	-1.948868	-1.329063
H	1.146006	2.950809	-0.677140
H	4.701422	-0.212443	-0.127980
H	3.572633	-2.381291	0.353323
H	1.108258	-2.484041	0.508296
H	-1.234941	0.930416	1.666107
H	-3.260962	-2.290562	0.377251

Energy = -540.678942314
Number of Imaginary Frequencies = 0

Phenanthrene + C_2H_4 [2,12] TS

C	-1.046102	2.076190	-0.030303
C	0.292243	2.087324	-0.213464
C	1.062040	0.855433	-0.327462
C	0.325483	-0.414566	-0.338284
C	-1.132726	-0.401185	-0.177967
C	-1.802841	0.841279	-0.004635
C	-3.201071	0.860096	0.167217
C	-3.939917	-0.312718	0.160732
C	-3.284962	-1.538939	-0.024238
C	-1.907301	-1.577635	-0.189837
C	1.104043	-1.543479	-0.361606
C	2.533798	-1.365015	-0.304319
C	3.060592	-0.247428	-1.076617
C	2.319749	0.881913	-1.060431
C	1.976410	0.559673	1.615766
C	2.725663	-0.642624	1.517092
H	-1.595355	3.009458	0.073320
H	0.832512	3.029992	-0.270040
H	-3.697705	1.818534	0.301675
H	-5.018036	-0.281790	0.292365
H	-3.855269	-2.463935	-0.039622
H	-1.422911	-2.537464	-0.340568
H	0.688102	-2.537596	-0.231936
H	3.134933	-2.272731	-0.283843
H	4.050531	-0.298994	-1.520793
H	2.660090	1.818097	-1.496112
H	2.503450	1.508044	1.634658
H	1.037758	0.557902	2.160338
H	3.809809	-0.555088	1.539193
H	2.361495	-1.504335	2.071494

Energy = -618.052185442
Number of Imaginary Frequencies = 1

Phenanthrene + C_2H_4 [2,12] Adduct

C	-1.015964	2.062147	-0.016344
C	0.323768	2.069967	-0.052635
C	1.147942	0.819727	-0.058875
C	0.321156	-0.477130	-0.101977
C	-1.148118	-0.428729	-0.052981
C	-1.801399	0.829655	-0.007438
C	-3.202962	0.882265	0.038963
C	-3.967516	-0.279931	0.038829
C	-3.327889	-1.522246	-0.009931

C	-1.938414	-1.589909	-0.055429
C	1.093883	-1.579926	-0.137850
C	2.584647	-1.323138	-0.126706
C	2.920359	-0.326317	-1.223174
C	2.181211	0.782793	-1.186139
C	2.012680	0.708856	1.275031
C	2.878060	-0.571564	1.226687
H	-1.567290	3.000403	0.001547
H	0.866741	3.013876	-0.064016
H	-3.690452	1.854124	0.074462
H	-5.051888	-0.220927	0.074878
H	-3.912259	-2.438531	-0.011974
H	-1.458952	-2.563470	-0.093773
H	0.713091	-2.596448	-0.127876
H	3.168739	-2.244009	-0.196219
H	3.720458	-0.512839	-1.933737
H	2.290859	1.628084	-1.859639
H	2.633434	1.606803	1.362847
H	1.326853	0.698338	2.127714
H	3.944531	-0.328520	1.279929
H	2.647469	-1.236009	2.065669

Energy = -618.087843993
Number of Imaginary Frequencies = 0

Phenanthrene + H_2 [11,14] TS

C	-3.486625	-0.261490	0.321987
C	-2.744358	0.878430	0.372215
C	-1.302432	0.856478	0.151974
C	-0.701054	-0.453897	-0.196909
C	-1.540637	-1.603164	-0.261296
C	-2.884021	-1.517882	-0.006670
C	-0.669474	2.020257	-0.529244
C	0.700987	-0.453923	-0.196874
C	1.302496	0.856469	0.151720
C	0.669488	2.020210	-0.529482
C	2.744428	0.878434	0.371895
H	3.215583	1.838362	0.570056
C	3.486652	-0.261508	0.321902
C	2.883963	-1.517951	-0.006361
C	1.540563	-1.603229	-0.260914
H	-1.286622	2.815438	-0.935020
H	4.557907	-0.220856	0.502833
H	-3.215480	1.838333	0.570576
H	-1.100876	-2.566866	-0.502781
H	-3.504034	-2.408669	-0.054850
H	1.286563	2.815342	-0.935463
H	4.557944	-0.220873	0.502696
H	3.503917	-2.408792	-0.054287
H	1.100751	-2.567004	-0.502000
H	0.559804	1.031085	1.307267
H	-0.559515	1.031098	1.307314

Energy = -540.592595060
Number of Imaginary Frequencies = 1

Phenanthrene + H_2 [11,14] Adduct

C	-3.550923	-0.270917	-0.120899
C	-2.879936	0.873451	0.091870
C	-1.400060	0.901760	0.374324
C	-0.686945	-0.439021	0.159194
C	-1.506823	-1.614923	-0.019115
C	-2.857192	-1.547238	-0.140360
C	-0.664919	2.019139	-0.352457
C	0.686945	-0.439020	0.159195
C	1.400060	0.901761	0.374326
C	0.664918	2.019140	-0.352457
C	2.879935	0.873452	0.091865
H	3.397692	1.830726	0.102994
C	3.550922	-0.270916	-0.120901
C	2.857193	-1.547238	-0.140356
C	1.506825	-1.614923	-0.019111
H	-1.248184	2.791208	-0.847857
H	-4.624953	-0.256386	-0.289859
H	-3.397694	1.830725	0.103005
H	-1.022439	-2.583865	-0.090164
H	-3.434629	-2.455820	-0.287665
H	1.248181	2.791209	-0.847857
H	4.624952	-0.256385	-0.289866
H	3.434631	-2.455821	-0.287656
H	1.022441	-2.583866	-0.090154
H	1.293125	1.140617	1.457182
H	-1.293121	1.140619	1.457180

Energy = -540.624757882
Number of Imaginary Frequencies = 0

Phenanthrene + C_2H_4 [11,14] TS

C	0.669611	-1.704076	-1.075200
C	-0.669611	-1.704075	-1.075200
C	-1.339177	-0.685493	-0.237628
C	-0.699557	0.648101	-0.254991
C	0.699557	0.648100	-0.254990
C	1.339177	-0.685494	-0.237629
C	2.801951	-0.705768	-0.210675
C	3.529469	0.426826	-0.033323
C	2.880418	1.704370	0.051353
C	1.521970	1.803217	-0.071982
C	-1.521970	1.803217	-0.071979
C	-2.880418	1.704371	0.051354
C	-3.529470	0.426827	-0.033322
C	-2.801951	-0.705767	-0.210676
C	-0.719617	-1.293338	1.510841
C	0.719617	-1.293326	1.510845
H	1.269703	-2.437945	-1.606018
H	-1.269705	-2.437943	-1.606019
H	3.295597	-1.669956	-0.315142
H	4.614601	0.379193	0.014498
H	3.481066	2.598821	0.191481
H	1.055184	2.782943	-0.029150
H	-1.055185	2.782945	-0.029156
H	-3.481065	2.598822	0.191491
H	-4.614602	0.379194	0.014495
H	-3.295597	-1.669955	-0.315144
H	-1.218033	-0.551570	2.129626
H	-1.207254	-2.264600	1.544300
H	1.218018	-0.551537	2.129618
H	1.207271	-2.264578	1.544325

Energy = -618.027012213
Number of Imaginary Frequencies = 1

Phenanthrene + C_2H_4 [11,14] Adduct

C	0.665751	-1.540815	-1.192205
C	-0.665763	-1.540867	-1.192160
C	-1.307066	-0.724885	-0.070910
C	-0.686766	0.675514	-0.070418
C	0.686775	0.675515	-0.070398

C	1.307060	-0.724884	-0.070921
C	2.806087	-0.725868	-0.106960
C	3.533107	0.405621	-0.052294
C	2.896434	1.709906	0.006805
C	1.542985	1.828922	-0.009076
C	-1.542974	1.828923	-0.009107
C	-2.896423	1.709917	0.006792
C	-3.533102	0.405635	-0.052296
C	-2.806094	-0.725863	-0.106947
C	-0.769935	-1.412899	1.266738
C	0.769928	-1.412934	1.266713
H	1.285268	-2.076351	-1.905429
H	-1.285287	-2.076430	-1.905360
H	3.294725	-1.697353	-0.162813
H	4.619513	0.358281	-0.063352
H	3.522475	2.596809	0.051537
H	1.090443	2.816531	0.018788
H	-1.090427	2.816534	0.018761
H	-3.522463	2.596820	0.051519
H	-4.619511	0.358294	-0.063349
H	-3.294738	-1.697345	-0.162799
H	-1.173759	-0.858723	2.118698
H	-1.167243	-2.431911	1.312525
H	1.173793	-0.858823	2.118695
H	1.167194	-2.431965	1.312446

Energy = -618.045618132
Number of Imaginary Frequencies = 0

Coronene (**8**)

C	3.424175	1.525600	0.000024
C	2.067812	1.959825	0.000013
C	1.036180	0.982144	0.000000
C	1.368547	-0.406191	-0.000003
C	2.731538	-0.810389	0.000000
C	3.743869	0.191103	0.000016
C	-0.332644	1.388129	-0.000008
C	0.332644	-1.388129	-0.000008
C	-1.036180	-0.982144	0.000000
C	-1.368547	0.406191	-0.000003
C	-2.067812	-1.959825	0.000012
C	-1.706377	-3.337314	0.000004
C	-0.390719	-3.727639	-0.000010
C	0.663723	-2.770565	-0.000014
C	2.037515	-3.146146	-0.000019
C	3.033384	-2.202067	-0.000010
H	4.076626	-2.508647	-0.000013
H	2.288134	-4.204263	-0.000030
H	4.211228	2.275862	0.000037
H	4.785166	-0.121866	0.000023
H	-2.497539	-4.083238	0.000008
H	-0.134603	-4.784460	-0.000020
C	1.706377	3.337314	0.000011
C	0.390718	3.727639	-0.000007
C	-0.663723	2.770565	-0.000017
H	2.497539	4.083238	0.000025
H	0.134603	4.784460	-0.000013
C	-2.037515	3.146146	-0.000025
C	-3.033384	2.202067	-0.000013
C	-2.731538	0.810389	0.000002
H	-2.288134	4.204263	-0.000044
H	-4.076626	2.508647	-0.000017
C	-3.424175	-1.525599	0.000027
H	-4.211228	-2.275862	0.000047
C	-3.743869	-0.191103	0.000022
H	-4.785166	0.121866	0.000034

Energy = -921.897984410
Number of Imaginary Frequencies = 0

Coronene + H_2 [1,20] TS

C	3.470579	1.469283	0.046870
C	2.859141	0.181648	-0.037258
C	1.448850	0.093790	0.008966
C	0.649102	1.277628	0.130230
C	1.287401	2.550950	0.149398
C	2.713849	2.607769	0.132553
C	0.816929	-1.184875	-0.084034
C	-0.772294	1.196651	0.140678
C	-1.437830	-0.107575	0.210325
C	-0.589763	-1.284061	-0.014971
C	-2.833032	-0.179883	-0.262912
C	-3.544051	1.048098	-0.495721
C	-2.948684	2.255832	-0.300115
C	-1.540967	2.368548	-0.003661
C	-0.888254	3.630086	0.038820
C	0.480054	3.718380	0.144464
H	0.964563	4.691293	0.177916
H	-1.489757	4.532941	-0.034840
H	4.555820	1.534012	0.024476
H	3.194379	3.582457	0.171886
H	-4.592174	0.989476	-0.779201
H	-3.519158	3.172910	-0.426549
C	3.619465	-1.020187	-0.175880
C	3.013401	-2.247789	-0.243244
C	1.592599	-2.373955	-0.176792
H	4.703415	-0.944799	-0.219745
H	3.614537	-3.149723	-0.330984
C	0.924389	-3.627930	-0.140192
C	-0.441468	-3.706107	0.043368
C	-1.213684	-2.522480	0.115144
H	1.516248	-4.537378	-0.211506
H	-0.927631	-4.674018	0.137069
C	-3.424571	-1.413826	-0.133209
H	-4.496089	-1.549798	-0.250321
C	-2.621642	-2.415041	0.526475
H	-2.310331	-1.584920	1.640089
H	-3.115054	-3.337366	0.830880
H	-1.815882	-0.614805	1.555034

Energy = -922.968011625
Number of Imaginary Frequencies = 1

Coronene + H_2 [1,20] Adduct

C	-3.710466	0.720362	0.012273
C	-2.476222	1.441967	0.058757
C	-1.260128	0.728321	0.117080
C	-1.277784	-0.712063	0.092813
C	-2.522080	-1.402480	-0.028075
C	-3.732880	-0.645413	-0.040595
C	-0.009914	1.438202	0.090335
C	-0.074134	-1.444935	0.136962
C	1.219879	-0.737497	0.494904
C	1.227332	0.741046	0.155070
C	2.473403	-1.465626	0.033499
C	2.375445	-2.909646	-0.101981
C	1.185749	-3.551995	-0.079137

C	-0.081498	-2.833374	-0.016239
C	-1.321032	-3.508282	-0.150226
C	-2.510713	-2.813853	-0.135575
H	-3.456717	-3.343020	-0.221484
H	-1.321086	-4.590023	-0.262618
H	-4.639424	1.285208	-0.010956
H	-4.678729	-1.178117	-0.104710
H	3.297383	-3.468014	-0.249703
H	1.147546	-4.633908	-0.184413
C	-2.447509	2.870316	-0.003640
C	-1.264403	3.549736	-0.069982
C	-0.014342	2.856321	-0.049634
H	-3.392422	3.407895	-0.029438
H	-1.255263	4.634298	-0.148384
C	1.222698	3.531936	-0.171432
C	2.407189	2.828673	-0.168979
C	2.424454	1.424143	0.001411
H	1.224838	4.613898	-0.280368
H	3.351332	3.356223	-0.286949
C	3.625422	-0.793140	-0.143614
H	4.531802	-1.342368	-0.394386
C	3.750926	0.692745	0.024752
H	4.275975	0.910883	0.972415
H	4.408546	1.104400	-0.755166
H	1.249867	-0.790133	1.603676

Energy = -923.033591132
Number of Imaginary Frequencies = 0

Coronene + C_2H_4 [1,20] TS

C	1.981959	3.006343	-0.379857
C	0.743237	3.614250	-0.412509
C	-0.449955	2.851320	-0.306877
C	-0.349194	1.434315	-0.219970
C	0.927165	0.821619	-0.271123
C	2.086701	1.598091	-0.299682
C	3.326976	0.855354	-0.049114
C	3.427311	-0.446335	-0.658608
C	2.301882	-1.235639	-0.624133
C	1.082622	-0.617014	-0.103617
C	-1.520298	0.634538	-0.037421
C	-1.405410	-0.792272	0.040787
C	-0.134011	-1.420771	-0.079013
C	2.309049	-2.660082	-0.831600
C	1.209137	-3.419114	-0.574768
C	-0.054006	-2.822099	-0.214163
C	-2.582910	-1.585626	0.157775
C	-2.458535	-2.999310	0.128489
C	-1.236550	-3.596747	-0.077218
C	-2.790116	1.254302	0.039868
C	-3.946086	0.434814	0.212632
C	-3.846178	-0.930425	0.266548
C	-2.870188	2.676008	-0.071809
C	-1.747859	3.443495	-0.242301
C	3.032994	0.364766	1.798729
C	1.848971	-0.426881	1.911061
H	2.886804	3.609087	-0.410196
H	0.668292	4.696660	-0.484967
H	4.237171	1.454601	-0.025366
H	4.401961	-0.869991	-0.887928
H	3.235220	-3.126513	-1.159397
H	1.249235	-4.499378	-0.694076
H	-3.354432	-3.606816	0.232234
H	-1.164574	-4.679144	-0.154442
H	-4.919012	0.915147	0.285207
H	-4.739484	-1.540569	0.377424
H	-3.849491	3.145834	-0.018046
H	-1.831833	4.525160	-0.317669
H	3.977059	-0.137099	1.999887
H	2.990714	1.361857	2.233276
H	1.940149	-1.494024	2.088406
H	0.951977	0.023781	2.323014

Energy = -1000.40971444
Number of Imaginary Frequencies = 1

Coronene + C_2H_4 [1,20] Adduct

C	1.986005	3.019021	-0.370264
C	0.739402	3.614141	-0.470682
C	-0.447394	2.851441	-0.342578
C	-0.339364	1.439764	-0.175140
C	0.938038	0.850429	-0.155442
C	2.084331	1.625497	-0.187594
C	3.318814	0.837546	0.188737
C	3.423993	-0.418302	-0.639918
C	2.325405	-1.202743	-0.619458
C	1.150607	-0.611775	0.162563
C	-1.509474	0.636757	0.024199
C	-1.386070	-0.794050	0.126648
C	-0.118284	-1.421526	0.043005
C	2.279046	-2.601407	-0.983362
C	1.206688	-3.372152	-0.682438
C	-0.044048	-2.798584	-0.200892
C	-2.570855	-1.588706	0.186771
C	-2.450138	-2.997422	0.109019
C	-1.225086	-3.581660	-0.125093
C	-2.778880	1.248414	0.045953
C	-3.939365	0.428868	0.210278
C	-3.838331	-0.934118	0.271734
C	-2.868262	2.667212	-0.129944
C	-1.753609	3.435712	-0.325525
C	3.018401	0.315779	1.659782
C	1.735029	-0.558910	1.656191
H	2.886988	3.626946	-0.409105
H	0.659021	4.689979	-0.607976
H	4.228825	1.443062	0.168878
H	4.378226	-0.746376	-1.044356
H	3.162182	-3.039354	-1.443247
H	1.222145	-4.438154	-0.897716
H	-3.347066	-3.608515	0.175904
H	-1.152065	-4.656259	-0.275841
H	-4.914173	0.908766	0.254055
H	-4.732608	-1.546874	0.358004
H	-3.853067	3.128227	-0.112861
H	-1.845873	4.511398	-0.456342
H	3.881523	-0.257840	2.011793
H	2.898066	1.178604	2.323174
H	1.942138	-1.583344	1.980522
H	0.966127	-0.145629	2.315833

Energy = -1000.43826915
Number of Imaginary Frequencies = 0

Coronene + H_2 [5,14] TS

C	2.460350	-2.846287	0.010161
C	2.509706	-1.433414	0.092600
C	1.282574	-0.713223	0.091919

C	0.050168	-1.422058	0.026133
C	0.024934	-2.830254	-0.110213
C	1.256162	-3.522783	-0.103928
C	1.282517	0.713321	0.091917
C	-1.164965	-0.690424	0.063200
C	-1.165020	0.690337	0.063206
C	0.050056	1.422058	0.026133
C	-2.473993	1.319579	-0.129168
C	-3.569494	0.673086	0.634214
C	-3.569449	-0.673365	0.634201
C	-2.473894	-1.319774	-0.129179
C	-2.433554	-2.777690	-0.282994
C	-1.262061	-3.469635	-0.271366
H	-1.279565	-4.552449	-0.377658
H	-3.375997	-3.310717	-0.383545
H	3.393682	-3.404272	0.012050
H	1.254244	-4.606317	-0.198141
H	-4.349090	1.277793	1.087017
H	-4.349006	-1.278129	1.086995
C	3.729441	-0.685020	0.144894
C	3.729386	0.685313	0.144891
C	2.509591	1.433610	0.092594
H	4.671309	-1.228242	0.167269
H	4.671211	1.228611	0.167263
C	2.460122	2.846479	0.010150
C	1.255881	3.522880	-0.103937
C	0.024706	2.830253	-0.110216
H	3.393410	3.404538	0.012035
H	1.253877	4.606413	-0.198153
C	-2.433785	2.777496	-0.282979
H	-3.376274	3.310444	-0.383516
C	-1.262344	3.469534	-0.271362
H	-1.279935	4.552347	-0.377649
H	-2.765005	-0.558375	-1.299638
H	-2.765081	0.558238	-1.299552

Energy = -922.957721965
Number of Imaginary Frequencies = 1

Coronene + H_2 [5,14] Adduct

C	2.473545	2.833295	-0.067052
C	2.511184	1.430010	-0.015051
C	1.276834	0.712418	0.057996
C	0.043337	1.419480	0.101952
C	0.039143	2.834569	0.003469
C	1.261217	3.516292	-0.072967
C	1.276842	-0.712404	0.057998
C	-1.182920	0.685917	0.209425
C	-1.182913	-0.685930	0.209424
C	0.043353	-1.419480	0.101953
C	-2.512690	-1.413871	0.338100
C	-3.588810	-0.666299	-0.440102
C	-3.588817	0.666261	-0.440103
C	-2.512705	1.413842	0.338103
C	-2.416078	2.886664	0.038321
C	-1.241647	3.528296	-0.069448
H	-1.220008	4.603431	-0.236535
H	-3.352105	3.436960	-0.034558
H	3.407876	3.386546	-0.123753
H	1.255621	4.601550	-0.145160
H	-4.344130	-1.243562	-0.967945
H	-4.344142	1.243516	-0.967946
C	3.735946	0.682027	-0.052023
C	3.735954	-0.681986	-0.052020
C	2.511200	-1.429982	-0.015047
H	4.674202	1.230362	-0.092920
H	4.674216	-1.230309	-0.092915
C	2.473577	-2.833268	-0.067044
C	1.261257	-3.516278	-0.072960
C	0.039175	-2.834569	0.003472
H	3.407914	-3.386508	-0.123742
H	1.255673	-4.601537	-0.145151
C	-2.416045	-2.886690	0.038310
H	-3.352066	-3.436995	-0.034583
C	-1.241607	-3.528309	-0.069454
H	-1.219955	-4.603443	-0.236547
H	-2.816556	1.335607	1.405123
H	-2.816539	-1.335646	1.405122

Energy = -923.004942284
Number of Imaginary Frequencies = 0

Coronene + C_2H_4 [5,14] TS

C	0.011380	1.503058	-3.525889
C	0.049048	2.708818	-2.844376
C	0.009128	2.755044	-1.431682
C	-0.087601	1.528966	-0.713184
C	-0.149967	0.295691	-1.422118
C	-0.083404	0.275235	-2.837013
C	-0.121803	-1.008977	-3.502031
C	-0.207076	-2.178356	-2.818270
C	-0.220718	-2.225324	-1.353130
C	-0.270725	-0.921579	-0.692036
C	-0.087601	1.528966	0.713184
C	-0.149967	0.295691	1.422118
C	-0.270725	-0.921579	0.692036
C	-0.989117	-3.281480	-0.673370
C	-0.989117	-3.281480	0.673370
C	-0.220718	-2.225324	1.353130
C	-0.083404	0.275235	2.837013
C	-0.121803	-1.008977	3.502031
C	-0.207076	-2.178356	2.818270
C	0.009128	2.755044	1.431682
C	0.049048	2.708818	2.844376
C	0.011380	1.503058	3.525889
C	0.077718	3.974788	0.684340
C	0.077718	3.974788	-0.684340
C	1.596761	-2.776978	-0.717120
C	1.596761	-2.776978	0.717120
H	0.057269	1.495881	-4.612573
H	0.122049	3.641524	-3.398624
H	-0.100179	-1.018624	-4.589896
H	-0.260711	-3.120906	-3.359210
H	-1.464781	-4.060611	-1.262999
H	-1.464781	-4.060611	1.262999
H	-0.100179	-1.018624	4.589896
H	-0.260711	-3.120906	3.359210
H	0.122049	3.641524	3.398624
H	0.057269	1.495881	4.612573
H	0.139979	4.913815	1.229434
H	0.139979	4.913815	-1.229434
H	1.653725	-3.741547	-1.214962
H	2.170899	-2.002970	-1.219258
H	1.653725	-3.741547	1.214962
H	2.170899	-2.002970	1.219258

Energy = -1000.39675146

Number of Imaginary Frequencies = 1

Coronene + C_2H_4 [5,14] Adduct

C	1.504249	-3.524576	-0.012630
C	2.720784	-2.842303	0.011370
C	2.772151	-1.435814	0.009728
C	1.542599	-0.712576	-0.016402
C	0.309991	-1.421071	-0.039143
C	0.283224	-2.835123	-0.038632
C	-1.021971	-3.492435	-0.074872
C	-2.189657	-2.818159	-0.097679
C	-2.272929	-1.318015	-0.056322
C	-0.902395	-0.682428	-0.071218
C	1.542547	0.712683	-0.016463
C	0.309883	1.421084	-0.039256
C	-0.902454	0.682361	-0.071291
C	-3.101333	-0.667704	-1.169864
C	-3.101815	0.667577	-1.169467
C	-2.273066	1.317877	-0.056147
C	0.283026	2.835139	-0.038719
C	-1.022237	3.492345	-0.074793
C	-2.189904	2.818024	-0.097418
C	2.772057	1.435998	0.009628
C	2.720574	2.842487	0.011186
C	1.503999	3.524681	-0.012788
C	3.996331	0.683288	0.034365
C	3.996379	-0.683015	0.034411
C	-2.956391	-0.774806	1.280208
C	-2.956241	0.774531	1.280430
H	1.501012	-4.612354	-0.012483
H	3.651372	-3.404521	0.031133
H	-1.030646	-4.580798	-0.091356
H	-3.129263	-3.367332	-0.131284
H	-3.655397	-1.281438	-1.874261
H	-3.656206	1.281323	-1.873596
H	-1.030984	4.580713	-0.091200
H	-3.129525	3.367179	-0.130837
H	3.651117	3.404784	0.030940
H	1.500676	4.612459	-0.012618
H	4.937497	1.227972	0.053692
H	4.937581	-1.227637	0.053766
H	-3.975954	-1.170030	1.333916
H	-2.400191	-1.170620	2.135137
H	-3.975724	1.169921	1.334422
H	-2.399769	1.170069	2.135311

Energy = -1000.42157610
Number of Imaginary Frequencies = 0

Coronene + H_2 [20,23] TS

C	1.347488	3.430245	0.317679
C	1.832558	2.102236	0.374268
C	0.868686	0.996167	0.321690
C	-0.494970	1.349715	-0.119552
C	-0.923155	2.697778	-0.210960
C	0.027699	3.725567	0.026814
C	1.404615	-0.306489	-0.119939
C	-1.404615	0.306489	-0.119939
C	-0.868686	-0.996167	0.321690
C	0.494970	-1.349715	-0.119552
C	-1.832558	-2.102236	0.374268
C	-3.214304	-1.803032	0.317979
C	-3.686885	-0.535839	0.027041
C	-2.798484	0.546353	-0.211096
C	-3.214304	1.888138	-0.456351
C	-2.309119	2.926463	-0.456373
H	-2.657399	3.948968	-0.582219
H	-4.274761	2.093728	-0.582050
H	2.062512	4.243076	0.427132
H	-0.290442	4.763052	-0.041409
H	-3.922162	-2.622076	0.427733
H	-4.758071	-0.362089	-0.040866
C	3.214304	1.803032	0.317979
C	3.686885	0.535839	0.027041
C	2.798484	-0.546353	-0.211096
H	3.922162	2.622076	0.427733
H	4.758071	0.362089	-0.040866
C	3.214304	-1.888138	-0.456351
C	2.309119	-2.926463	-0.456373
C	0.923155	-2.697778	-0.210960
H	4.274761	-2.093728	-0.582050
H	2.657399	-3.948968	-0.582219
C	-1.347488	-3.430245	0.317679
H	-2.062512	-4.243076	0.427132
C	-0.027699	-3.725567	0.026814
H	0.290442	-4.763052	-0.041409
H	0.413856	0.475901	1.524473
H	-0.413856	-0.475901	1.524473

Energy = -922.936520487
Number of Imaginary Frequencies = 1

Coronene + H_2 [20,23] Adduct

C	3.679941	-0.696852	-0.109022
C	2.511146	-1.446515	0.063342
C	1.258473	-0.724856	0.533399
C	1.227071	0.752997	0.188607
C	2.465784	1.435593	-0.030096
C	3.668191	0.693152	-0.112057
C	-0.035479	-1.439300	0.188860
C	0.035479	1.439300	0.188860
C	-1.258473	0.724856	0.533399
C	-1.227071	-0.752997	0.188607
C	-2.511146	1.446515	0.063342
C	-2.449101	2.833641	-0.109786
C	-1.240875	3.520914	-0.112446
C	0.004581	2.853334	-0.029829
C	1.240875	3.530638	-0.213933
C	2.431454	2.844875	-0.214153
H	3.368445	3.374267	-0.370568
H	1.228740	4.606778	-0.370350
H	4.612850	-1.222802	-0.301817
H	4.596998	1.234006	-0.277429
H	-3.372111	3.376555	-0.303034
H	-1.238837	4.595633	-0.278387
C	2.449101	-2.833641	-0.109786
C	1.240875	-3.520914	-0.112446
C	-0.004581	-2.853334	-0.029829
H	3.372111	-3.376555	-0.303034
H	1.238837	-4.595633	-0.278387
C	-1.240875	-3.530638	-0.213933
C	-2.431454	-2.844875	-0.214153
C	-2.465784	-1.435593	-0.030096
H	-1.228740	-4.606778	-0.370350
H	-3.368445	-3.374267	-0.370568
C	-3.679941	0.696852	-0.109022

H	-4.612850	1.222802	-0.301817
C	-3.668191	-0.693152	-0.112057
H	-4.596998	-1.234006	-0.277429
H	1.329004	-0.765461	1.644267
H	-1.329004	0.765461	1.644267

Energy = -922.981739854
Number of Imaginary Frequencies = 0

Coronene + C_2H_4 [20,23] TS

C	-3.498098	-1.235860	0.043730
C	-2.832196	-2.427529	-0.191359
C	-1.425410	-2.463681	-0.369377
C	-0.692357	-1.252834	-0.245651
C	-1.347402	0.000014	0.178736
C	-2.821177	0.000028	0.118231
C	-3.498074	1.235928	0.043725
C	-2.832149	2.427584	-0.191366
C	-1.425362	2.463708	-0.369380
C	-0.692332	1.252848	-0.245651
C	0.692225	-1.252830	-0.245601
C	1.347178	-0.000014	0.179557
C	0.692250	1.252817	-0.245598
C	1.425271	2.463656	-0.369350
C	2.821046	-0.000028	0.118101
C	3.497975	1.235815	0.043434
C	2.832077	2.427545	-0.191416
C	1.425223	-2.463683	-0.369355
C	2.832030	-2.427600	-0.191422
C	3.497951	-1.235883	0.043429
C	0.687875	-3.659379	-0.610956
C	-0.688082	-3.659388	-0.610941
C	-0.688010	3.659401	-0.610943
C	0.687947	3.659366	-0.610955
C	0.730389	-0.000006	1.977914
C	-0.729184	0.000005	1.979003
H	-4.585098	-1.233476	0.094342
H	-3.396796	-3.352695	-0.279618
H	-4.585075	1.233566	0.094336
H	-3.396731	3.352761	-0.279629
H	4.584994	1.233365	0.093710
H	3.396670	3.352711	-0.279692
H	3.396604	-3.352777	-0.279702
H	4.584970	-1.233455	0.093705
H	1.231833	-4.590764	-0.750429
H	-1.232038	-4.590779	-0.750379
H	-1.231948	4.590803	-0.750385
H	1.231923	4.590741	-0.750425
H	1.209008	-0.903522	2.350546
H	1.209024	0.903495	2.350559
H	-1.207482	-0.903534	2.351911
H	-1.207467	0.903556	2.351905

Energy = -1000.37977340
Number of Imaginary Frequencies = 1

Coronene + C_2H_4 [20,23] Adduct

C	3.495960	1.228141	0.083969
C	2.831362	2.416728	-0.200572
C	1.428906	2.453807	-0.391093
C	0.686578	1.256840	-0.202735
C	1.324697	-0.000663	0.335091
C	2.826046	-0.001321	0.208339
C	3.494793	-1.231460	0.084059
C	2.828985	-2.419313	-0.200770
C	1.426557	-2.454895	-0.391744
C	0.685361	-1.257238	-0.203580
C	-0.685464	1.257576	-0.202850
C	-1.324850	0.000687	0.334550
C	-0.686657	-1.256551	-0.203574
C	-1.429037	-2.453520	-0.391644
C	-2.826079	0.001384	0.208523
C	-3.496040	-1.228139	0.084609
C	-2.831387	-2.416588	-0.200390
C	-1.426657	2.455115	-0.391583
C	-2.829147	2.419324	-0.200996
C	-3.494874	1.231501	0.084055
C	-0.686909	3.633832	-0.703604
C	0.690343	3.633189	-0.703327
C	0.686805	-3.633601	-0.703906
C	-0.690452	-3.632951	-0.703805
C	-0.772913	-0.000261	1.872724
C	0.773874	-0.001130	1.871956
H	4.584226	1.225661	0.106265
H	3.404724	3.330746	-0.336281
H	4.583048	-1.230090	0.106671
H	3.401351	-3.333974	-0.336316
H	-4.584284	-1.225770	0.107579
H	-3.404660	-3.330711	-0.335774
H	-3.401640	3.333845	-0.336964
H	-4.583128	1.230095	0.106685
H	-1.228742	4.557058	-0.896135
H	1.233120	4.555921	-0.895570
H	1.228670	-4.556831	-0.896329
H	-1.233222	-4.555670	-0.896131
H	-1.175249	0.887338	2.368466
H	-1.176674	-0.887472	2.367991
H	1.177304	0.885745	2.368148
H	1.176345	-0.888840	2.367494

Energy = -1000.38768114
Number of Imaginary Frequencies = 0

Pyridine (**9**)

C	1.142344	-0.721742	0.000001
C	-1.142210	-0.721944	0.000012
C	-1.198732	0.672903	-0.000001
C	-0.000124	1.385651	-0.000010
C	1.198620	0.673090	0.000004
H	2.059783	-1.308831	0.000026
H	-2.059568	-1.309165	0.000020
H	-2.157921	1.182444	0.000008
H	-0.000197	2.472510	-0.000001
H	2.157706	1.182825	0.000020
N	0.000116	-1.421075	-0.000015

Energy = -248.284972858
Number of Imaginary Frequencies = 0

Pyridine + H_2 [C,N] TS

C	-1.169701	-0.700908	-0.199062
C	1.169701	-0.700909	-0.199062
C	1.220349	0.653014	-0.241977
C	0.000000	1.273406	0.248169
C	-1.220349	0.653015	-0.241977
H	-2.023501	-1.356286	-0.346707
H	2.023501	-1.356287	-0.346707
H	2.118686	1.222528	-0.454755

H	0.000000	2.341471	0.454673
H	-2.118686	1.222530	-0.454755
H	0.000000	0.501683	1.512849
H	0.000000	-0.511253	1.461354
N	0.000000	-1.304300	0.282501

Energy = -249.354066662
Number of Imaginary Frequencies = 1

Pyridine + H_2 [C,N] Adduct

C	0.701760	-1.199194	0.000000
C	0.701763	1.199193	0.000000
C	-0.638854	1.244360	0.000000
C	-1.504587	0.000002	0.000000
C	-0.638856	-1.244360	0.000000
H	1.314727	-2.095241	0.000000
H	1.314730	2.095239	0.000000
H	-1.124145	2.216229	0.000000
H	-2.183401	0.000005	-0.872728
H	-1.124151	-2.216226	0.000000
N	1.406638	-0.000001	0.000000
H	2.411818	-0.000003	0.000000
H	-2.183397	0.000000	0.872730

Energy = -249.455334195
Number of Imaginary Frequencies = 0

Pyridine + C_2H_4 [C,N] TS

C	0.881813	-0.530771	1.164918
C	0.617764	0.798460	1.215296
C	0.031108	1.333385	0.000000
C	0.617767	0.798460	-1.215296
C	0.881815	-0.530771	-1.164916
C	-1.690888	0.382118	-0.000001
C	-1.441874	-1.015260	-0.000001
H	1.157731	-1.120467	2.037234
H	0.684123	1.383904	2.127513
H	-0.260527	2.382063	0.000000
H	0.684127	1.383904	-2.127513
H	1.157735	-1.120467	-2.037232
H	-2.115490	0.806575	0.906714
H	-2.115488	0.806575	-0.906718
H	-1.570013	-1.587894	0.911056
H	-1.570011	-1.587894	-0.911058
N	0.651826	-1.251433	0.000000

Energy = -326.793130782
Number of Imaginary Frequencies = 1

Pyridine + C_2H_4 [C,N] Adduct

C	-0.689090	-1.188711	-0.715637
C	0.643260	-1.231550	-0.747303
C	1.276281	0.000017	-0.117191
C	0.643227	1.231572	-0.747290
C	-0.689122	1.188689	-0.715649
C	0.766379	0.000003	1.373937
C	-0.787601	-0.000005	1.322668
H	-1.375235	-1.958716	-1.057757
H	1.230524	-2.058247	-1.136060
H	2.367118	0.000032	-0.167759
H	1.230469	2.058291	-1.136038
H	-1.375286	1.958672	-1.057773
H	1.148663	-0.884467	1.894650
H	1.148652	0.884471	1.894662
H	-1.209393	-0.883575	1.809573
H	-1.209403	0.883567	1.809563
N	-1.276588	-0.000017	-0.110610

Energy = -326.833872086
Number of Imaginary Frequencies = 0

Pyridine + H_2 [C,C] TS

C	1.275082	0.442990	-0.235429
C	0.187763	1.269682	0.249367
C	-1.119022	0.833938	-0.189093
C	-1.285101	-0.516757	-0.204910
C	-0.118677	-1.257538	0.226238
H	2.239539	0.870471	-0.506445
H	0.370782	2.325768	0.430544
H	-1.919481	1.544781	-0.366843
H	-2.231847	-1.012388	-0.392696
H	-0.202831	-2.327432	0.406706
H	-0.001148	-0.531806	1.522192
H	0.155247	0.437929	1.526349
N	1.135638	-0.848745	-0.242406

Energy = -249.382247658
Number of Imaginary Frequencies = 1

Pyridine + H_2 [C,C] Adduct

C	1.448093	-0.084695	0.000000
C	-0.617625	-1.226491	0.000000
C	-1.469728	0.024486	0.000000
C	-0.636009	1.275989	0.000000
C	0.695759	1.220158	0.000000
H	2.120197	-0.136584	0.870697
H	-1.167446	-2.174261	0.000000
H	-2.143857	-0.003962	0.871844
H	1.290893	2.132163	0.000000
N	0.650958	-1.309367	0.000000
H	-1.155775	2.232078	0.000000
H	-2.143861	-0.003967	-0.871842
H	2.120205	-0.136585	-0.870692

Energy = -249.457534777
Number of Imaginary Frequencies = 0

Pyridine + C_2H_4 [C,C] TS

C	0.903756	0.943719	-0.912574
C	1.123121	-0.388938	-1.096249
C	0.596097	-1.253023	-0.080958
C	0.579998	-0.696391	1.243461
C	-1.525196	-0.872236	-0.400546
C	-1.697366	0.511668	-0.240955
H	1.159861	1.696977	-1.652091
H	1.575442	-0.796200	-1.996051
H	0.692934	-2.330215	-0.190807
H	0.668481	-1.342337	2.117765
H	-1.519066	-1.299984	-1.398068
H	-1.871342	-1.546429	0.376482
H	-1.858625	1.125113	-1.122215
H	-2.190112	0.873296	0.656625
H	-0.078598	2.345770	0.434283
N	0.362449	0.573347	1.439464
C	0.166903	1.298630	0.270793

Energy = -326.818123840
Number of Imaginary Frequencies = 1

Pyridine + C_2H_4 [C,C] Adduct

C	-0.528905	1.386257	-0.553661
C	0.800359	1.252363	-0.583121
C	1.278375	-0.040718	0.043512
C	0.597761	-0.156692	1.397738
C	0.631946	-1.209498	-0.797641
C	-0.907037	-1.056791	-0.730725
H	-1.081392	2.225284	-0.966012
H	1.495054	1.966016	-1.015761
H	2.365499	-0.133830	0.094809
H	1.167107	-0.390924	2.299579
H	0.997952	-1.146937	-1.826834
H	0.953560	-2.173630	-0.390239
H	-1.347615	-0.962073	-1.727818
H	-1.369387	-1.920107	-0.241542
H	-2.313951	0.373443	0.201126
N	-0.669537	-0.033945	1.463586
C	-1.235844	0.225142	0.111831

Energy = -326.867489454
Number of Imaginary Frequencies = 0

Pyrimidine (**10**)

C	0.000000	1.308948	0.000000
C	1.184573	-0.622359	0.000000
C	-0.000020	-1.356283	0.000000
C	-1.184578	-0.622359	0.000000
H	0.000026	2.397581	0.000000
H	2.154784	-1.117086	0.000000
H	-0.000009	-2.441571	0.000000
H	-2.154815	-1.117031	0.000000
N	1.199267	0.716446	0.000000
N	-1.199243	0.716472	0.000000

Energy = -264.323726321
Number of Imaginary Frequencies = 0

Pyrimidine + H_2 [C,N] TS

C	1.257489	0.527553	-0.231671
C	0.082356	1.240133	0.229245
C	-1.205669	-0.507298	-0.219212
C	1.076107	-0.815981	-0.166901
H	2.199195	1.017215	-0.451396
H	0.128870	2.307129	0.434519
H	-2.127211	-1.026999	-0.471673
H	1.854680	-1.560854	-0.301309
H	-0.140591	-0.449121	1.463739
H	-0.014498	0.539422	1.505435
N	-0.160070	-1.284026	0.291979
N	-1.148807	0.784993	-0.270276

Energy = -265.403933323
Number of Imaginary Frequencies = 1

Pyrimidine + H_2 [C,N] Adduct

C	0.731700	-1.129609	0.000000
C	0.583198	1.260704	0.000000
C	-0.749985	1.171838	0.000000
C	-1.438636	-0.179266	0.000000
H	1.411408	-1.983990	0.000000
H	1.128531	2.198561	0.000000
H	-1.353049	2.075053	0.000000
H	-2.104133	-0.276084	-0.873252
N	1.367044	0.100987	0.000000
N	-0.525445	-1.334279	0.000000
H	2.372517	0.153598	0.000000
H	-2.104123	-0.276090	0.873261

Energy = -265.501734235
Number of Imaginary Frequencies = 0

Pyrimidine + C_2H_4 [C,N] TS

C	0.614793	-0.753749	1.130968
C	-0.002685	1.243379	0.347422
C	0.841074	1.055963	-0.813692
C	1.140237	-0.247900	-1.048302
C	-1.666473	0.419873	-0.214493
C	-1.418054	-0.944762	-0.486945
H	0.761417	-1.499634	1.912096
H	-0.328648	2.252770	0.592115
H	1.087726	1.867069	-1.491327
H	1.635340	-0.607002	-1.948111
H	-2.243056	0.641699	0.680643
H	-1.909919	1.059555	-1.059281
H	-1.689106	-1.706340	0.234985
H	-1.332974	-1.297929	-1.507766
N	0.694777	-1.221232	-0.170508
N	0.300347	0.457373	1.470064

Energy = -342.844776908
Number of Imaginary Frequencies = 1

Pyrimidine + C_2H_4 [C,N] Adduct

C	0.611064	-0.262413	1.328121
C	-1.192534	0.366306	0.137807
C	-0.347289	1.443192	-0.507808
C	0.941798	1.103413	-0.548455
C	-1.022545	-0.916280	-0.746119
C	0.498718	-1.218277	-0.794620
H	1.220999	-0.598716	2.165847
H	-2.240972	0.643006	0.256003
H	-0.767098	2.366457	-0.894412
H	1.764872	1.676530	-0.964694
H	-1.580018	-1.741144	-0.290710
H	-1.435981	-0.737348	-1.743393
H	0.731628	-2.203910	-0.382140
H	0.898494	-1.175789	-1.810300
N	1.262679	-0.193853	0.027617
N	-0.623706	0.004606	1.465276

Energy = -342.885021280
Number of Imaginary Frequencies = 0

Pyrimidine + H_2 [C,C] TS

C	1.191997	0.607183	-0.210639
C	-0.000001	1.271354	0.262461
C	-1.191999	0.607181	-0.210639
C	0.000001	-1.231981	0.208008
H	2.091965	1.156896	-0.480137
H	-0.000002	2.341366	0.446721
H	-2.091967	1.156893	-0.480136
H	0.000002	-2.304978	0.383200
H	0.000000	-0.553080	1.523640
H	0.000000	0.410057	1.527376
N	1.208259	-0.694969	-0.229701
N	-1.208257	-0.694971	-0.229701

Energy = -265.429498764
Number of Imaginary Frequencies = 1

Pyrimidine + H_2 [C,C] Adduct

C	-1.403544	-0.000004	0.000000
C	0.585925	-1.243182	0.000000
C	1.443268	0.000003	0.000000
C	0.585919	1.243184	0.000000
H	-2.068383	-0.000001	-0.874489
H	1.107875	-2.205718	0.000000
H	2.114553	0.000000	-0.873054
N	-0.684104	-1.267635	0.000000
N	-0.684109	1.267631	0.000000
H	1.107864	2.205724	0.000000
H	-2.068367	0.000000	0.874500
H	2.114539	0.000009	0.873063

Energy = -265.500367649
Number of Imaginary Frequencies = 0

Pyrimidine + C_2H_4 [C,C] TS

C	0.768399	0.634525	1.191192
C	0.396116	1.333437	0.000000
C	0.768399	0.634525	-1.191192
C	-1.699589	0.620016	0.000000
C	-1.614689	-0.774662	0.000000
H	1.001474	1.168437	2.112421
H	0.324156	2.417071	0.000000
H	1.001474	1.168437	-2.112421
H	-1.947844	1.149077	0.914365
H	-1.947844	1.149077	-0.914365
H	-1.836196	-1.312803	0.916599
H	-1.836196	-1.312803	-0.916599
H	0.347062	-2.318698	0.000000
N	0.768399	-0.671077	-1.210435
C	0.404087	-1.233295	0.000000
N	0.768399	-0.671077	1.210435

Energy = -342.866250723
Number of Imaginary Frequencies = 1

Pyrimidine + C_2H_4 [C,C] Adduct

C	-0.750988	-0.584448	-1.200624
C	-1.261687	0.180433	-0.000074
C	-0.751117	-0.584308	1.200616
C	-0.419313	1.517893	-0.000103
C	1.076721	1.129051	-0.000027
H	-1.402890	-0.837867	-2.038198
H	-2.337700	0.363688	-0.000142
H	-1.403093	-0.837573	2.038179
H	-0.684253	2.106730	-0.883263
H	-0.684319	2.106816	0.882980
H	1.594346	1.508667	-0.885480
H	1.594288	1.508786	0.885409
H	2.190757	-0.785954	0.000105
N	0.486492	-0.892570	1.230459
C	1.159901	-0.431306	0.000085
N	0.486617	-0.892742	-1.230290

Energy = -342.916037500
Number of Imaginary Frequencies = 0

Pyrazine (**11**)

C	1.133254	-0.698363	0.000002
C	-1.133254	-0.698365	-0.000006
C	-1.133245	0.698378	-0.000006
C	1.133262	0.698350	0.000002
H	2.067241	-1.257285	0.000006
H	-2.067266	-1.257250	0.000028
H	-2.067251	1.257274	0.000036
H	2.067257	1.257260	0.000005
N	0.000003	1.409486	-0.000002
N	-0.000015	-1.409486	-0.000002

Energy = -264.317235092
Number of Imaginary Frequencies = 0

Pyrazine + H_2 [N,N] TS

C	-0.676418	1.158608	-0.220804
C	-0.676418	-1.158608	-0.220804
C	0.676418	-1.158608	-0.220804
C	0.676418	1.158608	-0.220804
H	-1.308045	2.023914	-0.393692
H	-1.308047	-2.023914	-0.393691
H	1.308045	-2.023914	-0.393692
H	1.308047	2.023914	-0.393691
H	0.514419	0.000000	1.455227
H	-0.514419	0.000000	1.455227
N	1.291414	0.000000	0.283115
N	-1.291414	0.000000	0.283115

Energy = -265.367213603
Number of Imaginary Frequencies = 1

Pyrazine + H_2 [N,N] Adduct

C	0.668931	1.210204	0.000003
C	0.668931	-1.210204	0.000003
C	-0.668931	-1.210204	0.000003
C	-0.668931	1.210204	0.000003
H	1.242827	2.128092	0.000014
H	1.242828	-2.128091	0.000015
H	-1.242827	-2.128092	0.000014
H	-1.242828	2.128091	0.000014
N	-1.401228	0.000000	-0.000005
N	1.401228	0.000000	-0.000005
H	2.403726	0.000001	-0.000023
H	-2.403726	0.000000	-0.000025

Energy = -265.464372427
Number of Imaginary Frequencies = 0

Pyrazine + C_2H_4 [N,N] TS

C	-0.749827	0.674755	1.155664
C	-0.747999	-0.676636	1.155682
C	-0.747999	-0.676635	-1.155682
C	-0.749828	0.674756	-1.155664
C	1.554106	-0.712271	0.000000
C	1.552438	0.715949	0.000000
H	-0.925180	1.290651	2.034474
H	-0.921673	-1.293016	2.034488
H	-0.921674	-1.293014	-2.034490
H	-0.925180	1.290653	-2.034473
H	1.847141	-1.228907	0.907616
H	1.847141	-1.228907	-0.907618
H	1.844157	1.233437	0.907554
H	1.844157	1.233437	-0.907554
N	-0.312900	1.329848	0.000000
N	-0.309133	-1.330397	0.000000

Energy = -342.809131302
Number of Imaginary Frequencies = 1

Pyrazine + C_2H_4 [N,N] Adduct

C	-0.665205	-1.181050	-0.714570
C	0.666753	-1.181301	-0.712879
C	0.666792	1.181310	-0.712827
C	-0.665166	1.181103	-0.714518
C	0.779614	-0.000041	1.316201
C	-0.782463	-0.000018	1.314661
H	-1.322374	-1.966127	-1.077386
H	1.324875	-1.965979	-1.075085
H	1.324940	1.965984	-1.074999
H	-1.322310	1.966220	-1.077299
H	1.188540	-0.885124	1.811705
H	1.188567	0.885008	1.811744
H	-1.192759	-0.885211	1.808755
H	-1.192732	0.885164	1.808795
N	-1.274824	0.000023	-0.115052
N	1.275009	-0.000018	-0.112467

Energy = -342.847269615
Number of Imaginary Frequencies = 0

Pyrazine + H_2 [C,C] TS

C	1.325265	0.139261	-0.221564
C	0.427431	1.179592	0.229150
C	-1.325265	-0.139261	-0.221564
C	-0.427431	-1.179592	0.229150
H	2.357991	0.339151	-0.500409
H	0.794259	2.184652	0.421922
H	-2.357991	-0.339152	-0.500409
H	-0.794259	-2.184652	0.421922
H	-0.199204	-0.435668	1.529458
H	0.199204	0.435668	1.529457
N	0.887199	-1.087563	-0.213784
N	-0.887199	1.087563	-0.213784

Energy = -265.426081990
Number of Imaginary Frequencies = 1

Pyrazine + H_2 [C,C] Adduct

C	1.413387	0.140769	0.000000
C	-0.675623	1.177135	0.000000
C	-1.413386	-0.140770	0.000000
C	0.675624	-1.177135	0.000000
H	2.083825	0.185229	-0.871756
H	-1.297506	2.079483	0.000000
H	-2.083826	-0.185228	-0.871755
H	1.297505	-2.079483	0.000000
N	-0.585317	-1.343399	0.000000
N	0.585316	1.343400	0.000000
H	-2.083814	-0.185235	0.871763
H	2.083818	0.185230	0.871761

Energy = -265.496158445
Number of Imaginary Frequencies = 0

Pyrazine + C_2H_4 [C,C] TS

C	0.770829	-0.784304	1.073474
C	0.407980	1.263516	0.228864
C	0.771248	0.784960	-1.072811
C	-1.664073	0.691782	0.086743
C	-1.663582	-0.693102	-0.088065
H	0.999630	-1.471950	1.887334
H	0.326948	2.333107	0.408303
H	1.000128	1.472828	-1.886460
H	-1.886016	1.105628	1.065527
H	-1.905485	1.338375	-0.750910
H	-1.904854	-1.339888	0.749473
H	-1.884661	-1.107184	-1.066951
H	0.329782	-2.332944	-0.408122
N	0.767621	-0.498574	-1.318633
C	0.409542	-1.263269	-0.228567
N	0.765645	0.499221	1.319201

Energy = -342.862569621
Number of Imaginary Frequencies = 1

Pyrazine + C_2H_4 [C,C] Adduct

C	0.595010	-0.740313	-1.188360
C	-1.246612	-0.135610	-0.030308
C	-0.589451	-0.741793	1.189773
C	-0.776244	1.361638	-0.046732
C	0.766061	1.367383	0.044463
H	1.184470	-1.137865	-2.016265
H	-2.334542	-0.222920	-0.035919
H	-1.175867	-1.143283	2.017820
H	-1.127288	1.814145	-0.979061
H	-1.235911	1.904676	0.784446
H	1.222027	1.912423	-0.787464
H	1.113652	1.824021	0.976089
H	2.335987	-0.205791	0.036632
N	0.686588	-0.757686	1.244616
C	1.247540	-0.126368	0.030240
N	-0.680925	-0.764461	-1.243293

Energy = -342.914900689
Number of Imaginary Frequencies = 0

Pyridazine (**12**)

C	0.000000	1.324754	0.000000
C	1.214569	0.630965	0.000000
C	1.143990	-0.751387	0.000000
C	-0.134925	-1.317865	0.000000
H	-0.029046	2.411808	0.000000
H	2.161263	1.163236	0.000000
H	2.031552	-1.377309	0.000000
H	-0.274537	-2.396309	0.000000
N	-1.196725	0.729996	0.000000
N	-1.264851	-0.604314	0.000000

Energy = -264.287587387
Number of Imaginary Frequencies = 0

Pyridazine + H_2 [C,N] TS

C	1.104376	0.810340	-0.225974
C	-0.174919	1.254697	0.259768
C	-1.256006	0.426066	-0.244546
C	1.222550	-0.545553	-0.193884
H	1.921513	1.489647	-0.441357
H	-0.358038	2.301893	0.480965
H	-2.216839	0.827484	-0.557529
H	2.149304	-1.093378	-0.333436
H	0.002302	-0.544559	1.470042
H	-0.143886	0.424134	1.530156
N	0.140015	-1.293413	0.273209
N	-1.101496	-0.860661	-0.233355

Energy = -265.374468064
Number of Imaginary Frequencies = 1

Pyridazine + H_2 [C,N] Adduct

C	0.000000	1.350461	0.000000
C	1.334938	0.627401	0.000000
C	1.100983	-0.866126	0.000000
C	-0.144145	-1.361646	0.000000
H	0.005428	2.439705	0.000000
H	1.930563	0.947436	0.873615
H	1.948765	-1.543349	0.000000
H	-0.363732	-2.424878	0.000000
N	-1.173366	0.825973	0.000000
N	-1.256216	-0.536207	0.000000
H	-2.195176	-0.895244	0.000000
H	1.930563	0.947436	-0.873615

Energy = -265.476461169
Number of Imaginary Frequencies = 0

Pyridazine + C_2H_4 [C,N] TS

C	0.549105	0.702351	1.226365
C	0.405606	1.283892	-0.088009
C	1.056142	0.498806	-1.095933
C	0.932822	-0.842867	-0.896681
C	-1.562114	0.734850	-0.343827
C	-1.635734	-0.663719	-0.190945
H	0.641258	1.311565	2.124121
H	0.375434	2.366322	-0.177252
H	1.479381	0.935226	-1.995051
H	1.202582	-1.592633	-1.636712
H	-1.980304	1.358793	0.441417
H	-1.668227	1.151117	-1.341636
H	-2.013242	-1.086358	0.732673
H	-1.741957	-1.299971	-1.061845
N	0.284462	-1.334224	0.223237
N	0.462696	-0.583482	1.383687

Energy = -342.813559244
Number of Imaginary Frequencies = 1

Pyridazine + C_2H_4 [C,N] Adduct

C	-0.586271	-0.498538	1.301549
C	-1.154112	-0.524038	-0.104688
C	-1.158300	0.909357	-0.581312
C	0.028581	1.489807	-0.391781
C	-0.034249	-1.268065	-0.923994
C	1.291518	-0.503117	-0.657961
H	-1.069670	-1.002618	2.138889
H	-2.120115	-1.026666	-0.173821
H	-2.034349	1.385233	-1.010674
H	0.308530	2.504087	-0.661075
H	0.033570	-2.311356	-0.598099
H	-0.302513	-1.264776	-1.984785
H	2.029377	-1.133012	-0.154197
H	1.738531	-0.124476	-1.580387
N	1.052692	0.681927	0.235784
N	0.532113	0.081094	1.503254

Energy = -342.859793497
Number of Imaginary Frequencies = 0

Pyridazine + H_2 [C,C] TS

C	1.104376	0.810340	-0.225974
C	-0.174919	1.254697	0.259768
C	-1.256006	0.426066	-0.244546
C	1.222550	-0.545553	-0.193884
H	1.921513	1.489647	-0.441357
H	-0.358038	2.301893	0.480965
H	-2.216839	0.827484	-0.557529
H	2.149304	-1.093378	-0.333436
H	0.002302	-0.544559	1.470042
H	-0.143886	0.424134	1.530156
N	0.140015	-1.293413	0.273209
N	-1.101496	-0.860661	-0.233355

Energy = -265.374468064
Number of Imaginary Frequencies = 1

Pyridazine + H_2 [C,C] Adduct

C	0.667404	1.228097	-0.117875
C	-0.669305	1.227097	-0.117927
H	1.257204	2.066346	-0.478628
H	-1.260320	2.064471	-0.478729
N	0.616981	-1.267311	-0.244311
N	-0.615000	-1.268308	-0.244363
C	-1.348528	-0.043677	0.271122
H	-2.376021	-0.116660	-0.092625
H	-1.377380	-0.186376	1.362526
C	1.348543	-0.041698	0.271088
H	1.377846	-0.184329	1.362495
H	2.376123	-0.113032	-0.092769

Energy = -265.461108633
Number of Imaginary Frequencies = 0

Pyridazine + C_2H_4 [C,C] TS

C	1.149231	0.681536	-0.905112
C	1.149249	-0.681485	-0.905134
C	0.375302	-1.277007	0.137550
C	-1.608211	-0.697928	-0.431118
C	-1.608197	0.697919	-0.431093
H	1.643281	1.289538	-1.656879
H	1.643314	-1.289440	-1.656930
H	0.286038	-2.357777	0.204191
H	-1.582570	-1.235170	-1.374037
H	-2.077917	-1.229923	0.389982
H	-1.582553	1.235185	-1.374000
H	-2.077935	1.229883	0.390010
H	0.286009	2.357773	0.204257
N	0.319028	0.642340	1.375534
C	0.375258	1.277005	0.137587
N	0.319050	-0.642385	1.375512

Energy = -342.829768411
Number of Imaginary Frequencies = 1

Pyridazine + C_2H_4 [C,C] Adduct

C	1.320822	0.670676	-0.581626
C	1.320942	-0.670194	-0.581994
C	0.104317	-1.250214	0.058055
C	-1.170593	-0.772400	-0.709534
C	-1.170700	0.772586	-0.709349
H	2.131886	1.297813	-0.938371
H	2.132081	-1.297000	-0.939133
H	0.127807	-2.331612	0.191165
H	-1.148018	-1.180314	-1.723695
H	-2.057438	-1.171129	-0.207030
H	-1.147427	1.180779	-1.723376
H	-2.057840	1.171082	-0.207223
H	0.127388	2.331567	0.192190
N	-0.082999	0.616742	1.439454
C	0.104055	1.250209	0.058637

N -0.082930 -0.617480 1.439166
Energy = -342.883896739
Number of Imaginary Frequencies = 0

1,2,3-Triazine (**13**)
C 0.000000 1.316739 0.000000
C 1.202184 0.623354 0.000000
C 1.076202 -0.758691 0.000000
H -0.047835 2.403152 0.000000
H 2.165806 1.123051 0.000000
H 1.936532 -1.423826 0.000000
N -0.118998 -1.366141 0.000000
N -1.227997 -0.636779 0.000000
N -1.185122 0.689950 0.000000
Energy = -280.296129825
Number of Imaginary Frequencies = 0

1,2,3-Triazine + H_2 [C,N], [1,4] TS
C 1.135862 0.739532 -0.203745
C -0.129775 1.226356 0.241938
C 1.176720 -0.623552 -0.155038
H 1.977668 1.382504 -0.431114
H -0.319572 2.275789 0.441223
H 2.064073 -1.232907 -0.295624
H -0.143959 -0.495133 1.473251
H -0.206184 0.453436 1.519248
N 0.043940 -1.291717 0.274863
N -1.153156 -0.728631 -0.269958
N -1.243480 0.529248 -0.291465
Energy = -281.393579478
Number of Imaginary Frequencies = 1

1,2,3-Triazine + H_2 [C,N], [1,4] Adduct
C 1.419918 -0.088332 0.000000
C 0.677513 1.222201 0.000000
C -0.656597 1.206249 0.000000
H 2.078715 -0.191021 0.875317
H 1.224975 2.159133 0.000000
H -1.285720 2.090411 0.000000
N -1.329634 -0.010641 0.000000
N -0.701654 -1.231660 0.000000
N 0.544394 -1.304108 0.000000
H -2.333444 -0.083344 0.000000
H 2.078723 -0.191022 -0.875312
Energy = -281.487815423
Number of Imaginary Frequencies = 0

1,2,3-Triazine + C_2H_4 [C,N], [1,4] TS
C 0.249480 1.266463 0.141838
C 1.106645 0.755030 -0.875839
C 1.143602 -0.607635 -0.878387
C -1.602086 0.631055 -0.387005
C -1.564315 -0.768912 -0.421099
H 0.086846 2.334604 0.249198
H 1.593917 1.385864 -1.611566
H 1.626669 -1.209631 -1.644264
H -2.121160 1.107571 0.440290
H -1.656260 1.172372 -1.327374
H -1.945151 -1.349529 0.410740
H -1.496672 -1.298279 -1.364205
N 0.445475 -1.311196 0.073127
N 0.377413 -0.677576 1.320892
N 0.307377 0.588919 1.373143
Energy = -358.834102239
Number of Imaginary Frequencies = 1

1,2,3-Triazine + C_2H_4 [C,N], [1,4] Adduct
C 0.066051 1.244292 -0.133217
C 1.312217 0.611486 -0.619421
C 1.307163 -0.719611 -0.426052
C -1.165748 0.610245 -0.835476
C -1.067725 -0.921454 -0.600709
H 0.054096 2.332649 -0.137284
H 2.162128 1.186891 -0.971380
H 2.147572 -1.387540 -0.599796
H -2.085165 1.025486 -0.409010
H -1.139367 0.866917 -1.897996
H -1.925223 -1.297850 -0.036204
H -1.015223 -1.473341 -1.542309
N 0.157986 -1.281239 0.179423
N -0.136362 -0.399339 1.525687
N -0.151705 0.794441 1.335352
Energy = -358.885360444
Number of Imaginary Frequencies = 0

1,2,3-Triazine + H_2 [C,N], [2,5] TS
C 1.170964 0.591519 -0.233833
C -0.000003 1.253848 0.278880
C -1.170968 0.591512 -0.233832
H 2.068401 1.111803 -0.556909
H -0.000006 2.312140 0.513845
H -2.068408 1.111792 -0.556907
H 0.000002 -0.567077 1.484982
H 0.000000 0.385379 1.539426
N 1.172545 -0.709977 -0.222164
N 0.000005 -1.290799 0.259796
N -1.172542 -0.709983 -0.222165
Energy = -281.398719124
Number of Imaginary Frequencies = 1

1,2,3-Triazine + H_2 [C,N], [2,5] Adduct
C 0.142060 0.577890 -1.200441
C -0.304700 1.375251 0.000000
C 0.142060 0.577890 1.200441
H -1.404337 1.464175 0.000000
H 0.484914 1.067131 2.108831
N 0.142060 -0.703859 1.200823
N -0.228291 -1.294171 0.000000
N 0.142060 -0.703859 -1.200823
H 0.484914 1.067131 -2.108831
H 0.065673 -2.263254 0.000000
H 0.101521 2.391863 0.000000
Energy = -281.505498103
Number of Imaginary Frequencies = 0

1,2,3-Triazine + C_2H_4 [C,N], [2,5] TS
C -0.886236 0.464459 -1.168968
C -0.577255 1.227728 0.000000
C -0.886235 0.464458 1.168969
C 1.525385 0.919993 0.000000
C 1.730050 -0.465063 0.000000
H -1.264787 0.909296 -2.086887
H -0.674383 2.308178 0.000001
H -1.264786 0.909294 2.086889

H	1.699419	1.479902	-0.913977
H	1.699420	1.479901	0.913977
H	2.007661	-0.972009	-0.916643
H	2.007662	-0.972010	0.916641
N	-0.130667	-1.347335	0.000000
N	-0.623556	-0.812905	1.173220
N	-0.623557	-0.812904	-1.173220

Energy = -358.838509995
Number of Imaginary Frequencies = 1

1,2,3-Triazine + C_2H_4 [C,N], [2,5] Adduct

C	-0.924030	-0.221728	-1.188110
C	-1.059273	0.692285	-0.000004
C	-0.924028	-0.221713	1.188115
C	0.273931	1.533655	-0.000010
C	1.440806	0.512988	-0.000004
H	-1.624159	-0.222403	-2.023155
H	-1.956485	1.311183	-0.000008
H	-1.624156	-0.222378	2.023160
H	0.294852	2.176529	-0.884837
H	0.294853	2.176540	0.884810
H	2.069956	0.603258	-0.887830
H	2.069958	0.603271	0.887818
N	0.907649	-0.894032	0.000006
N	0.091229	-0.995756	1.224004
N	0.091228	-0.995772	-1.223992

Energy = -358.885035350
Number of Imaginary Frequencies = 0

1,2,4-Triazine (**14**)

C	-1.258788	-0.358631	0.000004
C	-0.878839	0.987878	0.000000
C	1.252445	0.289177	-0.000009
H	-2.301127	-0.666050	0.000010
H	-1.615187	1.789963	0.000004
H	2.316315	0.513192	0.000081
N	0.405864	1.329884	-0.000006
N	-0.356352	-1.341422	0.000001
N	0.937787	-1.009556	-0.000006

Energy = -280.322076691
Number of Imaginary Frequencies = 0

1,2,4-Triazine + H_2 [N,N] TS

C	-1.205418	-0.533730	-0.222357
C	1.197158	0.468278	-0.223897
C	-1.045281	0.814481	-0.199723
H	-2.135459	-1.063908	-0.393983
H	2.125463	0.948753	-0.518477
H	-1.827818	1.547533	-0.365165
H	0.141927	0.424702	1.476605
H	0.000954	-0.566493	1.451925
N	0.172627	1.270301	0.302760
N	-0.126725	-1.277510	0.274095
N	1.099267	-0.819186	-0.259004

Energy = -281.392453549
Number of Imaginary Frequencies = 1

1,2,4-Triazine + H_2 [N,N] Adduct

C	-1.048639	0.878443	0.000047
C	0.189514	1.377259	0.000038
C	0.982272	-0.902638	0.000058
H	-1.933890	1.503176	0.000202
H	0.423548	2.431734	0.000166
H	1.829257	-1.583756	0.000202
N	1.283300	0.451688	-0.000093
N	-1.257646	-0.502412	-0.000191
N	-0.186859	-1.422192	0.000067
H	2.237475	0.765002	-0.000156
H	-2.166836	-0.924121	0.000250

Energy = -281.493873048
Number of Imaginary Frequencies = 0

1,2,4-Triazine + C_2H_4 [N,N] TS

C	0.758887	1.143649	-0.660235
C	1.148422	-0.094083	-1.054224
C	0.652902	-0.826223	1.034417
C	-1.363956	-0.913354	-0.559819
C	-1.660110	0.409630	-0.135078
H	0.912426	2.058026	-1.226189
H	1.684233	-0.312193	-1.974636
H	0.866663	-1.611967	1.756824
H	-1.310417	-1.144643	-1.617140
H	-1.629004	-1.752766	0.072995
H	-1.923903	1.142019	-0.891382
H	-2.198057	0.530792	0.799711
N	-0.075150	1.233157	0.454887
N	0.694973	-1.171003	-0.312270
N	0.291776	0.333991	1.475876

Energy = -358.835866884
Number of Imaginary Frequencies = 1

1,2,4-Triazine + C_2H_4 [N,N] Adduct

C	0.085165	-0.840642	1.201611
C	0.985921	1.119571	-0.316067
C	1.435290	-0.113646	-0.543384
C	-1.280093	0.518542	-0.647292
C	-0.754406	-0.913214	-0.961979
H	0.108614	-1.634559	1.946398
H	1.489393	2.056056	-0.535556
H	2.391923	-0.411942	-0.961263
H	-2.254051	0.497053	-0.151258
H	-1.360483	1.141400	-1.541840
H	-1.479711	-1.688414	-0.698770
H	-0.484652	-1.039870	-2.012726
N	0.504058	-1.158424	-0.149847
N	-0.325556	1.194902	0.296242
N	-0.355972	0.314466	1.504702

Energy = -358.875353020
Number of Imaginary Frequencies = 0

1,2,4-Triazine + H_2 [C,N] TS

C	-1.262569	-0.257896	-0.212947
C	1.295451	0.203088	-0.233893
C	0.342201	1.189380	0.234090
H	-2.267271	-0.584803	-0.466683
H	2.309596	0.431912	-0.548782
H	0.638740	2.208086	0.466177
H	0.159547	0.450089	1.526672
H	-0.176220	-0.448241	1.479528
N	-0.389045	-1.229696	0.283637
N	0.911977	-1.037774	-0.196653
N	-0.939345	1.001117	-0.255615

Energy = -281.422040660
Number of Imaginary Frequencies = 1

1,2,4-Triazine + H_2 [C,N] Adduct

C	0.795481	1.081646	0.000000
C	1.384170	-0.315163	0.000000
C	-0.844040	-1.023224	0.000000
H	1.466618	1.940293	0.000000
H	2.042342	-0.442616	0.874221
H	-1.634450	-1.776371	0.000000
N	0.378839	-1.386098	0.000000
N	-0.454754	1.362406	0.000000
N	-1.302312	0.274841	0.000000
H	2.042343	-0.442614	-0.874221
H	-2.282926	0.503711	0.000000

Energy = -281.522681346
Number of Imaginary Frequencies = 0

1,2,4-Triazine + C_2H_4 [C,N] TS

C	0.751277	0.846345	-1.011902
C	0.773740	-0.783609	1.002850
C	-1.598854	-0.781392	-0.167645
C	-1.658175	0.596799	0.079393
H	0.999288	1.552213	-1.801790
H	1.007603	-1.529284	1.760846
H	-1.717896	-1.165859	-1.173814
H	-1.796522	-1.492745	0.625759
H	-1.949292	1.256123	-0.733636
H	-1.970013	0.929480	1.065719
H	0.099530	2.301648	0.498350
N	0.711667	0.475339	1.336556
C	0.265732	1.249262	0.282812
N	0.830009	-0.424906	-1.279088
N	0.476178	-1.281292	-0.250966

Energy = -358.862780491
Number of Imaginary Frequencies = 1

1,2,4-Triazine + C_2H_4 [C,N] Adduct

C	-0.299762	-0.888397	1.143467
C	1.128939	0.507855	0.147785
C	0.994455	-0.375856	-1.068211
C	-0.028430	1.555188	0.000805
C	-1.327427	0.736208	-0.203773
H	-0.760230	-1.518568	1.903236
H	2.107893	0.976623	0.251025
H	1.770786	-0.469584	-1.826973
H	-0.063561	2.156699	0.914052
H	0.173547	2.224454	-0.840966
H	-2.088485	0.967671	0.545541
H	-1.763361	0.889081	-1.193800
N	-0.099666	-1.016600	-1.224602
N	0.816313	-0.305597	1.338960
N	-1.028538	-0.740140	-0.096152

Energy = -358.909485710
Number of Imaginary Frequencies = 0

1,2,4-Triazine + H_2 [C,C] TS

C	-0.525787	-1.103369	0.208347
C	1.324601	0.056043	-0.186088
C	0.488277	1.140434	0.242353
H	-1.021153	-2.053249	0.384418
H	2.363284	0.189430	-0.479460
H	0.872988	2.139539	0.418596
H	0.102075	0.426365	1.530138
H	-0.318385	-0.405651	1.527916
N	-0.822559	1.088701	-0.252858
N	-1.357017	-0.074455	-0.265438
N	0.790811	-1.136400	-0.191601

Energy = -281.438800048
Number of Imaginary Frequencies = 1

1,2,4-Triazine + H_2 [C,C] Adduct

C	-1.390174	-0.125856	0.000000
C	-0.669047	1.187547	0.000000
C	1.371618	0.096010	0.000000
H	-2.049581	-0.217642	-0.874064
H	-1.276514	2.099438	0.000000
H	2.032390	0.092941	-0.876462
N	0.595418	1.318312	0.000000
N	-0.526922	-1.342509	-0.000001
N	0.708149	-1.232407	-0.000001
H	2.032366	0.092922	0.876478
H	-2.049557	-0.217642	0.874081

Energy = -281.499935168
Number of Imaginary Frequencies = 0

1,2,4-Triazine + C_2H_4 [C,C] TS

C	1.012771	0.583612	-1.026670
C	0.303850	-1.268068	-0.013391
C	-1.707342	-0.564803	-0.217758
C	-1.611974	0.819984	-0.170766
H	1.480513	1.135273	-1.841125
H	0.125987	-2.338915	-0.038068
H	-1.836376	-1.062681	-1.173925
H	-2.069754	-1.107918	0.649041
H	-1.667299	1.401228	-1.085754
H	-1.884728	1.350537	0.735935
H	0.528255	2.312836	0.239817
N	0.627255	0.534638	1.328379
C	0.511630	1.232001	0.139128
N	0.897285	-0.716317	-1.118200
N	0.514002	-0.747852	1.254224

Energy = -358.876108482
Number of Imaginary Frequencies = 1

1,2,4-Triazine + C_2H_4 [C,C] Adduct

C	1.243851	-0.251774	-0.854720
C	-0.653647	-1.042826	0.037260
C	-1.477400	0.186456	-0.455101
C	-0.534101	1.405605	-0.433116
H	2.158570	-0.258969	-1.448157
H	-1.257094	-1.942773	0.146678
H	-1.842995	-0.032046	-1.462085
H	-2.342185	0.325423	0.199486
H	-0.445650	1.875336	-1.416264
H	-0.871150	2.167691	0.275837
H	1.614511	1.688052	0.102659
N	0.608614	0.329430	1.407401
C	0.873251	0.893938	0.022365
N	0.460376	-1.267063	-0.861869
N	-0.172666	-0.629668	1.411855

Energy = -358.930991418
Number of Imaginary Frequencies = 0

1,3,5-Triazine (**15**)

C	-1.264596	-0.275507	-0.000012
C	0.393677	1.232838	0.000000

C	0.870880	-0.957351	0.000012
H	-2.328236	-0.507249	0.000089
H	0.724743	2.269879	0.000000
H	1.603386	-1.762640	-0.000087
N	-0.418561	-1.310859	0.000000
N	1.344602	0.292963	0.000012
N	-0.925993	1.017915	-0.000012

Energy = -280.364778486
Number of Imaginary Frequencies = 0

1,3,5-Triazine + H_2 [C,N] TS

C	0.223728	-0.618004	-1.133065
C	0.223728	-0.618004	1.133065
C	-0.274016	1.197916	0.000000
H	0.495706	-1.220948	-1.995790
H	0.495706	-1.220948	1.995790
H	-0.522468	2.255773	0.000000
H	-1.528812	0.488252	0.000000
H	-1.439393	-0.490219	0.000000
N	0.223728	0.676939	-1.197870
N	0.223728	0.676939	1.197870
N	-0.239081	-1.294358	0.000000

Energy = -281.454086004
Number of Imaginary Frequencies = 1

1,3,5-Triazine + H_2 [C,N] Adduct

C	-0.618206	-1.191837	0.000000
C	1.398701	-0.000007	0.000000
C	-0.618192	1.191844	0.000000
H	-1.225211	-2.098591	0.000000
H	2.060102	-0.000012	-0.877348
H	-1.225186	2.098607	0.000000
N	-1.340359	0.000008	0.000000
N	0.649095	1.265246	0.000000
N	0.649079	-1.265255	0.000000
H	2.060093	-0.000007	0.877354
H	-2.348324	0.000014	0.000000

Energy = -281.551436153
Number of Imaginary Frequencies = 0

1,3,5-Triazine + C_2H_4 [C,N] TS

C	-0.908406	-0.401734	-1.131915
C	0.038866	1.252350	-0.000009
C	-0.908267	-0.401722	1.132000
C	1.705173	0.292100	-0.000067
C	1.404814	-1.083563	-0.000067
H	-1.298835	-0.899158	-2.019112
H	0.399212	2.278477	-0.000018
H	-1.298589	-0.899162	2.019234
H	2.123320	0.707915	-0.913610
H	2.123424	0.707896	0.913436
H	1.455192	-1.664310	-0.913742
H	1.455312	-1.664331	0.913587
N	-0.773284	-1.183398	0.000025
N	-0.538578	0.840859	-1.204077
N	-0.538439	0.840837	1.204134

Energy = -358.896876828
Number of Imaginary Frequencies = 1

1,3,5-Triazine + C_2H_4 [C,N] Adduct

C	-0.853435	-0.383553	1.157609
C	1.040914	-0.657508	-0.004648
C	-0.861343	-0.379861	-1.153070
C	1.272182	0.886009	-0.001696
C	-0.137128	1.526147	0.002002
H	-1.588658	-0.446670	1.958282
H	1.971466	-1.223068	-0.008840
H	-1.602120	-0.440574	-1.948784
H	1.849458	1.161454	0.885563
H	1.847320	1.166319	-0.888811
H	-0.314198	2.142930	0.885972
H	-0.318801	2.141989	-0.881696
N	-1.201377	0.431064	0.004779
N	0.275365	-0.964138	1.221651
N	0.267211	-0.959751	-1.226840

Energy = -358.935637120
Number of Imaginary Frequencies = 0

Tetrazine (**16**)

C	-1.265262	-0.000018	-0.000008
C	1.265262	-0.000010	0.000002
H	-2.351054	0.000003	0.000087
H	2.351054	0.000016	0.000034
N	-0.662946	-1.196247	-0.000006
N	0.662954	-1.196243	0.000000
N	0.662923	1.196257	0.000000
N	-0.662931	1.196254	-0.000006

Energy = -296.321147367
Number of Imaginary Frequencies = 0

Tetrazine + H_2 [N,N] TS

C	-0.034494	1.267558	-0.223926
C	0.034494	-1.267558	-0.223926
H	-0.166397	2.301855	-0.522836
H	0.166397	-2.301855	-0.522836
H	0.419812	-0.239122	1.482957
H	-0.419812	0.239122	1.482957
N	1.140701	-0.569690	0.289948
N	-1.140701	0.569690	0.289948
N	-1.140701	-0.719742	-0.235172
N	1.140701	0.719742	-0.235172

Energy = -297.414767056
Number of Imaginary Frequencies = 1

Tetrazine + H_2 [N,N] Adduct

C	0.020260	-1.319391	0.000000
C	-0.020260	1.319391	0.000000
H	0.136386	-2.401158	0.000000
H	-0.136386	2.401158	0.000000
N	-1.172851	0.585677	0.000000
N	1.172851	-0.585677	0.000000
H	2.087176	-1.001713	0.000000
H	-2.087176	1.001713	0.000000
N	-1.172851	-0.846574	0.000000
N	1.172851	0.846574	0.000000

Energy = -297.526797160
Number of Imaginary Frequencies = 0

Tetrazine + C_2H_4 [N,N] TS

C	-0.752498	-0.871095	0.918262
C	-0.752496	0.871102	-0.918258
C	1.597974	-0.682277	-0.174889
C	1.597978	0.682264	0.174881
H	-1.001014	-1.656481	1.627497

H	-1.001009	1.656491	-1.627491
H	1.850292	-1.426288	0.572684
H	1.812538	-0.971248	-1.197656
H	1.812548	0.971233	1.197647
H	1.850304	1.426272	-0.572694
N	-0.330371	1.262332	0.347638
N	-0.330389	-1.262329	-0.347638
N	-0.774571	0.367229	1.307546
N	-0.774584	-0.367223	-1.307540

Energy = -374.859074430
Number of Imaginary Frequencies = 1

Tetrazine + C_2H_4 [N,N] Adduct

C	0.700977	-0.968643	0.844925
C	0.700194	0.969202	-0.844924
C	-1.306271	0.709853	0.312796
C	-1.305700	-0.710892	-0.312803
H	1.081307	-1.839745	1.374827
H	1.079860	1.840602	-1.374813
H	-1.742991	0.730941	1.313894
H	-1.824691	1.444227	-0.308973
H	-1.823543	-1.445677	0.308960
H	-1.742394	-0.732328	-1.313904
N	0.124501	-1.172680	-0.460267
N	0.123557	1.172777	0.460268
N	0.749980	0.188312	1.379420
N	0.750141	-0.187715	-1.379415

Energy = -374.901727942
Number of Imaginary Frequencies = 0

Tetrazine + H_2 [C,C] TS

C	-1.209882	-0.000012	0.219777
C	1.209882	0.000006	0.219777
H	-2.279412	-0.000018	0.397283
H	2.279412	0.000016	0.397283
H	0.453265	0.000013	1.539215
H	-0.453265	0.000006	1.539216
N	0.643132	1.184079	-0.232512
N	-0.643149	1.184069	-0.232512
N	-0.643135	-1.184078	-0.232511
N	0.643152	-1.184068	-0.232511

Energy = -297.449411736
Number of Imaginary Frequencies = 1

Tetrazine + H_2 [C,C] Adduct

C	1.347383	0.000003	0.000019
C	-1.347383	-0.000006	0.000019
H	2.004506	0.000006	-0.878078
H	-2.004505	-0.000007	-0.878078
N	0.621634	-1.281591	-0.000015
N	-0.621625	-1.281595	-0.000015
N	-0.621633	1.281592	-0.000015
N	0.621625	1.281596	-0.000015
H	2.004430	0.000006	0.878173
H	-2.004431	-0.000007	0.878172

Energy = -297.500709083
Number of Imaginary Frequencies = 0

Tetrazine + C_2H_4 [C,C] TS

C	-0.422764	-1.231061	-0.000432
C	1.695297	-0.690228	-0.000280
C	1.695244	0.690407	0.000236
H	-0.338978	-2.312195	-0.000990
H	1.874680	-1.236191	0.920712
H	1.875761	-1.235637	-0.921387
H	1.875664	1.235839	0.921337
H	1.874520	1.236386	-0.920768
H	-0.339313	2.312171	0.000987
N	-0.789110	0.647329	-1.188377
C	-0.422967	1.231028	0.000441
N	-0.788966	-0.647418	1.188402
N	-0.788884	-0.646276	-1.188966
N	-0.788924	0.646187	1.188987

Energy = -374.887351813
Number of Imaginary Frequencies = 1

Tetrazine + C_2H_4 [C,C] Adduct

C	-0.323598	1.178622	-0.016608
C	1.218762	0.961065	-0.002665
C	1.448526	-0.558360	0.002347
H	-0.622318	2.224314	-0.032671
H	1.648763	1.444649	-0.883436
H	1.626419	1.445091	0.888642
H	1.980864	-0.900085	-0.889149
H	2.002396	-0.893072	0.883104
H	0.062781	-2.308836	0.032721
N	-0.656780	-0.712427	1.219888
C	0.039099	-1.221582	0.016599
N	-0.838548	0.486628	-1.219633
N	-0.847579	0.519200	1.199928
N	-0.656470	-0.746335	-1.199790

Energy = -374.944749153
Number of Imaginary Frequencies = 0

References

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S2. (a) Ess, D. H.; Houk, K. N. *J. Am. Chem. Soc.* **2007**, *129*, 10646–10647. (b) Ess, D. H.; Houk, K. N. *J. Am. Chem. Soc.* **2008**, *130*, 10187–10198. (c) Jones, G .O.; Houk, K. N. *J. Org. Chem.* **2008**, *73*, 1333–1342.