

Polycyclic Aromatic Hydrocarbon Formation Mechanism in the “Particle Phase”. A Theoretical Study

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SUPPLEMENTARY INFORMATION

INDEX

page

1. Comparison between the Frenklach and Bittner-Howard mechanisms	2
2. Results on the “perpendicular” arrangement	4
3. Table A. “Particle-phase” system in the $\perp$ arrangement. Free energy differences	5
4. Table B. “Gas-phase” system. Entropy differences	6
5. Table C. “Particle-phase” system in the $\parallel$ arrangement. Entropy differences	7
6. Table D. “Particle-phase” system in the $\perp$ arrangement. Entropy differences	8
7. GEOMETRIES and ENERGIES	
7.1. Complexes of Figure 1.	9
7.2. PAH growth in the “gas phase” (= without ovalene) --- Species of Table 1.	24
7.3. ADSORBED PHASE: growing system $\parallel$ to ovalene --- Species of Table 2.	33
7.4. Species of Table 3	72
7.5. Species of Table 4	94
7.6. ADSORBED PHASE: growing system approximately $\perp$ to ovalene	112

COMPARISON BETWEEN THE FRENKLACH AND BITTNER-HOWARD MECHANISMS

We could make reference to the paper by Kislov, Mebel & alii,^[1] namely to their Figure 1 (p 913) and Table 1, from which ΔE_{ZPE} values are obtained to draw **Figure 1 below** [G3(MP2,CC) data]. There, the process A3-A3a-A4b-A5-N1 (green) corresponds to the Bittner-Howard variant,^[2] while the sequence A3-A10-A11-A12-A13-N1 (magenta) corresponds to the steps suggested by Frenklach & coworkers.^[3] A branching occurs right from the beginning in the magenta curve, corresponding to simple H loss (upper curve) or to a +H/-H₂ process. A similar branching occurs in the green curve at the end. The first barrier is 4.5 kcal mol⁻¹ high for the Bittner-Howard curve, while it is 6.2 kcal mol⁻¹ for the Frenklach curve. Both curves converge to naphthalene (N1). The conclusion in ref. 1 is "The calculations allowed us, for the first time, to consider the HACA network as a whole, using the most reliable potential energy surfaces, which are expected to be accurate within 1-2 kcal/mol. ... the reactions involved in various HACA sequences are demonstrated to have relatively low barriers and high rate constants under combustion conditions. A comparison of the significance of different HACA mechanisms (e.g., Frenklach's, alternative Frenklach's, and Bittner and Howard's routes) in PAH growth can be made in the future...". Then, in another paper by Ahlrichs & coworkers^[4] is concluded that the two pathways are similarly viable ("As a summary, we find that the Bittner-Howard mechanism is slightly favored, ... This result is in line with that of Bauschlicher et al. [ref 5 here] for the analogous reaction of benzene and two acetylene to form naphthalene"). In conclusion, given that the purpose of this investigation is to assess if adsorption of the growing system R on a soot platelet P could affect (and how) the growth itself, we believe that any of the two variants discussed here was eligible.

[1] V.V. Kislov, N.I. Islamova, A.M. Kolker, S.H. Lin, A.M. Mebel, *J. Chem. Theory. Comput.* **2005**, 1, 908-924

[2] J.D. Bittner, J.B. Howard, *Symp. Int. Combust. Inst.* **1981**, 18, 1105-1116

[3] M. Frenklach, D.W. Clary, W.C. Gardiner, S.E. Stein, *Proc. Combust. Inst.* **1985**, 20, 887-901

[4] B. V. Unterreiner, M. Sierka and R. Ahlrichs "Reaction pathways for growth of polycyclic aromatic hydrocarbons under combustion conditions, a DFT study" *Phys. Chem. Chem. Phys.*, **2004**, 6, 4377-4384

[5] C.W. Bauschlicher, Jr., A. Ricca, *Chem. Phys. Lett.* **2000**, 326, 283-287

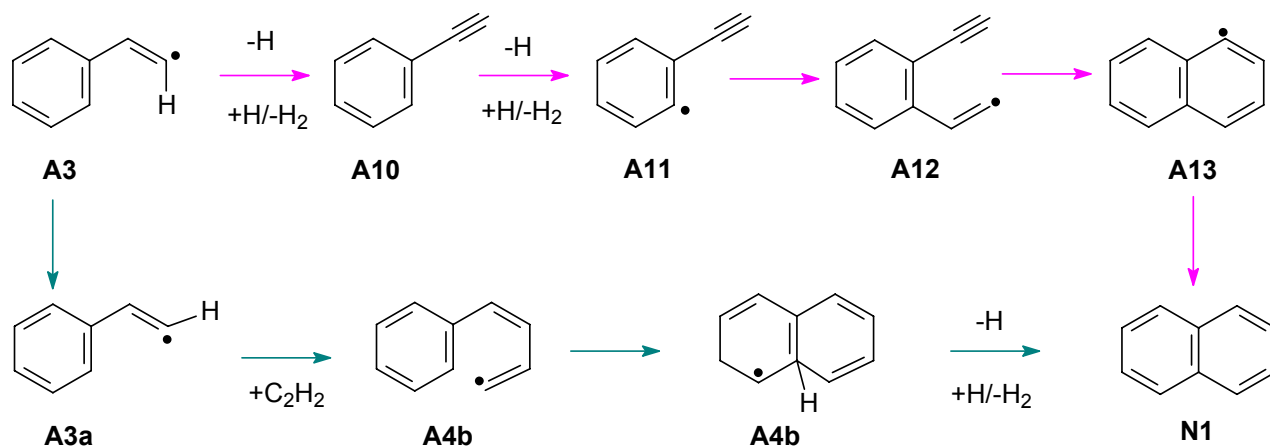
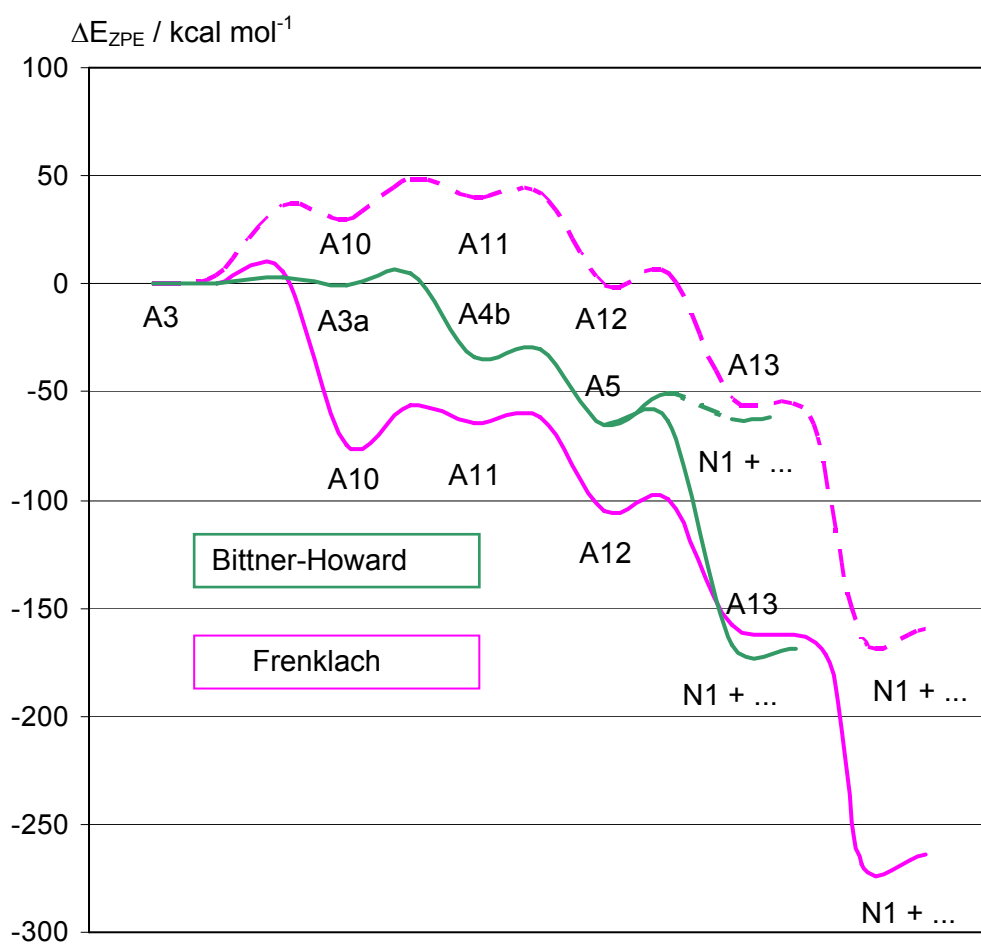


Figure 1

RESULTS ON THE “PERPENDICULAR” ARRANGEMENT

In the main text, emphasis is put on the results obtained for the || layout, because there is indication that this “graphite-like” arrangement is favoured as soon as the system’s size grows beyond some limit (with consequent higher probability of being adsorbed). Figure 1 in the paper, which has been obtained with a rather limited basis set, with the purpose of just seeing a trend [however, the data are corrected for the Basis Set Superposition Error (BSSE)].

For the $\perp$ adsorption (**Table A**), the reference is again the || complex **3**, because the $\perp$ complex **3** (4 kcal mol⁻¹ higher in terms of E, with BSSE correction) is kinetically very unstable.

1) The critical points and barriers for the channel **3-5-6** come out to be the very same already defined for the || arrangement, since the growing species slips sideways and abandons the $\perp$ orientation.

2) The ring closure **3-4** requires overcoming barriers higher, to some extent, than those assessed for the gas-phase and || cases.

3) As regards chain lengthening from **3** to **8**, estimates based on hypotheses A and B would indicate again that chain extension is not competitive, in particular at higher temperatures.

4) If we consider that, for larger growing systems, the || adsorption mode has to be expected to be more stable, the data collected for the $\perp$ case appear to be less important. For this reason, emphasis has been put, in the main text, on the results obtained for the || arrangement.

Table A. “Particle-phase” system in the $\perp$ arrangement. Free energy differences.

	ΔE_{ZPE}	ΔS	ΔG					
T/K:		300	300	700	1100	1500	1900	2300
cyclizations								
3 (complex)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TS 3-4	5.3	-4.4	6.9	9.1	11.8	14.8	18.1	21.5
4	-30.4	-4.0	-29.9	-28.0	-25.8	-23.6	-21.4	-19.2
H loss TS 4-7	-15.1	-8.7	-12.5	-8.5	-4.3	0.2	4.8	9.5
7 -H complex	-22.1	2.3	-26.4	-27.5	-28.9	-30.5	-32.1	-33.9
7 + H	-15.2	52.9	-31.4	-51.9	-71.5	-90.5	-109.1	-127.4
abstr.TS 4-7	-18.2	-10.0	-16.4	-11.8	-6.7	-1.5	3.9	9.4
7 ovalene-H	-39.1	-5.8	-38.9	-36.0	-32.8	-29.5	-26.2	-22.8
chain extension								
A: TS 3-8	4.1	-36.3	14.4	28.9	43.3	57.6	71.8	86.0
B-complex	-0.9	-27.9	7.7	18.3	28.2	37.7	46.9	55.9
B: TS 3-8	4.1	-36.9	14.6	29.3	44.0	58.5	72.9	87.3
8	-44.6	-46.3	-32.6	-13.2	6.7	26.7	46.7	66.6

TABLE B. “Gas-phase” system. Entropy differences.

	ΔS					
T/K :	300	700	1100	1500	1900	2300
cyclizations						
3	0.0	0.0	0.0	0.0	0.0	0.0
TS 3-4	-8.1	-9.4	-10.2	-10.8	-11.2	-11.6
4	-10.0	-11.0	-11.1	-11.1	-11.0	-11.0
TS 3-5	-7.0	-7.9	-8.2	-8.6	-8.9	-9.2
5	-1.9	-2.2	-2.3	-2.3	-2.3	-2.4
TS 5-6	-7.1	-8.8	-9.7	-10.3	-10.8	-11.2
6	-9.4	-11.0	-11.3	-11.4	-11.4	-11.4
H loss TS 4-7	-11.0	-12.1	-12.5	-12.8	-13.1	-13.4
H loss TS 6-7	-10.1	-11.1	-11.5	-11.8	-12.1	-12.4
7 + H	10.5	10.7	10.9	10.9	10.8	10.7
chain extension						
TS 3-8	-34.0	-33.6	-33.2	-32.9	-32.7	-32.5
8	-41.8	-42.8	-42.2	-42.5	-40.8	-40.3

S in cal mole⁻¹ K⁻¹

TABLE C. “Particle-phase” system in the || arrangement. Entropy differences.

	ΔS					
T/K:	300	700	1100	1500	1900	2300
cyclizations						
3	0.0	0.0	0.0	0.0	0.0	0.0
TS 3-4	-0.9	-2.4	-3.2	-3.8	-4.2	-4.6
4	0.0	-0.5	-0.5	-0.5	-0.5	-0.5
TS 3-5	-1.9	-2.8	-3.2	-3.5	-3.8	-4.1
5	-1.6	-1.9	-2.0	-2.1	-2.1	-2.1
TS 5-6	-6.2	-8.0	-8.9	-9.6	-10.1	-10.4
6	-11.2	-13.4	-13.9	-14.1	-14.1	-14.2
H losses						
H abstr.TS 4-7	-10.0	-12.3	-12.9	-13.3	-13.6	-13.9
H loss TS 6-7	-9.5	-10.9	-11.4	-11.8	-12.2	-12.5
7 -H complex	2.3	3.2	3.8	4.1	4.3	4.4
7 + H	52.7	49.4	47.7	46.5	45.4	44.6
H abstr.TS 6-7	-13.6	-16.3	-17.0	-17.4	-17.8	-18.1
7 + ovalene-H	-4.4	-6.4	-6.6	-6.7	-6.7	-6.8
chain extension						
A : TS 3-8	-34.7	-34.4	-34.1	-33.8	-33.6	-33.4
B -complex	-32.2	-30.3	-29.2	-28.3	-27.7	-27.1
B : TS 3-8	-38.0	-38.0	-37.7	-37.4	-37.2	-37.1
8	-39.8	-41.0	-40.4	-39.7	-39.1	-38.6

S in cal mole⁻¹ K⁻¹

Table D. “Particle-phase” system in the $\perp$ arrangement. Entropy differences.

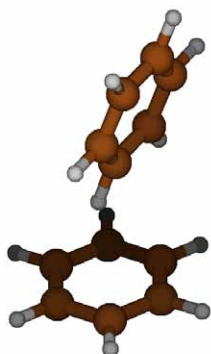
	ΔS					
T/K:	300	700	1100	1500	1900	2300
cyclizations						
3 (complex)	0.0	0.0	0.0	0.0	0.0	0.0
TS 3-4	-4.4	-6.3	-7.2	-7.9	-8.4	-8.8
4	-4.0	-5.3	-5.5	-5.5	-5.5	-5.5
H loss TS 4-7	-8.7	-10.4	-11.0	-11.3	-11.7	-12.0
7 -H complex	2.3	3.2	3.8	4.1	4.3	4.4
7 + H	52.9	49.9	48.3	47.0	46.0	45.2
abstr.TS 4-7	-10.0	-12.3	-12.9	-13.3	-13.6	-13.9
7 ovalene-H	-5.8	-7.9	-8.2	-8.3	-8.3	-8.3
chain extension						
A: TS 3-8	-36.3	-36.2	-35.9	-35.6	-35.4	-35.3
B-complex	-27.9	-25.5	-24.2	-23.3	-22.7	-22.1
TS 3-8	-36.9	-36.8	-36.5	-36.2	-36.0	-35.8
8	-46.3	-49.5	-50.0	-50.0	-49.9	-49.7

S in cal mole⁻¹ K⁻¹

GEOMETRIES and ENERGIES

Complexes of Figure 1.

1. BENZENE DIMER (A) in the "PERPENDICULAR" COMPLEX

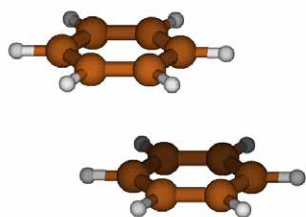


$E_{\text{raw}} = -464.518858953 \text{ a.u.}$

$E_{\text{BSSE-corrected}} = -464.516996 \text{ a.u.}$

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C,1.6953875048,-0.170714751,2.0294831608
C,2.7320468738,-0.1386970198,1.0925336088
C,2.4409142434,0.0054996003,-0.2674562345
C,1.1124792814,0.1168434505,-0.6882421554
C,-2.1556621418,1.2217297839,4.0973091412
C,-0.9090890445,1.6942012294,4.5185952652
C,0.0379506165,0.8045063361,5.0325367495
C,-0.2584907037,-0.5586506763,5.1210283529
C,-1.5033107156,-1.0322076971,4.6969828837
C,-2.4529683051,-0.1411496135,4.1871647784
H,-0.6743072644,2.7527176487,4.4410957879
H,-2.8889562974,1.9131372919,3.6893779356
H,1.0070147751,1.1730449809,5.3597774594
H,-3.4175750344,-0.510825228,3.8476957941
H,0.479543131,-1.2518825474,5.5172605093
H,-1.7318673574,-2.0931576522,4.7604431461
H,1.9124888845,-0.2795413183,3.0888099321
H,-0.4333191299,-0.0834805336,2.3436884384
H,3.7656769802,-0.2252186198,1.4204432407
H,3.2469066738,0.031164098,-0.9973241934
H,0.8848661019,0.229119018,-1.7459324588
H,-0.9563454625,0.1706859626,-0.0775765776

2. BENZENE DIMER in the "PARALLEL" COMPLEX

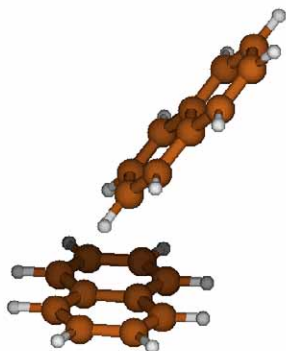


$E_{\text{raw}} = -464.517993424$

$E_{\text{BSSE-corrected}} = -464.514307 \text{ a.u.}$

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 C,-0.1844470984,0.3260263003,1.5955769927
 C,1.0220939198,0.2224844933,2.2941706081
 C,2.1817876406,-0.1803784359,1.6276897633
 C,2.1367782809,-0.4821418378,0.2645042253
 C,0.9324936915,-0.377433141,-0.4330611122
 C,0.2436883731,-3.6720130211,-0.2273499709
 C,0.2886713851,-3.3707815496,1.1359559041
 C,1.4930370459,-3.4753252623,1.8333766136
 C,2.6538179244,-3.8804811102,1.1687907866
 C,2.6101391971,-4.1775426241,-0.1956588134
 C,1.4034860585,-4.0741779242,-0.8941069586
 H,-1.1664915126,0.1068120459,-0.3124309451
 H,-1.0874740148,0.6402652596,2.1133351064
 H,1.0571677954,0.4549602294,3.3557557375
 H,3.1184481363,-0.2688692927,2.1722241572
 H,3.0329925222,-0.8196992273,-0.247657753
 H,0.8954262666,-0.6262090014,-1.4900056869
 H,-0.6930502846,-3.5836675013,-0.7717647858
 H,-0.6076820912,-3.0338696964,1.6483311635
 H,1.5300567713,-3.2270200678,2.8904345197
 H,3.5922055782,-3.958721628,1.7123866179
 H,3.5132610478,-4.4912301565,-0.7136297413
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3. NAPHTHALENE DIMER (B) in the "PERPENDICULAR" COMPLEX

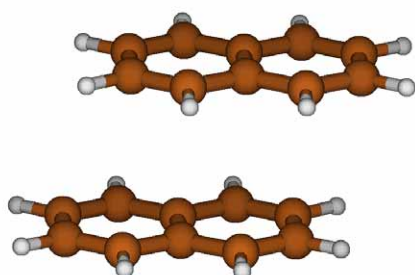


$E_{\text{raw}} = -771.828234011 \text{ a.u.}$

$E_{\text{BSSE-corrected}} = -771.825474 \text{ a.u.}$

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C,2.4312599345,0.7515732275,1.2923594032
C,2.4372846207,1.2809408594,-0.0233491656
C,1.2510353127,1.5287209826,-0.6776307506
C,-1.2339329833,1.5218122092,-0.6935281983
C,-2.4270615958,1.267471211,-0.0544323512
C,-2.4349576137,0.738219334,1.2613161032
C,-1.2488084894,0.4751299253,1.9118080835
H,3.3840653843,1.4949992002,-0.5117534653
H,3.3734712361,0.5613219722,1.7994269472
H,1.2276448414,0.0795518846,2.9381157034
H,-1.2487509082,0.0728733611,2.9223524646
H,-3.3825123894,0.5428220373,1.7563244109
H,-3.3686883283,1.4762689696,-0.5549369694
H,-1.2216333024,1.9370540468,-1.6983104009
C,-0.7202661366,4.1279577896,1.4941149132
C,0.6982554471,4.1317617445,1.5048942694
C,-1.4145505153,5.264370105,1.1437746241
C,1.3916901977,5.2719045871,1.1651487689
C,0.7053335048,6.4607773211,0.7976909268
C,-0.7290618934,6.4568996569,0.7867182945
C,-1.4155667567,7.6443650091,0.4162540486
C,-0.7217719139,8.7838634073,0.0720895774
C,0.6964572257,8.7876976106,0.0829562465
C,1.3910290819,7.6519300338,0.4377305126
H,1.2311499425,3.2246098352,1.770977728
H,-1.2522556963,3.2179863691,1.7521992011
H,-2.5024950926,5.265352842,1.1294317458
H,-2.5034734849,7.6355777608,0.4099337358
H,-1.2593227968,9.6857645757,-0.2091747468
H,1.2333875861,9.6924871717,-0.1900964832
H,2.4789362084,7.6489608311,0.4480060475
H,2.4797103753,5.2787049034,1.1673081063
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4. NAPHTHALENE DIMER (B) in the "PARALLEL" COMPLEX

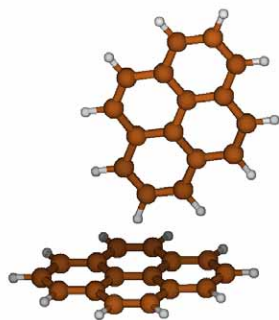


$E_{\text{raw}} = -771.830684819 \text{ a.u.}$

$E_{\text{BSSE-corrected}} = -771.824766 \text{ a.u.}$

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C,2.466747799,-0.0614013482,1.5056499108
C,2.5022202254,-0.0077674218,0.1299891401
C,1.3126953272,0.2241689071,-0.6064237664
C,-1.1737775589,0.5303976319,2.1724344432
C,-1.2069840287,0.4621097187,3.5473312009
C,-0.0206654849,0.2156110925,4.2821797271
C,1.1768170236,0.0452086474,3.6261055479
C,0.8265023704,-3.2937908664,5.1647382321
C,0.8858303681,-3.2448412977,3.7466158256
C,-0.3194688328,-3.0014329668,3.0106590937
C,-1.5345484456,-2.8254999516,3.7224525535
C,-1.5617844936,-2.8807406306,5.0982294353
C,-0.3679602064,-3.1140395613,5.8272500154
C,2.1015127426,-3.4187265304,3.0330691936
C,2.1265525193,-3.3481449317,1.658094289
C,0.9361136299,-3.0993397702,0.9307624023
C,-0.2572680552,-2.9290347936,1.5942681527
H,3.0141020606,-3.6039290709,3.595712334
H,3.0641932238,-3.4716928206,1.1230202554
H,0.974978439,-3.0159631032,-0.1509444624
H,-1.1710392224,-2.718446036,1.0445458592
H,-2.4434271533,-2.6333024356,3.1576695276
H,-2.4985564326,-2.7415612502,5.6317002492
H,-2.0831007727,0.7140932021,1.6040424142
H,-2.1479142264,0.5859908612,4.0765584002
H,-0.0657922145,0.1338961846,5.3637908009
H,2.0874029422,-0.1634789735,4.1817725873
H,1.745083356,-3.4761452225,5.7184336852
H,-0.4006174366,-3.1545384615,6.9130728964
H,-0.801207753,0.585147127,-0.5107018507
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H,3.4422161236,-0.1473880348,-0.3976660513
H,3.3722636223,-0.252643299,2.0761077526

5. PYRENE DIMER (C) in the "PERPENDICULAR" COMPLEX



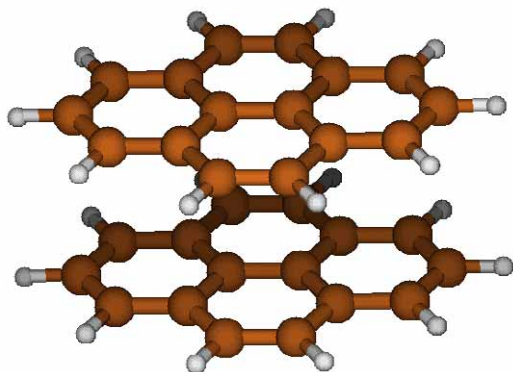
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$E_{\text{BSSE-corrected}} = -1231.614524 \text{ a.u.}$

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 C,2.7246748052,0.0074977376,1.790110446
 C,2.8034553346,0.0086122277,0.388302897
 C,1.6469152851,-0.0337442277,-0.3909494806
 C,1.333713866,-0.0392203444,3.8343335757
 C,2.5135278013,0.0049984133,4.6389033868
 C,3.7929946793,0.0495624116,3.9844498873
 C,3.8942734199,0.0507688468,2.6257945253
 C,0.0482230271,-0.0842062562,4.4568462335
 C,-0.0309872773,-0.0834272141,5.8591342567
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 C,2.3851098214,0.0041536204,6.0361595397
 C,-1.0201405752,-0.1263716952,2.2614221042
 C,-1.1202741689,-0.1279465028,3.6202920712
 C,2.3132020143,-0.0286752688,9.8592162435
 C,2.9738231586,-1.2624679519,9.5744004153
 C,4.2969325752,-1.2356441701,9.1058570929
 C,4.9605169418,-0.0232078634,8.9136663291
 C,4.318198598,1.1867962641,9.1791144861
 C,2.9954839572,1.208287548,9.6493892272
 C,0.9597088197,-0.0304492427,10.3116897325
 C,0.2675365348,-1.266866376,10.4895326882
 C,0.9609848151,-2.4929668927,10.2005081553
 C,2.2510390731,-2.4908597986,9.7631204469
 C,0.2896754009,1.2047974723,10.5659230685
 C,1.0057630176,2.4336998918,10.3541848329
 C,2.295562593,2.4353978996,9.9161861406
 C,-1.0434593245,1.1786349982,11.0051339868
 C,-1.7099437664,-0.03354295,11.1867303849
 C,-1.0650414048,-1.2439258366,10.9305885491
 H,4.8358829162,2.1293262047,9.0191562262
 H,5.9843941593,-0.021297012,8.5494728058
 H,4.7979170157,-2.1755617045,8.8879650191
 H,2.7603762803,-3.4253224097,9.5408293498
 H,0.4248951124,-3.4294421214,10.3340604834
 H,-1.5912953288,-2.1854470694,11.067507773
 H,-2.7419588437,-0.034876834,11.526983888
 H,-1.5530585066,2.1191992143,11.1995107996
 H,0.4874677211,3.3696693181,10.5480012566
 H,2.8226201954,3.372526232,9.7546451719

H,3.2759340158,0.0377669339,6.6581194652
H,-1.0086405159,-0.1173837329,6.3343286639
H,1.0767854291,-0.0366587827,7.7161230518
H,4.6845141097,0.0828104964,4.6064965331
H,4.8683398589,0.0851028411,2.1432225716
H,3.7821086348,0.0433284775,-0.0846843723
H,1.7274132419,-0.0320972779,-1.4748100532
H,-0.5100615569,-0.1111663883,-0.4030936739
H,-1.9126288314,-0.1594204657,1.6407889593
H,-2.0945817548,-0.1623313789,4.1023532469

6. PYRENE-DIMERS (C) in the "PARALLEL" COMPLEX



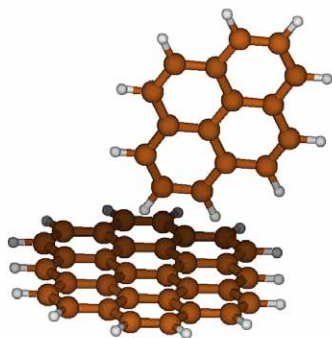
$E_{\text{raw}} = -1231.62366340 \text{ a.u.}$

$E_{\text{BSSE-corrected}} = -1231.616155 \text{ a.u.}$

C,0.0107805952,-0.1209248706,-0.0349963172
C,0.0098982452,-0.1199796039,1.3926026299
C,1.2469998558,-0.1194221633,2.1051259305
C,2.4491740603,-0.1189246501,1.3817570015
C,2.4419543449,-0.1195230324,-0.0124409183
C,1.2378589836,-0.1204010334,-0.7152742986
C,-1.2496053904,-0.121986849,-0.7247959609
C,-2.4285858354,-0.1194407676,-0.0436897035
C,-2.4608080623,-0.1158033529,1.3927312521
C,-1.2237069782,-0.1178763796,2.1052620275
H,3.3911450552,-0.1235046311,1.9251032566
H,3.3830274039,-0.1252162128,-0.5559724318
H,1.2374625166,-0.1271367527,-1.8026930016
H,-1.2390807052,-0.1310603179,-1.8122119845
H,-3.375744818,-0.1255884477,-0.57810781
C,0.0130766693,-3.7289950978,-0.0326001079
C,0.011458794,-3.7282737184,1.3950185601
C,-1.22249748,-3.728195668,2.1071194261
C,-2.4592339893,-3.7283608115,1.3939801917
C,-2.4262747988,-3.7254073339,-0.0424379042
C,-1.2469692125,-3.725986771,-0.7230016242
H,-3.3731557629,-3.7175279289,-0.5773159251
H,-1.2359371407,-3.717980205,-1.8104245191
C,1.2404836734,-3.7330425112,-0.7122848725
C,2.4442263538,-3.7350961226,-0.0088450949
C,2.4507335822,-3.7334012028,1.3853606757
C,1.2481930353,-3.7299688536,2.1081496187
H,3.3924344957,-3.7296113658,1.9291818613
H,3.3855874946,-3.7322212451,-0.5519129287
H,1.2406281587,-3.7281426898,-1.7997181225

C,1.2147953577,-0.1195957093,3.5415546081
 C,0.0358078457,-0.1180156727,4.2226797145
 C,-1.2245879097,-0.1159151416,3.5328714173
 C,-2.4516775283,-0.1113193038,4.213140063
 C,-3.6557819802,-0.108656622,3.5102951357
 C,-3.6629969405,-0.1106494372,2.1160824758
 C,1.2152485986,-3.7287374587,3.5445756543
 C,0.0359395025,-3.7292741798,4.2251594749
 C,-1.2241145414,-3.7302824143,3.534745111
 C,-2.4515389691,-3.7337392675,4.2144286527
 C,-3.6552916448,-3.734395513,3.5109764229
 C,-3.6617901915,-3.7317424771,2.1167536508
 H,-4.604975625,-0.1135568101,1.5727231762
 H,-4.5968635176,-0.1106831737,4.0538470321
 H,-2.4512920693,-0.1159934571,5.3005666398
 H,0.0252937143,-0.1241708491,5.3101213695
 H,2.1619482582,-0.1262448417,4.07598524
 H,0.0249131953,-3.7229301284,5.3125997161
 H,2.1621428261,-3.7225111864,4.0794621226
 H,-2.451692241,-3.7297108317,5.3018653939
 H,-4.5966553793,-3.7313246364,4.0540396211
 H,-4.6034948783,-3.7271730523,1.5729362783

7. PYRENE-OVALENE (D) in the "PERPENDICULAR" COMPLEX



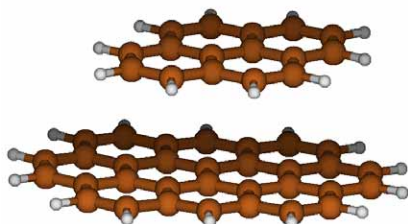
$E_{\text{raw}} = -1843.89522047 \text{ a.u.}$

$E_{\text{BSSE-corrected}} = -1843.893026 \text{ a.u.}$

C,3.6385537901,1.4633248896,-2.1176732133
 C,2.983607314,1.4035941872,-0.845623081
 C,2.6267945188,0.1479057436,-0.293116157
 C,2.898349309,-1.0437647145,-1.0105797605
 C,3.5512953685,-0.9774413581,-2.283660394
 C,3.9098508941,0.2728342107,-2.8045812533
 C,2.681723233,2.6045049766,-0.1378139984
 C,2.0176930271,2.5421833888,1.1225964457
 C,1.659443876,1.2784937755,1.678497857
 C,1.9628405235,0.0848551447,0.9781399836
 C,0.9878551996,1.2134779505,2.9423396076
 C,0.6391068431,-0.0380105269,3.4688979011
 C,0.9173909259,-1.2293041807,2.7842313267
 C,1.5849838222,-1.1691125427,1.5182133577
 C,2.5110454032,-2.305472914,-0.4696394813
 C,1.8540841935,-2.3678170183,0.7941195683
 C,-0.8896858089,0.0755961766,-0.9121265557

C,-1.6788781685,0.0751453796,-2.0622237678
 C,-3.0756880411,-0.0434457167,-1.9755760488
 C,-3.6814496614,-0.1657768141,-0.6876941687
 C,-2.865350195,-0.1619419902,0.4833804819
 C,-1.4739974428,-0.0385726671,0.3484163809
 C,-3.9234340494,-0.0490068991,-3.1369147859
 C,-5.276589618,-0.1685086406,-3.0263467561
 C,-5.9132986511,-0.2950621902,-1.7431548538
 C,-5.0965634394,-0.2922101099,-0.5709552893
 C,-5.6991793425,-0.4171921216,0.718720918
 C,-7.0949266036,-0.5413386864,0.8081867265
 C,-7.8860139834,-0.5430780073,-0.3410631841
 C,-7.3048320732,-0.4212751894,-1.6035911217
 C,-3.4987002729,-0.2892124665,1.7675738347
 C,-4.851027826,-0.4113305424,1.8803497821
 H,4.4061229006,0.3210628204,-3.771663583
 H,-0.8654676249,-0.0384107248,1.2470436743
 H,-1.2168672783,0.1647123427,-3.042597047
 H,0.188053665,0.1618589895,-0.9866917058
 H,0.188053665,0.1618589895,-0.9866917058
 H,-2.8640498106,-0.2866339015,2.6507899549
 H,-5.3192753856,-0.5076195852,2.8573312594
 H,-7.554018746,-0.6365177619,1.7895524811
 H,-8.96493195,-0.6404276995,-0.2519890938
 H,-7.9264793467,-0.4233318482,-2.4959771604
 H,-5.9055636281,-0.1711958669,-3.9134571805
 H,-3.4553295789,0.0447591349,-4.1141069245
 C,3.98723022,2.7513651776,-2.644684584
 C,3.6997649173,3.8986259717,-1.9616451352
 C,3.0371104515,3.8655753483,-0.691254727
 C,2.7213803942,5.0414104705,0.0291281945
 C,2.0766986112,4.9809848895,1.2493373168
 C,1.7100434915,3.740889127,1.8230039116
 C,1.0383633204,3.6488675557,3.0860304541
 C,0.6923773204,2.4413700989,3.6222583946
 C,3.8069294121,-2.2035783729,-2.9838111588
 C,3.4342909982,-3.4092529507,-2.4614969419
 C,2.7740279383,-3.5015826085,-1.192857799
 C,2.373100181,-4.7391512097,-0.6368559323
 C,1.7352086132,-4.7994589726,0.586733759
 C,1.4609661257,-3.6261498547,1.3278505538
 C,0.7981049599,-3.6595896867,2.5978716601
 C,0.5383817927,-2.5147353101,3.2955559413
 H,4.4871914155,2.7942711845,-3.6092281134
 H,3.9689972079,4.8672258867,-2.3762429509
 H,2.9946543776,6.0035648771,-0.397445483
 H,1.839668638,5.8951307506,1.7880734342
 H,0.8062707912,4.5710026409,3.6134265476
 H,0.1818284281,2.3883715299,4.5807523016
 H,0.1308361312,-0.0870217856,4.4301736431
 H,0.0304833177,-2.5571393982,4.2561499635
 H,0.5000856612,-4.625837951,2.9976163492
 H,1.4314197721,-5.7589694123,0.9982684306
 H,2.574910546,-5.650939302,-1.1936017055
 H,3.6325870455,-4.3293159611,-3.006244411
 H,4.304982579,-2.1503801578,-3.9488979331

8. PYRENE-OVALENE (D) in the "PARALLEL" COMPLEX



$E_{\text{raw}} = -1843.90624198 \text{ a.u.}$

$E_{\text{BSSE-corrected}} = -1843.404042 \text{ a.u.}$

C,-0.00296,-0.05984,-0.03646
C,-0.00469,-0.07783,1.39601
C,1.24058,-0.06872,2.0821
C,2.46138,-0.05151,1.34617
C,2.43646,-0.04724,-0.08519
C,1.16324,-0.0461,-0.74537
C,1.26822,-0.09031,3.50693
C,0.05001,-0.13119,4.23937
C,-1.17437,-0.14329,3.53098
C,-1.20058,-0.11468,2.14976
C,0.1071,-0.16209,5.67141
C,1.30018,-0.15284,6.33602
C,2.54752,-0.1141,5.62728
C,2.51665,-0.08363,4.19582
C,3.72926,-0.06233,3.46424
C,4.9697,-0.06879,4.14865
C,4.99437,-0.09132,5.57995
C,3.78383,-0.11337,6.28587
C,6.1904,-0.07416,3.41214
C,7.4362,-0.09862,4.09723
C,7.4349,-0.106,5.53036
C,6.2679,-0.10288,6.24042
C,6.16226,-0.07598,1.98693
C,7.37998,-0.10711,1.25337
C,8.60535,-0.12993,1.96103
C,8.63271,-0.12377,3.34192
C,4.91372,-0.06006,1.29857
C,3.70129,-0.0529,2.0307
C,3.64578,-0.05343,-0.79037
C,4.88203,-0.06643,-0.13244
C,6.12784,-0.09734,-0.84178
C,7.32198,-0.11891,-0.17845
H,1.32664,-0.17579,7.42291
H,3.80504,-0.13462,7.37368
H,6.28355,-0.1128,7.32774
H,8.39242,-0.11811,6.046
H,9.5831,-0.141,3.87035
H,9.53414,-0.15183,1.39566
H,8.25832,-0.14306,-0.73125
H,-0.96041,-0.06772,-0.55198

H,-2.15078,-0.12271,1.62077
H,-2.10362,-0.17393,4.09527
H,-0.82974,-0.19248,6.22306
H,6.10064,-0.10472,-1.92887
H,3.62471,-0.05932,-1.87821
H,1.14823,-0.0425,-1.83259
C,3.71624,-3.66231,2.1212
C,3.75055,-3.63843,3.54866
C,4.99427,-3.62131,4.19948
C,6.18171,-3.62284,3.46816
C,6.15622,-3.64206,2.07359
C,4.93666,-3.66303,1.37956
C,2.46555,-3.68327,1.43803
C,1.24533,-3.67716,2.17982
C,1.31106,-3.64691,3.61511
C,2.5064,-3.62983,4.26816
C,2.43138,-3.71035,0.01053
C,3.67576,-3.70853,-0.70863
C,4.87097,-3.68507,-0.05608
C,1.18828,-3.73711,-0.63991
C,0.00085,-3.73331,0.09161
C,0.02564,-3.70158,1.48551
H,7.08456,-3.63365,1.508
H,5.80512,-3.67552,-0.61231
H,3.63974,-3.72458,-1.79559
H,1.16228,-3.75842,-1.72699
H,-0.95259,-3.75165,-0.42995
H,-0.9028,-3.68988,2.05092
H,0.37709,-3.63336,4.17126
H,2.5416,-3.60186,5.35433
H,5.0203,-3.59781,5.286
H,7.13488,-3.59966,3.98884
--- end of complexes of Figure 1 ---

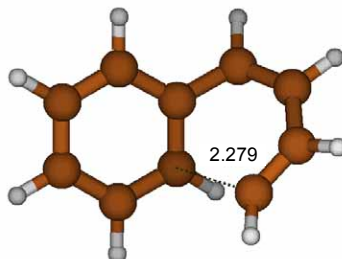
PAH growth in the "gas phase" (= without ovalene) --- Species of Table 1.

3

E = -386.373808502 a.u.

C,0.1893214156,-0.0000608393,-0.5914369759
C,0.4375278145,0.0009803241,0.7945088045
C,1.3063077517,-0.0004669599,-1.4563922554
C,1.7402949916,0.0015331086,1.2897934511
C,2.6074445781,0.0000774937,-0.9636187123
C,2.8312844005,0.0010784086,0.4168413714
C,-1.1330430272,-0.0007207397,-1.2126447351
C,-2.4013321979,-0.0010869164,-0.7296973674
H,-0.4039884939,0.001378909,1.4852527241
H,1.1365726448,-0.0012382366,-2.5310145662
H,1.9036281912,0.0023380888,2.3645450579
H,3.4471499409,-0.0002698154,-1.653779322
H,3.8455789427,0.0015137965,0.8074468834
H,-1.0790155339,-0.0010587627,-2.301504254
H,-3.1705714732,-0.001638722,-1.499707054
C,-2.9719017802,-0.0010136866,0.6170359327
C,-2.4103513301,-0.0001741483,1.8164581123
H,-4.0713049186,-0.0018045751,0.6097342705
H,-2.7813649991,-0.0000969511,2.8339405058

TS 3 --> 4



E = -386.367825174 a.u.

C,0.1154296848,-0.5488949948,-0.7972257801
C,0.0649665726,-0.4484027822,0.6241179924
C,1.2437562881,-0.1478200236,1.3234431888
C,2.4364429957,0.0987263259,0.646720924
C,2.4788741779,0.0241912012,-0.7553962449
C,1.3414383786,-0.3269886326,-1.4677816111
C,-1.215996078,-0.553097852,1.3138176454
C,-2.3624903752,-0.0070286511,0.8382401273
C,-2.4583207506,0.8394765679,-0.3532828484
C,-1.5411566618,0.9294185292,-1.3117895497
H,1.2108785941,-0.0779049862,2.4084259067
H,3.3345080518,0.3486856456,1.204983283
H,3.4136195111,0.2083318296,-1.278721442
H,1.3865136347,-0.4472931654,-2.5470622063
H,-0.6557154852,-1.1222934588,-1.3011828186
H,-1.2240467562,-1.0050501416,2.3048101372
H,-3.2623363112,-0.0887083904,1.4443354003
H,-3.3426775059,1.4859633648,-0.3953155938
H,-1.4784091261,1.5407911738,-2.2054557292

4

E = -386.426356137 a.u.

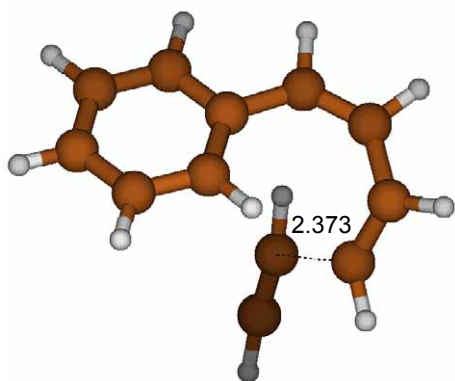
C,-0.6277054621,0.1309686671,0.4477778284
C,-0.444388529,0.0171981318,1.8396446019
C,0.8182273645,-0.0956778401,2.3942953599
C,1.9827070139,-0.1714364123,1.54989989
C,1.8904820908,0.0184902896,0.2114707179
C,0.5856105998,0.4351324692,-0.4222273229
H,-1.3263067135,-0.0535053903,2.4739515144
H,0.9313871587,-0.2182598264,3.4677060304
H,2.9415963365,-0.4151252141,2.0017573976
H,2.7631606673,-0.0542714144,-0.4336266986
H,0.6295190355,1.5560753734,-0.4627724136
C,-1.884580193,0.0013264258,-0.1744880003
C,-2.0001997009,-0.1271066659,-1.5473635682
H,-2.7694297928,-0.0698585356,0.4556669859
H,-2.9784204801,-0.261457867,-2.0002167474
C,-0.8240440455,-0.2029858488,-2.3753695746
C,0.4111835944,0.0017995646,-1.8573978642
H,-0.9396805321,-0.4585587199,-3.4262464095
H,1.304417923,-0.0712910928,-2.473672067

H loss TS 4-7

E = -386.409083066 a.u.

C,0.0042595836,-0.0590826557,0.1224552237
C,0.1225963492,-0.0602465785,1.5339238026
C,1.387756145,0.2517889164,2.1268033193
C,2.4886039757,0.5467597769,1.2793200236
C,2.3442732802,0.540569542,-0.0913396294
C,1.0897723418,0.2366611466,-0.6755640744
C,-0.9819468148,-0.3771170488,2.3882652711
C,-0.8478793399,-0.2836834958,3.7702151735
C,0.4040072008,0.0206312193,4.3460616715
C,1.4992489155,0.2740544101,3.5441928603
H,0.9868255226,0.2354066686,-1.7573939315
H,3.1933660925,0.7691508488,-0.7299484118
H,3.4482380099,0.781048813,1.7345127004
H,2.4638876963,0.5123367502,3.9863110862
H,0.5014709804,0.0617266567,5.4276029231
H,-1.7056087053,-0.4757336667,4.4085130073
H,-1.9642955379,-0.4991565047,1.94002731
H,-0.9587239444,-0.3018493922,-0.3208679703
H,-0.9645296129,-2.3512474894,2.2179881971

Ethyne addition TS 3 --> 8



E = -463.701457109 a.u.

C,-2.0062816059,1.3313187825,-1.85421508
 C,-2.0191228656,1.1025293907,-0.474030156
 C,-0.8314912491,0.8882352872,0.2203975964
 C,0.4052628375,0.9048455512,-0.4513779588
 C,0.4029292315,1.1589700728,-1.8361245221
 C,-0.7871430902,1.360331048,-2.5341104516
 C,1.7077951811,0.7228996345,0.2052868255
 C,2.0593043765,0.2033456345,1.4043642845
 C,1.2800929496,-0.4836342447,2.443775988
 C,0.2459424959,-1.298712235,2.289571342
 C,0.1207620131,-2.4127240862,0.1975155164
 C,-0.6349069567,-3.3675521757,0.2260011047
 H,1.3528530138,1.1948039756,-2.3655069722
 H,-0.761196245,1.5452432768,-3.6048944898
 H,-2.9376254587,1.4890343969,-2.391746746
 H,-2.9629519643,1.0889199306,0.0650863459
 H,-0.8550315412,0.7090577913,1.2877109971
 H,2.5391265495,1.1006263838,-0.3906605947
 H,3.1165962876,0.29390971,1.6545669274
 H,1.6841886348,-0.3595640016,3.4584404693
 H,-0.3319863772,-1.8829445192,2.9943306226
 H,0.829958536,-1.6826789476,-0.1320870762
 H,-1.3327913414,-4.1555239542,0.4024335825

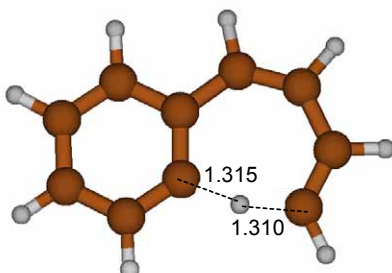
8

E = -463.783012374 a.u.

C,-2.088686891,-0.9840568252,-2.0019675802
 C,-2.079123926,-0.7848963686,-0.6174667936
 C,-0.8758798605,-0.7224973025,0.0808545622
 C,0.3532511338,-0.8662030869,-0.5909305383
 C,0.325313149,-1.0855270316,-1.9815942706
 C,-0.878471523,-1.1347993001,-2.6829671857
 C,1.6610728187,-0.8580375831,0.0763876593
 C,2.0455392108,-0.4307933901,1.3013427319
 C,1.3273518919,0.2914446228,2.3525748831
 C,0.5373066139,1.3822290023,2.2293740548
 C,0.2261442071,2.0592286759,0.9785267459
 C,-0.6196262457,3.0708616845,0.8630946613
 H,1.2664014635,-1.2168643395,-2.5116256051
 H,-0.8717325406,-1.2978646871,-3.7576393353
 H,-3.0305999449,-1.0259339736,-2.5426073603

H,-3.0163412526,-0.6759842946,-0.0777084684
H,-0.8799606582,-0.5689329274,1.1529297417
H,2.4488491906,-1.3144156873,-0.5234911781
H,3.0735478128,-0.6770873017,1.57355105
H,1.5442814742,-0.0462159712,3.3665985654
H,0.1079041776,1.8149188538,3.1304841501
H,0.7390230858,1.6877050464,0.0854353882
H,-0.986516282,3.6989566976,0.0606994717

TS 3 --> 5



E = -386.363223668 a.u.

C,0.204690284,0.0104364539,-0.7894694422
C,0.2522277811,-0.0073785678,0.6107157997
C,1.5390033582,-0.0113720885,1.1992648736
C,2.6889746843,0.0017731506,0.4164640809
C,2.5950400138,0.0194385101,-0.9812815484
C,1.3351618911,0.0237752148,-1.5916323721
C,-0.920082823,-0.0214159677,1.4763740596
C,-2.2415641229,-0.0206706332,1.1655258416
C,-2.9029851721,-0.005529878,-0.1346900582
C,-2.3194915709,0.0108987802,-1.3378803664
H,1.6183517755,-0.0248890375,2.28469879
H,3.6655023233,-0.00161204,0.8934613446
H,3.4958649523,0.0297324683,-1.5900968556
H,1.2476933582,0.0373914022,-2.6756295876
H,-0.6807615222,-0.0342446085,2.5391935148
H,-2.9237940343,-0.0333561387,2.0134273936
H,-3.9955332442,-0.0084259791,-0.0889598483
H,-2.8075488771,0.0223446517,-2.3084714717
H,-1.0102278165,0.0133247814,-1.2914635006

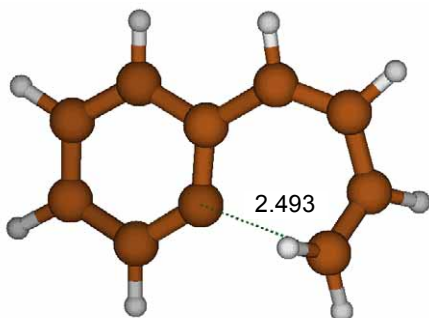
5

E = -386.374886689 a.u.

C,0.2937345414,-0.0560837549,-0.7941066649
C,0.2677420658,0.0333219555,0.5930072159
C,1.5435997676,0.0241039308,1.2093439727
C,2.7157432675,-0.0661394397,0.4590723362
C,2.6631816175,-0.1507174725,-0.9358316247
C,1.4152486563,-0.1401115374,-1.5847891936
C,-0.9219863611,0.0994073764,1.4433513021
C,-2.2312849908,-0.0304517546,1.1317921042
C,-2.8706966961,-0.1942666247,-0.1728157831
C,-2.5455466355,0.4333557317,-1.3134554976
H,1.5970097005,0.0911351822,2.2947754609
H,3.677100451,-0.068974857,0.9656634785

H,3.5788721505,-0.2219060118,-1.5182124066
H,1.3515722863,-0.199797123,-2.6689616146
H,-0.6889399209,0.2029035637,2.5026766066
H,-2.9164432301,-0.0669084532,1.9794647112
H,-3.7299364597,-0.8673371128,-0.1815879878
H,-3.0891766904,0.2366528456,-2.2343838851
H,-1.7584696825,1.1797215034,-1.352843367

TS 5 --> 6



E = -386.37327056 a.u.

C,-0.1123600185,0.0717804581,0.1169078784
C,-0.0614835718,0.1349839684,1.5089988237
C,1.231650983,0.0462992614,2.0760856832
C,2.3639466071,-0.0938702395,1.2758150503
C,2.2477744578,-0.1519458871,-0.1160599269
C,0.9791507674,-0.0605126084,-0.712128106
C,-1.2308861151,0.2269356694,2.3861512405
C,-2.5298440245,0.0272051738,2.048870628
C,-3.0059473414,-0.211737894,0.6983102716
C,-2.5259765992,0.4330448038,-0.3937922092
H,1.3362768749,0.0893747417,3.1589960139
H,3.3444619554,-0.1569786722,1.7400039289
H,3.1340939043,-0.2601838991,-0.7370176713
H,0.873522274,-0.094619924,-1.7941379784
H,-0.9989133364,0.3581667954,3.4421238138
H,-3.2549756075,-0.0521016943,2.858658214
H,-3.7424144603,-1.005816599,0.5675995127
H,-2.8300454741,0.1449694431,-1.396772713
H,-1.9916400806,1.3717571025,-0.307602896

6

E = -386.468369284 a.u.

C,0.023274707,0.0532385207,-0.6902449525
C,0.0642400895,-0.0553130547,0.7271542077
C,1.3215891352,-0.1361939171,1.3676082259
C,2.5017488761,-0.1116500954,0.6362061534
C,2.4547429974,-0.0055742278,-0.7606825857
C,1.2192490654,0.0754206394,-1.4077134391
C,-1.1578060058,-0.0824868641,1.4797864535
C,-2.4072188383,-0.0052094213,0.8362786709
C,-2.5116069364,0.1009205256,-0.5289792351
C,-1.3039861117,0.1434822293,-1.4210418453
H,1.3491885345,-0.2190078551,2.4519881141
H,3.4590257491,-0.1750275288,1.1471753759

H,3.3738752389,0.013740925,-1.3401035267
H,1.1824321274,0.1577962609,-2.4926725092
H,-1.1006060682,-0.1658823312,2.5616360174
H,-3.3114424991,-0.0309256739,1.4406391821
H,-3.4879860567,0.1592041716,-1.0031041253
H,-1.366004066,-0.6674572607,-2.1690693765
H,-1.3238448307,1.0677532852,-2.0267190739

H loss TS 6-7

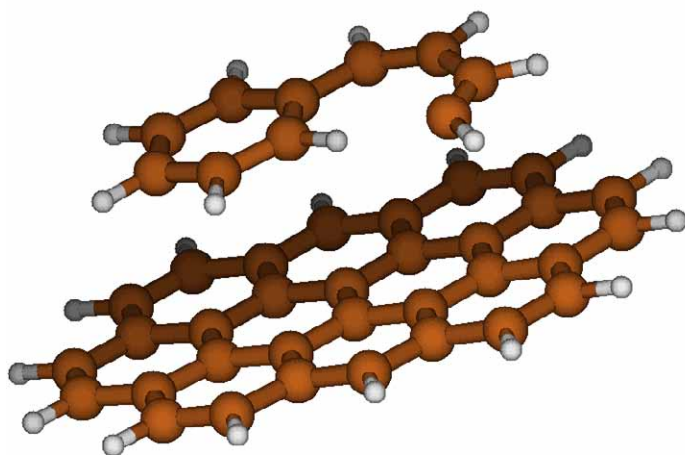
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C,0.0710385442,-0.182966743,1.4747671739
C,1.3758357745,-0.108398121,2.1206160135
C,2.4958884175,0.2765448591,1.3444880786
C,2.3897074825,0.4498081614,-0.0194776775
C,1.1521330976,0.214057884,-0.6830108569
C,-1.0108819296,-0.7924827775,2.2154230094
C,-0.8677866154,-1.0831265111,3.5461109354
C,0.3700002792,-0.8471397099,4.2093239845
C,1.4632731469,-0.3863280771,3.5065069701
H,1.1050018614,0.2890594886,-1.7662939331
H,3.2633727981,0.7300373972,-0.6015422856
H,3.4537546171,0.4056890407,1.8435959011
H,2.422525434,-0.2560165733,4.0027244503
H,0.4596465419,-1.0704862764,5.2688972075
H,-1.6977925034,-1.5109866994,4.1023039132
H,-1.9511661273,-0.9675383947,1.6987621022
H,-0.9177374696,-0.3036452852,-0.4651580664
H,-0.3759848709,1.4045387555,1.7480206896

--- end of Species of Table 1 ---

ADSORBED PHASE: growing system PARALLEL to ovalene --- Species of Table 2

3



E = -1614.48092325 a.u.

C,-0.0403472569,0.3053777639,0.2084254465
C,-0.0202089916,0.2112326843,1.6375189555
C,1.2350288944,0.1425632356,2.3015988639
C,2.4439715332,0.1830830833,1.54879769
C,2.3979135682,0.2925048498,0.1228828926
C,1.1161853383,0.3449827276,-0.5170266062
C,3.6939181161,0.1433496943,2.2128616863
C,3.7435339458,0.0620847758,3.6431914575
C,2.5422253437,0.0352970463,4.3927876027
C,1.2835839278,0.0742827059,3.7242458523
C,2.72571359,3.5629363522,0.7407908508
C,1.4184348658,3.4610296325,1.2048128281
C,1.174062363,3.2915105459,2.5699947024
C,2.2500637659,3.2334928738,3.4583746947
C,3.5577848889,3.3367125328,2.9915708045
C,3.8282843068,3.5005769553,1.619840298
C,3.5962995237,0.3655180696,-0.5978020634
C,4.8420390742,0.3346246421,0.0411037517
C,4.8948401123,0.2145199221,1.4661745976
C,6.1529940332,0.1920080881,2.1349427907
C,6.203243962,0.1019714957,3.5557318973
C,4.9938425148,0.0477720886,4.308609638
C,5.0398551674,0.0086593665,5.7396533918
C,3.840724758,-0.0149920409,6.4636716642
C,2.5945247163,0.0003054196,5.8236522951
C,7.4589633937,0.1049147033,4.2230673243
C,7.4793824224,0.0496210586,5.6544238611
C,6.3231049857,0.0088608789,6.3814016807
C,5.1591807597,3.5931282421,1.0272628275
C,6.4191554652,3.5442124696,1.5280660192
C,6.9664630471,3.357789877,2.8695936003
C,6.3805869989,3.2277800092,4.0492038308
H,2.9127829949,3.6764195852,-0.3245207681

H,0.591464363,3.4868334727,0.5013269621
 H,0.1571931679,3.1768733556,2.9348863645
 H,2.071477446,3.080430448,4.5189416888
 H,4.3879787811,3.2749974338,3.6928706811
 H,5.1222437997,3.7136580126,-0.0551693147
 H,7.1998047839,3.6279361317,0.7749914009
 H,8.0619566015,3.2799745355,2.8727799446
 H,6.7203747491,3.0167583816,5.0550147375
 H,6.3550009528,-0.0248285676,7.4678428629
 H,8.4444422022,0.0493744268,6.1561314166
 C,7.357965401,0.2940496797,1.3884741299
 C,1.3584864278,-0.0011224995,6.5523191333
 H,3.8781312722,-0.0382005306,7.550899801
 H,3.558284241,0.4572309658,-1.6814772218
 H,-1.005400313,0.3527207891,-0.2909661055
 H,1.0852261858,0.424567135,-1.6011375771
 C,7.279503253,0.4092221349,-0.0373245887
 C,8.5935419535,0.2890556561,2.0777998785
 H,8.2074623922,0.4843164205,-0.5995979529
 C,6.0764932914,0.4283192972,-0.6828244908
 H,6.0320954283,0.5182306493,-1.7656680981
 C,8.6427009314,0.1930707695,3.4547585743
 H,9.5127846648,0.3636811715,1.5013170492
 H,9.6007606094,0.1934659509,3.9694526629
 C,0.1553975997,0.0391909949,5.9069861887
 H,1.4017446853,-0.0295531281,7.6384648328
 H,-0.7728497165,0.043386052,6.4736268927
 C,0.0772029543,0.0835098401,4.4766304155
 C,-1.1581017192,0.1499244425,3.7897306518
 C,-1.2049973736,0.2093493122,2.4103303138
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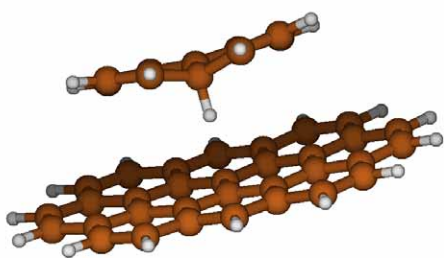
TS 3 --> 4

E = -1614.47179738 a.u.

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 C,2.2960807024,0.1130209824,1.2660504794
 C,2.279827594,0.1620191784,-0.1553930167
 C,1.0361118371,0.253367115,-0.8234387697
 C,1.084027692,0.0710682793,3.4160203505
 C,-0.1473130911,0.0715508033,4.1456061613
 C,-1.3766810158,0.1607313888,3.4118482044
 C,-1.3843583175,0.234925231,2.0481601067
 C,3.5336441542,-0.0078133486,1.962685384
 C,3.5451977147,-0.0906850495,3.3767363033
 C,2.3134944496,-0.0454097587,4.1079150924
 C,2.322902908,-0.1642437977,5.5196761413
 C,1.0886735306,-0.1573655849,6.2439608251
 C,-0.1170084631,-0.0368082648,5.5412141724
 C,3.555846343,-0.3354611248,6.2137934103
 C,4.7790642947,-0.3972374478,5.4855226557
 C,4.7703415653,-0.268337217,4.0651381266
 C,5.995724678,-0.3594116247,3.3294189799

C,5.9643672021,-0.2627967355,1.9321268475
 C,4.762376732,-0.0922948576,1.2328989442
 C,4.71279506,-0.0220564416,-0.1994385286
 C,3.525026078,0.1003189671,-0.8622079832
 C,3.5651542308,-0.4821918679,7.6284046437
 C,2.3187585235,-0.4463547631,8.3331655954
 C,1.132858125,-0.2964714106,7.6712939244
 C,4.7989268768,-0.6856567936,8.2883706539
 C,5.9837235807,-0.7519209814,7.5819832047
 C,6.0044274279,-0.6121995641,6.1746245381
 C,7.2178980311,-0.6884325871,5.4164959491
 C,7.2151730095,-0.566764453,4.0562397145
 C,1.718881219,-3.1753488542,2.1340586881
 C,0.7245828109,-3.1602824947,3.1269895155
 C,1.080864547,-3.2195793009,4.4722540824
 C,2.426511774,-3.3096720374,4.8554992797
 C,3.4342621341,-3.3029801297,3.8508203901
 C,3.059644317,-3.2217291366,2.4908428658
 C,2.8050451461,-3.4674280265,6.2528321562
 C,3.7912870501,-4.3002963857,6.6656543138
 C,4.51786891,-5.2414150515,5.8066148462
 C,4.5618491654,-5.2039710347,4.4778947392
 H,0.314839218,-3.1897139023,5.2425712963
 H,-0.3209830166,-3.0708463323,2.8459766416
 H,1.4376309521,-3.0920979929,1.0876875899
 H,3.8315057042,-3.1454309657,1.7302579559
 H,4.4356919633,-2.9996592043,4.1333385834
 H,2.2125127508,-2.939582349,6.9972851211
 H,3.9850829833,-4.3765473084,7.7335728558
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 H,8.1497852269,-0.8527664574,5.9522802067
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 H,-1.0546448422,-0.0386683079,6.0935310535
 H,-2.3247190756,0.2977218287,1.5054838366
 H,-2.3098984372,0.1624618189,3.9700588168
 H,2.3353000704,-0.5551353138,9.415108235
 H,0.193361875,-0.2829840818,8.218750007
 H,4.7997349932,-0.7991649714,9.3698914534
 H,6.9234328517,-0.9173829179,8.1034505364
 H,5.6488914641,-0.0775750422,-0.7499293712
 H,3.5029253677,0.144721765,-1.9485770931
 H,1.0289324603,0.2919973808,-1.9101739492
 H,-1.0996594095,0.3480970135,-0.6480582088

4 (with H-inner)



E = -1614.52882905 a.u.

C,-1.2611160263,0.7020767254,3.0431141492
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 C,-1.2202240567,-1.9777467176,2.0854273356
 C,-2.4090156554,-1.3490558188,2.4066004079
 C,-2.4053716307,-0.0195674721,2.9608582619
 C,1.2986204596,0.7241164576,2.983965635
 C,2.4478842469,0.0147537342,2.8692618243
 C,2.447944689,-1.3222027927,2.3347724307
 C,1.2560781087,-1.9659879684,2.0564391504
 C,2.4537454484,-0.4983262212,-0.9649498783
 C,3.6831227655,-1.2124024482,-0.9587575424
 C,4.8930142692,-0.4934013564,-0.8181833269
 C,4.8949129936,0.8809007839,-0.6797157502
 C,3.686771876,1.6164178445,-0.6723597294
 C,2.4556780555,0.9191946752,-0.8175300203
 C,1.2196987404,-1.2012253094,-1.08541096
 C,1.2154071721,-2.6284221597,-1.1932217109
 C,2.4731140282,-3.3176017339,-1.1985725392
 C,3.6528459472,-2.6395080445,-1.084704331
 C,-0.006382701,-0.4943365517,-1.0432175849
 C,-0.0056106954,0.9327821628,-0.8925240464
 C,1.2227062269,1.6338076614,-0.7867270337
 C,1.2194730069,3.0534301062,-0.600873189
 C,2.4795178213,3.7284202504,-0.4772920686
 C,3.6584500268,3.0398887143,-0.5108311461
 C,-1.2331724997,-1.200459769,-1.0802493237
 C,-1.230387473,-2.6277231651,-1.1876075429
 C,-0.0078135301,-3.3072446026,-1.2527406579
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 C,-1.2285092551,3.0551006258,-0.6025273747
 C,-1.233225607,1.6352468046,-0.786647088
 C,-2.4670156623,0.9218497931,-0.8157873168
 C,-2.466455987,-0.4962428422,-0.9589639829
 C,-3.6966097914,-1.209072626,-0.9513657929
 C,-3.6676489379,-2.6364960085,-1.0743281809
 C,-2.4886887535,-3.3158259264,-1.1891022513
 C,-4.9058864827,-0.4880977438,-0.8148708608
 C,-4.9064881495,0.8866839715,-0.6814066295
 C,-3.6975246894,1.6209362557,-0.6742892892
 C,-3.6676771514,3.0448115471,-0.5165159393
 C,-2.4878864707,3.7318913105,-0.4822965229

H,1.2597842762,-3.007917657,1.7458710801
 H,3.389973575,-1.8479052109,2.2140853036
 H,3.3890101723,0.4422491527,3.2075680861
 H,1.2912629645,1.7296265252,3.3984112405
 H,-0.0202149264,0.6124504722,1.3830425677
 H,-1.2221115762,-3.0174891322,1.7673855503
 H,-3.3491151985,-1.8835652599,2.310351327
 H,-3.3379622777,0.3901271477,3.3422891328
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 H,-5.8439336132,-1.0382795413,-0.8124052637
 H,-5.8448981137,1.4255093469,-0.5735283996
 H,2.4738297535,4.8077649741,-0.3456029408
 H,4.6051899743,3.564811956,-0.4067321721
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4 (with H-outer)

E = -1614.53384086 a.u.

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 C,2.4301202593,0.0025473865,1.3834885419
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 C,1.2733297725,-0.055489492,3.5630921084
 C,0.062382264,-0.1004937717,4.3235341474
 C,-1.1871059863,-0.0897202227,3.6202045064
 C,-1.2314803923,-0.0520515024,2.2559778529
 C,3.6891745931,-0.0271089429,2.0512840775
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 C,6.1316434917,-0.0901330505,1.968039611
 C,4.9042280915,-0.0463529822,1.2937646114
 C,4.8164317117,-0.0335508497,-0.1384198975
 C,3.6076144226,-0.0127710197,-0.7735834984
 C,3.8837125521,-0.2667978366,7.7260936003
 C,2.6537975326,-0.3090144758,8.4600641411
 C,1.4459378879,-0.2704127978,7.8242063596
 C,5.1450606261,-0.3333431947,8.3629202726

C,6.3167850456,-0.3115655644,7.6313551625
C,6.2953687726,-0.2220753273,6.2192970457
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C,7.4517290555,-0.1744376429,4.0705080136
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C,0.3855634062,-3.2425883672,2.6132454499
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H-loss TS 4

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C,2.4879468893,-0.5001066151,1.358587676
C,2.3502704108,-0.7958188989,0.019925165
C,1.1441272675,-0.483166116,-0.6667339155
C,-0.8586187577,1.054442329,2.1055193722
C,-0.6692220231,1.4638414828,3.3978444127
C,0.5367495411,1.1530142722,4.0853810146
C,1.5606445082,0.4967668055,3.4374701973
C,0.6290166091,4.2369274967,2.6846365915
C,0.7541115484,4.5935953668,4.0547751551
C,-0.3660292169,5.1375565784,4.726146682
C,-1.5694893076,5.3221639574,4.0735563923

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 C,-0.748898337,4.03777605,0.6467963799
 C,-2.0039462664,4.1995153548,-0.0238571193
 C,-3.1007277776,4.7669930585,0.7070584037
 C,-2.9648090444,5.1367242048,2.0146576187
 C,2.6834842728,2.663762679,-0.0369836003
 C,3.9189028326,2.4463116378,0.6516179687
 C,4.0335404569,2.8355619692,1.9918086285
 C,-2.1260531305,3.7880892101,-1.3576063176
 C,-1.0514020473,3.2197026471,-2.0541970155
 C,0.2058468908,3.0546789882,-1.3886287201
 C,1.3039582589,2.4563153416,-2.0729870286
 C,2.5426884946,2.2605700389,-1.3964823257
 C,3.6248309673,1.6285839915,-2.0673171834
 C,4.853523224,1.4269761927,-1.3583478214
 C,4.9957601485,1.819764243,-0.0583777703
 C,3.4472267055,1.2032064593,-3.4047321968
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 H,-0.4977101853,-1.2458906671,1.8700347932
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 H,-0.8384671654,0.3163229305,-0.5123512373
 H,-2.1216520996,2.9083319045,-3.9186611879
 H,-0.2183474404,1.8657373931,-5.0931982411
 H,-3.0815979466,3.9082644501,-1.8639749532
 H,4.9724992767,2.6650882194,2.5147450748
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 H,4.2772406512,0.7178166238,-3.9127899925
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H Abstraction TS 4-7

E = -1614.50931643 a.u.

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 C,1.2806996041,-0.0826747948,3.4803611006
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 C,-1.1752206743,-0.0564978803,3.4959257605
 C,-1.1681454462,-0.032265341,2.0959060178
 C,0.0861670149,-0.0878260524,5.6341427364
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 C,-2.3681244339,-0.0085896801,5.6237732408
 C,-2.3904907412,-0.0179894113,4.2590695415
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 C,1.3285443836,-0.1125905692,6.3421181232
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 C,5.0123455878,-0.0617103515,4.1734102267
 C,4.9997699267,-0.0436381538,5.5842962241
 C,3.7584046272,-0.0672664128,2.0469685858
 C,3.7324950498,0.0540254468,-0.7701988031
 C,4.9352150228,0.0110362984,-0.0986429176
 C,4.9820554971,-0.0471460772,1.3170303902
 C,6.2278530496,-0.0613384091,3.4143224309
 C,6.2109853386,-0.0524269371,2.0447206133
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 H,4.7208998675,-0.0895308379,8.2865750221
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Complex 7 + ovalene-H
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C,1.5868037302,-2.7643530492,-0.8978358834
C,2.8752058147,-3.383549042,-0.7891796407
C,0.2443939303,-0.6905419751,-0.8615891111
C,-0.9439151545,-1.4683671472,-1.03576537
C,-0.851371886,-2.8828850984,-1.1425251819
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C,1.2455271974,2.9234212869,-0.5371998874
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C,2.6092926004,0.8515713374,-0.5526442119
C,3.7907704528,1.6280603174,-0.3760767373
C,3.6715086854,3.0446514146,-0.2975874363
C,2.4403884542,3.6650738492,-0.3895422888
C,5.1182061225,-0.4179233096,-0.351823962
C,5.0386946055,0.9573298861,-0.27745408
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 H,4.9792521619,-3.1255939416,-0.5307696787
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TS 3 --> 5

E = -1614.47022152 a.u.

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C,-0.2216941959,3.1071192913,-3.7555934031
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5

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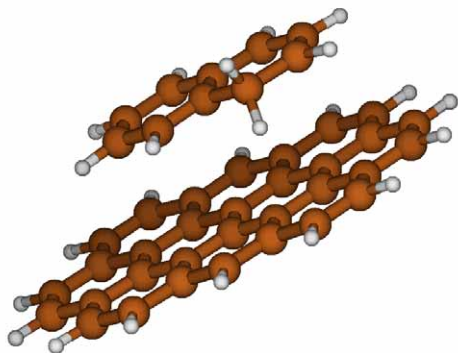
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6

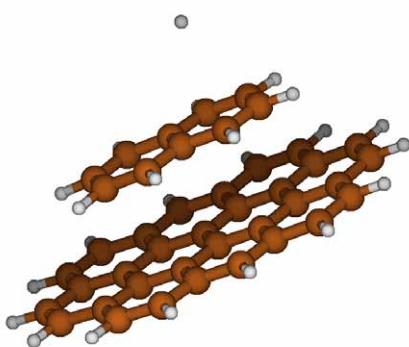


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Complex 7 + H + ovalene



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H Abstraction TS 6-7

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H,-0.0578909085,4.6421399538,-0.7730343137
H,-5.5172771244,-1.5240144005,-1.7800246813
H,-5.6631928156,0.9470590021,-1.6376902662
H,-4.5761886423,3.1523456457,-1.277638753
H,-2.5578642952,4.5193667101,-1.0049986964
H,-2.5897541592,-1.7981645524,1.7777533556
H,-4.143988898,0.0861896838,2.1652708252
H,2.3750491719,4.7500154326,-0.3469353582
H,4.5747367943,3.6364463598,-0.1706141283
H,5.9391325597,1.5510679088,-0.1384924972
H,6.0823189728,-0.9147157111,-0.2702783313

H,4.9792521619,-3.1255939416,-0.5307696787
H,2.9318037285,-4.4680557886,-0.845852985
H,0.4673013374,-4.5907710359,-1.1185840131
H,-1.9762474339,-4.7210410838,-1.4255433991
H,-4.1631401519,-3.6091275483,-1.6860826274
H,-0.8573595312,2.5742547695,3.4202678022
H,-3.2820446242,2.2686072329,3.011159131
H,1.4564544721,1.6916351326,3.3175378811
H,3.0141110839,-0.1719810429,2.8326429258
H,2.1358137361,-2.3779515018,2.0891001566
H,-0.2938848106,-2.7138716312,1.7864845694

Complex 7 + ovalene-H

E = -1614.5446025 a.u.

C,4.0104234385,-2.6382298666,-0.6139597362
C,3.9595668858,-1.2123097682,-0.5371047447
C,2.6924106776,-0.5663338689,-0.643947457
C,1.5104041831,-1.3371939151,-0.8235618022
C,1.5868037302,-2.7643530492,-0.8978358834
C,2.8752058147,-3.383549042,-0.7891796407
C,0.2443939303,-0.6905419751,-0.8615891111
C,-0.9439151545,-1.4683671472,-1.03576537
C,-0.851371886,-2.8828850984,-1.1425251819
C,0.4078387885,-3.5064770382,-1.0516876356
C,0.1707628916,0.7089511026,-0.7091246026
C,-1.1641248265,1.3572189887,-0.4902516344
C,-2.334802741,0.5745983465,-1.0175718452
C,-2.2226912493,-0.8225394121,-1.156146696
C,-3.5613739478,1.2232510541,-1.2058197514
C,-3.6112412511,2.6728882193,-1.1294408662
C,-2.4904456692,3.434085253,-0.9653686116
C,-1.1978612596,2.8440656204,-0.768781757
C,-0.0298031029,3.5564473039,-0.6930156073
C,1.2455271974,2.9234212869,-0.5371998874
C,1.3333314863,1.4894400255,-0.5979580676
C,-4.7095169634,0.4446780669,-1.4928334107
C,-4.627077485,-0.9322436235,-1.5799608246
C,-3.3890620567,-1.5968307579,-1.4224845346
C,-3.2653412909,-3.023075035,-1.5033551681
C,-2.0554770884,-3.638559081,-1.3583231507
C,2.6092926004,0.8515713374,-0.5526442119
C,3.7907704528,1.6280603174,-0.3760767373
C,3.6715086854,3.0446514146,-0.2975874363
C,2.4403884542,3.6650738492,-0.3895422888
C,5.1182061225,-0.4179233096,-0.351823962
C,5.0386946055,0.9573298861,-0.27745408
C,-1.2435462468,1.6161136015,3.0803167504
C,-0.3249483617,0.5563227969,2.8487986343
C,-0.8275067187,-0.7086230205,2.3959284705
C,-2.2206570167,-0.8498646677,2.1598468627
C,-3.0846722045,0.2014851186,2.3761829564
C,-2.5929688754,1.4441895786,2.8494703199
C,1.0773695957,0.7212139807,3.0057269377
C,1.9414106952,-0.3176739188,2.7412120876
C,1.4411309816,-1.5764352037,2.32255288

C,0.0887750457,-1.7665915253,2.1560296948
 H,-1.312005825,1.3094194577,0.6094596826
 H,-0.0578909085,4.6421399538,-0.7730343137
 H,-5.5172771244,-1.5240144005,-1.7800246813
 H,-5.6631928156,0.9470590021,-1.6376902662
 H,-4.5761886423,3.1523456457,-1.277638753
 H,-2.5578642952,4.5193667101,-1.0049986964
 H,-2.5897541592,-1.7981645524,1.7777533556
 H,-4.143988898,0.0861896838,2.1652708252
 H,2.3750491719,4.7500154326,-0.3469353582
 H,4.5747367943,3.6364463598,-0.1706141283
 H,5.9391325597,1.5510679088,-0.1384924972
 H,6.0823189728,-0.9147157111,-0.2702783313
 H,4.9792521619,-3.1255939416,-0.5307696787
 H,2.9318037285,-4.4680557886,-0.845852985
 H,0.4673013374,-4.5907710359,-1.1185840131
 H,-1.9762474339,-4.7210410838,-1.4255433991
 H,-4.1631401519,-3.6091275483,-1.6860826274
 H,-0.8573595312,2.5742547695,3.4202678022
 H,-3.2820446242,2.2686072329,3.011159131
 H,1.4564544721,1.6916351326,3.3175378811
 H,3.0141110839,-0.1719810429,2.8326429258
 H,2.1358137361,-2.3779515018,2.0891001566
 H,-0.2938848106,-2.7138716312,1.7864845694

Ethyne addition TS 3-8 (A process)

E = -1691.8093118 a.u.

C,-0.0162329448,-0.0102390534,0.0363649304
 C,-0.0160918647,-0.037861029,1.4506418648
 C,1.2256296654,0.02545434,2.1399349173
 C,2.4429523297,0.1164246923,1.4050654131
 C,2.4141082077,0.131465661,-0.0162914692
 C,1.1642302546,0.068537025,-0.67671652
 C,1.2560888288,-0.0413486173,3.5627519916
 C,0.0376165658,-0.1737834825,4.3008051618
 C,-1.1984039823,-0.2218663992,3.5762987657
 C,-1.2230217285,-0.1552682567,2.2124379998
 C,3.690575278,0.1505848125,2.0942360172
 C,3.7195494222,0.0984912973,3.5092227121
 C,2.4949617796,-0.0022913896,4.2475755184
 C,2.5257752659,-0.089617333,5.6602832183
 C,1.3043566835,-0.2294508276,6.3924330103
 C,0.0893916449,-0.266891596,5.6971219132
 C,3.7729169756,-0.0609716746,6.3499827964
 C,4.9903870609,0.0407502518,5.6167762771
 C,4.9598847906,0.1101433893,4.1928325028
 C,6.183204102,0.1725147211,3.4512601903
 C,6.1341578214,0.2186734424,2.0519624123
 C,4.9173357229,0.2057869796,1.3575348693
 C,4.852296463,0.2309947329,-0.0756000172
 C,3.6545967608,0.1944047786,-0.7312488576
 C,3.8056217188,-0.1646107904,7.7675571956
 C,2.5687351386,-0.3006054228,8.4785103826
 C,1.3723797611,-0.3339781139,7.8213768093
 C,5.0569366632,-0.1436243387,8.4271362628

C,6.2376114338,-0.0371573585,7.7164985992
 C,6.2352081869,0.0482517085,6.3043356791
 C,7.4451278711,0.1213424791,5.5403363154
 C,7.4215726037,0.1770102735,4.1758035443
 C,1.3384074038,-3.1295880602,1.7901528584
 C,0.3633241671,-3.3479654637,2.764518294
 C,0.7321177994,-3.4593565603,4.1025536056
 C,2.0784730265,-3.3611199231,4.5077289767
 C,3.0473209283,-3.1428525187,3.508638484
 C,2.6785768318,-3.0272821516,2.1717685487
 C,2.3433264658,-3.4438592959,5.9476264925
 C,3.4606266656,-3.3257167886,6.7047362026
 C,4.8782711643,-3.1523006002,6.374094153
 C,5.5772866931,-3.6889041353,5.3845662156
 H,-0.0335542842,-3.6028088634,4.8615551918
 H,-0.6849013943,-3.4073078473,2.4861909131
 H,1.0564524692,-3.0135498085,0.7474755439
 H,3.4427008152,-2.8363169413,1.4237487944
 H,4.0893798308,-3.0554972351,3.7850475306
 H,1.4281516334,-3.5613174362,6.527672169
 H,3.2764160961,-3.3054349287,7.7783338838
 H,5.4222483693,-2.5377207528,7.1022408441
 H,6.6259425374,-3.6294240414,5.1215304993
 H,8.3484979962,0.2265441688,3.6094202184
 H,8.3921403583,0.1257882987,6.0750240945
 H,7.0648523409,0.2596590492,1.4897257566
 H,-0.8380892508,-0.3748988454,6.255930642
 H,-2.168174425,-0.1987350855,1.6760717698
 H,-2.1224896653,-0.3192344419,4.1412129768
 H,2.6043188458,-0.3802117002,9.5625978048
 H,0.4419463151,-0.4405988849,8.3740551503
 H,5.0766363297,-0.2180092947,9.5119205012
 H,7.1912690192,-0.0276653182,8.2390605132
 H,5.7852687928,0.2746347871,-0.6323905711
 H,3.6219080605,0.2078517213,-1.8182004179
 H,1.1471161735,0.0808421482,-1.7639859423
 H,-0.9683741047,-0.0606818139,-0.4867510649
 C,4.6805502874,-5.7269880364,4.5771002432
 C,5.470078379,-6.3648634426,3.9028173299
 H,3.7973361792,-5.4361564441,5.1081082547
 H,6.2674441945,-6.7873271054,3.3330723841

Ethyne Addition TS 3-8 (B process)

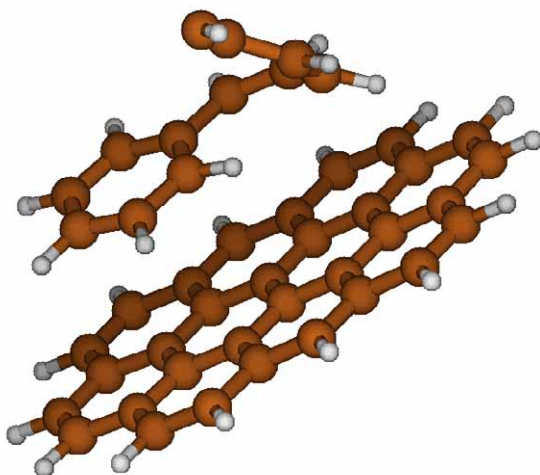
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 C,2.439730,0.029737,-0.016458
 C,1.205626,0.019768,-0.696681
 C,3.664057,0.061375,-0.805159
 C,4.985356,0.082685,-0.496711
 C,5.810492,0.056536,0.712783
 C,5.687055,0.251606,2.026155
 C,4.355637,0.902182,3.730457

C,4.109200,2.104134,3.772964
 C,2.685702,-3.170826,1.157750
 C,2.991050,-3.003553,2.548344
 C,4.339520,-2.894153,2.968887
 C,5.394205,-2.973930,2.013223
 C,5.089278,-3.127705,0.630668
 C,3.732051,-3.220696,0.205585
 C,6.747417,-2.853110,2.432946
 C,7.023069,-2.653070,3.824433
 C,6.016084,-2.558542,4.742798
 C,4.639757,-2.674359,4.352454
 C,1.942537,-2.903117,3.495452
 C,2.247917,-2.674001,4.875724
 C,3.587681,-2.563076,5.272598
 C,6.138537,-3.149216,-0.327755
 C,7.476460,-3.036207,0.118342
 C,7.772640,-2.896800,1.460335
 C,1.337009,-3.252050,0.733241
 C,0.282970,-3.177415,1.688418
 C,0.585028,-2.997041,3.069140
 C,-0.468594,-2.865059,4.014336
 C,-0.137240,-2.645484,5.391041
 C,1.161267,-2.552165,5.804536
 C,-1.807545,-2.937193,3.562295
 C,-2.099812,-3.122720,2.225124
 C,-1.071554,-3.239568,1.260734
 C,-1.348232,-3.387615,-0.136394
 C,-0.340918,-3.451679,-1.056314
 C,1.034629,-3.380505,-0.659065
 C,2.083179,-3.417970,-1.586398
 C,3.422798,-3.337843,-1.186498
 C,5.803633,-3.269349,-1.715501
 C,4.504937,-3.359604,-2.127184
 H,1.204020,0.016799,-1.784513
 H,-0.939394,-0.026486,-0.545181
 H,-0.937964,-0.028135,1.945279
 H,1.232155,-0.018872,3.171352
 H,3.353504,-0.031345,1.917775
 H,3.468101,0.050348,-1.877592
 H,5.620247,0.054141,-1.380984
 H,6.839739,-0.226158,0.450787
 H,6.504372,0.139461,2.729487
 H,6.240924,-2.394323,5.793893
 H,8.061187,-2.563441,4.136011
 H,3.817164,-2.388035,6.321720
 H,1.850830,-3.505558,-2.645852
 H,-2.387535,-3.437240,-0.452868
 H,-0.565913,-3.552663,-2.115386
 H,6.613714,-3.283851,-2.441026
 H,4.265758,-3.447167,-3.184381
 H,8.275732,-3.057196,-0.618893
 H,8.806232,-2.805321,1.785884
 H,1.396303,-2.379335,6.851961
 H,-0.950227,-2.547294,6.106625
 H,-2.610073,-2.839203,4.289551
 H,-3.134377,-3.170890,1.893460

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H,4.333352,-0.106935,4.096169

8



E = -1691.89000342 a.u.

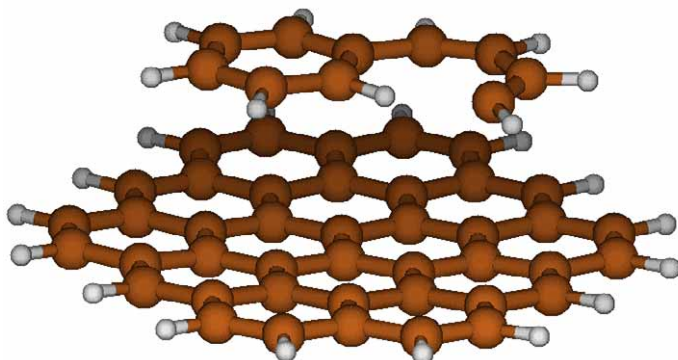
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C,2.3867521647,0.1399545966,-0.0283250741
C,1.1322019185,0.0735904339,-0.6794439573
C,1.2556983043,-0.0350861295,3.559373275
C,0.0425557521,-0.166238956,4.3064607203
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C,3.6793157814,0.1558642475,2.0723624682
C,3.7191669614,0.0968511874,3.4868164636
C,2.4998799266,0.0017058559,4.234870324
C,2.5412939381,-0.0917441173,5.6468807651
C,1.3244899369,-0.2204129638,6.3887677196
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C,3.7946412536,-0.0896131862,6.3257667363
C,5.0074266514,-0.0035069437,5.5826196875
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C,6.1231356183,0.2068457552,2.0103556879
C,4.9004745583,0.2080025591,1.3260633574
C,4.8243703654,0.2395252847,-0.1063805007
C,3.6215607452,0.2058682672,-0.7526846244
C,3.8381081087,-0.2043542047,7.7422866637
C,2.605046896,-0.3187268543,8.4637422545
C,1.4027072046,-0.3278854693,7.8169336186
C,5.0953490885,-0.2162913631,8.3902430053
C,6.2716711482,-0.1271752603,7.67013328
C,6.2586275921,-0.0245026894,6.2591019912

C,7.4627643913,0.044734112,5.4853204654
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 C,0.7061389505,-3.5137728745,4.0616563685
 C,2.0269092015,-3.3449971591,4.5203616529
 C,3.0236125521,-3.0729523794,3.5629777807
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 C,2.2459784141,-3.386125512,5.9690656547
 C,3.3629383907,-3.3258709074,6.7297031295
 C,4.7850915942,-3.30549054,6.3911267606
 C,5.4632079787,-4.137490503,5.5696964746
 H,-0.0816121146,-3.6931151971,4.7899952343
 H,-0.6415830801,-3.5474209866,2.385510739
 H,1.1505519875,-3.0779595488,0.7181645102
 H,3.4901372969,-2.7558988538,1.4942841012
 H,4.0386188675,-2.8890975459,3.8858268731
 H,1.3135556509,-3.3994882295,6.5326787734
 H,3.1780917153,-3.2122636482,7.7983821615
 H,5.3699369017,-2.5776163884,6.951564418
 H,6.5363166672,-3.9924478266,5.4590390677
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 H,8.4143467386,0.0283960524,6.011529694
 H,7.0493909818,0.2449115254,1.4406801014
 H,-0.8194480487,-0.3557603242,6.2688347382
 H,-2.1818618018,-0.2043990761,1.6977453555
 H,-2.1183586693,-0.3160403708,4.1629277598
 H,2.6486875246,-0.4034245951,9.5471337186
 H,0.4753498046,-0.4210282502,8.377146356
 H,5.1233396334,-0.3021783471,9.4739567926
 H,7.2298360065,-0.1418952534,8.1841893432
 H,5.7530777572,0.2831478485,-0.6702082687
 H,3.5804347463,0.2220593552,-1.8392977445
 H,1.1069227626,0.0866094138,-1.7665355072
 H,-0.9982929791,-0.0643747182,-0.4736683735
 C,4.8692747826,-5.244633253,4.8227472133
 C,5.5321766691,-6.0010810064,3.9627691964
 H,3.8089642386,-5.4267189276,5.0015595422
 H,6.5455850719,-6.0522936156,3.5801393488

--- end of Species of Table 2 ---

Species of Table 3

3 adsorbed on P2 (tetrabenzovalene)



E = -1987.45374050 a.u.

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C,2.4949806065,0.0047783039,1.3452167562
C,2.472982972,-0.0030344239,-0.0927630762
C,1.188809291,-0.0051618012,-0.7548723373
C,1.3080678339,-0.0445557395,3.4997139785
C,0.093206245,-0.1166912753,4.2328274189
C,-1.1570418812,-0.1346320024,3.540562679
C,-1.1637678002,-0.073459559,2.1296340707
C,3.7389134177,-0.0212134316,2.0296838718
C,3.7683258401,-0.0469723692,3.4585575024
C,2.5598666699,-0.063453441,4.1886147211
C,2.5894540927,-0.1406654531,5.6151867342
C,1.3737399787,-0.2229457087,6.3466699515
C,0.1234394702,-0.2176467125,5.6573792276
C,3.8321194773,-0.1841180424,6.2988374438
C,5.0491082715,-0.1606313168,5.5651146317
C,5.0200120339,-0.1024807947,4.1463482026
C,6.2364497166,-0.1323555904,3.4091894009
C,6.2073425753,-0.1053314721,1.980558543
C,4.9554640108,-0.0533274661,1.2928023575
C,4.9233937975,-0.0491201347,-0.1375804925
C,3.6743716726,-0.0241585765,-0.7974088029
C,3.8540263025,-0.2998338727,7.7305408749
C,2.6526706434,-0.3707300274,8.4315263704
C,1.4060007475,-0.3435798028,7.7714710806
C,5.1363519603,-0.3620415988,8.3915718631
C,6.3008663915,-0.3282152175,7.6905964089
C,6.3113985985,-0.2372264264,6.2497568641
C,7.4925340099,-0.2501765857,5.5119639305
C,7.4876249704,-0.2030297582,4.0993697225
C,1.1532737411,-3.0948186858,1.9631904099
C,0.127088792,-3.1653245103,2.9086889041
C,0.4326552961,-3.2313389355,4.2641237377
C,1.7704162284,-3.2383807988,4.7176011253
C,2.7879601541,-3.1627561391,3.7464435117
C,2.4836720684,-3.0934496826,2.3896347383
C,1.9873240094,-3.2998043031,6.1614213278
C,3.0936217164,-3.3626614754,6.9414333886

C,4.5287438681,-3.3545521866,6.6612548934
 C,5.1967225942,-3.240502763,5.5275239595
 H,-0.3700960012,-3.2494981776,4.9979513405
 H,-0.9107976645,-3.1321356249,2.590632739
 H,0.9188620364,-3.0010970605,0.9062751354
 H,3.2867036354,-3.0013683971,1.6635945816
 H,3.8277193804,-3.1325104141,4.0716819638
 H,1.0512717775,-3.2891697872,6.7211876831
 H,2.8859588905,-3.3961090819,8.0093337059
 H,5.1383924294,-3.405573925,7.5747214008
 H,6.2425289144,-3.1503818356,5.2618581019
 C,8.6908818593,-0.2327081689,3.3271015279
 H,8.4462548976,-0.3088397776,6.0332245737
 C,7.4231516803,-0.1424726979,1.2432550796
 C,-1.0905279935,-0.3457018199,6.3871339732
 H,-2.1180558624,-0.0917410641,1.6063353395
 C,-2.3590518817,-0.253143403,4.3048808204
 H,2.6728639583,-0.4658375112,9.5157052949
 C,0.167205551,-0.4619076071,8.4749667391
 H,5.1467021812,-0.4404590262,9.4766044885
 H,7.257679348,-0.3801339707,8.205565762
 C,6.1645420421,-0.0819642975,-0.8471330948
 H,3.6540964632,-0.0295987545,-1.8855713271
 H,1.176401162,-0.0067718438,-1.8425340534
 H,-0.9318423229,-0.0150301857,-0.5665865121
 C,7.3637746815,-0.1248826272,-0.1827392615
 C,8.6582361456,-0.2024706977,1.9560891519
 C,-2.3258042089,-0.3586495733,5.6723742401
 C,-1.0316510242,-0.4664520096,7.8081502876
 H,6.1377828883,-0.0747314141,-1.9344157294
 H,8.298302208,-0.151121767,-0.7388626269
 H,9.5834596629,-0.2277697417,1.3845579544
 H,9.6411987668,-0.2825732471,3.8538344745
 H,-3.3088724522,-0.2673196939,3.7750019751
 H,-3.2495599462,-0.4560956163,6.2385122064
 H,-1.9655310701,-0.5642090393,8.3573571572
 H,0.1951983313,-0.5559883348,9.5582350361

TS 3-4 adsorbed on P2 (tetrabenzo-ovalene)

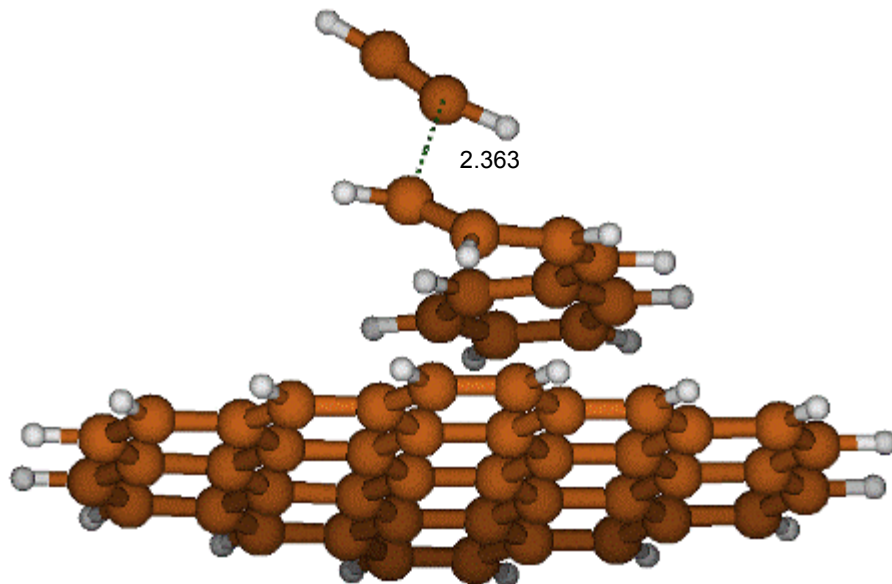
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C,0.0592324453,0.1206761575,0.138512778
 C,0.0768301193,0.1212753742,1.5274415304
 C,1.2997065665,0.0953134289,2.2180371165
 C,2.4999457316,0.0426950563,1.5123154472
 C,2.5044711097,-0.0002971052,0.1104715087
 C,1.2670862957,0.0478086974,-0.5885220287
 C,3.7478270413,-0.1369430735,-0.6418811019
 C,3.8760811623,-0.9493551697,-1.7153073363
 C,2.8515762003,-1.8892934579,-2.1922778652
 C,1.5630353593,-1.8537598925,-1.8782999187
 C,3.086590244,3.0678262632,-0.0174091835
 C,1.7121235685,3.1696214589,0.362638604
 C,1.35599745,3.2268692459,1.744882096
 C,2.3684534692,3.179165617,2.7414033434
 C,3.7418036352,3.0809228157,2.3617533301

C,4.0986536404,3.0271553238,0.9794621533
 C,2.0080604538,3.1888071341,4.1253394288
 C,0.641956364,3.2447123331,4.4805672919
 C,-0.3640849884,3.2867072061,3.5182710727
 C,-0.0109713226,3.2797473182,2.1243693553
 C,-1.0262531606,3.2791269981,1.1290813642
 C,-2.4136932374,3.2951945144,1.5076183208
 C,-2.7360243437,3.3256698705,2.915375047
 C,-1.7652829583,3.3197469922,3.8673834275
 C,0.7042686225,3.1630234905,-0.6255561815
 C,-0.6723004275,3.2188229864,-0.2444837422
 C,-1.688516406,3.1621144869,-1.2378857463
 C,-3.066181951,3.1918691141,-0.8524853084
 C,-3.3950171149,3.2612941358,0.5194487622
 C,-1.3344748181,3.0497493098,-2.6180940306
 C,0.0413794859,2.9842705332,-2.9988263276
 C,1.0581350506,3.0408049018,-2.0055433382
 C,2.4237743871,2.9364579463,-2.382928179
 C,3.4395049204,2.9566437578,-1.3879899451
 C,4.8221647202,2.8319283634,-1.7630442781
 C,5.8014651812,2.8174721597,-0.7732814563
 C,5.4720086868,2.9022778944,0.5979354182
 C,5.140478905,2.6979415135,-3.1648667908
 C,4.1691104018,2.6736423364,-4.115530967
 C,2.7713868904,2.7871586033,-3.7706059033
 C,1.7620380629,2.7492444837,-4.7297184661
 C,0.3974763778,2.8422925828,-4.3772261163
 H,3.4479522605,0.0461561105,2.0443763221
 H,1.310498628,0.1561768637,3.3027393726
 H,-0.8538596287,0.2079534901,2.0819565113
 H,-0.8791620663,0.2350146377,-0.3969653615
 H,1.2777120985,0.3696600629,-1.6240454912
 H,4.618672908,0.4015804767,-0.2732557682
 H,4.8467307695,-1.0094420559,-2.2047911351
 H,3.23431795,-2.711926475,-2.8105419779
 H,0.7300528245,-2.501266421,-2.1296101972
 C,-0.6497242181,2.7878488839,-5.3495731766
 H,2.0277093408,2.6344923652,-5.7787678431
 C,-2.3510383196,2.9839082159,-3.6106120124
 C,4.7529409012,3.0099360603,3.3599657009
 H,0.3718648413,3.2477557995,5.5348688812
 C,3.049527804,3.1238361392,5.1028524677
 H,6.8471642685,2.7192185654,-1.0585186938
 C,6.4636050541,2.8478988724,1.6269328878
 H,6.1880892991,2.6062002911,-3.4426967203
 H,4.4265870719,2.5626910339,-5.1664100243
 C,-4.0622655922,3.1327945162,-1.8768302762
 H,-4.4439505556,3.2750947503,0.8092887378
 H,-3.7863291842,3.3453610114,3.1975733711
 H,-2.0270504275,3.3342926132,4.9230711833
 C,-3.7172642642,3.0354016894,-3.2008099199
 C,-1.9687174919,2.8576192532,-4.980029835
 C,4.3678327872,3.0400039942,4.7337580006
 C,6.1163388865,2.8986374553,2.9528022223
 H,2.7722510443,3.1373272622,6.1544354275
 H,7.507058876,2.7568712491,1.3340657507

H,6.8827572205,2.848658051,3.7230579603
H,5.1477587745,2.9873590045,5.4901386706
H,-5.1085967879,3.1620204958,-1.5815224154
H,-0.3763960236,2.6836668648,-6.3970577667
H,-2.7526892713,2.8106000373,-5.732601533
H,-4.4881663733,2.9875639527,-3.9667059235

TS 3-8 adsorbed on P2 (tetrabenzo-ovalene)



E_{raw} = -2064.42010378 a.u.

C,-0.0003044876,0.0216734786,0.0265120822
C,0.0320339015,0.0311689676,1.4174080182
C,1.2508326618,-0.0009613676,2.1011899145
C,2.443702927,-0.0387838044,1.3782897315
C,2.4126291738,-0.0411753982,-0.0142197593
C,1.1936074637,-0.0163182219,-0.7227939959
C,1.2767966628,0.0203009306,-2.1881262997
C,0.3496419172,0.0895830193,-3.1705089458
C,-1.1182932016,0.0899685892,-3.1519944945
C,-1.9372097364,-0.6151055883,-2.3903888204
C,1.0197338037,3.082057567,2.098240548
C,2.0737559805,3.0331132682,3.0745213944
C,3.3995478735,3.0272621226,2.6511578022
C,3.7412287975,3.053171735,1.2812247727
C,2.6998176858,3.1068522565,0.3036797119
C,1.3409290084,3.1267951575,0.7167724309
C,5.0966290082,2.9937419629,0.8316018433
C,5.403308954,2.9801640222,-0.5054224585
C,4.3820421425,3.0330136436,-1.5011142229
C,3.0231591119,3.1008258025,-1.087477526
C,1.9810915216,3.13955003,-2.0634109433
C,2.30326229,3.1244981104,-3.4572471291
C,3.679746429,3.0616232212,-3.8384312086
C,4.676907165,3.0144499067,-2.8976829418
C,0.6218644262,3.1695215431,-1.6512852043
C,0.2981564087,3.1481369143,-0.2599766326
C,-0.340201216,3.0394470727,2.5102864514
C,-0.6724865169,2.9415223113,3.9059857128

C,0.4086123975,2.9065987742,4.8638730209
 C,1.7091449744,2.9528845984,4.4697069008
 C,-1.3763110584,3.0483678244,1.5392033705
 C,-1.0528144221,3.1126282187,0.1485343672
 C,-2.7359047551,2.9644299849,1.9491815795
 C,-3.0569567872,2.8776251272,3.3407466138
 C,-2.0097718102,2.8678359266,4.2891631988
 C,-0.4135677685,3.1781052651,-2.6227354438
 C,-1.7737212059,3.1437564267,-2.2122238699
 C,-2.0953429948,3.0993946351,-0.8292225317
 C,-3.4548717671,3.0216728849,-0.418819066
 C,-3.7786272223,2.9537863616,0.9716969467
 C,-5.1376210561,2.8671051091,1.3821605611
 C,-5.431381845,2.7908949031,2.776954159
 C,-4.4336011966,2.7939622676,3.7183341921
 C,-0.0798900456,3.1799514138,-4.0206452193
 C,1.2587537094,3.1560867364,-4.405771184
 C,-1.1592723253,3.1812054629,-4.9798977068
 C,-2.4617590653,3.1577222052,-4.5867351137
 C,-2.8279372515,3.1247921469,-3.1901678551
 C,-4.153837929,3.0573212392,-2.7689239675
 C,-4.4965419785,3.0009943656,-1.3994438912
 C,-5.8520402719,2.9185180455,-0.9514644527
 C,-6.1581535593,2.8546205485,0.3841959404
 C,-0.9723054518,-2.6127800162,-1.5764794444
 C,-1.7996805751,-3.4046164292,-1.1712526539
 H,3.344992995,-0.0287272682,-0.5746757738
 H,3.3979649151,-0.0328348537,1.8968772979
 H,1.2680885883,0.0352256328,3.1870183481
 H,-0.8996252158,0.0877533838,1.9729941465
 H,-0.9516022228,0.0536303099,-0.4882973109
 H,2.3079133719,0.0616974577,-2.5418020308
 H,0.7561558671,0.2296836293,-4.1719351581
 H,-1.5611713877,0.7268844222,-3.9290565964
 H,-3.0180184459,-0.6819503265,-2.3594770775
 H,-4.9492894657,3.0405936488,-3.5115569622
 H,4.1959493978,2.980873042,3.3916429059
 H,1.5086591887,3.1489308911,-5.4651617025
 H,-0.9021217054,3.1952103245,-6.036779386
 H,-3.2613949627,3.1530362915,-5.324182066
 H,-2.257952795,2.7930268062,5.3461876773
 H,0.1528193737,2.8372322773,5.9188036466
 H,2.51052306,2.9202908391,5.204593934
 H,-0.0431435085,-2.1577345649,-1.8565247218
 H,-2.6305862383,-3.9887347693,-0.8429801442
 H,-6.4733038463,2.7258373884,3.0825812298
 H,-7.1949271993,2.7903805512,0.7070029521
 H,-4.6754646365,2.7302800737,4.7768157783
 H,-6.6427350696,2.9056374127,-1.6981579926
 H,6.4399811634,2.9285605139,-0.8308527797
 H,5.7190738768,2.9625719028,-3.2051257421
 H,5.8869641125,2.9511828184,1.5776587318
 H,3.9221267265,3.0482056025,-4.8986788872

3 adsorbed on P3 (tribenzo-corannulene)
 E = -1460.69667504 a.u.

C,-3.9013081553,-0.0179979724,1.4445998076
 C,-4.3604824639,-1.0904316052,0.8188941141
 C,-3.842760737,-2.4551167176,0.7358769023
 C,-2.6659257989,-3.0254392424,1.0954764096
 C,-1.463355529,-2.5119881251,1.7478042628
 C,-1.4024829729,-1.3315904297,2.5105143634
 C,-0.198472125,-0.8981935883,3.064777401
 C,0.9726599629,-1.6347361049,2.8772122069
 C,0.9273610636,-2.8247259521,2.1444266042
 C,-0.2759904482,-3.2593280972,1.5988648985
 H,-2.3062652534,-0.7481044977,2.6592962957
 H,-0.1749443605,0.0267044379,3.6345312324
 H,1.9132782498,-1.283308352,3.2922874495
 H,1.8335071253,-3.4019146966,1.9827870487
 H,-0.3039446153,-4.1766676959,1.0157461011
 H,-2.5703705835,-4.0715711179,0.8036305921
 H,-4.5300052613,-3.1282961671,0.2260875622
 H,-5.2827758489,-0.9490252799,0.2384283755
 H,-4.2018047551,1.0192380985,1.5119956436
 C,4.488956361,-1.1805632255,-0.7163083069
 C,4.8656635803,0.0833655559,-0.2759475036
 C,3.9016705361,1.0471652326,0.1112695027
 C,2.5475202573,0.6481636912,0.1611391607
 C,2.1580531273,-0.6552925703,-0.3043444155
 C,3.1252202139,-1.5554634152,-0.8017951504
 C,2.6492795421,-2.7462463822,-1.4791603956
 C,1.3288935907,-2.9432701444,-1.7918728802
 C,0.3110556693,-1.9963597405,-1.3898854656
 C,0.7727459204,-0.9649290422,-0.4991138364
 C,4.1988184263,2.4484043671,0.3345171897
 C,3.2231625522,3.4059438757,0.4387935806
 C,1.8187999256,3.0560343592,0.4064048238
 C,1.5503943808,1.6413751605,0.4411643009
 C,0.2330128672,1.2401613377,0.4178654877
 C,-0.1484251115,-0.0477342551,-0.0543888738
 C,-1.4283734151,0.0439764541,-0.6140642042
 C,-1.8628362755,-0.8161032928,-1.6236950534
 C,-0.9977750894,-1.9211908974,-1.9200510803
 C,-2.9701028349,-0.2847105514,-2.3979318387
 C,-3.3714840659,1.0405624298,-2.2953624734
 C,-2.7254086841,1.9785222933,-1.3961478727
 C,-1.8446400902,1.3994216766,-0.501585296
 C,0.7552040276,3.9590321012,0.1643735732
 C,-0.57878063,3.4968660036,-0.0908157266
 C,-1.6415724836,4.147367951,-0.8401790094
 C,-2.6540749698,3.4278423616,-1.4584882524
 C,-0.8112905411,2.1375946937,0.1443745765
 H,-3.3598153909,3.9671814032,-2.0869342597
 H,-1.5932121388,5.2211219734,-1.0085439783
 H,0.9952767606,5.0121514718,0.0294529826
 H,3.5036104411,4.4548450992,0.5038805503
 H,5.2439803141,2.7500599752,0.3330897746
 H,5.9164677425,0.3640335313,-0.2878942686
 H,5.2498763898,-1.8747836504,-1.0660689953
 H,3.3918938536,-3.4625284813,-1.8239722972

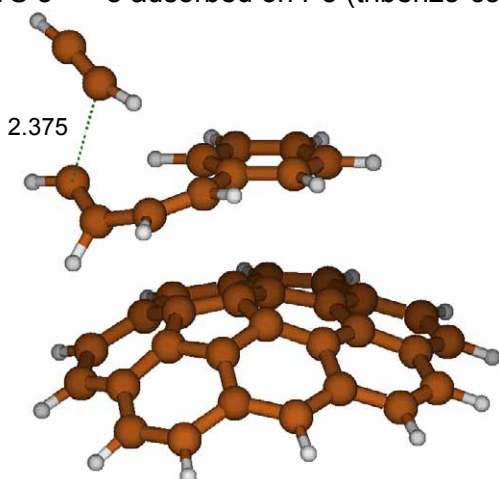
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H,-1.2934761079,-2.6518335805,-2.670680812
H,-3.4353158763,-0.907625673,-3.1590468582
H,-4.1346898423,1.4029218581,-2.980993463

TS 3 --> 4 adsorbed on P3 (tribenzo-corannulene)
Eraw=-1460.68800846 a.u.

C,0.910535597,0.0904754671,-2.1306587848
C,0.946628476,0.2099066034,-0.7321710599
C,2.1287707287,0.1514521105,-0.0268550999
C,3.3576109418,0.1999693158,-0.776114043
C,3.3124802081,0.113043205,-2.1887369017
C,2.0749547435,-0.0642460677,-2.8909389009
C,2.0631527123,-0.2849666215,1.3382806703
C,3.2679337442,-0.4168071935,2.0636126687
C,4.5059748726,-0.1147105719,1.3731589508
C,4.5600992956,0.1412373394,0.0273490082
C,0.8359113921,-0.8129475202,1.8685310117
C,0.8181134374,-1.45520921,3.1254421106
C,2.0112517469,-1.4543431798,3.8899254511
C,3.2007136525,-0.9529303543,3.3738454151
C,-0.2659391565,-0.3203700902,-0.2055185255
C,-0.3243745196,-0.9110553615,1.0344247651
C,-1.4010424021,-1.8314851713,1.2855290706
C,-1.4185461321,-2.3890540037,2.6201584627
C,-0.3832548526,-2.1773301364,3.4940030185
C,-1.0613989036,-0.7596768168,-1.2736462747
C,-1.9881339811,-1.7964392844,-1.1298092841
C,-2.2282163578,-2.2416126349,0.2136391176
C,-0.3312168282,-0.51979588,-2.4716113777
C,-0.4872704683,-1.3021428526,-3.6009360031
C,-1.608951415,-2.2217649232,-3.5482151522
C,-2.3245012787,-2.4523144119,-2.3816459348
C,1.8471303648,-0.6787238813,-4.1885366331
C,0.6360361306,-1.266932358,-4.5209762153
C,-2.4510205936,1.8242733951,0.4149786064
C,-1.2125446142,2.5277601971,0.4303164369
C,-0.4374736607,2.5468442429,1.6106327604
C,-0.8959365949,1.9158111965,2.7600558517
C,-2.1095995357,1.2102930859,2.7413948523
C,-2.8713826808,1.1614051174,1.574119093
C,-3.2871533244,1.869508002,-0.7793858897
C,-3.4703321477,2.995718204,-1.5094850038
C,-2.9601999621,4.3248650867,-1.1527729253
C,-2.0002248303,4.5725477752,-0.2672013436
H,-0.7247540982,2.7253581476,-0.517891852
H,0.5364277619,3.0283385758,1.6010753536
H,-0.2914183515,1.9257444481,3.6629978338
H,-2.4438679358,0.6819231226,3.6293884256
H,-3.8061223301,0.6066167731,1.5554413817
H,-3.8456813499,0.9720997163,-1.0397477301
H,-4.1426993119,2.9528963765,-2.3639078767
H,-3.4779043235,5.1642531362,-1.6328099815
H,-1.5622171689,5.4916471141,0.105078054
H,0.5628864871,-1.7990639947,-5.4670789362

H,2.6770058928,-0.7721424944,-4.8857306943
H,4.2539611864,0.0350871496,-2.7294709859
H,5.5254036079,0.2607889581,-0.459361472
H,5.4311976144,-0.1801368302,1.9414323178
H,4.11398689,-1.0298708225,3.9595404815
H,2.0071254168,-1.9164162412,4.8746505571
H,-0.4145173935,-2.6374496367,4.479260664
H,-2.2513874562,-3.0229790698,2.9162398842
H,-2.9649533406,-3.021065352,0.3994968221
H,-3.0906518444,-3.2247341671,-2.3891687083
H,-1.843322777,-2.822405823,-4.42452535

TS 3 --> 8 adsorbed on P3 (tribenzo-corannulene)



E = -1538.02512053 a.u.

C,-0.9206941205,0.8265516725,0.945861902
C,0.0907848304,0.1023450251,0.3041128834
C,0.7220318803,-0.9566238219,0.9115515395
C,0.15136923,-1.4628618023,2.1308064615
C,-0.9015636059,-0.7513120359,2.7533924453
C,-1.3824350285,0.4909646578,2.2207080758
C,2.0477234618,-1.2741793025,0.4715383181
C,2.7393642265,-2.3205950108,1.1194001218
C,2.0555924386,-3.013709952,2.1929802702
C,0.8518363181,-2.5941626159,2.6982315224
C,2.7389902351,-0.393175863,-0.4303255794
C,4.1217073179,-0.5574490343,-0.6664717809
C,4.7637038785,-1.6882614254,-0.1024959197
C,4.0922287681,-2.5449544147,0.7621218409
C,0.7676460656,0.9715313154,-0.5982714933
C,2.101332129,0.8040633988,-0.8990873239
C,2.8344000729,1.9586027256,-1.3513379009
C,4.2277685417,1.7100313163,-1.6551367169
C,4.8175253119,0.5078850533,-1.3609410079
C,0.1827074024,2.2441961341,-0.507862288
C,0.9087640459,3.4145074882,-0.7494769998
C,2.2251077071,3.2355364312,-1.2908670745
C,-0.8625001164,2.1606228871,0.4556258227
C,-1.2704006123,3.2443986278,1.2091105387
C,-0.6999450566,4.5149777656,0.7944493062
C,0.3285209139,4.5972017702,-0.132594529
C,-2.0344521607,1.592794042,2.9066789354

C,-1.9762355753,2.8954487157,2.4298235625
 C,-1.6500327258,-1.3314557392,-1.6925069424
 C,-2.2199257726,-2.0383423051,-0.616695376
 C,-1.603815448,-3.1820114565,-0.1136162726
 C,-0.4160564765,-3.6588940664,-0.6717317135
 C,0.1493624682,-2.9852929804,-1.7577252077
 C,-0.4661255853,-1.8448960755,-2.2637678049
 C,-2.1281572442,-0.050592334,-2.2240243162
 C,-2.950175017,0.9016719307,-1.7245873877
 C,-3.7818694915,0.9489096682,-0.514520665
 C,-4.6094053964,0.0239730415,-0.0546281477
 H,-3.1380812757,-1.6841099588,-0.1687586337
 H,-2.0532631338,-3.6994742433,0.7296385402
 H,0.0674417945,-4.5409759778,-0.261535273
 H,1.0771271428,-3.3393872771,-2.1987343968
 H,-0.0060037948,-1.3051877281,-3.0882036074
 H,-1.6220928611,0.2334704684,-3.1466086712
 H,-2.9668987224,1.834856895,-2.288689058
 H,-3.7420996337,1.9125228701,0.0117396022
 H,-5.2897119816,0.0033980917,0.7875087267
 H,-2.3956041761,3.6887052311,3.0451331277
 H,-2.4979467541,1.4185139995,3.8754400402
 H,-1.2486954614,-1.0912988439,3.7274153147
 H,0.4316770388,-3.0920762452,3.5692942929
 H,2.5697644525,-3.8485816408,2.6642196672
 H,4.6314101505,-3.3671611025,1.2274202502
 H,5.820784911,-1.8485280903,-0.3024170109
 H,5.8743047704,0.365564581,-1.5760742684
 H,4.8244847977,2.511264656,-2.0852441005
 H,2.8324674426,4.1068389762,-1.5293081346
 H,0.7742099401,5.5706998681,-0.3255253916
 H,-1.0211971557,5.4281272774,1.2910989245
 C,-5.3164031923,-1.535752921,-1.7003002476
 C,-6.2785850432,-2.199555497,-1.3558395022
 H,-4.5120942326,-1.1320454956,-2.2815058171
 H,-7.1081207095,-2.697946393,-0.9057922139

3 adsorbed on P4 (7-H-ovalene)

E = -1615.05644323 a.u.

C,5.0460062927,-0.0626086517,-0.7085353771
 C,3.8593532697,-0.8278554759,-0.9304359773
 C,2.5914044332,-0.1836410257,-0.8359252971
 C,2.5278967884,1.207247474,-0.5246839413
 C,3.7274192897,1.9411662371,-0.2966339558
 C,4.979996514,1.2705010664,-0.3980247325
 C,1.3914173918,-0.9351016235,-1.0099755363
 C,1.4735741072,-2.3174093421,-1.2656684963
 C,2.728307532,-2.9285294442,-1.3811117396
 C,3.9014306123,-2.2074086392,-1.2198785809
 C,1.2654105307,1.8530996487,-0.4162318698
 C,0.0626720139,1.1114591048,-0.6253833734
 C,0.1183066807,-0.2740549401,-0.9066739415
 C,-1.1000001439,-1.0184162691,-1.0825875709
 C,-1.0744156731,-2.4073548534,-1.3156710589
 C,0.2293954491,-3.1644280059,-1.351999418

C,-2.3552638103,-0.3452147013,-1.0004833212
 C,-2.4037028152,1.0527912055,-0.7228153994
 C,-1.1967270473,1.7766815774,-0.5195804364
 C,-1.2476266721,3.1661990433,-0.1855447008
 C,-0.0500204824,3.8698980543,0.0290081348
 C,1.2023792625,3.2421638894,-0.0819148014
 C,2.4240672226,3.9509588407,0.1389354817
 C,3.6380188512,3.3230445876,0.0353401954
 C,-3.569519712,-1.0751941794,-1.1542670755
 C,-3.5034560654,-2.4630299334,-1.3984462956
 C,-2.2782244851,-3.1060809367,-1.4756958912
 C,-4.8155642743,-0.383386369,-1.0438838229
 C,-4.8569220179,0.9607024956,-0.7798994677
 C,-3.660433188,1.7120623377,-0.603490741
 C,-3.6847849203,3.0972223568,-0.2774573173
 C,-2.5245298133,3.7983506465,-0.0707139609
 C,2.5837826933,-1.0529787963,2.2108963533
 C,2.2424824379,-2.396287168,2.0365133011
 C,0.9037600109,-2.7753895488,2.015443271
 C,-0.1351176401,-1.8309516461,2.1617997602
 C,0.2335570572,-0.4849933411,2.3505905067
 C,1.5721841012,-0.103444335,2.3730049725
 C,-1.5059845223,-2.3275843257,2.0843541574
 C,-2.723579031,-1.7295982908,2.0920902189
 C,-3.1623026246,-0.3386918855,2.1785115115
 C,-2.510253619,0.7756962805,2.4683332704
 H,0.6421269202,-3.8221895961,1.8727570345
 H,3.018805596,-3.142696014,1.8956701782
 H,3.6253031189,-0.745044881,2.1981905557
 H,1.8269817748,0.9454225536,2.4944841982
 H,-0.5439297386,0.2662730765,2.4730685152
 H,-1.5491245663,-3.4103764274,1.9646391645
 H,-3.5573850843,-2.4162159277,1.9613440127
 H,-4.2250007305,-0.2144396669,1.9299084053
 H,-2.7655253169,1.8280399551,2.4729161161
 H,-2.5555275073,4.8551703051,0.1834126247
 H,-4.6494284976,3.5913948359,-0.18653204
 H,-0.0933255692,4.9255540909,0.2878430229
 H,0.2410250393,-3.871349462,-0.5061412886
 H,4.8671813585,-2.7000659583,-1.3035305855
 H,2.7737955064,-3.9962427254,-1.5861872361
 H,-4.4282557967,-3.0217658928,-1.5205300671
 H,-2.2410032826,-4.1783061486,-1.6576256874
 H,-5.7346372831,-0.9507292276,-1.1702283257
 H,-5.8104792694,1.4764789701,-0.6915935557
 H,2.3687753344,5.0063323781,0.3946717756
 H,4.5591582733,3.8747854538,0.2082882542
 H,5.8888406321,1.841707805,-0.2234330944
 H,6.0070842207,-0.5657119361,-0.7843037499
 H,0.26818096,-3.7936922699,-2.2543304486

TS 3 --> 4 adsorbed on P4 (7-H-ovalene)

E = -1615.04705296 a.u.

C,-1.3164384844,-2.1393941574,0.7937095859
 C,-1.0916961635,-2.2513973301,2.1595141414

C,0.2206802297,-2.3229758027,2.6540743442
 C,1.3007974368,-2.3088667873,1.7718408799
 C,1.0978412589,-2.2436173508,0.3868313757
 C,-0.2323390596,-2.1496750323,-0.1118891682
 C,2.2107968722,-2.3236041878,-0.5498800695
 C,2.1605794527,-3.0335346852,-1.7026636113
 C,1.0569435401,-3.9109396102,-2.1073580259
 C,-0.1675365271,-3.9037224112,-1.5889732158
 C,1.7133809134,0.8872886188,0.0865925337
 C,0.3230142255,0.9789086029,0.4471013092
 C,-0.064463755,1.0037051456,1.831912772
 C,0.8999137481,0.9579486633,2.8572963035
 C,2.3721230417,0.882998413,2.5403247634
 C,2.7179140453,0.8337113829,1.0729982768
 C,0.4898527829,0.9540062937,4.1965568555
 C,-0.8521315386,0.986805637,4.5423958327
 C,-1.8478835367,1.0282673686,3.5441404239
 C,-1.448945376,1.0402765461,2.1755640526
 C,-2.4429718591,1.0570520505,1.1524336403
 C,-3.8243470386,1.0686868436,1.5012334434
 C,-4.1920182479,1.0672217727,2.8770479354
 C,-3.2409813102,1.0467962123,3.8632416224
 C,-0.6681428373,0.9907807178,-0.5628421825
 C,-2.0529513262,1.0323389708,-0.2152805692
 C,-3.0511415199,1.0149399419,-1.2393496997
 C,-4.4283533368,1.0424414264,-0.8568655625
 C,-4.7983474035,1.0679614077,0.4624285774
 C,-2.657860439,0.9525000377,-2.5867807135
 C,-1.3033505275,0.8889447534,-2.9557390389
 C,-0.296592777,0.9062864213,-1.9402314882
 C,1.0756322063,0.8072737608,-2.3027336696
 C,2.0806541444,0.8007302411,-1.2897158994
 C,3.4520202813,0.6764438879,-1.6601322597
 C,4.4300701231,0.6401520942,-0.6446510484
 C,4.0605094933,0.7126138976,0.6903834444
 C,3.7924311254,0.5697639774,-3.0435924193
 C,2.8236159944,0.5773852723,-4.0122587453
 C,1.4455276128,0.6942462221,-3.6735866101
 C,0.4246301201,0.694099106,-4.6660913659
 C,-0.8984832581,0.7889270013,-4.3228618984
 H,2.3188341868,-2.3631132545,2.1514818894
 H,0.3945217524,-2.3667468935,3.7254003878
 H,-1.9292527781,-2.2264174153,2.851195594
 H,-2.3244968881,-1.9978257096,0.4151222538
 H,-0.3776807043,-1.7330096475,-1.1019119852
 H,3.1416654894,-1.836094564,-0.2681586232
 H,3.0480436451,-3.0543281592,-2.3316056144
 H,1.3166405283,-4.6647868512,-2.8607029799
 H,-1.0481008341,-4.5079687448,-1.775239676
 H,-1.6698348168,0.780727831,-5.0890971502
 H,0.7174062148,0.6102643593,-5.7100738663
 H,-3.4204460159,0.9363035178,-3.3622378257
 H,2.7923980097,-0.0079414241,3.0326070019
 H,-1.1522038632,0.9781302919,5.5874697525
 H,1.2480914487,0.914774224,4.9761184871
 H,5.4767344764,0.5434827705,-0.922587614

H,4.823684734,0.6717292347,1.4650294992
H,4.8420866227,0.4763038283,-3.3116468971
H,3.092873976,0.4910158528,-5.0623818241
H,-5.1811273812,1.0347835507,-1.6413925981
H,-5.8500906751,1.0817342943,0.7388346437
H,-5.2495066706,1.0781300161,3.1306380969
H,-3.5310373247,1.0409751317,4.9112141642
H,2.8890829107,1.7372257592,3.0070557689

TS 3-8 adsorbed on P4 (7-H-ovalene)

E = -1692.38500486 a.u.

C,-1.1622214411,-2.0947377768,1.1769779515
C,-1.147726822,-2.0556738523,2.5737209014
C,0.0748283947,-1.9969725755,3.2441655529
C,1.2634441703,-1.9746291612,2.518448212
C,1.2705328643,-2.0045488673,1.1087418402
C,0.0254244844,-2.0697743593,0.4522952685
C,2.5780513301,-1.9164855826,0.4508841881
C,2.9753918224,-1.8309072824,-0.8418758423
C,2.2527712113,-1.881217269,-2.1155044922
C,1.2124387346,-2.6270434596,-2.4582823285
C,-1.6493381173,1.0570920679,2.1266351106
C,-2.0527926185,1.0992861968,3.4931229211
C,-3.4341226493,0.9240083585,3.8157058368
C,-4.3669334618,0.7053507049,2.8359779708
C,-3.9929588789,0.6554557502,1.4623223092
C,-2.6255709189,0.840855443,1.1090505166
C,-0.2715197799,1.1889530144,1.7822109751
C,0.6833620883,1.3499003458,2.8043095006
C,0.2664478233,1.4115785881,4.1400083996
C,-1.0705759473,1.2918282034,4.4864755906
C,0.1227545677,1.1419879475,0.3995769497
C,-0.8530391008,0.9492034736,-0.6066213017
C,-2.2272445571,0.7818622408,-0.2552527871
C,-3.2027656927,0.5391227981,-1.2721190389
C,-4.5669859974,0.3583671247,-0.8850440858
C,-4.9451624286,0.4149137321,0.4312728579
C,1.507011493,1.2861198047,0.0369387979
C,2.5037371263,1.434266796,1.0209930755
C,2.1568904067,1.3940175249,2.4883198678
C,-2.798720898,0.4788770786,-2.6169864563
C,-1.4554945623,0.655353451,-2.9906542742
C,-0.4709320179,0.8938060928,-1.9817429576
C,0.8921340378,1.0654316035,-2.3492217582
C,1.8806918032,1.2637177883,-1.340193902
C,3.2494220718,1.4047714282,-1.7124286238
C,4.2173773049,1.5681256794,-0.6988987942
C,3.8432377314,1.5787459961,0.6356286858
C,3.600525182,1.3653959277,-3.0972869436
C,2.6461641831,1.1783845831,-4.0639966776
C,1.2740031935,1.0137951728,-3.7205941108
C,0.2746480002,0.7781291583,-4.7067059318
C,-1.0388063954,0.6008959329,-4.3570788607
H,2.2142199373,-1.9185969988,3.04516914
H,0.1021820839,-1.9492839729,4.3289946306

H,-2.0806456194,-2.0506874946,3.1299443495
 H,-2.1084890667,-2.1236183698,0.6450496484
 H,-0.0085934969,-2.0939361547,-0.6283689899
 H,3.3949502203,-1.8373949024,1.1686443666
 H,4.039683546,-1.6382744071,-0.9729881119
 H,2.6965736237,-1.2460350297,-2.8920136556
 H,0.6698211493,-2.7290552978,-3.3896340923
 H,-1.7928262858,0.4183079849,-5.1189389675
 H,0.5763661226,0.7366027238,-5.7507937862
 H,-3.5439855325,0.2929066866,-3.3871930169
 H,2.625766139,0.498946545,2.9300216798
 H,-1.3753945361,1.3337554447,5.5294154145
 H,1.0166767822,1.5421773173,4.917320745
 H,5.2617408785,1.6809428051,-0.9797827428
 H,4.6004768258,1.6963837285,1.4082187134
 H,4.6468995709,1.4822839369,-3.3689944097
 H,2.9254020424,1.1435178275,-5.1145153748
 H,-5.3033211588,0.1726898445,-1.663235238
 H,-5.9866515905,0.2735061443,0.7107274083
 H,-5.4142856426,0.5649512023,3.0930447554
 H,-3.7291826003,0.9598703292,4.8616946355
 H,2.6236387321,2.2471966142,3.0038083437
 C,1.0380635266,-4.6378932648,-1.2252131758
 C,0.2920686196,-5.4532339817,-1.7389068615
 H,1.7327455015,-4.1753428707,-0.5542973982
 H,-0.3948269442,-6.0407090915,-2.3063425017
 --- end of complexes of Table 3 ---

Species of Table 4

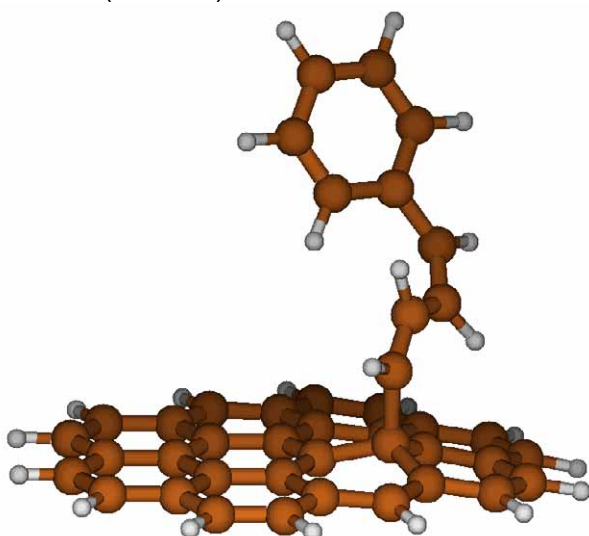
TS 3-9 on P1 (ovalene)

E = -1614.46037394 a.u.

C,3.4659540766,-1.8846646124,-1.6746287187
C,3.2542622231,-0.4827386161,-1.4841238229
C,1.9356606074,-0.0201011901,-1.2178110579
C,0.8553054828,-0.9440588194,-1.143713729
C,1.0920997019,-2.3409151634,-1.3419759093
C,2.4315965344,-2.7750614932,-1.6112593256
C,-0.4488380522,-0.4860880705,-0.8246022468
C,-0.6691820221,0.895129424,-0.5599174192
C,0.3858273149,1.8248246694,-0.6905243774
C,1.697971868,1.3691265711,-1.0129709819
C,2.9287526269,-2.1879385879,2.0448506313
C,4.2594451045,-1.7780059806,2.0035495187
C,4.570040279,-0.4163949096,1.9646789402
C,3.537280124,0.5250664258,1.9633247884
C,2.2075287019,0.1150062149,2.0080743147
C,1.8754252561,-1.2541428679,2.0611505677
C,0.01776721,-3.2362938023,-1.2535159786
C,-1.2850036732,-2.8001766511,-0.9693873392
C,-1.5238651869,-1.4116848652,-0.7406977269
C,-2.8380299831,-0.9579176718,-0.4060434133
C,-3.070042096,0.4120552261,-0.122360151
C,-1.9494746181,1.3373011337,-0.0528212716
C,-2.2317286651,2.7724040055,-0.0717230607
C,-1.1778414769,3.662443765,-0.2354516635
C,0.1382594864,3.2237138265,-0.4972106428
C,-4.3793692369,0.8760486313,0.1426481533
C,-4.5900844857,2.2865181765,0.3356680489
C,-3.5739431368,3.1901060439,0.2007443901
C,0.4998471791,-1.7577774655,2.0428412916
C,-0.6531684625,-1.0794192873,2.2007020782
C,-0.7991714377,0.3257591499,2.6159026564
C,-1.4840813904,1.2865848983,2.0088038322
H,2.6878645186,-3.2485815527,2.0550558239
H,5.0534585316,-2.5204670377,1.9898603854
H,5.6062293806,-0.0916185675,1.9178426084
H,3.7653760289,1.5846647821,1.8912420579
H,1.419960369,0.8547002957,1.9432929125
H,0.4136298534,-2.8124084449,1.7860500738
H,-1.5780772961,-1.6156543382,2.0012958711
H,-0.2697604448,0.6005022527,3.5383658477
H,-1.5917834286,2.3173524862,2.3273659689
H,-3.7712091547,4.2557881915,0.2917226873
H,-5.6010790623,2.6278212006,0.5454210889
C,-3.9204144741,-1.8820936916,-0.3555595868
C,1.2366557295,4.1289462258,-0.6101338337
H,-1.370289992,4.7313654699,-0.1649644519
H,0.1978795386,-4.2975469846,-1.413003518
H,4.4781342175,-2.2304617669,-1.8701972259
H,2.608524841,-3.8379451373,-1.7575190962
C,-3.6541391559,-3.2688589993,-0.6031773843
C,-5.2159990365,-1.4014502967,-0.055889035

H,-4.4843597798,-3.9694765404,-0.5533050405
 C,-2.3935367078,-3.7094813906,-0.8879423107
 H,-2.2053511213,-4.765655263,-1.0656519139
 C,-5.4417066385,-0.0575489713,0.1741334376
 H,-6.0401379491,-2.109788167,-0.0168296825
 H,-6.4469655591,0.3006084199,0.3831074067
 C,2.5038126845,3.6833841939,-0.8852986425
 H,1.0474095326,5.1900828941,-0.4656465157
 H,3.3296964018,4.3873460893,-0.9558775621
 C,2.7756130814,2.2944000326,-1.0917299665
 C,4.0773332264,1.8057396243,-1.3612933946
 C,4.309028199,0.4576232425,-1.5465471563
 H,4.8998184814,2.5151503967,-1.4159336833
 H,5.3159515249,0.0980128618,-1.7442690602

9 on P1 (ovalene)

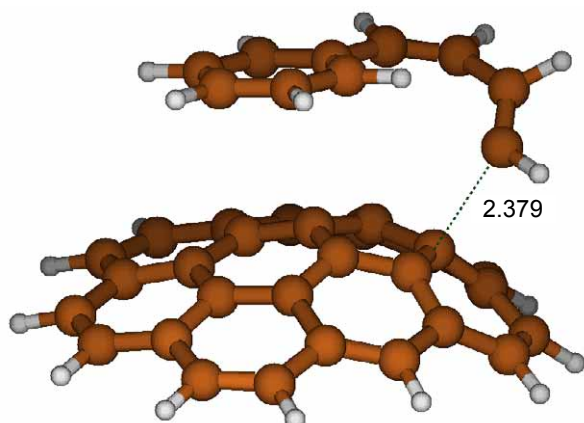


E = -1614.48559078 a.u.

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 C,2.4764461134,3.5638776354,1.3192636402
 C,3.3299904224,4.5824268751,1.7864360049
 C,4.302811098,5.1419816862,0.9614185819
 C,4.4582634958,4.6819169203,-0.3500789085
 C,1.4662172838,3.0125910793,2.2281001105
 C,0.2745426749,2.4556668714,1.9169115232
 C,-0.3197701241,2.4363986323,0.5834467993
 C,-1.2327762826,1.6182578897,0.0281580209
 C,-1.8597479764,0.279942917,0.5091095055
 C,-1.2535805725,-0.7172840008,-0.4610635818
 C,-0.0012314376,-1.2967126403,-0.1571928634
 C,0.5422384135,-1.2013554998,1.1605600683
 C,-0.2341894375,-0.6110935518,2.21557774
 C,-1.4788300174,-0.0077390104,1.9412707101
 C,-2.2871764232,0.4737422067,2.9805523973
 C,-1.8027896145,0.4097230409,4.30967557
 C,-0.5533687557,-0.1133880519,4.5847261836
 C,0.2519708475,-0.6476650144,3.5540187372
 C,1.5463204079,-1.21025934,3.806244935
 C,2.2958652637,-1.7427221508,2.7983764607

C,1.8057956649,-1.7876734256,1.4478674176
 C,2.5207921861,-2.4343102184,0.4222381685
 C,1.9943679209,-2.5702501985,-0.8691820719
 C,2.6886982287,-3.2627654044,-1.9154055187
 C,2.1373631,-3.4106315002,-3.1593200222
 C,0.8460527668,-2.8815312523,-3.468926288
 C,0.1354016972,-2.1741131105,-2.4544133273
 C,0.7070457367,-2.0142139691,-1.1601676286
 C,-1.1570365118,-1.6443504101,-2.7285287212
 C,-1.8519639329,-0.9118191456,-1.717631841
 C,-3.1706837441,-0.4041299559,-1.984172531
 C,-3.9055328592,0.215596917,-0.9247732324
 C,-3.362391245,0.4542071154,0.3105167133
 C,-4.116673849,0.9684536171,1.4159155988
 C,-3.5974148054,1.0153054615,2.6744167958
 C,-3.7307839712,-0.6151278244,-3.2651606036
 C,-3.0426547708,-1.2919590649,-4.2534034627
 C,-1.74450646,-1.8259729088,-4.0141813239
 C,-1.0123123654,-2.531312468,-5.0054041338
 C,0.2423066546,-3.0402580074,-4.7408803194
 H,2.6765220219,-3.9443590459,-3.9384706702
 H,0.7874806877,-3.5794957199,-5.5119542197
 H,-1.46183733,-2.6656234889,-5.9863366053
 H,-3.4915811684,-1.4349403303,-5.2331789425
 H,-4.7298671247,-0.2336729744,-3.4628027734
 H,-4.9511609656,0.4624332408,-1.1022697913
 H,-5.1404168947,1.2873895456,1.2321933238
 H,-4.1923578597,1.3996499551,3.4992724347
 H,-2.4254624588,0.7945643858,5.1137932316
 H,-0.1792936481,-0.1327856411,5.6055737399
 H,0.0276859116,3.2378575934,-0.0688873913
 H,-0.3050522124,2.0589678062,2.7410210957
 H,1.7221972647,3.0706042954,3.2855001912
 H,3.2728521468,-2.1727984082,3.004610238
 H,-1.5590073044,1.8467420714,-0.9846125371
 H,2.0613941517,2.2644780151,-0.352827387
 H,3.2123864873,4.9389692181,2.8074054027
 H,4.9433265222,5.9340961779,1.3409628413
 H,5.2204197915,5.1128246799,-0.9940093315
 H,3.7721595955,3.2703933328,-1.8296978882
 H,3.4924318909,-2.868260608,0.6480618619
 H,3.6691567432,-3.677713858,-1.694680211
 H,1.9182117578,-1.2076186893,4.8281153324

TS 3 --> 10 on P3 (tribenzo-corannulene)



E = -1460.69252342 a.u.

C,3.4852928544,0.7508774661,-1.3234779572
 C,4.2733456512,-0.3080248992,-1.4356394596
 C,4.0547393805,-1.6942224241,-1.0002404874
 C,2.9699401882,-2.4985389217,-1.0297628847
 C,1.6235540496,-2.3356887757,-1.5876894956
 C,1.249952378,-1.3244332132,-2.4926129826
 C,-0.0568299549,-1.2443646032,-2.968061512
 C,-1.0241794704,-2.1641973464,-2.5516283787
 C,-0.6647168487,-3.1844951618,-1.6692363943
 C,0.6460868628,-3.2731001246,-1.2055081796
 H,1.9830925252,-0.5910682802,-2.8030843332
 H,-0.3272639856,-0.4453116624,-3.6532283405
 H,-2.048272505,-2.0799337775,-2.9046930023
 H,-1.4076111879,-3.900964723,-1.3291850655
 H,0.9206185628,-4.0629819004,-0.5104213625
 H,3.1159184027,-3.4734428866,-0.5637130849
 H,4.9542226611,-2.1498325556,-0.5845114903
 H,5.2828012008,-0.1294254413,-1.8363134078
 H,3.6456327432,1.792156631,-1.5765743891
 C,-4.6210940311,-0.9766133035,0.827148156
 C,-4.8990631874,0.2271071756,0.1912443331
 C,-3.8607781812,1.0610706279,-0.2957316558
 C,-2.5357600673,0.5755873777,-0.2338152863
 C,-2.2479671608,-0.6668611623,0.4317338736
 C,-3.2879869426,-1.4192005269,1.0197175393
 C,-2.9146001218,-2.5208975714,1.8839001979
 C,-1.6190861799,-2.754951625,2.2687611193
 C,-0.5291044488,-1.9471908879,1.7671107718
 C,-0.8933913151,-1.0307953107,0.7220711884
 C,-4.0562410373,2.4275359285,-0.7355408286
 C,-3.0153361118,3.2953936217,-0.9453124389
 C,-1.6403934221,2.8662466277,-0.8087236758
 C,-1.4673041729,1.4515061118,-0.6174792261
 C,-0.1792547366,0.9779641396,-0.4811279378
 C,0.1027566597,-0.2458918095,0.1879512992
 C,1.3743684091,-0.1636146473,0.7588455428
 C,1.7130505435,-0.8818438153,1.9073434473
 C,0.7680490598,-1.8730380028,2.3299677086
 C,2.8135882326,-0.3000943404,2.6564199316
 C,3.2882544754,0.9764527018,2.3861143067
 C,2.7508610029,1.7937266493,1.3218653794

C,1.9164536937,1.1209114895,0.425738925
 C,-0.5226012066,3.7253318425,-0.6655126332
 C,0.7682897876,3.2224956575,-0.3001838869
 C,1.8485640273,3.9137261583,0.3878790279
 C,2.7729266483,3.2321597956,1.1685485022
 C,0.9147725902,1.8328168178,-0.3203053772
 H,3.4784144888,3.8152084528,1.7571568684
 H,1.8685039367,5.0013286011,0.3912188872
 H,-0.6925389327,4.8000726966,-0.6932242256
 H,-3.2222122423,4.3377594411,-1.1770781554
 H,-5.0782403136,2.7908453876,-0.8185626336
 H,-5.9285252546,0.5708072192,0.1196882022
 H,-5.4364417142,-1.5626321717,1.2454830964
 H,-3.713839015,-3.1272385359,2.3045908884
 H,-1.4071635892,-3.533314941,2.9984792997
 H,0.9886697919,-2.4902862506,3.198968471
 H,3.2018300148,-0.8242927883,3.5269122334
 H,4.0274570249,1.405437187,3.0594681125

10 on P3 (tribenzo-corannulene)

E = -1460.74452612 a.u.

C,-0.6535233974,1.7500500854,-0.4138453477
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 C,-2.7383535107,0.7401558474,-1.1670777836
 C,-3.262602694,2.0465198328,-1.4139637419
 C,-2.4861370125,3.173452626,-1.0313607571
 C,-1.2094382803,3.0310264216,-0.4172611123
 C,-3.5652400027,-0.418605029,-1.0240402937
 C,-4.929171357,-0.3230388805,-1.3797286839
 C,-5.410035565,0.9505962761,-1.8624499761
 C,-4.6384081102,2.0855385778,-1.8483691122
 C,-3.0828668617,-1.5680603729,-0.2989493975
 C,-3.970928472,-2.6072728486,0.0581352657
 C,-5.3041515197,-2.546971005,-0.4309196615
 C,-5.7676793086,-1.4423268959,-1.1257070017
 C,-0.9371428934,-0.4903172482,-0.0268003224
 C,-1.7752297785,-1.5562367178,0.2819830146
 C,-1.4033429393,-2.3900437219,1.3809991398
 C,-2.3034870299,-3.4837195665,1.6570921965
 C,-3.5029618915,-3.597357242,0.999779354
 C,0.1356877669,-0.1163500676,0.7597398323
 C,0.3778667975,-0.7623732727,1.9759271999
 C,-0.3293236636,-1.9741426981,2.213586877
 C,0.5257759223,1.3073544,0.4319416781
 C,0.6112293351,2.1360560529,1.6947822328
 C,1.0645992726,1.4520987246,2.8557625391
 C,1.0414120015,0.0637551299,2.981898233
 C,-0.5927582028,3.9623228506,0.5275089866
 C,0.2063350133,3.49320341,1.5719526881
 C,1.8390693364,1.5478315606,-0.3102415961
 C,2.8521688376,0.710529978,-0.5999538937
 C,2.9438301191,-0.7245700604,-0.3846674918
 C,4.071598614,-1.4673470306,-0.4699370844
 C,5.4541548546,-1.0109564391,-0.6533811027
 C,5.9305772318,0.2166087444,-0.1525228799

C,7.2560038656,0.6026849705,-0.3506796676
 C,8.13897321,-0.230516761,-1.0427611567
 C,7.6886093889,-1.4641022615,-1.523173353
 C,6.3656376842,-1.8514798483,-1.321610517
 H,5.2626764264,0.8497543432,0.4218188284
 H,7.6037296589,1.5520706889,0.0488348947
 H,9.1719321152,0.0715934054,-1.1940796381
 H,8.3707645976,-2.1255161085,-2.0513008961
 H,6.0182696383,-2.8126722581,-1.6939031895
 H,3.9546959663,-2.5490960322,-0.4102460625
 H,2.0185960413,-1.2568842381,-0.1949127976
 H,3.7112816881,1.1623516421,-1.0927314711
 H,1.950893948,2.5937124473,-0.5887333695
 H,0.4561379727,4.1849794253,2.3752332409
 H,-0.9176832748,4.9996769016,0.5407266985
 H,-2.9535904235,4.155595287,-1.0673430707
 H,-5.0776151606,3.040303429,-2.128182866
 H,-6.4515060663,1.0161770187,-2.1695374164
 H,-6.810728506,-1.3965246903,-1.4304762768
 H,-5.9866562694,-3.3604112257,-0.1954457163
 H,-4.1731911196,-4.4170689198,1.2491062231
 H,-2.0409947847,-4.2023671925,2.4299867042
 H,-0.155972812,-2.5184634736,3.1397940224
 H,1.3398374713,-0.3841321034,3.9263260099
 H,1.3594822626,2.0406997349,3.7233640371

TS 3 --> 11 on P4 (7-H-ovalene)

E = -1615.04871905 a.u.

C,5.1199029557,0.5586307765,-0.6175036637
 C,3.9720174293,-0.2559286926,-0.8809351476
 C,2.6717031284,0.3098887713,-0.7264163322
 C,2.5380891421,1.6675805664,-0.3054463182
 C,3.7005887413,2.4549817904,-0.0516163999
 C,4.9880296584,1.8611671591,-0.2207076465
 C,1.5107597481,-0.4789170915,-0.9871334432
 C,1.6595205102,-1.8242020885,-1.3790278198
 C,2.9443660629,-2.360100146,-1.5285373595
 C,4.0809221814,-1.6000497043,-1.2893613991
 C,1.2444085097,2.2287559107,-0.1268077707
 C,0.081974797,1.4306239998,-0.3769734649
 C,0.2051696103,0.1061316632,-0.8184824548
 C,-0.9774637611,-0.6793477906,-1.1013020251
 C,-0.8764028595,-2.0200226919,-1.4916472289
 C,0.4589710658,-2.7142408604,-1.5766817036
 C,-2.2676070255,-0.0791819376,-0.9678119644
 C,-2.3963193963,1.257668692,-0.4981545536
 C,-1.2226456602,1.9864948664,-0.0870929035
 C,-1.3385260083,3.4002697386,0.2185873565
 C,-0.1898979291,4.1478651402,0.430633594
 C,1.1088880713,3.5868592333,0.2852345051
 C,2.2841236676,4.3490880339,0.5223403837
 C,3.5376507307,3.8002623656,0.3631696501
 C,-3.4406874433,-0.8334506154,-1.2615968935
 C,-3.2984527611,-2.1822821003,-1.6644044687

C,-2.0453813935,-2.7547214406,-1.7660747088
 C,-4.7166777895,-0.2206764558,-1.1014077621
 C,-4.8280759485,1.0785930217,-0.6692650813
 C,-3.673774704,1.8472141529,-0.3580748768
 C,-3.7689901518,3.2038359836,0.1005973593
 C,-2.6564685018,3.9504176162,0.3603861881
 C,1.604722143,-4.3591227157,1.631531138
 C,0.3652416738,-5.0091913379,1.635776612
 C,-0.8127470654,-4.2673538745,1.6904904573
 C,-0.789382364,-2.8595517901,1.7493372314
 C,0.4678496288,-2.2222163369,1.7277242552
 C,1.6469432302,-2.9635704791,1.675411369
 C,-2.0622985499,-2.1346814012,1.723084571
 C,-2.2867283317,-0.8284773737,1.9674917317
 C,-1.3184750605,0.1321596294,2.5210446019
 C,-1.1031871568,1.3701190139,2.1029674237
 H,-1.7747674494,-4.7750957542,1.6794830147
 H,0.3183020864,-6.0945389734,1.590493235
 H,2.5251879586,-4.9345936507,1.5785631528
 H,2.5998923889,-2.4443185683,1.6272305242
 H,0.5207049616,-1.1420846093,1.6859292847
 H,-2.9080138936,-2.7242880794,1.3735430209
 H,-3.2749077549,-0.4371774882,1.7366340654
 H,-0.7114662142,-0.2431075388,3.3571641455
 H,-0.403528257,2.1246296013,2.4474216102
 H,-2.7477749991,4.9893248549,0.6679359473
 H,-4.759575659,3.6387159074,0.2119338667
 H,-0.2789370028,5.1941314143,0.7150525036
 H,0.4871071442,-3.505401435,-0.8103077906
 H,5.0695235327,-2.0361878842,-1.4115582121
 H,3.0440871141,-3.4012331036,-1.827582023
 H,-4.1911674327,-2.7634518751,-1.8830095872
 H,-1.9471057612,-3.7970819814,-2.0614100817
 H,-5.6052073466,-0.806069256,-1.3255979258
 H,-5.806572848,1.5387471379,-0.5533688501
 H,2.174670684,5.3843810432,0.8363706055
 H,4.4259966387,4.3979650203,0.5534065156
 H,5.8675012906,2.4701007007,-0.0247014332
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 H,0.5409056577,-3.2370105401,-2.5419974029

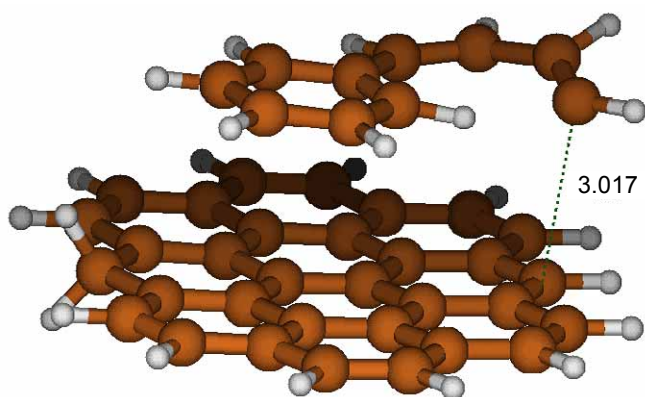
11 on P4 (7-H-ovalene)

E = -1615.09494957 a.u.

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 C,3.2238985888,-4.0018677578,-0.1738026314
 C,3.6877548205,-2.688221144,-0.1198796399
 C,2.9184237357,-1.6178627594,-0.6162766363
 C,3.4456724354,-0.256731418,-0.4627427901
 C,2.9782628664,0.9022301552,-0.9620858454
 C,1.8976131124,1.0623322848,-1.9577885299
 C,0.6824528055,1.6107761857,-1.833364303
 C,-0.0661051437,2.1113396815,-0.5719027302
 C,0.9032542481,2.4468337471,0.5418238121

C,1.3317431167,1.4320636587,1.4283592185
 C,0.7252332586,0.1349922613,1.4052346301
 C,-0.4773295348,-0.0739297242,0.5941902132
 C,-0.9544306279,0.9237298379,-0.2244801473
 C,-2.2088210806,0.7857389057,-0.9043076563
 C,-2.9292961621,-0.4332996361,-0.8044985168
 C,-2.3998736752,-1.5049815757,-0.0265500698
 C,-1.1794608523,-1.3321004772,0.6889574643
 C,-3.0985372997,-2.7472512365,0.035889025
 C,-4.3361879912,-2.8827494135,-0.6793808455
 C,-4.8514555985,-1.8501804517,-1.4079779207
 C,-4.1706652399,-0.5913154327,-1.4961896744
 C,-4.6756552685,0.493305967,-2.2366101924
 C,-3.9893570017,1.7002586283,-2.2907848618
 C,-2.7574162722,1.8725435235,-1.6359346674
 C,-2.0742585281,3.1503741162,-1.6238985805
 C,-0.8593417833,3.3276976894,-1.045462099
 C,-0.1963081317,4.609543446,-0.978213136
 C,0.9292795928,4.7845408562,-0.2448127603
 C,1.4676864173,3.7213142472,0.5945864398
 C,2.5291683198,3.9754944171,1.5030464549
 C,3.0020221496,2.9822810167,2.3305526698
 C,2.4160270528,1.6914037366,2.3188951413
 C,2.9069310793,0.6284729966,3.1256711106
 C,2.3455229169,-0.6222366926,3.0450024425
 C,1.240199336,-0.880660019,2.1917729377
 C,0.6809058212,-2.2785017353,2.129332382
 C,-0.6536457898,-2.4016769346,1.4374385029
 C,-1.350146371,-3.6144088723,1.4818099351
 C,-2.5499944949,-3.7900981412,0.8010018813
 H,4.6594421482,-2.4747767484,0.3202763317
 H,3.8401233698,-4.8084996786,0.2157382693
 H,1.592857775,-5.2987422698,-0.7488287941
 H,0.1877578102,-3.4226929003,-1.5923657575
 H,1.0125240658,-1.1113583012,-1.4975083172
 H,-4.860736837,-3.8336991923,-0.6220391162
 H,4.2966283395,-0.1863215135,0.2132098393
 H,-3.0765499101,-4.7400952603,0.8555091461
 H,-0.9332781045,-4.4363691075,2.0597712394
 H,3.4590043079,1.8171943842,-0.6186895217
 H,1.4077819727,-2.9105653771,1.593738239
 H,0.6151058167,-2.6968647945,3.1443164894
 H,2.735251619,-1.43767343,3.6501263336
 H,3.74151371,0.8210374963,3.7958337981
 H,2.1236302559,0.6506264995,-2.9443419062
 H,0.0369939233,1.6165137237,-2.7101074855
 H,-5.6213386841,0.3783691748,-2.7607302024
 H,-5.793176658,-1.9647007152,-1.9396548423
 H,-4.4069585412,2.5373332795,-2.8456207178
 H,-2.5815850472,4.0003221571,-2.0780774155
 H,-0.6481295297,5.4455688849,-1.5078023582
 H,1.4116665066,5.758041904,-0.1986675488
 H,2.9676607762,4.9703462179,1.5299314712
 H,3.8323467956,3.1741463361,3.0061527085

TS 3 --> 12 on P4 (7-H-ovalene)



E = -1615.094957 a.u.

C,5.14163,0.32727,-0.90759
 C,4.09747,-0.62743,-1.1114
 C,2.73976,-0.20374,-1.00831
 C,2.44823,1.15515,-0.68539
 C,3.51102,2.07951,-0.46861
 C,4.85684,1.63096,-0.59735
 C,1.67931,-1.14201,-1.18867
 C,1.9893,-2.48937,-1.45913
 C,3.32894,-2.88663,-1.56155
 C,4.36743,-1.98269,-1.39576
 C,1.09733,1.57689,-0.54801
 C,0.03279,0.64345,-0.74455
 C,0.31467,-0.70595,-1.05633
 C,-0.76296,-1.64963,-1.19835
 C,-0.50896,-3.00967,-1.46027
 C,0.90172,-3.52452,-1.60639
 C,-2.11106,-1.20937,-1.03448
 C,-2.38836,0.15727,-0.73506
 C,-1.31748,1.07972,-0.57932
 C,-1.59486,2.42974,-0.21171
 C,-0.52797,3.31997,0.00582
 C,0.80968,2.92374,-0.1722
 C,1.89548,3.82883,0.03236
 C,3.19621,3.42189,-0.11436
 C,-3.1868,-2.14018,-1.13782
 C,-2.89204,-3.49346,-1.40435
 C,-1.5784,-3.90942,-1.55994
 C,-4.52731,-1.67685,-0.95751
 C,-4.78857,-0.36117,-0.67992
 C,-3.73401,0.58813,-0.55343
 C,-3.98346,1.94674,-0.21936
 C,-2.95213,2.83298,-0.04351
 C,1.73007,-1.78458,1.95181
 C,0.55219,-2.53105,1.86467
 C,-0.68086,-1.90687,2.0253
 C,-0.77796,-0.52272,2.28202
 C,0.42016,0.21339,2.34957
 C,1.6552,-0.41116,2.1955
 C,-2.12053,0.03146,2.43817
 C,-2.59798,1.23259,2.84772
 C,-1.95737,2.47955,3.26524
 C,-0.75904,2.9736, 2.99357

H,-1.59525,-2.48859,1.93615
H,0.59341,-3.59614,1.65135
H,2.69438,-2.25947,1.79346
H,2.56239,0.18561,2.2242
H,0.37349,1.29071,2.48327
H,-2.89826,-0.69609,2.20798
H,-3.68334,1.28494,2.90914
H,-2.61997,3.11923,3.86684
H,-0.23735,3.88348,3.2638
H,-3.15143,3.86309,0.24018
H,-5.01397,2.2669,-0.08339
H,-0.74504,4.34522,0.29368
H,1.06735,-4.31865,-0.86034
H,5.40127,-2.30971,-1.47578
H,3.55071,-3.9314,-1.77017
H,-3.70899,-4.20665,-1.48259
H,-1.36379,-4.95754,-1.75908
H,-5.33825,-2.39624,-1.04297
H,-5.8118,-0.0199,-0.54048
H,1.6659, 4.8541, 0.31288
H,4.01371,4.12082,0.04663
H,5.65899,2.34748,-0.43613
H,6.17235,-0.00753,-0.9963
H,1.00685,-4.02797,-2.5809

12

E = -1615.13923710 a.u.

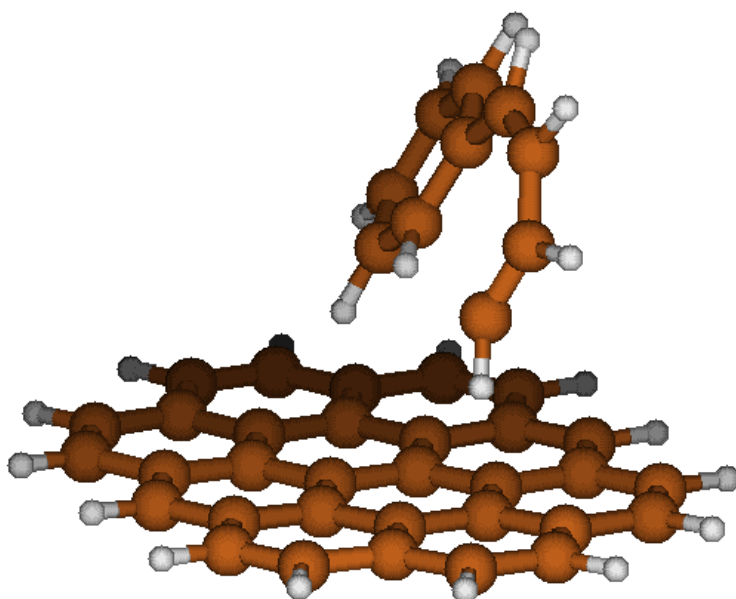
C,2.7010342069,4.3081107359,1.3716856648
C,1.6618454119,4.0336603727,0.4657032285
C,1.4452413948,2.6852359881,0.0517759696
C,2.2755983778,1.6402989619,0.5544110456
C,3.3029591578,1.9540365646,1.4591768829
C,3.5008493847,3.2841059004,1.8543111633
C,2.0453391781,0.274497244,0.1164458653
C,1.019536543,-0.0153517325,-0.7768855063
C,0.1642591193,1.0419540149,-1.2851675352
C,0.392530733,2.3872346395,-0.8667022069
C,0.7949535331,-1.3789607402,-1.2232604953
C,1.6476101281,-2.4200414728,-0.7473219792
C,2.701535685,-2.1220534799,0.1698820611
C,2.9084543439,-0.7826058212,0.6140094697
C,1.4515180122,-3.7635996459,-1.1839332845
C,0.4094484648,-4.0390520078,-2.0864742319
C,-0.4181218061,-3.0225396776,-2.5335824589
C,-0.2451022397,-1.6966036451,-2.1112214581
C,-1.207937206,-0.6424731803,-2.6346212193
C,-0.8859333366,0.7693328442,-2.1745594843
C,2.3189470301,-4.7953217435,-0.6937698103
C,3.3227467124,-4.5117370087,0.1818779845
C,3.5459746956,-3.1714331284,0.6411944565
C,4.5762029188,-2.8605020898,1.5456026579
C,4.7666268125,-1.5552920287,1.9715576207
C,3.9475732509,-0.5117751781,1.5192052381
C,4.2040782084,0.8855509885,2.0272153846
C,-1.6820845434,1.8195409739,-2.6529690172

C,-1.4641816847,3.1299846251,-2.2619643318
C,-0.4310391317,3.4414781336,-1.3608625206
C,-0.1866495517,4.7865020367,-0.9270564473
C,0.8165355471,5.0707366578,-0.0509116135
C,-2.6580798748,-1.0164392001,-2.3190616874
C,-3.2160927597,-1.013959047,-1.0944423878
C,-2.5149061628,-0.727301626,0.1462787816
C,-3.0826614709,-0.4750320604,1.3471529748
C,-4.5066565169,-0.30020106,1.6545407955
C,-5.417361617,0.2765375702,0.7480489654
C,-6.7627530588,0.423655629,1.0844773835
C,-7.2270863613,0.0095832938,2.3358383031
C,-6.3300553819,-0.5405950618,3.2567894985
C,-4.9852776039,-0.6841651793,2.9219228077
H,-4.2884703853,-1.110180188,3.6402844271
H,-6.6791997219,-0.8538975909,4.2374055069
H,-8.2753499638,0.1281379298,2.5971744304
H,-7.4479534645,0.8771633425,0.3726452618
H,-5.0541825253,0.6386504703,-0.2079437482
H,0.9974135582,6.091954413,0.276051693
H,-2.4156192306,-0.4013487951,2.2054476299
H,2.8684847359,5.3345464915,1.6891189473
H,4.3024271481,3.5078064906,2.5553566649
H,-1.4311421523,-0.7743705515,0.1110898708
H,4.115978171,0.8890548233,3.1253563751
H,5.2530090732,1.1547287707,1.8283234716
H,5.5673296928,-1.3258585194,2.6717693779
H,5.2214541805,-3.6577251229,1.9068337844
H,-4.2695813025,-1.2728709378,-1.0128220603
H,-3.2764210783,-1.2971721119,-3.1686862396
H,-2.0931669354,3.9307312754,-2.643451236
H,-0.8261072549,5.5755076926,-1.3157216715
H,-2.4970708407,1.5852453457,-3.3331546034
H,-1.1246017615,-0.6497902195,-3.7313796146
H,-1.232743019,-3.2486988738,-3.2169990524
H,0.2588390544,-5.0612470889,-2.4251025961
H,2.152955083,-5.812907929,-1.0393842483
H,3.9772076865,-5.2974672754,0.5517684645

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ADSORBED PHASE: growing system approximately
PERPENDICULAR to ovalene

3



E = -1614.47014431 a.u.

C,0.27289903,-1.0851798955,0.5540811808
C,0.2929621863,-1.2867960485,-0.8657404577
C,-0.955967098,-1.1209184483,1.2573068227
C,-0.9152101845,-1.5323356378,-1.564875689
C,-2.1721361628,-1.3743505459,0.5561205052
C,-2.1517765579,-1.5775270014,-0.8551214425
C,1.4768124216,-0.8059771795,1.246928107
C,1.5169845947,-1.2113668628,-1.577465988
C,2.7083905059,-0.7250790291,0.5325044382
C,2.7296849001,-0.9302637637,-0.8789535348
C,-3.4078779138,-1.3999162776,1.2594637942
C,-3.3672073688,-1.8067254957,-1.5575406655
C,-4.6017530826,-1.6311110895,0.535985136
C,-4.5817207834,-1.8278379462,-0.8326889886
C,3.9126410935,-0.4107956554,1.2216391827
C,3.956471345,-0.8339079719,-1.5923338815
C,5.1182325536,-0.3224952114,0.4862250836
C,5.1400069236,-0.5304370909,-0.8792201567
C,0.223386091,-0.6143420449,3.336193998
C,0.3289181816,-1.6561355757,-3.6658711104
C,1.4475296913,-0.562766142,2.657077902
C,1.5328214492,-1.4006780183,-2.9968942985
C,2.6803468796,-0.2564295589,3.3224005981
C,2.7896686985,-1.3109015928,-3.6831164381
C,3.8585902484,-0.1843092112,2.635678543
C,3.947312027,-1.0392050992,-3.0107754691
C,-0.9776925027,-0.8853151858,2.6692319097
C,-0.893465747,-1.7210229135,-2.9843200924
C,-2.2408074602,-0.9243330856,3.3485807152
C,-2.1364930888,-1.9614351512,-3.6596330801
C,-3.4016957057,-1.1717330932,2.6739304162

C,-3.3186677901,-2.0011043623,-2.9770248303
 H,0.2038107508,-0.4247883731,4.4073033801
 H,0.3412642493,-1.7984178773,-4.744461979
 H,-2.2533754484,-0.7448483746,4.42073744
 H,-2.1168268457,-2.1073651039,-4.736892097
 H,-4.3516229352,-1.1936165244,3.2026002665
 H,-4.2528638229,-2.179198542,-3.5042710691
 H,-5.5449014347,-1.6476210503,1.0768105541
 H,-5.5089436789,-2.0013501884,-1.3734208901
 H,2.6546497864,-0.0732798513,4.3937416215
 H,2.7986701739,-1.45928641,-4.7601624599
 H,4.7839924094,0.0545365534,3.1545455296
 H,4.8908688876,-0.968288613,-3.5466566782
 H,6.036584553,-0.0833595595,1.0173148044
 H,6.0756138753,-0.4568267463,-1.4284258687
 C,0.9207111712,2.161307317,-0.0378276795
 C,1.966829909,2.8117819622,0.6186212577
 C,1.738741942,4.0629800173,1.1998604434
 C,0.4733812808,4.6393178943,1.1318913672
 C,-0.6050377026,3.9790107096,0.5034598682
 C,-0.349935325,2.7311347086,-0.0948975286
 C,-1.8994125908,4.6592715149,0.5086092232
 C,-3.1725679492,4.2284128793,0.33276243
 C,-3.7594993345,2.9087188467,0.0968558238
 C,-3.2238771184,1.7526661601,-0.2630409357
 H,1.0924434416,1.1905888392,-0.480880152
 H,2.9459471378,2.3435236788,0.6721744434
 H,2.5456361433,4.5887783502,1.7041864256
 H,0.2983643308,5.6142223208,1.5822150743
 H,-1.1477701316,2.2109247956,-0.6167358324
 H,-1.8166266364,5.7199152221,0.7479430492
 H,-3.9287831258,5.0043755706,0.441328431
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 H,-3.6030155552,0.7523757105,-0.4223791227

TS 3 --> 4

E = -1614.46879031 a.u.

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 C,-1.3666991779,0.2878025866,-1.3233152442
 C,-0.1142249597,-0.3160330791,-1.0466202884
 C,-0.0603840804,-1.5725786506,-0.3575989312
 C,-1.2590807662,-2.2139645522,0.0406329905
 C,1.0847803466,0.3465127515,-1.4076184077
 C,2.3451625982,-0.2319424806,-1.0791231346
 C,2.3985893446,-1.4823511762,-0.3971659903
 C,1.1918700694,-2.1538475993,-0.0428028078
 C,-1.4166399908,1.5573884429,-1.9837894496
 C,-1.2023527021,-3.4624954393,0.7408901996
 C,1.0278492101,1.618538034,-2.0628014863
 C,1.2428537396,-3.3966959955,0.6660509961
 C,2.2607453043,2.2768500294,-2.3847734174
 C,3.4655580629,1.7164313766,-2.0716869675
 C,3.548623487,0.4508325356,-1.406002833
 C,-2.4360504357,-4.0828109427,1.131093851

C,-3.6406329375,-3.498492861,0.860895889
 C,-3.7239037709,-2.2413096233,0.1775035245
 C,-2.6994714649,2.1528506198,-2.2223404567
 C,-3.8525642058,1.5349589331,-1.830109099
 C,-3.8298520061,0.2664932536,-1.1630132668
 C,2.5285170944,-3.9440690665,0.9924410854
 C,3.6818171817,-3.2953802887,0.6540686889
 C,3.6566262972,-2.0441555716,-0.044593176
 C,4.8383977712,-1.3442873765,-0.3841469497
 C,4.7858934777,-0.1328709959,-1.0462574335
 C,-0.2198340132,2.1891565246,-2.3446521139
 C,0.0462009181,-4.026723582,1.0330373155
 C,-4.9596833764,-1.6079315862,-0.0940588683
 C,-5.0110317489,-0.3892903171,-0.7423178178
 H,-2.7328790264,3.1191585136,-2.7192293476
 H,-0.2603408486,3.1605168196,-2.8324528611
 H,2.2128100153,3.2428046603,-2.8813355768
 H,4.3918131384,2.2308234829,-2.3167097332
 H,5.7038454089,0.393414582,-1.2971315178
 H,5.7978420262,-1.7771326186,-0.1109934845
 H,4.6484544205,-3.7193553171,0.9157827539
 H,2.5642865449,-4.8900880146,1.5272662091
 H,0.0882847464,-4.9715223234,1.5710120315
 H,-2.3894826036,-5.0334717116,1.6567777755
 H,-4.5663365544,-3.9793096466,1.1681808721
 H,-5.8774500188,-2.0975333966,0.2228662203
 H,-5.969338208,0.0857520256,-0.9382726076
 H,-4.8170625345,2.0019364301,-2.0149875456
 C,-1.6922924546,2.8030928473,1.4084788607
 C,-2.0020600859,3.9414427173,2.141862686
 C,-0.9755915546,4.783559452,2.6052699521
 C,0.3600093124,4.4660824612,2.3547886341
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 C,-0.3426594736,2.4549020643,1.1803140327
 C,2.0856058634,2.8687584947,1.4998893013
 C,2.4888103779,1.5831713296,1.6519971265
 C,1.6408660448,0.4755612892,2.1022941466
 C,0.3124162574,0.4814896871,2.1280075086
 H,-2.4772108201,2.1820882647,0.9847666484
 H,-3.0406181358,4.2030032257,2.3299512064
 H,-1.2227067285,5.6858617564,3.1587093873
 H,1.1530938772,5.1151314741,2.7202218285
 H,-0.1093733079,1.7755567303,0.3761895279
 H,2.8393933044,3.6370642757,1.3326765013
 H,3.5455799029,1.3552158877,1.5350952662
 H,2.1823103535,-0.4018467356,2.4731653326
 H,-0.4217217665,-0.2574505157,2.4257987726

4

E = -1614.52737134 a.u.

C,-0.0153086282,-1.5508497688,0.2552411257
 C,-0.0094138868,-0.3446545807,1.0311595104
 C,1.2092717661,-2.1524594114,-0.1298560332
 C,-1.2455099684,-2.1301593962,-0.1458177888
 C,1.2212521816,0.2526352684,1.4004744389

C,-1.233756756,0.2750087851,1.3843357646
C,-2.4777837868,-1.5063254814,0.2116097017
C,2.4479233311,-1.5512370008,0.2440021175
C,-2.4711928395,-0.301701683,0.9734924849
C,2.4532843501,-0.3466544596,1.0059772464
C,1.1999636654,-3.3533314897,-0.9110090816
C,-1.247787972,-3.3310611553,-0.9269860769
C,1.2246347034,1.4825216925,2.1331461528
C,-1.2243706813,1.5047880235,2.1171483261
C,-0.0267453767,-3.9170380017,-1.285655557
C,0.0031468658,2.0772725755,2.4771851531
C,-3.69823518,0.3388302737,1.2974371327
C,3.6874331518,0.2714278499,1.3461358884
C,-3.7119096997,-2.0724379353,-0.2121229415
C,3.6770052695,-2.1398661032,-0.1634285629
C,-3.6620444721,1.5634993865,2.0398871774
C,3.6637891883,1.496744346,2.088033635
C,-3.6878003119,-3.280819,-0.9823991579
C,3.6410094502,-3.3476463381,-0.9341826187
C,-2.4795847531,2.1224280048,2.4318919726
C,2.486653258,2.0772542609,2.4643696132
C,-2.5109264694,-3.8842191432,-1.3234654559
C,2.4579202753,-3.9294632162,-1.2908919748
C,-4.9109862053,-0.2464832704,0.8638935274
C,4.8949148627,-0.336033446,0.9286346431
C,-4.9182324783,-1.4185405603,0.1327515531
C,4.8904074835,-1.5081315715,0.1975307523
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H,0.0081430873,3.0182018652,3.0231265532
H,-2.5098463282,-4.797918,-1.9127916767
H,2.4479412312,-4.8430336689,-1.8803331639
H,-2.4678597832,3.0574578533,2.9863619307
H,2.484689007,3.0124810733,3.0186269681
H,-4.6055179647,2.0474312786,2.2808442382
H,4.6126720742,1.9634416496,2.3414294652
H,-4.6364685137,-3.7089478523,-1.2974860508
H,4.5857798254,-3.7930545502,-1.2367791392
H,-5.8596323259,-1.8536857105,-0.1940790623
H,5.8279389881,-1.9604580429,-0.1168550334
H,-5.8469709339,0.2469842867,1.1145917899
H,5.8363689005,0.1402704569,1.1917450149
C,0.0273760658,2.0284201237,-1.2886119688
C,0.0381946887,3.49515422,-1.6907982054
C,1.2985598948,1.2981701231,-1.6324692373
C,-1.2448128005,1.3109616642,-1.6551283579
C,1.2837123892,4.1386557713,-1.8235847374
C,-1.1984486911,4.1512462973,-1.8435684879
C,2.4523909801,1.9805112095,-1.8295186122
C,-2.3883487211,2.0048897357,-1.8708660755
C,2.4672033694,3.420268322,-1.8532873785
C,-2.3884328771,3.4447639987,-1.893031661
H,0.0176908542,2.0640685268,-0.1721513948
H,1.2751074808,0.2126403174,-1.6258108132
H,-1.2317580087,0.2252379831,-1.6511726123
H,3.3820133041,1.4411807024,-1.9960395966
H,-3.3202660225,1.4750529366,-2.0541923011

H,3.4132051083,3.9394401345,-1.9806985693
H,-3.3269793179,3.9734711785,-2.035486594
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H,-1.1996834851,5.2311264119,-1.9838324883

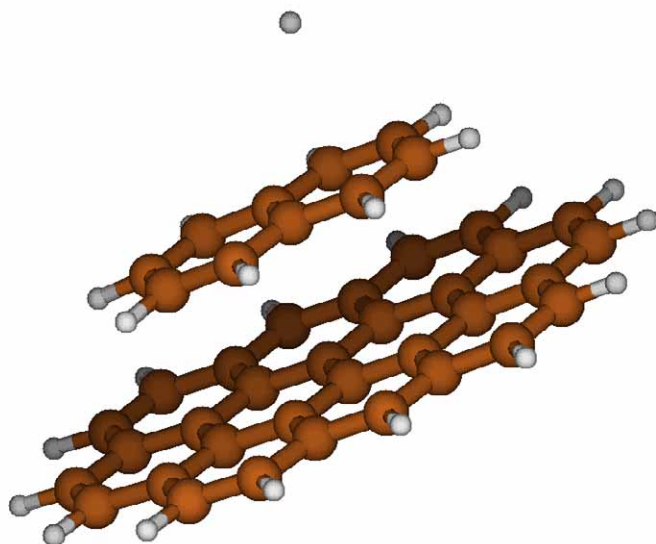
H loss TS 4-7

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C,1.7128714722,-1.3322666411,-0.6164221324
C,0.4283630602,-0.7208955017,-0.6672837571
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C,0.1549760104,0.60806247,2.8414900566
C,2.4048924533,-3.6517961005,3.4612717708
C,3.3132225105,-3.9143164626,2.406315661
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C,2.8817932108,-3.1547635681,4.6993745995
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C,5.1307668031,-4.344321741,0.2846368476
C,5.6001312762,-3.9117950411,1.4924315796
C,0.9984901213,-3.8342057294,3.2559114018
C,0.5179177677,-4.2924565294,2.0047246614
C,1.4311389973,-4.557498662,0.9437686355
C,0.9460126589,-4.9725751083,-0.3264827306
C,1.8701606088,-5.1876830498,-1.3756997238
C,3.2245778903,-4.995125021,-1.1848995239
C,0.0851649198,-3.523556143,4.2936159155
C,0.5640328503,-3.0194064826,5.5378954839
C,1.9627202633,-2.8324912337,5.7398937562
C,2.435834232,-2.2979566644,6.9699078818
C,3.844400767,-2.0923220165,7.1360155776
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C,0.1470355806,-2.1658325618,7.7896563227
C,1.5015458961,-1.9762127147,7.9822413452
C,-1.3210175008,-3.6912983858,4.0818093333
C,-2.218017368,-3.3563780346,5.149585024
C,-1.7545522582,-2.8740121359,6.340150998
C,-0.8892575854,-4.4544906361,1.7980410423
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C,-0.465222324,-5.1435641493,-0.5043761467
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Complex 7 + H + ovalene

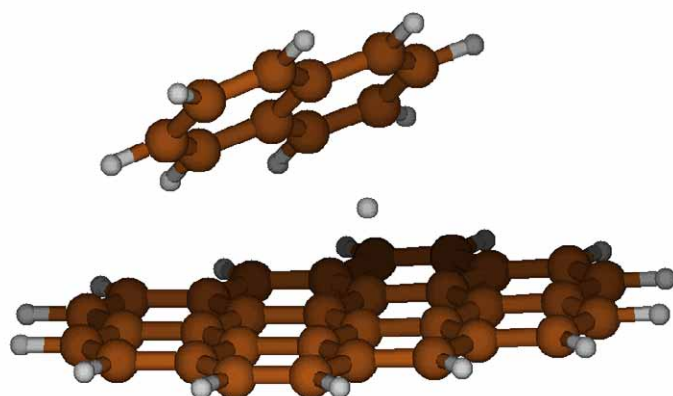


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 C,0.4491599231,-4.3923421047,2.0966344424
 C,1.3449950226,-4.6029213617,1.0078746939
 C,0.8468260163,-5.0382423208,-0.2506865499
 C,1.7528807002,-5.2108971731,-1.3232577623
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H Abstraction TS 4-7



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C,1.2806996041,-0.0826747948,3.4803611006
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C,-2.3904907412,-0.0179894113,4.2590695415
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C,3.7808736537,-0.07331387,3.4619914189
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C,3.7584046272,-0.0672664128,2.0469685858
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Complex 7 + ovalene-H

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 C,3.7907704528,1.6280603174,-0.3760767373
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Ethyne Addition TS 3-8 (A process)

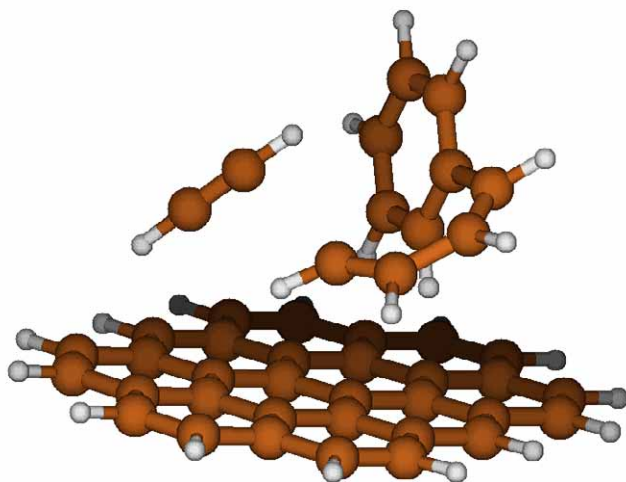
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H,-2.1727701523,0.0185303052,1.6252118059
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H,8.3623327095,-0.12398691,3.52023628
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H,-1.5298844588,4.758145732,3.270837415

H,-1.0408546165,2.7585768832,2.056375247
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Complex [3 + Ethyne(ads)] in the B process

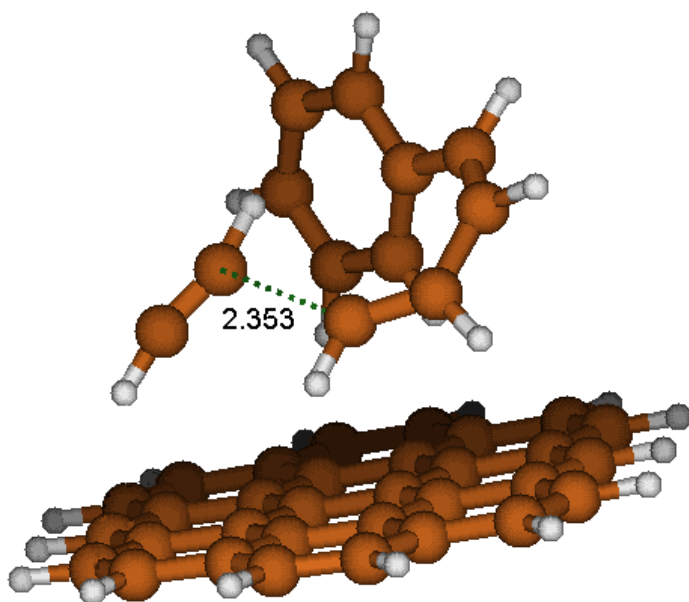


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C,5.2641936862,0.2124233417,-0.4451756467
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C,1.277177696,-0.7399023977,-1.5440826806
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C,0.2250691056,0.1632022447,-1.2523488883
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C,-1.3853475206,-1.4001106796,-2.2724701241
C,-0.3336085871,-2.2869290139,-2.5370656871
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C,-0.5480218487,2.2945006015,-0.2751137769
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C,-1.8883116395,1.9671954461,-0.6355348163
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 C,-1.5245104555,-4.0833027802,1.7546966907
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Ethyne Addition TS 3-8 (B process)

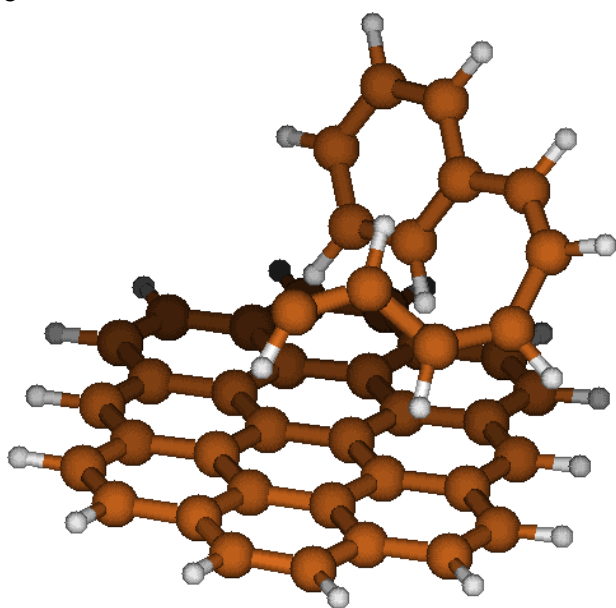


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8



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