PCCP

Supporting material (ESI) for PCCP

Do defects in PAHs promote catalytic activity in space? Stone-Wales pyrene as a test case

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Dealing with biradical systems

In order to produce a correct UHF wavefunction for singlet states open-shell biradical systems, we mixed HOMO and LUMO in order to destroy α-β orbitals and spatial symmetries (keyword guess=mix implemented in Gaussian16) doing a constrained optimization of the geometry when the hydrogen is distant more than 3 Å from the carbon site taken in exam. We verified the correctness of the calculation for singlet closed shell biradicals analyzing the eigenvalue S^2 (i.e. close to 1) and verifying that the molecular orbitals (MOs) and, specifically, alpha orbital and beta orbital are distinguishable and separated upper the Fermi level (i.e. the MOs of pyrene are separated by the MO of the radical hydrogen upper the Fermi level). We optimized the geometry of TS controlling the initial guess with the correct wave function (using the keyword guess=read implemented in gaussian16 after having recorded the correct wave function in a appropriate chk format from the constrained optimization done in the precedent step).

Mulliken Spin analysis

Mulliken Spin partitioning scheme, employing the M06-2X/pcseg-1 theory level, for each atoms of the minima optimized structures of single extra hydrogenated species of SW-pyrene and pristine pyrene are reported (Fig. S2 and S3)

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Crossover temperature

Table S1 Crossover temperatures (Tc) and imaginary frequencies (*ifreq*) of the transition state for the extraction of molecular hydrogen promoted by the carbon pairs located in the Stone-Wales and pristine pyrene.

STONE-WALES C pairs	Tc (K)	*ifreq* (cm^{-1})
C(12)-C(10)	502	i2192.9714
C(8)-C(11)	488	i2132.8003
C(5)-C(8)	421	i1838.1007
C(2)-C(4)	400	i1747.8361
C(5)-C(2)	511	i2230.0669
C(8)|C(3)	534	i2330.1100
C(12)|C(4)	427	i1863.5223
C(5)|C(13)	397	i1733.7670
C(11)|C(2)	444	i1940.0362
PRISTINE		
C(12)'-C(10)'	506	i2210.3011
C(8)'-C(11)'	571	i2494.1826
C(2)'-C(4)'	481	i2100.1131
C(5)'|C(13)'	401	i1750.1005

We report in Table S1 the values of crossover temperatures along with the imaginary frequencies (*ifreq*) of the transition states, for each carbon pairs, of the process related to the molecular hydrogen extraction by Stone-Wales and pristine pyrene.

The crossover temperature (Tc) has been calculated with the following equation:

$$Tc = (\hbar * \mathrm{freq})/k_b$$

$\hbar$=h/2π is the reduced Planck's constant, *ifreq* is the module of the imaginary frequency of the transition state and k_b is the Boltzmann's constant.

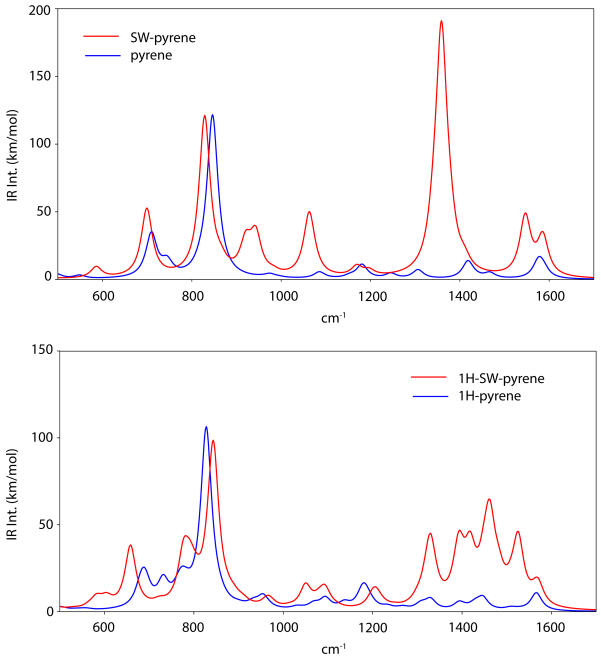


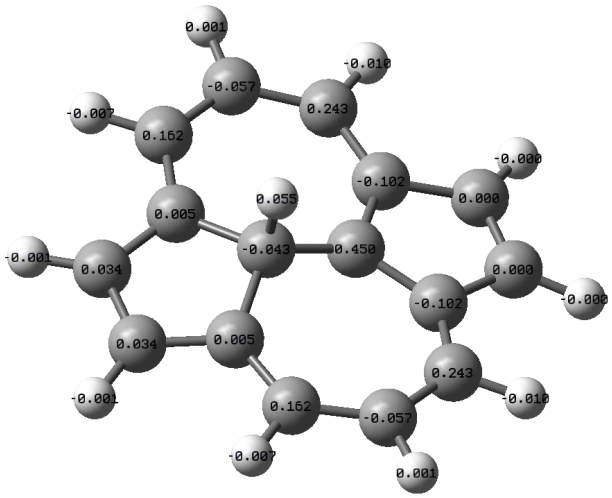
Fig. S1 Top panel. Comparison between the infrared spectrum obtained at B3LYP/4-31G level of Stone-wales pyrene (red) an pristine pyrene (blue). Bottom panel. Comparison between 1H-C2-SW pyrene and its pristine isomer.

Infrared spectroscopy of pristine and Stone-Wales pyrene

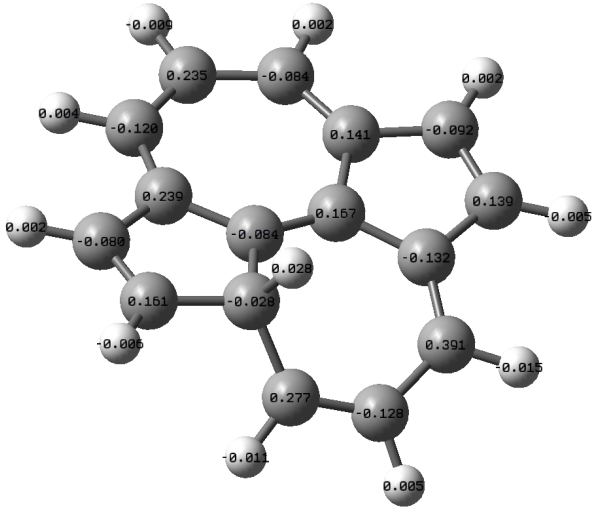
The harmonic infrared spectra of pristine, Stone-Wales pyrene and their singly hydrogenated isomers were calculated with B3LYP/4-31G and a triple scaling factor scheme developed especially for PAH molecules[1]. The spectra were convoluted with a Gaussian line shape with a Full Width Half Maximum of 30 cm^{-1} and are represented in Fig. S1. Stone-Wales pyrene possesses a very strong C-C mode at 1357 cm^{-1} and other less strong modes at 1062 cm^{-1} (C-H in plane) and 940 cm^{-1} (C-C skeleton mode) which are not present in pristine pyrene and can help distinguishing between the two structures. As for the singly hydrogenated molecules, 1H-C2-SW pyrene shows strong infrared activity in the 1300-1600 cm^{-1}, with a combination of C-C stretch and C-H in plane modes.

References

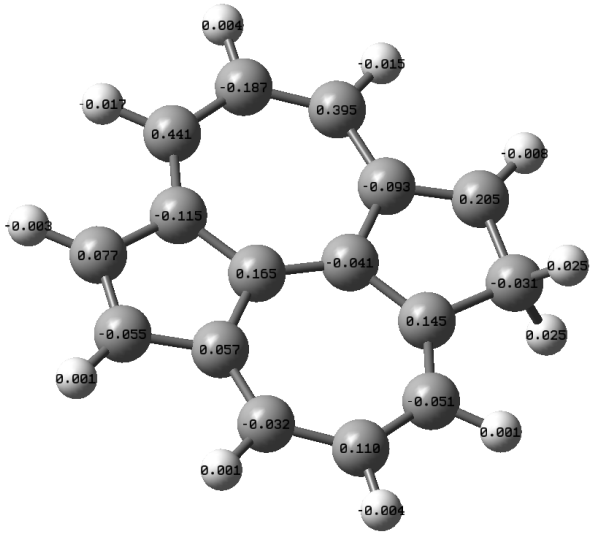
1 C. W. Bauschlicher, A. Ricca, C. Boersma and L. J. Allamandola, *The Astrophysical Journal Supplement Series*, 2018, **234**, 32.



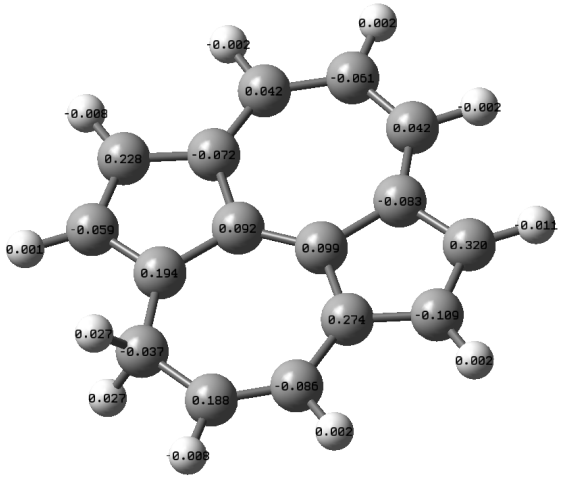
(a) 1H-C2-SW-pyrene



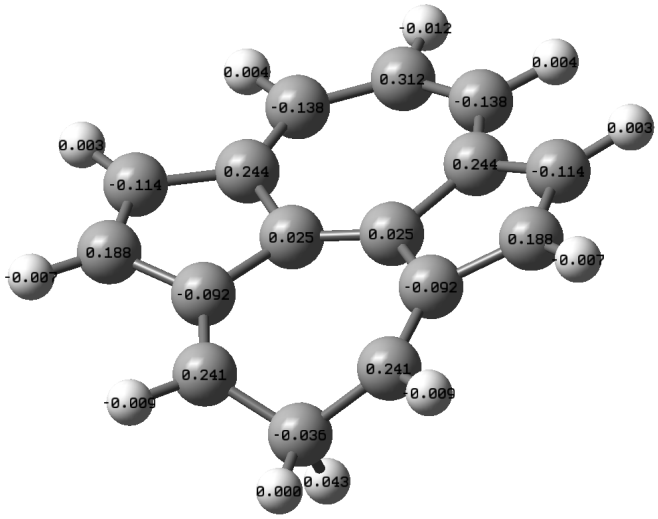
(b) 1H-C5-SW-pyrene



(c) 1H-C12-SW-pyrene

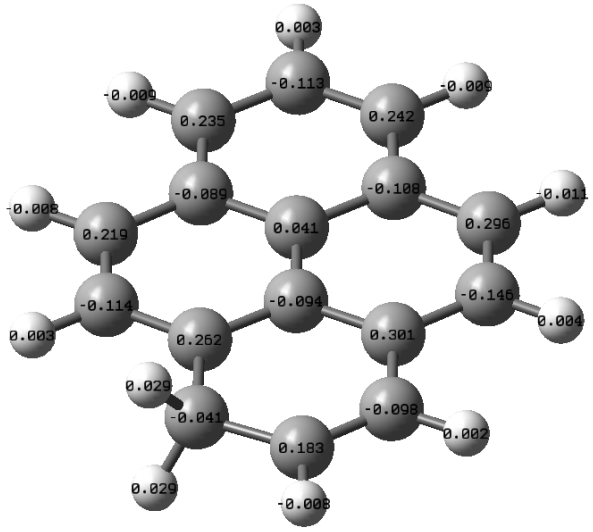


(d) 1H-C8-SW-pyrene

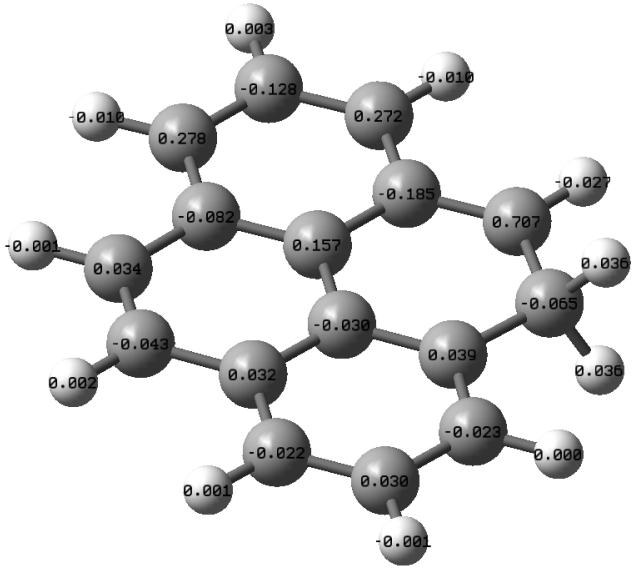


(e) 1H-C11-SW-pyrene

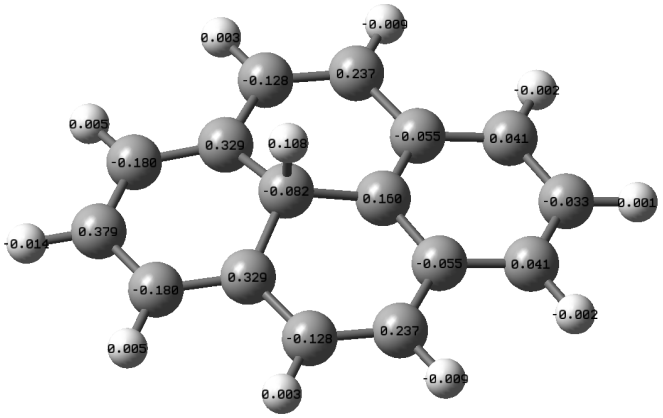
Fig. S2 Mulliken Spin partitioning scheme of several species of SW-pyrene with one hydrogen chemisorbed.



(a) 1H-C8-pyrene



(b) 1H-C12-pyrene



(c) 1H-C1-pyrene

Fig. S3 Mulliken Spin partitioning scheme of several species of pyrene with one hydrogen chemisorbed.

Optimized geometries

Stone-Wales formation by Pyrene

M06-2X/pcseg-1 optimized structure of Pyrene

C	0.000000	0.713974	-0.000000
C	-0.000000	-0.713974	0.000000
C	2.461789	0.676944	-0.000000
C	-2.461789	-0.676944	-0.000000
C	-2.461789	0.676944	-0.000000
C	2.461789	-0.676944	0.000000
C	1.230398	1.425253	-0.000000
C	-1.230398	-1.425253	0.000000
C	-1.230398	1.425253	-0.000000
C	1.230398	-1.425253	0.000000
C	1.207779	2.824376	-0.000000
C	-1.207779	-2.824376	0.000000
C	-1.207779	2.824376	-0.000000
C	1.207779	-2.824376	0.000000
C	0.000000	3.513428	-0.000000
C	-0.000000	-3.513428	0.000000
H	3.399866	1.228705	-0.000000
H	-3.399866	-1.228705	-0.000000
H	-3.399866	1.228705	-0.000000
H	3.399866	-1.228705	0.000000
H	2.149515	3.369672	-0.000000
H	-2.149515	-3.369672	0.000000
H	-2.149515	3.369672	-0.000000
H	2.149515	-3.369672	0.000000
H	0.000000	4.600664	-0.000000
H	-0.000000	-4.600664	0.000000

M06-2X/pcseg-1 optimized structure of Intermediate

C	-0.392036	-0.457218	0.459236
C	0.392036	0.457218	0.459237
C	-1.024119	2.640623	-0.562101
C	1.024119	-2.640624	-0.562098
C	-0.425642	-2.658669	-0.347374
C	0.425643	2.658668	-0.347376
C	-1.924959	1.803751	-0.066583
C	1.924959	-1.803751	-0.066581
C	-1.147609	-1.588874	0.090184
C	1.147609	1.588874	0.090184
C	-2.887077	1.085360	0.467435
C	2.887077	-1.085360	0.467437
C	-2.600720	-1.441033	0.018486
C	2.600720	1.441033	0.018486
C	-3.313232	-0.304189	0.170098
C	3.313231	0.304189	0.170099
H	-1.390892	3.355781	-1.301919
H	1.390893	-3.355782	-1.301915
H	-0.957624	-3.536454	-0.711999
H	0.957625	3.536453	-0.712001
H	-3.471725	1.578587	1.251053
H	3.471724	-1.578586	1.251056
H	-3.159952	-2.353968	-0.185281
H	3.159952	2.353968	-0.185281
H	-4.397247	-0.419711	0.134404
H	4.397247	0.419711	0.134406

M06-2X/pcseg-1 optimized structure of TS1

C	-0.478625	0.337058	-0.196438
C	0.534840	-0.343960	-0.172913
C	-0.931105	-2.594438	0.495077
C	0.976891	2.615562	0.395042
C	-0.460732	2.633752	0.206773
C	0.509429	-2.620462	0.331639
C	-1.806424	-1.677171	0.072593
C	1.858764	1.680767	0.028288
C	-1.222980	1.516540	-0.024957
C	1.275822	-1.514373	0.063136
C	-2.889737	-1.082921	-0.402389
C	2.949552	1.066361	-0.401811
C	-2.670919	1.415618	0.036013
C	2.722587	-1.410297	0.143560
C	-3.379878	0.276132	-0.135092
C	3.434696	-0.279281	-0.066259
H	-1.343053	-3.373387	1.141250
H	1.378355	3.422612	1.012698
H	-0.970318	3.570716	0.426523
H	1.014958	-3.546540	0.601248
H	-3.475438	-1.654869	-1.129111
H	3.547422	1.605637	-1.143450
H	-3.218511	2.344117	0.189178
H	3.267227	-2.330863	0.346915
H	-4.464808	0.376314	-0.160216
H	4.519857	-0.380074	-0.068907

M06-2X/pcseg-1 optimized structure of TS2

C	0.226999	0.570790	-0.051930
C	-0.287846	-0.536279	-0.052860
C	0.764119	-2.863371	0.573073
C	-0.843013	2.905272	0.512913
C	0.590051	2.844457	0.334031
C	-0.662854	-2.805048	0.350103
C	1.579477	-1.894369	0.140301
C	-1.645051	1.930818	0.067670
C	1.155874	1.624252	0.073330
C	-1.220289	-1.588278	0.057256
C	2.637928	-1.283594	-0.378596
C	-2.687428	1.313460	-0.475418
C	2.562078	1.297061	-0.052783
C	-2.621962	-1.262940	-0.115463
C	3.143624	0.084205	-0.250036
C	-3.197036	-0.052733	-0.345280
H	1.163909	-3.634839	1.233545
H	-1.262496	3.684792	1.151348
H	1.203989	3.727483	0.498694
H	-1.281665	-3.686079	0.507027
H	-3.275129	1.934094	-1.159606
H	3.234671	2.154650	-0.057221
H	-3.294273	-2.120644	-0.129643
H	4.218264	0.132784	-0.427035
H	-4.265828	-0.103709	-0.554147
H	3.245973	-1.912549	-1.036918

M06-2X/pcseg-1 optimized structure of SW-pyrene

C	0.003865	2.907318	0.684306
C	0.000897	0.688519	-0.000325
C	0.003697	2.906671	-0.687052
C	-0.000893	-0.688519	0.000325
C	0.001896	1.566485	-1.171292
C	0.002182	1.567591	1.169812
C	-0.001892	-1.566485	1.171292
C	0.001312	1.244708	-2.525528
C	0.001931	1.247091	2.524351
C	-0.003694	-2.906670	0.687052
C	-0.000383	-0.001483	-3.141942
C	-0.003862	-2.907318	-0.684306
C	-0.001927	-1.247091	-2.524351
C	-0.002179	-1.567590	-1.169812
H	-0.005078	-3.782468	-1.326753
H	-0.003130	-2.109163	-3.192414
H	-0.004752	-3.781213	1.330325
H	-0.000516	-0.001996	-4.229432
H	0.002351	2.106149	-3.194405
C	-0.001309	-1.244707	2.525528
C	0.000387	0.001483	3.141942
H	0.004756	3.781214	-1.330325
H	0.005081	3.782468	1.326753
H	0.003133	2.109164	3.192414
H	0.000520	0.001997	4.229432
H	-0.002347	-2.106148	3.194405

M06-2X/pcseg-1 optimized structure of TS 1h

C	0.724824	-0.080920	0.389585
C	-0.639401	-0.149539	0.784570
C	0.616088	-2.479149	-0.090675
C	-0.698415	2.634857	0.114301
C	0.658721	2.430393	0.364177
C	-0.736158	-2.468764	0.094929
C	1.384399	-1.273567	0.003689
C	-1.644499	1.698703	-0.210560
C	1.392337	1.181111	0.302147
C	-1.408472	-1.271743	0.497593
C	2.765269	-1.220810	-0.287149
C	-2.815805	1.181101	-0.580431
C	2.757615	1.177896	0.032393
C	-2.839197	-1.134197	0.433474
C	3.440850	-0.018387	-0.235590
C	-3.449277	-0.010016	-0.047223
H	1.125350	-3.399419	-0.370053
H	-1.069602	3.652963	0.255757
H	1.252704	3.323978	0.546234
H	-1.320740	-3.371612	-0.072436
H	-3.326442	1.626841	-1.442648
H	3.290110	2.125429	-0.027019
H	-3.458372	-2.019864	0.575963
H	4.505879	0.013657	-0.451886
H	-4.522047	-0.076794	-0.227095
H	3.285835	-2.136057	-0.562026
H	-1.034654	0.585963	1.474537

Stone-Wales formation catalyzed by H

M06-2X/pcseg-1 optimized structure of 1H-pyrene

C	0.516256	-0.002375	0.743689
C	0.190692	-0.001924	-0.728334
C	0.081665	2.472660	0.696072
C	0.111145	-2.466582	-0.662344
C	0.077822	-2.476727	0.695406
C	0.114966	2.462832	-0.661692
C	0.120609	1.263795	1.459380
C	0.088879	-1.221903	-1.416374
C	0.118622	-1.268113	1.459051
C	0.090771	1.218396	-1.416048
C	-0.095247	1.219300	2.821958
C	-0.085917	-1.206869	-2.806298
C	-0.097182	-1.223647	2.821614
C	-0.084049	1.203998	-2.805980
C	-0.150496	-0.002211	3.512929
C	-0.163053	-0.001282	-3.493958
H	-0.011244	3.415984	1.232304
H	0.069092	-3.400595	-1.218731
H	-0.016534	-3.420048	1.231390
H	0.074345	3.397060	-1.217824
H	-0.273951	2.149464	3.359251
H	-0.166467	-2.150645	-3.342253
H	-0.277372	-2.153663	3.358667
H	-0.163136	2.148041	-3.341683
H	-0.326872	-0.002224	4.585048
H	-0.296030	-0.001037	-4.572999
H	1.636568	-0.003265	0.779716

M06-2X/pcseg-1 optimized structure of Int 1h

C	0.750566	0.105516	-0.348003
C	-0.586651	0.244431	-0.761846
C	0.720663	2.485506	0.197060
C	-0.788096	-2.643817	-0.078899
C	0.593146	-2.417398	-0.332800
C	-0.637650	2.518734	0.013588
C	1.450938	1.266199	0.069562
C	-1.715895	-1.814169	0.434574
C	1.358565	-1.194425	-0.255674
C	-1.327376	1.357459	-0.439299
C	2.831837	1.151754	0.366493
C	-2.683159	-1.036027	0.866640
C	2.723826	-1.244182	0.017741
C	-2.780175	1.194119	-0.368779
C	3.454351	-0.076038	0.299959
C	-3.352482	0.101623	0.185947
H	1.253948	3.382208	0.506946
H	-1.152676	-3.639591	-0.341895
H	1.169794	-3.314487	-0.551651
H	-1.196663	3.428423	0.224945
H	-3.038401	-1.208193	1.890048
H	3.219368	-2.211566	0.077327
H	-3.431274	2.021899	-0.651755
H	4.516121	-0.156020	0.520005
H	-4.436823	0.117508	0.305691
H	3.389275	2.039799	0.657626
H	-1.069578	-0.561562	-1.294616

M06-2X/pcseg-1 optimized structure of TS 2h

C	0.466857	-0.242681	-0.694743
C	-0.670786	0.339499	-0.983428
C	0.849530	2.666899	0.004495
C	-0.701082	-2.537926	0.733981
C	0.654657	-2.415543	0.297581
C	-0.569574	2.470295	0.253616
C	1.767013	1.718865	0.128500
C	-1.787261	-1.873977	0.329108
C	1.246406	-1.289376	-0.373017
C	-1.270731	1.382987	-0.152820
C	2.891136	1.097268	0.441665
C	-2.894782	-1.315548	-0.096027
C	2.707521	-1.214074	-0.470083
C	-2.690483	1.211418	0.183930
C	3.432086	-0.132377	-0.126121
C	-3.378465	0.054343	0.204229
H	1.170280	3.641519	-0.373184
H	-0.865834	-3.248895	1.547558
H	1.343862	-3.173177	0.664768
H	-1.114680	3.289344	0.724926
H	-3.534689	-1.908627	-0.759542
H	3.234078	-2.135448	-0.718433
H	-3.224108	2.115377	0.481004
H	4.517010	-0.227988	-0.113686
H	-4.441340	0.117786	0.441200
H	3.430251	1.493032	1.307697
H	-1.252501	-0.005187	-1.842666

M06-2X/pcseg-1 optimized structure of TS 3h

C	0.158178	0.639625	-1.172297
C	-0.133885	-0.522411	-0.621204
C	1.488796	-2.331157	0.590736
C	-1.582344	2.136246	0.772660
C	-0.175621	2.446023	0.490892
C	0.181855	-2.639778	0.417504
C	1.937895	-1.046734	0.193971
C	-2.367773	1.314347	0.111925
C	0.644151	1.751651	-0.320528
C	-0.712720	-1.617342	-0.134080
C	3.006180	-0.340067	-0.167843
C	-3.169109	0.472204	-0.492638
C	2.090370	2.023142	-0.390078
C	-2.171385	-1.837779	-0.102002
C	3.080273	1.102702	-0.373391
C	-3.195788	-0.986825	-0.282917
H	2.177848	-3.019718	1.081878
H	-1.995838	2.585694	1.677846
H	0.258350	3.255070	1.079805
H	-0.226868	-3.598521	0.728877
H	3.946241	-0.885329	-0.310691
H	-3.892703	0.876629	-1.205083
H	2.387358	3.071841	-0.442157
H	-2.442025	-2.883043	0.053400
H	4.094357	1.486702	-0.479603
H	-4.191864	-1.428503	-0.313178
H	0.216539	0.749338	-2.258917

M06-2X/pcseg-1 optimized structure of Int 2h

C	0.416447	-0.396819	-0.785039
C	-0.499107	0.450468	-1.154229
C	0.918808	2.393098	0.828997
C	-0.834621	-2.414043	0.903964
C	0.574456	-2.260662	0.691429
C	-0.524321	2.183547	0.663928
C	1.910541	1.898608	0.121743
C	-1.835152	-1.844141	0.235088
C	1.194439	-1.222389	-0.058355
C	-1.171024	1.324085	-0.149268
C	2.917831	1.354056	-0.513297
C	-2.856522	-1.319149	-0.396393
C	2.671719	-1.097583	-0.009943
C	-2.636416	1.179815	-0.046128
C	3.418038	-0.006383	-0.233110
C	-3.359693	0.055462	-0.196346
H	1.203132	2.999550	1.691541
H	-1.123658	-3.045730	1.746904
H	1.227464	-2.913833	1.265889
H	-1.139513	2.750199	1.363347
H	-3.379163	-1.935627	-1.134390
H	3.194985	-2.027796	0.213469
H	-3.185909	2.095836	0.177282
H	4.501401	-0.127207	-0.238243
H	-4.445715	0.151898	-0.166156
H	3.408055	1.920867	-1.308243
H	-0.914829	0.436005	-2.165182

M06-2X/pcseg-1 optimized structure of Int 3h

C	0.134754	-0.538929	0.670232
C	0.311787	0.744576	0.270656
C	1.255960	2.758935	-0.385462
C	-1.166081	-2.588283	-0.751790
C	0.214260	-2.720128	-0.321451
C	-0.099062	2.950140	-0.204290
C	1.574480	1.382004	-0.135122
C	-2.047340	-1.690306	-0.323800
C	0.921408	-1.675825	0.236268
C	-0.733325	1.735144	0.185141
C	2.822876	0.815340	-0.121774
C	-2.952800	-0.897329	0.217506
C	2.361241	-1.642958	0.230624
C	-2.160773	1.597483	0.255823
C	3.173317	-0.549099	0.112677
C	-3.055830	0.560632	0.267272
H	1.977105	3.513564	-0.682324
H	-1.455405	-3.202046	-1.609394
H	0.762917	-3.587348	-0.686498
H	-0.629973	3.882888	-0.374628
H	3.656644	1.484206	-0.335375
H	-3.754193	-1.409332	0.763222
H	2.853572	-2.616305	0.255678
H	-2.652463	2.571909	0.282502
H	4.242280	-0.754672	0.107717
H	-4.087318	0.886246	0.401741
H	-0.775087	-0.763818	1.208030

M06-2X/pcseg-1 optimized structure of 1H-SW-pyrene

C	0.231437	2.853301	0.706675
C	-0.443393	0.727116	-0.000000
C	0.231437	2.853301	-0.706675
C	-0.053971	-0.710749	0.000000
C	-0.078814	1.596477	-1.187695
C	-0.078814	1.596477	1.187695
C	0.032480	-1.551319	1.152881
C	-0.119572	1.264040	-2.561857
C	-0.119572	1.264040	2.561856
C	0.222164	-2.915418	0.676288
C	-0.182845	0.016214	-3.137382
C	0.222164	-2.915418	-0.676287
C	-0.090405	-1.239288	-2.500556
C	0.032480	-1.551319	-1.152881
H	0.348519	-3.772225	-1.330828
H	-0.070225	-2.098569	-3.171289
H	0.348519	-3.772225	1.330828
H	-0.227217	-0.011296	-4.224213
H	-0.046985	2.113104	-3.242210
C	-0.090405	-1.239287	2.500556
C	-0.182845	0.016214	3.137382
H	0.464505	3.708764	-1.335037
H	0.464505	3.708764	1.335036
H	-0.046985	2.113104	3.242210
H	-0.227217	-0.011296	4.224213
H	-0.070225	-2.098569	3.171289
H	-1.557722	0.744585	-0.000000

Hydrogenation of SW-pyrene

M06-2X/pcseg-1 optimized structure of 1H-C11-SW

C	0.283340	2.893567	0.679582
C	-0.073517	0.688637	-0.018430
C	0.407339	2.890334	-0.671779
C	-0.077601	-0.678189	-0.020328
C	0.105768	1.563447	-1.193056
C	-0.013663	1.566912	1.159455
C	-0.023005	-1.560074	1.155113
C	-0.053886	1.270260	-2.504121
C	-0.197707	1.254837	2.494459
C	0.266069	-2.887142	0.671553
C	-0.666477	0.011188	-3.042560
C	0.390098	-2.880896	-0.679794
C	-0.061424	-1.253012	-2.507626
C	0.096464	-1.550789	-1.197381
H	0.603099	-3.736608	-1.312840
H	0.174548	-2.037692	-3.226502
H	0.370168	-3.751203	1.321124
H	-0.599157	0.012503	-4.133896
H	0.186775	2.055511	-3.220817
C	-0.205191	-1.250615	2.490979
C	-0.346666	0.001704	3.098353
H	0.625454	3.746513	-1.302447
H	0.392595	3.755183	1.331549
H	-0.192953	2.109679	3.172012
H	-0.495065	0.000652	4.175453
H	-0.205550	-2.107348	3.166156
H	-1.746141	0.014079	-2.801508

M06-2X/pcseg-1 optimized structure of TS 1H-C11-SW

C	0.283340	2.893567	0.679582
C	-0.073517	0.688637	-0.018430
C	0.407339	2.890334	-0.671779
C	-0.077601	-0.678189	-0.020328
C	0.105768	1.563447	-1.193056
C	-0.013663	1.566912	1.159455
C	-0.023005	-1.560074	1.155113
C	-0.053886	1.270260	-2.504121
C	-0.197707	1.254837	2.494459
C	0.266069	-2.887142	0.671553
C	-0.666477	0.011188	-3.042560
C	0.390098	-2.880896	-0.679794
C	-0.061424	-1.253012	-2.507626
C	0.096464	-1.550789	-1.197381
H	0.603099	-3.736608	-1.312840
H	0.174548	-2.037692	-3.226501
H	0.370168	-3.751203	1.321124
H	-0.599157	0.012502	-4.133896
H	0.186775	2.055511	-3.220817
C	-0.205191	-1.250615	2.490979
C	-0.346666	0.001704	3.098353
H	0.625454	3.746513	-1.302447
H	0.392595	3.755183	1.331549
H	-0.192953	2.109679	3.172012
H	-0.495065	0.000652	4.175453
H	-0.205550	-2.107348	3.166156
H	-2.911202	0.017198	-2.541389

M06-2X/pcseg-1 optimized structure of 1H-C12-SW

C	0.078646	2.903106	0.674848
C	-0.009949	0.701282	0.007057
C	0.062401	2.925597	-0.698903
C	-0.061218	-0.693636	-0.024944
C	0.007796	1.592095	-1.179578
C	0.035614	1.559595	1.155035
C	-0.078939	-1.585319	1.166309
C	-0.020271	1.282721	-2.530643
C	0.041811	1.260458	2.532028
C	-0.131291	-2.875484	0.739245
C	-0.073495	0.034117	-3.149556
C	-0.153201	-2.971720	-0.741706
C	-0.111032	-1.207179	-2.527325
C	-0.105885	-1.526987	-1.174154
H	0.703949	-3.539396	-1.136896
H	-0.150724	-2.067269	-3.197682
H	-0.154322	-3.733817	1.405106
H	-0.087101	0.031514	-4.237093
H	0.002935	2.145918	-3.196593
C	-0.048855	-1.235585	2.561674
C	0.003716	0.005518	3.149918
H	0.086527	3.803975	-1.335365
H	0.118395	3.770704	1.327534
H	0.081550	2.125163	3.192233
H	0.017539	0.013772	4.238543
H	-0.071857	-2.094199	3.231026
H	-1.058961	-3.475105	-1.114990

M06-2X/pcseg-1 optimized structure of TS 1H-C12-SW

C	-0.005334	2.898308	0.678895
C	-0.011167	0.681288	-0.008696
C	0.001888	2.901645	-0.692227
C	-0.016887	-0.696818	-0.014227
C	-0.000944	1.562552	-1.178740
C	-0.011455	1.556958	1.161729
C	-0.013431	-1.579375	1.157353
C	0.009086	1.245051	-2.533686
C	-0.014814	1.235927	2.516306
C	-0.006989	-2.911172	0.680183
C	0.005602	0.000462	-3.153430
C	-0.061840	-2.918033	-0.704812
C	-0.012861	-1.245989	-2.537147
C	-0.019726	-1.565499	-1.184455
H	0.076458	-3.785950	-1.342209
H	-0.028965	-2.107679	-3.205580
H	0.006248	-3.786530	1.321711
H	0.012326	0.001783	-4.240818
H	0.018963	2.108380	-3.199968
C	-0.012203	-1.256304	2.516207
C	-0.013440	-0.012305	3.131792
H	0.009621	3.777526	-1.333504
H	-0.004349	3.771676	1.323789
H	-0.016414	2.096730	3.185696
H	-0.014297	-0.012888	4.219337
H	-0.010806	-2.118561	3.183650
H	-1.926141	-3.239127	-1.018230

The intermediate 1H-C2-SW C(2) is the same of 1H-SW-pyrene that you can find in section "Stone-Wales formation catalyzed by H".

M06-2X/pcseg-1 optimized structure of TS 1H-C2-SW

C	0.012093	2.898515	0.687657
C	-0.126676	0.683058	0.000001
C	0.012094	2.898515	-0.687658
C	-0.013227	-0.703579	0.000000
C	-0.046121	1.567920	-1.176172
C	-0.046123	1.567920	1.176171
C	0.003658	-1.574026	1.167806
C	-0.036822	1.242100	-2.531094
C	-0.036826	1.242100	2.531094
C	0.049597	-2.918580	0.684343
C	-0.055453	-0.005167	-3.140568
C	0.049596	-2.918580	-0.684343
C	-0.034992	-1.252599	-2.520983
C	0.003656	-1.574026	-1.167805
H	0.077645	-3.791718	-1.328875
H	-0.035506	-2.113619	-3.190241
H	0.077648	-3.791718	1.328875
H	-0.064321	-0.009494	-4.228077
H	-0.004918	2.101517	-3.201545
C	-0.034989	-1.252599	2.520983
C	-0.055453	-0.005166	3.140568
H	0.054600	3.774294	-1.327834
H	0.054598	3.774294	1.327833
H	-0.004926	2.101517	3.201545
H	-0.064320	-0.009493	4.228077
H	-0.035501	-2.113619	3.190242
H	-1.973401	0.889338	0.000000

M06-2X/pcseg-1 optimized structure of 1H-C5-SW

C	-0.188159	2.921842	0.620183
C	-0.173743	0.674640	0.014461
C	-0.486700	2.910578	-0.688537
C	-0.102866	-0.696452	-0.007221
C	-0.547949	1.499447	-1.207972
C	-0.011525	1.563203	1.120586
C	-0.047032	-1.589072	1.173677
C	0.295758	1.254148	-2.430559
C	0.261289	1.255857	2.457975
C	-0.226205	-2.922668	0.683335
C	0.428322	0.045528	-3.020999
C	-0.327432	-2.895898	-0.679342
C	-0.006542	-1.217195	-2.507165
C	-0.207107	-1.542323	-1.171689
H	-0.436565	-3.761487	-1.326685
H	-0.022157	-2.050092	-3.208863
H	-0.251147	-3.804723	1.315222
H	0.944629	0.013152	-3.980624
H	0.763632	2.122349	-2.891956
C	0.158197	-1.257776	2.493270
C	0.345067	0.015558	3.070073
H	-0.674607	3.779099	-1.312988
H	-0.091940	3.804160	1.247475
H	0.394210	2.117603	3.112949
H	0.543919	0.024147	4.139493
H	0.190593	-2.099679	3.185514
H	-1.594683	1.233522	-1.452732

M06-2X/pcseg-1 optimized structure of TS 1H-C5-SW

C	-0.041135	2.899819	0.648378
C	-0.066954	0.672578	-0.012369
C	-0.097880	2.902547	-0.715121
C	-0.028918	-0.702555	-0.015457
C	-0.165480	1.550582	-1.201862
C	-0.033642	1.556825	1.139397
C	-0.009802	-1.580021	1.162074
C	0.036805	1.231322	-2.555972
C	0.007667	1.242421	2.498926
C	-0.032049	-2.920994	0.679823
C	0.081116	-0.015511	-3.157010
C	-0.056402	-2.917970	-0.690911
C	0.000803	-1.260316	-2.536390
C	-0.047664	-1.576502	-1.178999
H	-0.070298	-3.792875	-1.333863
H	0.012165	-2.124053	-3.201657
H	-0.028646	-3.795787	1.322389
H	0.185210	-0.025480	-4.239763
H	0.105583	2.093371	-3.219209
C	0.011049	-1.252197	2.510433
C	0.026104	0.002473	3.119671
H	-0.115205	3.773843	-1.361878
H	-0.005830	3.774463	1.290728
H	0.026900	2.107321	3.162819
H	0.052349	0.008102	4.206891
H	0.018735	-2.108324	3.185869
H	-1.962642	1.367988	-1.023660

M06-2X/pcseg-1 optimized structure of TS 1H-C8-SW

C	0.027158	2.917725	0.686025
C	-0.008324	0.701712	-0.005663
C	0.014729	2.918333	-0.687286
C	-0.020214	-0.676733	-0.008224
C	-0.005221	1.581611	-1.169034
C	0.011215	1.577360	1.167705
C	-0.028090	-1.555856	1.161298
C	-0.064606	1.263392	-2.534240
C	0.010611	1.253888	2.521277
C	-0.029031	-2.895097	0.675690
C	-0.001539	0.005248	-3.153903
C	-0.014607	-2.892205	-0.697136
C	0.013719	-1.232623	-2.538058
C	-0.011160	-1.553231	-1.178424
H	-0.007386	-3.766084	-1.341256
H	0.046575	-2.095135	-3.204423
H	-0.036008	-3.771001	1.316986
H	0.009386	0.009835	-4.241389
H	0.013196	2.123097	-3.200876
C	-0.027471	-1.237443	2.516550
C	-0.010249	0.006851	3.136037
H	0.014823	3.793637	-1.329647
H	0.045333	3.791887	1.329444
H	0.026188	2.114236	3.191335
H	-0.010416	0.004729	4.223514
H	-0.037857	-2.100503	3.183209
H	-1.974395	1.507935	-2.789786

M06-2X/pcseg-1 optimized structure of 1H-C8-SW

C	-0.188159	2.921842	0.620183
C	-0.173743	0.674640	0.014461
C	-0.486700	2.910578	-0.688537
C	-0.102866	-0.696452	-0.007221
C	-0.547949	1.499447	-1.207972
C	-0.011525	1.563203	1.120586
C	-0.047032	-1.589072	1.173677
C	0.295758	1.254148	-2.430559
C	0.261289	1.255857	2.457975
C	-0.226205	-2.922668	0.683335
C	0.428322	0.045528	-3.020999
C	-0.327432	-2.895898	-0.679342
C	-0.006542	-1.217195	-2.507165
C	-0.207107	-1.542323	-1.171689
H	-0.436565	-3.761487	-1.326685
H	-0.022157	-2.050092	-3.208863
H	-0.251147	-3.804723	1.315222
H	0.944629	0.013152	-3.980624
H	0.763632	2.122349	-2.891956
C	0.158197	-1.257776	2.493270
C	0.345067	0.015558	3.070073
H	-0.674607	3.779099	-1.312988
H	-0.091940	3.804160	1.247475
H	0.394210	2.117603	3.112949
H	0.543919	0.024147	4.139493
H	0.190593	-2.099679	3.185514
H	-1.594683	1.233522	-1.452732

M06-2X/pcseg-1 optimized structure of 2H-C12C4-SW

C	0.605186	2.869799	-0.543713
C	-0.057982	0.701342	0.101173
C	-0.728512	2.866817	-0.373630
C	-0.041136	-0.709831	0.627624
C	-1.157374	1.519610	0.046351
C	1.110568	1.529445	-0.212561
C	1.184755	-1.542591	0.253368
C	-2.529924	1.224639	0.390539
C	2.435652	1.282703	-0.052331
C	0.838020	-2.724316	-0.276713
C	-3.113326	0.006903	0.402665
C	-0.638435	-2.875722	-0.442109
C	-2.486627	-1.243455	0.022059
C	-1.182928	-1.554408	0.057121
H	-0.925368	-3.076845	-1.483305
H	-3.164664	-2.014449	-0.349247
H	1.554333	-3.488939	-0.570773
H	-4.178931	-0.038187	0.623726
H	-3.158570	2.088789	0.605800
C	2.575552	-1.165537	0.464317
C	3.109804	0.065977	0.345020
H	-1.409911	3.699506	-0.521304
H	1.235686	3.696266	-0.854987
H	3.096483	2.128904	-0.243759
H	4.183970	0.157172	0.495932
H	3.258973	-1.989370	0.672978
H	-1.022733	-3.714082	0.158643
H	-0.117419	-0.681019	1.729572

M06-2X/pcseg-1 optimized structure of 2H-C5C2-SW

C	0.728580	2.569929	0.477847
C	-0.781844	0.706629	0.137023
C	0.290419	2.683991	-0.777837
C	-0.213149	-0.684093	0.038611
C	-0.785223	1.658771	-1.100731
C	0.075123	1.455844	1.154452
C	-0.179145	-1.524969	1.122961
C	-0.679907	1.199332	-2.526686
C	0.151926	1.160900	2.468696
C	0.335729	-2.839434	0.693646
C	-0.213730	0.069899	-3.076790
C	0.633942	-2.783709	-0.616135
C	0.269762	-1.134438	-2.428089
C	0.269773	-1.446961	-1.113752
H	1.046370	-3.570323	-1.239480
H	0.637983	-1.906784	-3.103994
H	0.466147	-3.687265	1.359491
H	-0.207602	0.033322	-4.165390
H	-0.998102	1.969582	-3.232503
C	-0.543201	-1.225546	2.488418
C	-0.403119	-0.018617	3.091475
H	0.619515	3.426596	-1.500925
H	1.469957	3.207534	0.952595
H	0.698881	1.847991	3.115003
H	-0.604059	0.036936	4.160841
H	-0.849636	-2.070750	3.105158
H	-1.741259	2.205710	-1.061048
H	-1.804500	0.615536	0.528858

M06-2X/pcseg-1 optimized structure of 2H-C11C2-SW

C	0.333425	2.868801	0.685966
C	-0.573929	0.740534	0.034641
C	0.243467	2.890548	-0.657331
C	-0.098307	-0.685368	0.031737
C	-0.182360	1.593840	-1.172034
C	-0.051397	1.571628	1.210085
C	-0.007447	-1.508778	1.125139
C	-0.181304	1.298276	-2.477776
C	-0.002037	1.251848	2.521741
C	0.331637	-2.870570	0.670670
C	-0.489790	-0.005338	-3.144557
C	0.407571	-2.884397	-0.669430
C	-0.101712	-1.276417	-2.464491
C	0.104074	-1.528636	-1.158490
H	0.641899	-3.723757	-1.316007
H	-0.010094	-2.134286	-3.133660
H	0.489280	-3.707801	1.344418
H	-0.021014	-0.005338	-4.136120
H	0.085943	2.110419	-3.155287
C	-0.261154	-1.231271	2.520215
C	-0.276888	-0.024661	3.131454
H	0.511300	3.723100	-1.302678
H	0.673310	3.685876	1.316867
H	0.302031	2.048670	3.201565
H	-0.425857	-0.016051	4.210239
H	-0.406233	-2.110154	3.148237
H	-1.572734	-0.065492	-3.358817
H	-1.677996	0.757986	0.088691

M06-2X/pcseg-1 optimized structure of 2H-C8C3-SW

C	-0.525634	2.873962	0.737445
C	-0.086868	0.744820	-0.040451
C	-0.371134	2.956564	-0.745278
C	0.085633	-0.686110	-0.054422
C	-0.057748	1.544883	-1.140552
C	-0.332255	1.597696	1.149168
C	0.377188	-1.540510	1.106074
C	0.373968	1.104637	-2.506030
C	-0.291837	1.207512	2.544759
C	0.470638	-2.913632	0.604900
C	-0.534000	0.023743	-3.033481
C	0.152873	-2.904392	-0.706091
C	-0.649823	-1.171307	-2.433439
C	-0.095212	-1.522640	-1.139925
H	0.082358	-3.766029	-1.363495
H	-1.245030	-1.944983	-2.920448
H	0.700863	-3.773977	1.224581
H	-1.092163	0.211113	-3.950077
H	1.400737	0.709068	-2.441013
C	0.373111	-1.231227	2.425814
C	0.053443	0.018437	3.084952
H	0.442259	3.641294	-1.032217
H	-0.739053	3.718529	1.386043
H	-0.532846	2.010329	3.241838
H	0.062201	-0.030410	4.172375
H	0.573152	-2.061910	3.103744
H	0.393575	1.958842	-3.190325
H	-1.280896	3.331714	-1.239475

M06-2X/pcseg-1 optimized structure of 2H-C2C4-SW

C	0.357717	2.801395	0.693315
C	-0.571558	0.768728	-0.002748
C	0.358831	2.801926	-0.695766
C	-0.569652	-0.778225	-0.003339
C	-0.083506	1.566100	-1.193031
C	-0.085416	1.565190	1.188926
C	-0.079867	-1.573594	1.188009
C	-0.154274	1.252197	-2.548367
C	-0.158362	1.250251	2.543905
C	0.364325	-2.812127	0.689548
C	-0.254257	-0.002073	-3.144592
C	0.365441	-2.811597	-0.696275
C	-0.143663	-1.258421	-2.546471
C	-0.077949	-1.572683	-1.194504
H	0.697021	-3.630992	-1.328428
H	0.008787	-2.097082	-3.226637
H	0.694887	-3.632005	1.321607
H	-0.274303	-0.002794	-4.233356
H	-0.015320	2.093627	-3.227979
C	-0.147755	-1.260364	2.540108
C	-0.259306	-0.004474	3.139011
H	0.688959	3.622714	-1.326869
H	0.686831	3.621700	1.325574
H	-0.020498	2.091161	3.224383
H	-0.281102	-0.006027	4.227740
H	0.003601	-2.099546	3.219877
H	-1.638740	1.049592	-0.003496
H	-1.635964	-1.061958	-0.004306

M06-2X/pcseg-1 optimized structure of 2H-C8C11-SW

C	-0.227639	2.918744	0.713626
C	-0.055479	0.719305	-0.023495
C	-0.139546	2.892024	-0.683608
C	0.019209	-0.669566	-0.009841
C	-0.036871	1.575721	-1.147853
C	-0.159586	1.602885	1.182277
C	0.148962	-1.529295	1.125264
C	0.183649	1.192611	-2.579991
C	-0.170091	1.250942	2.530812
C	0.288918	-2.904686	0.634441
C	-0.695338	0.043604	-3.065271
C	0.206056	-2.927343	-0.705810
C	-0.341800	-1.286037	-2.475887
C	-0.012672	-1.562810	-1.200100
H	0.250865	-3.798988	-1.350951
H	-0.391342	-2.145156	-3.147547
H	0.421384	-3.759346	1.291347
H	-0.633113	-0.032530	-4.156685
H	1.238666	0.917309	-2.732641
C	0.127850	-1.230595	2.481723
C	-0.032940	0.000178	3.117440
H	-0.139120	3.766219	-1.330139
H	-0.318124	3.798928	1.340920
H	-0.274280	2.091528	3.218075
H	-0.042314	-0.023204	4.205145
H	0.238395	-2.091247	3.142146
H	-0.002481	2.073102	-3.206019
H	-1.749220	0.263192	-2.828547

M06-2X/pcseg-1 optimized structure of 2H-C12C10-SW

C	-2.952188	0.697294	-0.019846
C	-0.755859	-0.000410	-0.000004
C	-2.951437	-0.700462	0.019530
C	0.630143	0.000336	0.000031
C	-1.636899	-1.170152	0.022304
C	-1.638162	1.168399	-0.022407
C	1.487366	1.175484	0.094451
C	-1.306194	-2.552083	0.085142
C	-1.308912	2.550689	-0.085060
C	2.917243	0.707588	0.288080
C	-0.082591	-3.148412	0.062418
C	2.917939	-0.704491	-0.288161
C	1.180652	-2.499338	-0.053266
C	1.488601	-1.173900	-0.094355
H	3.137153	-0.673447	-1.365646
H	2.037533	-3.171194	-0.124124
H	3.642910	1.376722	-0.183333
H	-0.057789	-4.234356	0.114697
H	-2.170234	-3.214182	0.152548
C	1.177968	2.500600	0.053476
C	-0.085963	3.148314	-0.062169
H	-3.828731	-1.339477	0.044685
H	-3.830179	1.335348	-0.045088
H	-2.173657	3.211872	-0.152460
H	-0.062342	4.234290	-0.114306
H	2.034119	3.173381	0.124384
H	3.644417	-1.372856	0.183098
H	3.136681	0.676833	1.365528

H_2 promoted by SW-pyrene

M06-2X/pcseg-1 optimized structure of 2H-C5C13-SW

C	-0.218752	2.915581	0.589920
C	-0.243800	0.659934	0.014921
C	-0.435709	2.901260	-0.730987
C	-0.185887	-0.722658	-0.002227
C	-0.493117	1.488718	-1.240217
C	-0.097583	1.547549	1.110591
C	0.043136	-1.615301	1.172729
C	0.454813	1.159984	-2.375671
C	0.117522	1.256764	2.454990
C	0.034948	-2.927207	0.684827
C	0.424741	-0.026275	-2.976748
C	-0.175663	-2.882393	-0.700035
C	-0.540920	-1.109194	-2.552524
C	-0.314452	-1.558912	-1.135030
H	-0.222082	-3.748605	-1.355409
H	-0.461903	-1.974691	-3.217509
H	0.175367	-3.817640	1.288053
H	1.132079	-0.242464	-3.776370
H	1.180484	1.917740	-2.667511
C	0.226601	-1.250656	2.504149
C	0.258859	0.017246	3.077732
H	-0.563600	3.768155	-1.372673
H	-0.142275	3.798946	1.218529
H	0.186232	2.124646	3.111667
H	0.419871	0.046171	4.153482
H	0.367822	-2.085876	3.191451
H	-1.522219	1.267635	-1.577550
H	-1.570773	-0.728671	-2.660312

M06-2X/pcseg-1 optimized structure of TS H_2-C12C10-SW

C	2.941232	-0.693971	-0.017366
C	0.736839	0.004084	0.001263
C	2.944559	0.691526	0.020508
C	-0.649140	0.007417	0.001073
C	1.621482	1.170627	0.027334
C	1.615869	-1.166703	-0.024563
C	-1.502419	-1.182909	0.025952
C	1.309678	2.546046	0.041630
C	1.297456	-2.540603	-0.038955
C	-2.889043	-0.689696	0.169007
C	0.086414	3.165424	0.010286
C	-2.885615	0.715295	-0.167479
C	-1.173678	2.534903	-0.045005
C	-1.496674	1.201833	-0.024045
H	-3.353474	1.069523	-1.081213
H	-2.033115	3.205125	-0.095119
H	-4.341462	-0.496502	-0.185950
H	0.082395	4.252709	0.010301
H	2.181859	3.200434	0.064673
C	-1.185842	-2.517517	0.046995
C	0.071217	-3.154091	-0.007953
H	3.822167	1.330154	0.040954
H	3.815765	-1.336813	-0.037568
H	2.166485	-3.199180	-0.061761
H	0.061968	-4.241343	-0.007976
H	-2.048506	-3.183598	0.096872
H	-4.339089	0.529033	0.187073
H	-3.358827	-1.041648	1.082633

M06-2X/pcseg-1 optimized structure of TS H_2-C8C11-SW

C	-0.062994	2.888848	0.720589
C	-0.134677	0.673975	0.007915
C	-0.016008	2.869659	-0.665851
C	-0.000366	-0.709204	0.026395
C	-0.102442	1.544341	-1.133138
C	-0.109261	1.564422	1.196984
C	0.111497	-1.558715	1.191274
C	-0.020106	1.186552	-2.536214
C	-0.119325	1.239759	2.551800
C	0.253387	-2.921132	0.726735
C	-0.523665	-0.098259	-3.065046
C	0.211682	-2.955940	-0.627551
C	-0.248304	-1.349704	-2.452306
C	0.045061	-1.614983	-1.138815
H	0.274165	-3.836997	-1.258422
H	-0.402158	-2.227951	-3.083761
H	0.360454	-3.772053	1.392652
H	-0.467395	0.971286	-4.329048
H	0.900545	1.562797	-2.978808
C	0.058703	-1.243186	2.544372
C	-0.063622	-0.003808	3.165896
H	0.043200	3.739249	-1.313998
H	-0.054194	3.769656	1.354135
H	-0.150450	2.100968	3.220456
H	-0.082166	-0.008796	4.253289
H	0.130355	-2.102274	3.212375
H	-0.586343	1.761498	-3.681972
H	-1.441919	-0.130686	-3.643246

M06-2X/pcseg-1 optimized structure of TS H_2-C2C4-SW

C	-0.694540	-2.805080	-0.436920
C	0.000000	-0.773910	0.496750
C	0.694540	-2.805080	-0.436920
C	0.000000	0.773040	0.497770
C	1.190980	-1.569910	0.008150
C	-1.190980	-1.569910	0.008150
C	-1.191260	1.568880	0.008530
C	2.546140	-1.255620	0.080600
C	-2.546140	-1.255620	0.080600
C	-0.692910	2.808440	-0.432920
C	3.141800	-0.001310	0.183430
C	0.692910	2.808440	-0.432930
C	2.543290	1.255010	0.074730
C	1.191260	1.568880	0.008520
H	1.325010	3.628700	-0.762450
H	3.223260	2.094220	-0.075590
H	-1.325020	3.628700	-0.762450
H	4.230550	-0.000210	0.204360
H	3.226180	-2.096530	-0.059390
C	-2.543290	1.255010	0.074740
C	-3.141800	-0.001320	0.183430
H	1.326230	-3.625000	-0.768090
H	-1.326220	-3.625010	-0.768090
H	-3.226180	-2.096530	-0.059400
H	-4.230550	-0.000220	0.204360
H	-3.223260	2.094220	-0.075580
H	0.084150	-0.559110	1.914440
H	-0.020140	0.371040	1.938680

M06-2X/pcseg-1 optimized structure of TS H_2-C5C8-SW

C	-0.222325	-2.996972	-0.135865
C	0.077323	-0.687314	-0.001141
C	1.122895	-2.758895	-0.028965
C	-0.155338	0.710242	0.035308
C	1.330787	-1.344738	0.041268
C	-0.914891	-1.743495	-0.101170
C	-1.457746	1.362889	0.108664
C	2.686116	-0.722585	0.289857
C	-2.309147	-1.647192	-0.121972
C	-1.229010	2.781476	0.110117
C	3.056008	0.600505	-0.228427
C	0.113307	3.000361	-0.011792
C	2.212974	1.658477	-0.306048
C	0.811608	1.744005	-0.052465
H	0.604091	3.967641	-0.078547
H	2.673763	2.601305	-0.606055
H	-2.014003	3.528268	0.161377
H	4.110957	0.737320	-0.446697
H	3.453738	-1.493403	0.197924
C	-2.728866	0.805149	0.100681
C	-3.122040	-0.529977	-0.012988
H	1.912508	-3.505352	-0.009319
H	-0.705602	-3.964274	-0.219531
H	-2.826663	-2.603183	-0.213153
H	-4.194426	-0.712707	-0.026137
H	-3.541603	1.530331	0.161995
H	2.005010	-0.920389	1.385406
H	2.892299	-0.557176	1.582367

M06-2X/pcseg-1 optimized structure of TS H_2-C5C2-SW

C	0.150153	2.891646	0.595601
C	-0.306636	0.691262	-0.031235
C	0.053415	2.902785	-0.766647
C	-0.047840	-0.727753	-0.058711
C	-0.136008	1.572395	-1.290335
C	0.009424	1.567127	1.106445
C	-0.073225	-1.570382	1.103798
C	0.051215	1.204004	-2.634154
C	0.007967	1.250773	2.465464
C	0.049901	-2.940667	0.649066
C	0.108627	-0.057631	-3.207259
C	0.136110	-2.935339	-0.704387
C	0.108166	-1.292035	-2.564759
C	0.062203	-1.567211	-1.194720
H	0.257993	-3.798470	-1.352547
H	0.178419	-2.167564	-3.209355
H	0.085309	-3.800482	1.309887
H	0.190234	-0.078619	-4.292063
H	0.110784	2.051788	-3.317044
C	-0.169967	-1.253668	2.457980
C	-0.118117	0.002321	3.061078
H	0.123834	3.782149	-1.400983
H	0.309834	3.763810	1.222322
H	0.120642	2.100538	3.137857
H	-0.136859	0.002852	4.149909
H	-0.226556	-2.106574	3.133004
H	-1.469422	1.507818	-0.938008
H	-1.640659	0.937898	0.021448

M06-2X/pcseg-1 optimized structure of TS H_2-C8C3-SW

C	-0.159550	2.872501	0.714281
C	0.177548	0.703937	-0.013391
C	-0.001561	2.879231	-0.705439
C	0.091176	-0.707442	0.009344
C	0.316865	1.533925	-1.110106
C	-0.024343	1.575647	1.181707
C	0.099379	-1.568200	1.170099
C	0.026273	1.289523	-2.531088
C	-0.053460	1.234304	2.551000
C	0.045795	-2.939852	0.685733
C	-0.101125	0.008086	-3.117189
C	-0.028862	-2.929692	-0.665537
C	-0.119709	-1.223099	-2.492601
C	-0.006922	-1.551105	-1.131921
H	-0.101441	-3.790340	-1.323022
H	-0.216268	-2.082305	-3.157086
H	0.047736	-3.810238	1.334484
H	-0.191530	-0.008659	-4.202650
H	0.443833	2.038808	-3.208838
C	0.117070	-1.259855	2.513155
C	0.053213	-0.000757	3.145277
H	0.328805	3.770596	-1.241872
H	-0.308964	3.744003	1.345458
H	-0.167631	2.084755	3.224077
H	0.042208	-0.016470	4.232882
H	0.144134	-2.119310	3.183933
H	-1.222729	2.055234	-2.454945
H	-1.181929	2.707865	-1.613346

M06-2X/pcseg-1 optimized structure of TS H_2-C5C13-SW

C	0.256706	2.930908	0.198625
C	-0.029766	0.651012	-0.072379
C	-1.086102	2.724996	0.146245
C	0.169944	-0.708209	-0.126762
C	-1.367321	1.310593	-0.023106
C	0.964576	1.685550	0.043420
C	1.451807	-1.437999	-0.130559
C	-2.518616	0.856316	-0.759601
C	2.350830	1.565588	-0.013196
C	1.127955	-2.805820	-0.005498
C	-2.958080	-0.421029	-0.655885
C	-0.249836	-2.943890	0.124601
C	-2.265319	-1.371540	0.175516
C	-0.864991	-1.679711	0.019722
H	-0.783752	-3.878334	0.269935
H	-2.865783	-2.225055	0.499285
H	1.854970	-3.611459	0.005078
H	-3.938132	-0.691496	-1.043341
H	-3.132792	1.608967	-1.250416
C	2.736335	-0.906646	-0.192911
C	3.141488	0.426366	-0.156398
H	-1.856257	3.488230	0.194377
H	0.750377	3.891338	0.317750
H	2.893681	2.508832	0.060471
H	4.214648	0.598146	-0.199566
H	3.537928	-1.645477	-0.233406
H	-1.761836	0.501209	1.259266
H	-2.092323	-0.384896	1.314542

M06-2X/pcseg-1 optimized structure of TS H_2-C12C4-SW

C	0.375136	3.010828	0.250469
C	-0.085191	0.716019	0.073745
C	-0.964460	2.846430	0.143268
C	0.096398	-0.709592	0.143919
C	-1.283050	1.427983	0.031326
C	1.000477	1.704923	0.174624
C	1.321917	-1.415545	-0.265893
C	-2.628746	0.979182	-0.149472
C	2.352270	1.532306	0.098371
C	1.026921	-2.765575	-0.298255
C	-3.096008	-0.284986	-0.325743
C	-0.331377	-2.947418	0.086747
C	-2.346625	-1.506151	-0.306795
C	-1.019882	-1.679711	-0.130465
H	-0.843074	-3.906167	0.091253
H	-2.925860	-2.421901	-0.427622
H	1.761662	-3.558779	-0.401931
H	-4.166833	-0.394686	-0.483992
H	-3.371344	1.776724	-0.175909
C	2.658627	-0.913910	-0.357089
C	3.115552	0.351532	-0.163229
H	-1.714023	3.632369	0.126326
H	0.921131	3.945175	0.327065
H	2.939442	2.446839	0.191862
H	4.190149	0.499711	-0.244862
H	3.405883	-1.671250	-0.596743
H	-0.092351	-2.340992	1.425040
H	0.151820	-1.271469	1.478246

M06-2X/pcseg-1 optimized structure of TS H_2-C11C2-SW

C	-0.752252	-2.830924	-0.339605
C	0.084775	-0.663599	0.121057
C	0.558507	-2.836068	-0.679899
C	-0.002772	0.738789	-0.164325
C	1.152190	-1.546590	-0.395646
C	-1.157189	-1.513459	0.090924
C	-1.113574	1.586920	-0.179144
C	2.475127	-1.282784	-0.210155
C	-2.459498	-1.170541	0.292940
C	-0.632057	2.927335	-0.460717
C	2.852724	-0.103471	0.508731
C	0.724342	2.939657	-0.543479
C	2.435421	1.228859	0.100822
C	1.190704	1.594996	-0.303098
H	1.366283	3.798438	-0.706000
H	3.178183	2.021554	0.204742
H	-1.286945	3.789329	-0.554606
H	3.857172	-0.123428	0.932039
H	3.209470	-2.074159	-0.347626
C	-2.472914	1.315508	0.166260
C	-3.058607	0.117815	0.439162
H	1.119150	-3.680068	-1.070283
H	-1.435713	-3.672288	-0.406313
H	-3.161241	-2.005920	0.261873
H	-4.118401	0.126662	0.683313
H	-3.113327	2.196226	0.223260
H	0.822165	-0.493442	1.444666
H	1.802258	-0.259096	1.533466

Pristine Pyrene

M06-2X/pcseg-1 optimized structure of 1H-C8-pyrene

C	-0.005501	0.698110	0.017650
C	-0.006044	-0.727573	0.005249
C	2.420212	0.675640	0.043043
C	-2.458904	-0.706925	-0.020447
C	-2.452111	0.672368	-0.008383
C	2.435638	-0.702909	0.031220
C	1.219138	1.398809	0.036660
C	-1.241390	-1.443944	-0.014011
C	-1.253964	1.399431	0.010577
C	1.225258	-1.441530	0.012030
C	1.251895	2.905770	0.050108
C	-1.213689	-2.850480	-0.025948
C	-1.240869	2.848353	0.023313
C	1.201250	-2.855892	-0.000519
C	-0.098645	3.551681	0.041478
C	-0.003142	-3.539988	-0.019172
H	3.361915	1.222960	0.057735
H	-3.400352	-1.251489	-0.035113
H	-3.394099	1.217919	-0.013577
H	3.380978	-1.241437	0.036510
H	1.833215	3.266083	-0.813801
H	-2.154891	-3.395877	-0.040619
H	-2.200347	3.363340	0.017670
H	2.144143	-3.398473	0.004711
H	-0.132506	4.639508	0.050581
H	-0.005022	-4.627331	-0.028646
H	1.814797	3.250902	0.932222

M06-2X/pcseg-1 optimized structure of TS 1H-C8-pyrene

C	-0.005501	0.698110	0.017650
C	-0.006044	-0.727573	0.005249
C	2.420212	0.675640	0.043043
C	-2.458904	-0.706925	-0.020447
C	-2.452111	0.672368	-0.008383
C	2.435638	-0.702909	0.031220
C	1.219138	1.398809	0.036660
C	-1.241390	-1.443944	-0.014011
C	-1.253964	1.399431	0.010577
C	1.225258	-1.441530	0.012030
C	1.251895	2.905770	0.050108
C	-1.213689	-2.850480	-0.025948
C	-1.240869	2.848353	0.023313
C	1.201250	-2.855892	-0.000519
C	-0.098645	3.551681	0.041479
C	-0.003142	-3.539988	-0.019172
H	3.361915	1.222960	0.057735
H	-3.400352	-1.251489	-0.035113
H	-3.394099	1.217919	-0.013577
H	3.380978	-1.241437	0.036510
H	1.833215	3.266083	-0.813801
H	-2.154891	-3.395877	-0.040619
H	-2.200347	3.363340	0.017671
H	2.144143	-3.398473	0.004711
H	-0.132506	4.639508	0.050582
H	-0.005022	-4.627331	-0.028645
H	2.018192	3.375609	1.250958

1H-C2-pyrene is the same of 1H-pyrene in section "Stone-Wales formation catalyzed by H".

M06-2X/pcseg-1 optimized structure of 1H-C2-pyrene

C	0.155164	-0.711238	-0.000000
C	0.030592	0.731763	0.000000
C	-0.008693	-0.672208	2.464756
C	0.018562	0.682851	-2.460866
C	-0.008693	-0.672208	-2.464756
C	0.018562	0.682851	2.460866
C	-0.005390	-1.425590	1.242317
C	0.005725	1.434536	-1.227869
C	-0.005390	-1.425590	-1.242317
C	0.005725	1.434536	1.227869
C	-0.071171	-2.816921	1.211767
C	-0.048969	2.833045	-1.207519
C	-0.071171	-2.816921	-1.211767
C	-0.048969	2.833045	1.207519
C	-0.078337	-3.505111	-0.000000
C	-0.074074	3.521904	0.000000
H	-0.040913	-1.218756	3.405384
H	0.017611	1.235290	-3.398374
H	-0.040913	-1.218756	-3.405384
H	0.017611	1.235290	3.398374
H	-0.133509	-3.364454	2.150219
H	-0.071313	3.377065	-2.149667
H	-0.133509	-3.364454	-2.150219
H	-0.071313	3.377065	2.149667
H	-0.127760	-4.591026	-0.000000
H	-0.115207	4.608326	0.000000
H	1.818377	-0.728069	-0.000000

M06-2X/pcseg-1 optimized structure of 1H-C12-pyrene

C	0.670535	0.011817	0.077114
C	-0.768873	-0.024681	0.031055
C	0.680578	-2.449093	0.023220
C	-0.856690	2.431040	0.082382
C	0.625710	2.557147	0.131794
C	-0.673378	-2.475377	-0.019924
C	1.398608	-1.205924	0.073176
C	-1.521960	1.202591	0.034405
C	1.370387	1.242462	0.126227
C	-1.442035	-1.260457	-0.017331
C	2.805945	-1.173172	0.118136
C	-2.932427	1.122452	-0.011716
C	2.752209	1.234906	0.169494
C	-2.855181	-1.288226	-0.062378
C	3.473294	0.031320	0.165646
C	-3.580541	-0.106311	-0.059157
H	1.251980	-3.375341	0.020780
H	-1.446869	3.344841	0.083946
H	0.971664	3.168586	-0.717376
H	-1.206510	-3.423424	-0.057568
H	-3.508490	2.045476	-0.009502
H	3.287554	2.182712	0.207202
H	-3.363446	-2.249070	-0.099522
H	4.559750	0.053666	0.200288
H	-4.666881	-0.138990	-0.094038
H	3.356033	-2.112085	0.114745
H	0.916782	3.130105	1.027132

M06-2X/pcseg-1 optimized structure of 1H-C12-pyrene

C	0.670535	0.011817	0.077114
C	-0.768873	-0.024681	0.031055
C	0.680578	-2.449093	0.023220
C	-0.856690	2.431040	0.082382
C	0.625710	2.557147	0.131794
C	-0.673378	-2.475377	-0.019924
C	1.398608	-1.205924	0.073176
C	-1.521960	1.202591	0.034405
C	1.370387	1.242462	0.126227
C	-1.442035	-1.260457	-0.017331
C	2.805945	-1.173172	0.118136
C	-2.932427	1.122452	-0.011716
C	2.752209	1.234906	0.169494
C	-2.855181	-1.288226	-0.062378
C	3.473294	0.031320	0.165646
C	-3.580541	-0.106311	-0.059157
H	1.251980	-3.375341	0.020780
H	-1.446869	3.344841	0.083946
H	0.971664	3.168586	-0.717376
H	-1.206510	-3.423424	-0.057568
H	-3.508490	2.045476	-0.009502
H	3.287554	2.182712	0.207202
H	-3.363446	-2.249070	-0.099522
H	4.559750	0.053666	0.200288
H	-4.666881	-0.138990	-0.094038
H	3.356033	-2.112085	0.114745
H	0.916782	3.130105	1.027132

M06-2X/pcseg-1 optimized structure of 2H-C2C4-pyrene

C	0.688401	-0.005427	0.779180
C	0.686402	-0.005734	-0.790581
C	-0.005512	2.419309	0.693372
C	-0.007586	-2.436992	-0.697187
C	-0.005824	-2.436720	0.688506
C	-0.007292	2.419035	-0.703958
C	0.167363	1.260198	1.436329
C	0.156284	-1.267926	-1.448079
C	0.159955	-1.267360	1.438520
C	0.163690	1.259632	-1.446897
C	-0.061772	1.211413	2.815409
C	-0.087146	-1.220614	-2.813120
C	-0.080001	-1.219512	2.804157
C	-0.068955	1.210306	-2.825371
C	-0.115336	-0.000206	3.494575
C	-0.124243	-0.001580	-3.503923
H	-0.224430	3.344429	1.224672
H	-0.218239	-3.362943	-1.230411
H	-0.215121	-3.362461	1.222627
H	-0.227563	3.343946	-1.235061
H	-0.287331	2.137399	3.342126
H	-0.337197	-2.142588	-3.335778
H	-0.328723	-2.141279	3.327811
H	-0.295858	2.136085	-3.351875
H	-0.319259	-0.002364	4.562756
H	-0.330884	-0.004157	-4.571580
H	1.746716	-0.008919	-1.089077
H	1.749471	-0.008499	1.074977

M06-2X/pcseg-1 optimized structure of TS 1H-C12-pyrene

C	0.656676	0.015752	0.044131
C	-0.772540	-0.018972	0.013871
C	0.677136	-2.445410	0.093876
C	-0.804900	2.439308	-0.080100
C	0.559776	2.483061	0.042130
C	-0.676347	-2.477440	0.077241
C	1.395701	-1.197231	0.073394
C	-1.514666	1.194122	-0.053930
C	1.340935	1.258355	0.036883
C	-1.452507	-1.264702	0.029464
C	2.795079	-1.142479	0.083716
C	-2.913378	1.133858	-0.102174
C	2.735978	1.271497	0.048053
C	-2.852786	-1.278599	-0.012855
C	3.455014	0.079324	0.067154
C	-3.571572	-0.090642	-0.078264
H	1.250688	-3.369812	0.123199
H	-1.376760	3.362035	-0.151814
H	1.087371	3.425966	-0.088836
H	-1.206216	-3.427870	0.093355
H	-3.481376	2.060433	-0.156066
H	3.258227	2.226336	0.049863
H	-3.373511	-2.233956	0.001749
H	4.541849	0.105896	0.074302
H	-4.657856	-0.119032	-0.112477
H	3.361368	-2.071432	0.105769
H	0.752437	2.818756	1.874977

M06-2X/pcseg-1 optimized structure of 2H-C12C10-pyrene

C	0.670752	0.035720	0.036042
C	-0.777488	0.005240	0.010396
C	0.674598	-2.422241	0.010897
C	-0.768578	2.488976	-0.374408
C	0.557987	2.523283	0.377238
C	-0.678695	-2.449918	0.078640
C	1.394935	-1.177334	-0.004136
C	-1.519461	1.204637	-0.121052
C	1.361942	1.267176	0.146167
C	-1.450396	-1.236106	0.072104
C	2.805131	-1.137368	-0.018868
C	-2.899473	1.150161	-0.106653
C	2.743030	1.270133	0.132220
C	-2.861037	-1.254814	0.086650
C	3.467122	0.069100	0.032707
C	-3.572813	-0.078134	0.014170
H	1.245034	-3.348956	-0.010244
H	-1.390439	3.348942	-0.103661
H	1.143492	3.403588	0.091225
H	-1.209941	-3.399133	0.116236
H	-3.471196	2.071397	-0.205759
H	3.275747	2.216037	0.214947
H	-3.376440	-2.211404	0.146836
H	4.554041	0.095768	0.017124
H	-4.659904	-0.096609	0.029681
H	3.360054	-2.072509	-0.062460
H	0.358687	2.603837	1.456670
H	-0.572420	2.558842	-1.455160

M06-2X/pcseg-1 optimized structure of 2H-C8C11-pyrene

C	0.000000	0.713974	0.000000
C	0.000000	-0.713974	0.000000
C	2.461789	0.676944	0.000000
C	-2.461789	-0.676944	0.000000
C	-2.461789	0.676944	0.000000
C	2.461789	-0.676944	0.000000
C	1.230398	1.425253	0.000000
C	-1.230398	-1.425253	0.000000
C	-1.230398	1.425253	0.000000
C	1.230398	-1.425253	0.000000
C	1.207779	2.824376	0.000000
C	-1.207779	-2.824376	0.000000
C	-1.207779	2.824376	0.000000
C	1.207779	-2.824376	0.000000
C	0.000000	3.513428	0.000000
C	0.000000	-3.513428	0.000000
H	3.399866	1.228705	0.000000
H	-3.399866	-1.228705	0.000000
H	-3.399866	1.228705	0.000000
H	3.399866	-1.228705	0.000000
H	1.804682	3.378205	-0.721938
H	-2.149515	-3.369672	0.000000
H	-2.149515	3.369672	0.000000
H	2.149515	-3.369672	0.000000
H	-0.167163	4.307658	-0.723420
H	0.000000	-4.600664	0.000000
H	1.371796	2.918495	1.072456
H	0.186230	3.702531	1.056163

M06-2X/pcseg-1 optimized structure of TS H_2-C2C4-pyrene

C	-0.784880	0.000740	0.599790
C	0.702310	0.113070	0.101420
C	-0.698670	2.424220	-0.098420
C	0.692850	-2.431800	-0.089890
C	-0.692850	-2.431800	-0.089900
C	0.698660	2.424220	-0.098430
C	-1.441620	1.265280	0.075620
C	1.443300	-1.262290	0.072800
C	-1.443300	-1.262290	0.072800
C	1.441610	1.265280	0.075610
C	-2.820390	1.215800	-0.155190
C	2.808640	-1.215150	-0.168970
C	-2.808640	-1.215150	-0.168980
C	2.820390	1.215810	-0.155190
C	-3.499250	0.003960	-0.207410
C	3.499250	0.003960	-0.207410
H	-1.229870	3.348840	-0.319700
H	1.226520	-3.358020	-0.298180
H	-1.226520	-3.358030	-0.298190
H	1.229860	3.348840	-0.319700
H	-3.347000	2.141270	-0.383100
H	3.331800	-2.137470	-0.416680
H	-3.331800	-2.137470	-0.416690
H	3.347000	2.141270	-0.383110
H	-4.567170	0.001210	-0.412690
H	4.567170	0.001220	-0.412690
H	-0.333310	-0.152120	1.831160
H	-1.243870	-0.155120	1.844910

M06-2X/pcseg-1 optimized structure of 2H-C5C13-pyrene

C	0.032044	0.693503	0.248001
C	0.015785	-0.722126	0.118705
C	2.437443	0.668581	0.022735
C	-2.469559	-0.669505	0.049057
C	-2.488858	0.655324	0.212677
C	2.451567	-0.700021	-0.037620
C	1.223001	1.382733	0.165937
C	-1.222710	-1.436543	0.059390
C	-1.252431	1.455544	0.513157
C	1.238201	-1.433306	-0.005440
C	1.222857	2.892802	0.216586
C	-1.209419	-2.809104	-0.054780
C	-1.216931	2.808395	-0.164510
C	1.205589	-2.850805	-0.108949
C	-0.072284	3.472298	-0.288962
C	0.010061	-3.520475	-0.122188
H	3.371672	1.224997	-0.035817
H	-3.395352	-1.216918	-0.121268
H	-3.434426	1.196268	0.185419
H	3.391788	-1.239635	-0.133068
H	2.070162	3.280067	-0.360889
H	-2.152984	-3.349000	-0.108317
H	-2.154982	3.230130	-0.524377
H	2.146293	-3.392575	-0.185671
H	-0.052400	4.456167	-0.754745
H	-0.006900	-4.604534	-0.203782
H	1.386494	3.224792	1.255430
H	-1.277156	1.655227	1.602808

M06-2X/pcseg-1 optimized structure of TS H_2-C12C10-pyrene

C	0.724390	-0.041760	-0.000680
C	-0.724390	-0.041760	0.000680
C	0.676040	-2.498950	-0.046490
C	-0.670390	2.444530	-0.363400
C	0.670390	2.444530	0.363400
C	-0.676040	-2.498950	0.046490
C	1.422010	-1.269280	-0.064650
C	-1.443280	1.173980	-0.106720
C	1.443280	1.173980	0.106720
C	-1.422010	-1.269280	0.064650
C	2.832220	-1.258640	-0.105590
C	-2.823620	1.148210	-0.066800
C	2.823620	1.148210	0.066800
C	-2.832220	-1.258640	0.105590
C	3.520300	-0.066760	-0.056380
C	-3.520300	-0.066760	0.056380
H	1.226350	-3.437160	-0.086120
H	-0.390540	3.828680	0.207750
H	0.382190	3.790490	-0.017150
H	-1.226350	-3.437160	0.086120
H	-3.377580	2.082020	-0.147410
H	3.377580	2.082020	0.147410
H	-3.366430	-2.204750	0.167450
H	4.607060	-0.062670	-0.092200
H	-4.607060	-0.062670	0.092200
H	3.366430	-2.204750	-0.167450
H	0.492990	2.519760	1.447030
H	-0.492990	2.519760	-1.447030

M06-2X/pcseg-1 optimized structure of TS H_2-C8C11-pyrene

C	0.644187	0.008014	0.017331
C	-0.775225	0.004287	0.038898
C	0.601357	-2.464206	-0.170569
C	-0.751115	2.446027	-0.097448
C	0.608505	2.444589	-0.174476
C	-0.744580	-2.454924	-0.083731
C	1.378620	-1.240841	-0.080744
C	-1.493542	1.228658	0.021443
C	1.355856	1.225458	-0.080072
C	-1.497828	-1.223494	0.030589
C	2.743874	-1.263123	-0.090254
C	-2.900467	1.206125	0.075034
C	2.771173	1.229735	-0.094039
C	-2.885667	-1.203324	0.079600
C	3.498271	-0.049838	0.205997
C	-3.588534	0.007657	0.117541
H	1.140800	-3.403684	-0.272526
H	-1.297241	3.386588	-0.138519
H	1.151905	3.381956	-0.278680
H	-1.300671	-3.391243	-0.116978
H	-3.441158	2.150473	0.070307
H	3.336358	2.120965	-0.341508
H	-3.429748	-2.146988	0.074513
H	4.558393	-0.019361	-0.033282
H	-4.674428	0.002081	0.158762
H	3.287560	-2.196815	-0.198921
H	3.748476	-0.091002	1.593288
H	3.124098	0.817061	1.131550

M06-2X/pcseg-1 optimized structure of TS H_2-C5C13-pyrene

C	0.662030	-0.036730	0.184350
C	-0.755810	-0.018200	0.082450
C	0.625450	-2.445990	0.007050
C	-0.697070	2.465100	-0.037180
C	0.630760	2.483110	0.100110
C	-0.744110	-2.456640	-0.026250
C	1.345930	-1.231400	0.112310
C	-1.467510	1.221310	0.012710
C	1.432990	1.250110	0.409200
C	-1.472960	-1.240390	-0.003660
C	2.856690	-1.235390	0.133420
C	-2.842080	1.210440	-0.074330
C	2.772180	1.196710	-0.293950
C	-2.892110	-1.205010	-0.080070
C	3.430060	0.047590	-0.408780
C	-3.558310	-0.007700	-0.103780
H	1.177790	-3.383070	-0.043940
H	-1.244930	3.389230	-0.214980
H	1.173910	3.426120	0.043650
H	-1.288320	-3.396720	-0.092590
H	3.230010	-2.095190	-0.434700
H	-3.380080	2.154610	-0.135890
H	3.189600	2.126080	-0.680410
H	-3.438120	-2.145190	-0.127640
H	4.404550	0.015220	-0.893220
H	-4.643700	0.011340	-0.164490
H	2.540130	-0.345300	1.437660
H	2.109140	0.369220	1.551570