Electronic Supplementary Material (ESI) for Chemical Communications

Supporting Information

π-Depletion as criterion to predict π-stacking ability

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Computational Details

All monomers were optimized with B3LYP[1-3]/6-31G* with Gaussian 09[4], 2-methylene-1,2-dihydronaphthalene, tetra- and hexahydrotriphenylene being constrained to be planar. Interaction energies were computed at the PBE0[5-7]/def2-TZVP, PBE0-dDsC[8, 9]/def2-TZVP, HF/def2-TZVP and MP2/def2-TZVP (for molecules of the validation set) levels in a development version of Q-Chem[10] for frozen monomers, separated by a vertical distance of 3.5 Å except otherwise noted. dDsC[8, 9] is a density-dependant dispersion correction developped in our laboratory, that is based on a damping function, which performs well in both inter- and intramolecular cases. Interaction energies with caffeine were computed with geometries fully relaxed at the PBE0-dDsC/def2-SVP level of theory. To assess the accuracy of the dDsC dispersion correction on these complexes, their interaction energies were also computed at the B97[11]-dDsC/def2-TZVP, PBE[5]/def2-TZVP, M06-2X[12]/def2-TZVP (using a Lebedev[13] grid with 99 radial and 590 angular[14] points), MP2/def2-TZVP and SCS-MP2[15]/def2-TZVP. All MP2 computations make use of the RI[16] approximation to speed up computations, with the cc-pVTZ[17] auxiliary basis set. BSSE counterpoise corrections were applied for all interaction energies, and DFT computations use a Lebedev[18] grid with 75 radial and 302 angular[14] points unless otherwise specified.

Energy decomposition analysis was performed on the same geometries and at vertical distances of 3.3 Å and 3.7 Å at the SAPT0[19] level using the aug-cc-pVDZ basis set. The resolution of the identity with appropriate auxiliary basis functions was applied to speed up computations.[20]

The LOL function[21] relies on the consideration of the electron kinetic energy density $\tau = \sum_i |\nabla \psi_i|^2$:

$$LOL = \frac{1}{1 + \frac{\tau}{D_0}}$$

where $D_0 = \frac{3}{5}(6\pi^2)^{2/3}\rho^{5/3}$ is the corresponding kinetic energy density in the uniform electron gas. Therefore, LOL>0.5 reveals electrons slower (less kinetic energy) than in the uniform electron gas, and LOL<0.5 electrons faster than in the uniform electron gas.

Electronic densities were obtained with Gaussian09[4] at the PBE[5]/cc-pVTZ level and their LOL was computed in Dgrid[22] using all orbitals of π-symmetry, with a grid mesh of 0.05 Bohrs.

Only LOL values above 0.55 are taken into account so that LOLIPOP is proportional to the portion of localized electronic density in space. The integration starts at a distance of 0.5 Å from the molecular plane where the most important contributions from the bonding basins are present. The chosen integration radius of 1.94 Å corresponds to the average between the C and H radii in benzene but the use of other radius within a small range does not alter the observed trend.

The script to obtain LOLIPOP values and detailed instructions to obtain them is available free of charge and without any warranty on our website: **http://lcmd.epfl.ch**

Validation set

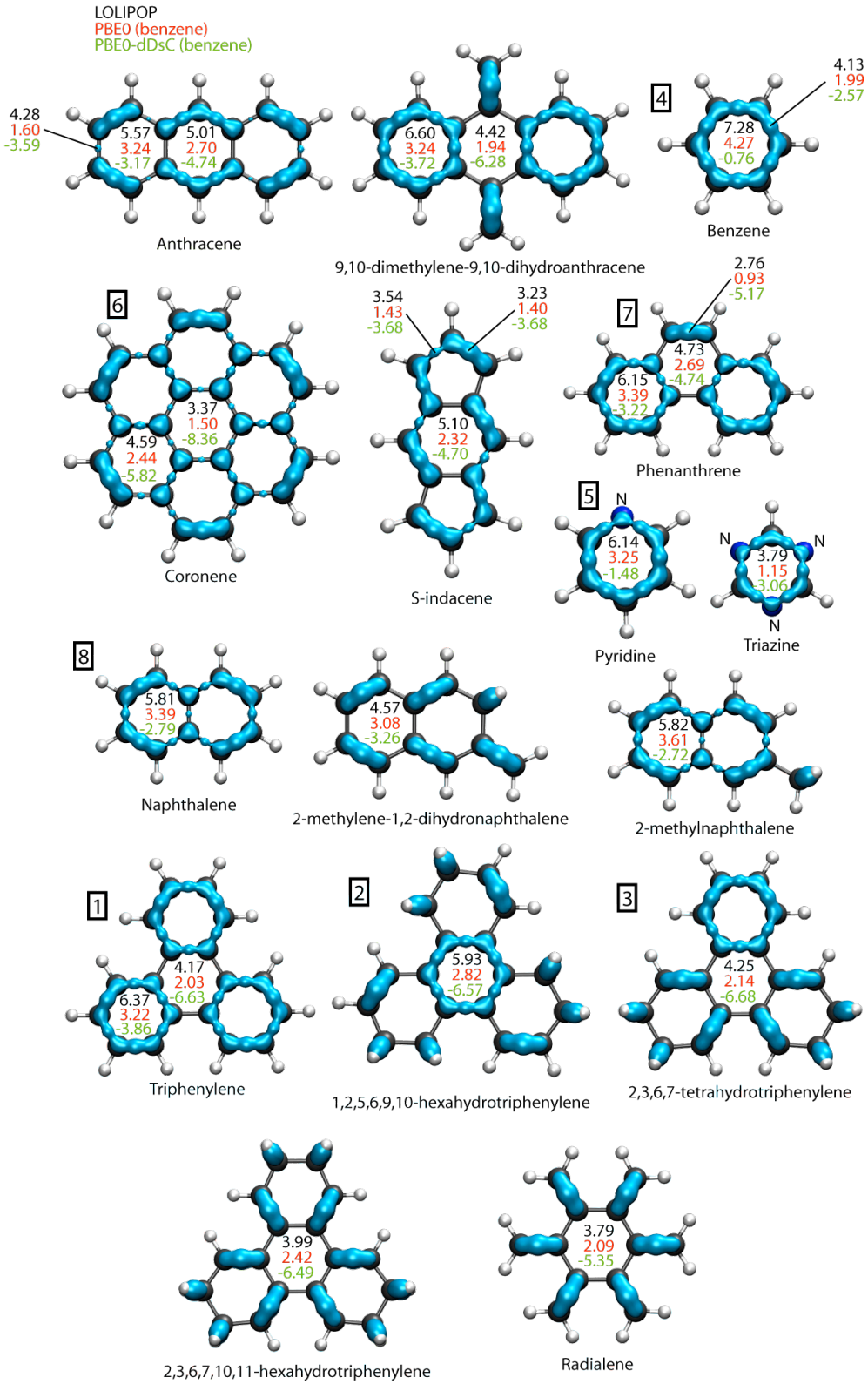

Fig. S1 LOLIPOP index (black), PBE0 interaction energies (for benzene) without (red) and with (green) dispersion correction and LOL isovalues of 0.55 obtained from the π-density. Nitrogen atoms are explicitly indicated and values corresponding to stacking on bonds are noted outside molecules.

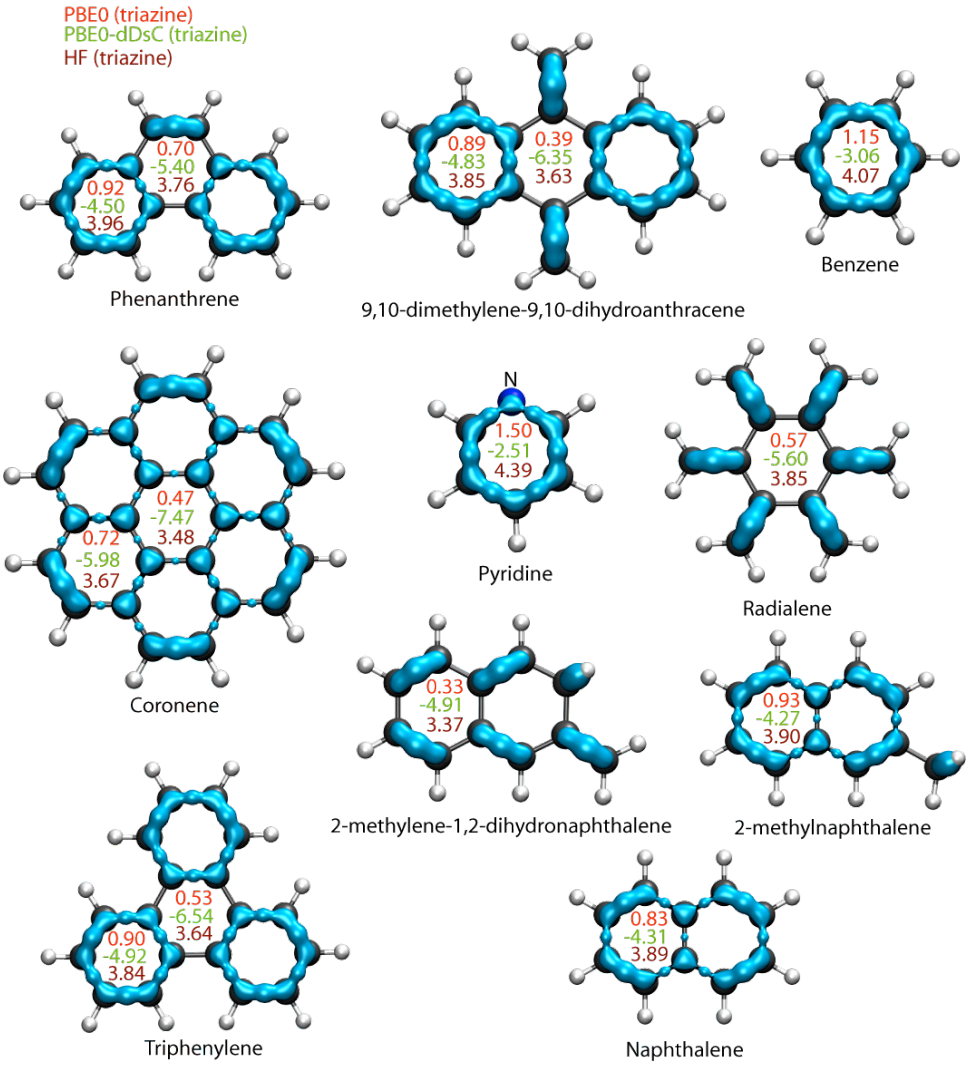

Fig. S2 HF (brown) and PBE0 interaction energies (for triazine) without (red) and with (green) dispersion correction and LOL isovalues of 0.55 obtained from the π-density. Nitrogen atoms are explicitly indicated.

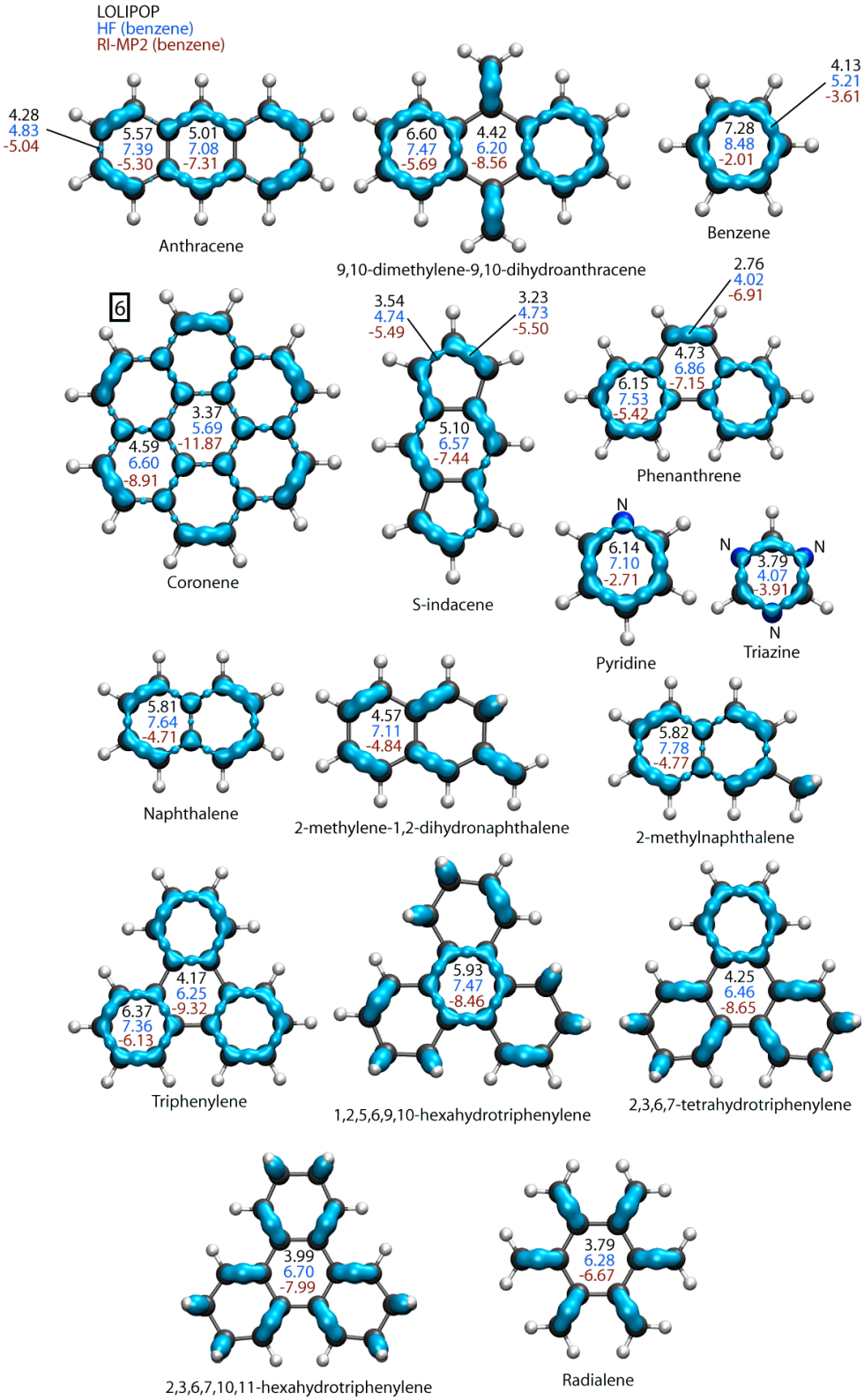

Fig. S3 LOLIPOP index (black), HF (blue) and RI-MP2 (brown) interaction energies for benzene and LOL isovalues of 0.55 obtained from the π-density. Nitrogen atoms are explicitly indicated and values corresponding to stacking on bonds are noted outside molecules.

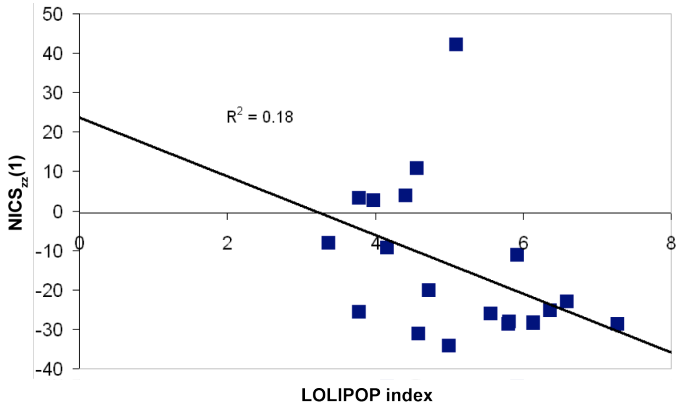

Fig. S4 $NICS_{zz}(1)$ plotted against LOLIPOP for molecular rings in Fig. S1. Linear regression show no significant correlation between the two indices.

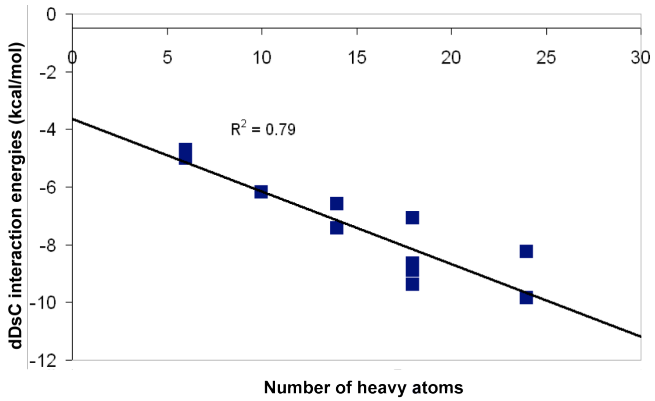

Fig. S5 dDsC contribution to the interaction energy plotted against the number of heavy atoms[23] for molecules in Fig. 1 (see article). Dispersion energies are linked to molecular size.

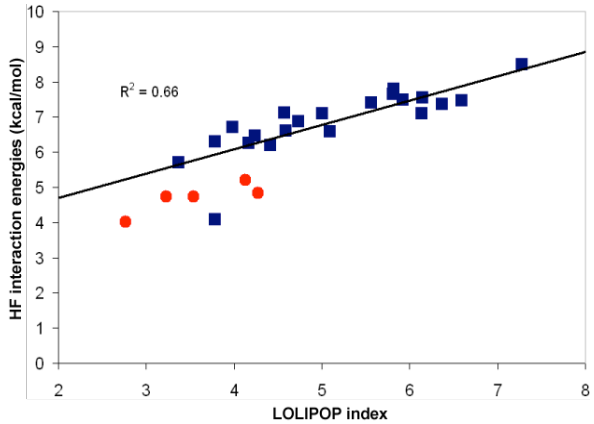

Fig. S6 HF interaction energies plotted against LOLIPOP index for parallel stacked (blue squares) and parallel displaced (red circles) benzene geometries. Linear regression takes only parallel stacked geometries into account.

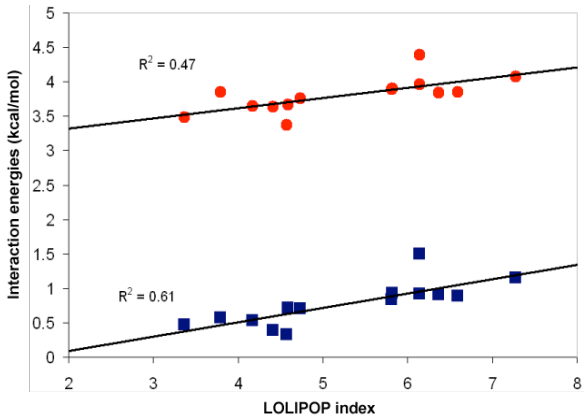

Fig. S7 HF (red circles) and PBE0 (blue squares) interaction energies plotted against LOLIPOP index for parallel stacked triazine geometries.

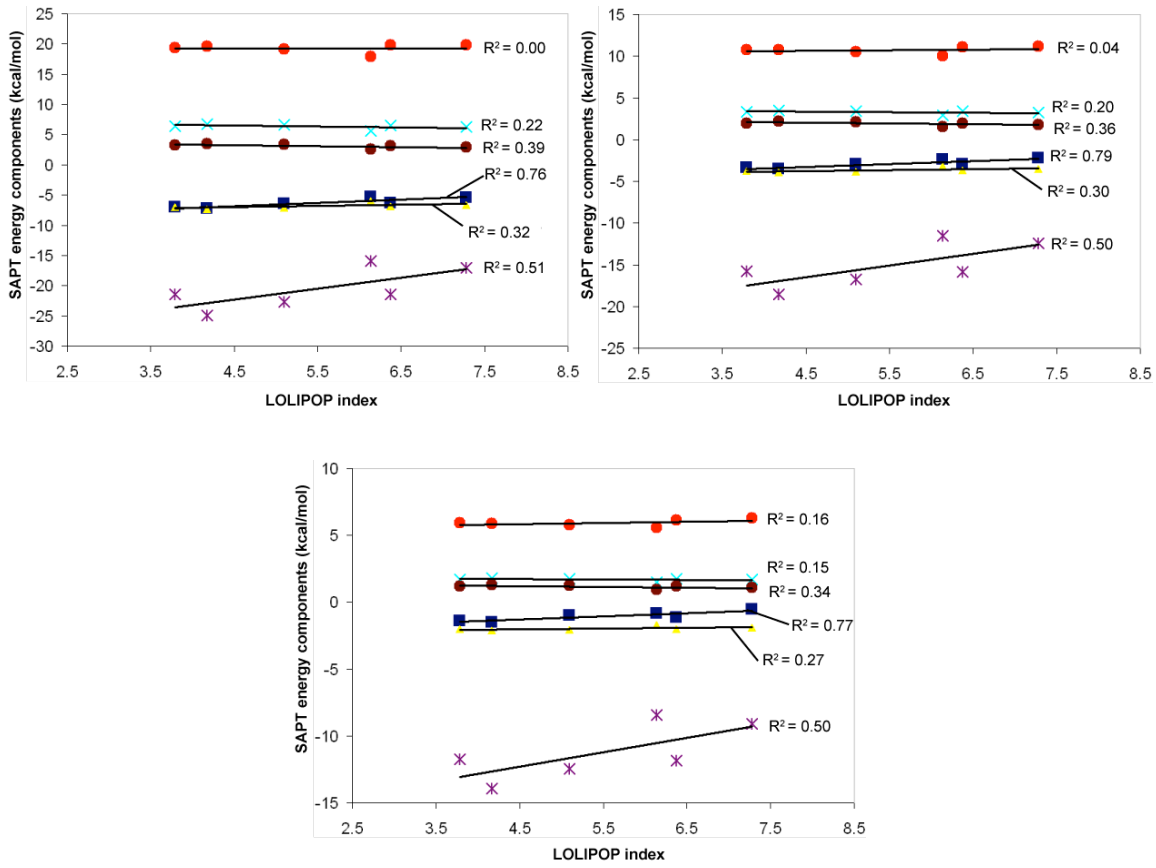

Fig. S8 SAPT0/aug-cc-pVDZ energy components plotted against LOLIPOP index for parallel stacked complexes of benzene: E^1_{elst} (blue squares), E^1_{exch} (red circles), E^2_{ind} (yellow triangles), $E^2_{exch\text{-}ind}$ (light blue crosses), E^2_{disp} (purple stars) and $E^2_{exch\text{-}disp}$ (brown circles) for vertical distance of 3.3 Å (top left), 3.5 Å (top right) and 3.7 Å (bottom). R^2 values indicate in all cases that the best correlation is between LOLIPOP and E^1_{elst}.

SAPT energy components

Table S1 SAPT0/aug-cc-pVDZ energy components and HF/aug-cc-pVDZ interaction energy for parallel stacked complexes with benzene at 3.3, 3.5 and 3.7 Å.

SAPT (kcal/mol)	E^1_{elst}	E^1_{exch}	$E^2_{ind.}$	$E^2_{exch-ind}$	E^2_{disp}	$E^2_{exch-disp}$	HF	HF + disp
Vertical distance 3.3 Å								
Benzene	-5.38	19.83	-6.63	6.24	-17.05	2.91	14.05	-0.09
Pyridine	-5.33	17.90	-5.95	5.58	-15.92	2.58	12.21	-1.13
Radialene	-7.04	19.42	-6.98	6.41	-21.42	3.21	11.81	-6.40
S-indacene	-6.47	19.12	-7.17	6.60	-22.64	3.38	12.08	-7.17
Triphenylene ext. ring	-6.37	19.77	-6.90	6.48	-21.38	3.19	12.98	-5.21
Triphenylene central ring	-7.29	19.60	-7.29	6.75	-24.88	3.50	11.77	-9.61
Vertical distance 3.5 Å								
Benzene	-2.20	11.19	-3.57	3.25	-12.39	1.79	8.67	-1.92
Pyridine	-2.42	10.02	-3.17	2.89	-11.53	1.57	7.32	-2.65
Radialene	-3.39	10.77	-3.75	3.33	-15.78	1.96	6.96	-6.85
S-indacene	-2.92	10.55	-3.85	3.41	-16.73	2.07	7.19	-7.47
Triphenylene ext. ring	-2.99	11.05	-3.71	3.37	-15.85	1.96	7.72	-6.16
Triphenylene central ring	-3.57	10.78	-3.92	3.50	-18.52	2.14	6.79	-9.59
Vertical distance 3.7 Å								
Benzene	-0.52	6.27	-1.94	1.68	-9.07	1.09	5.49	-2.49
Pyridine	-0.87	5.57	-1.70	1.47	-8.43	0.94	4.48	-3.01
Radialene	-1.39	5.93	-2.03	1.70	-11.73	1.18	4.21	-6.34
S-indacene	-1.01	5.78	-2.09	1.73	-12.48	1.25	4.41	-6.81
Triphenylene ext. ring	-1.16	6.13	-2.02	1.73	-11.86	1.19	4.68	-5.99
Triphenylene central ring	-1.51	5.87	-2.13	1.78	-13.92	1.29	4.01	-8.61

Interaction energies with caffeine

Table S2 Interaction energies of caffeine-candidate complexes computed with PBE0-dDsC/def2-TZVP, B97-dDsC/def2-TZVP, PBE-dDsC/def2-TZVP, M06-2X/def2-TZVP, RI-MP2/def2-TZVP and RI-SCS-MP2/def2-TZVP. All geometries optimized with PBE0-dDsC/def2-SVP.

Interaction energies (kcal/mol)	PBE0-dDsC	B97-dDsC	PBE-dDsC	M06-2X	RI-MP2	SCS-RI-MP2
Candidate A	-14.77	-13.98	-13.10	-11.91	-17.65	-11.49
Candidate B	-14.95	-13.77	-13.01	-13.86	-19.12	-12.22
Candidate C	-16.46	-15.69	-14.48	-14.21	-20.42	-13.39
Candidate D	-16.33	-15.55	-14.68	-13.20	-19.64	-12.88
Candidate E	-15.14	-14.53	-13.58	-12.22	-17.93	-11.96

Candidate chemosensors

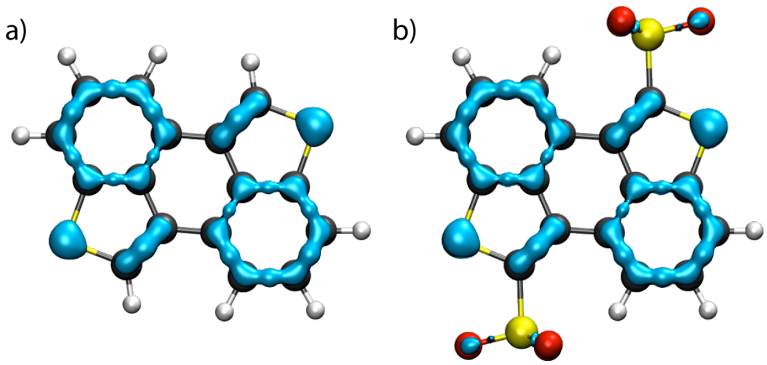

Fig. S9 LOL isosurfaces (isovalue 0.55) obtained from the π-density for molecules **C** and **C-dye**. The sulfonyl groups do not affect the LOL_{π} isosurface.

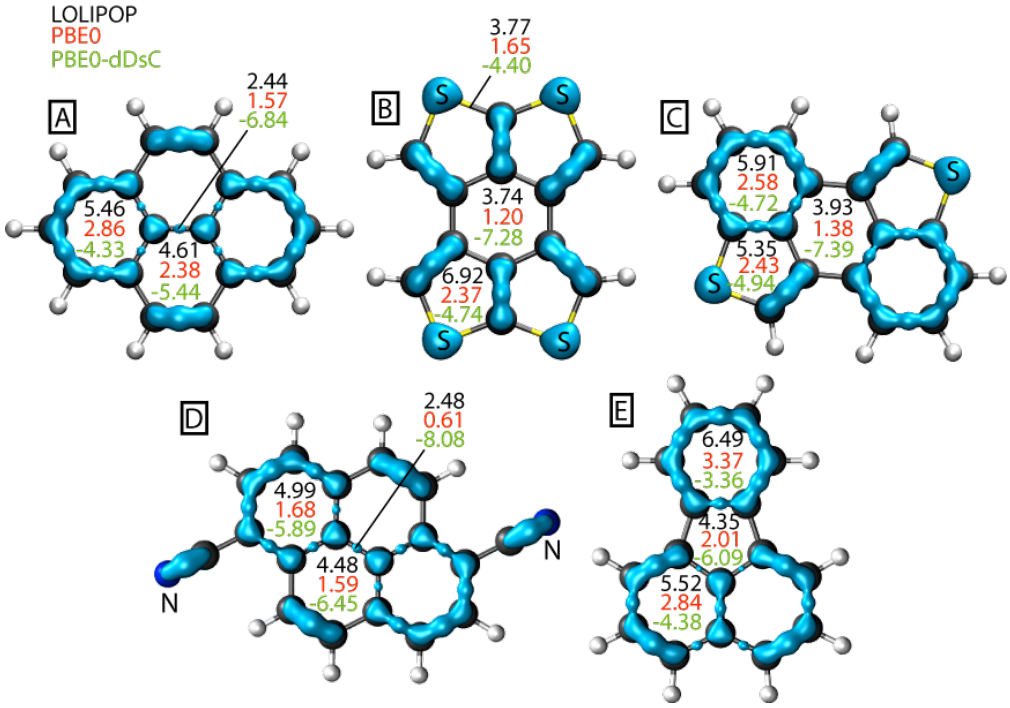

Fig. S10 LOLIPOP index (black), PBE0 interaction energies (for benzene) without (red) and with (green) dispersion correction and LOL isovalues of 0.55 obtained from the π-density. Nitrogen and sulfur atoms are explicitly indicated and values corresponding to stacking on bonds are noted outside molecules.

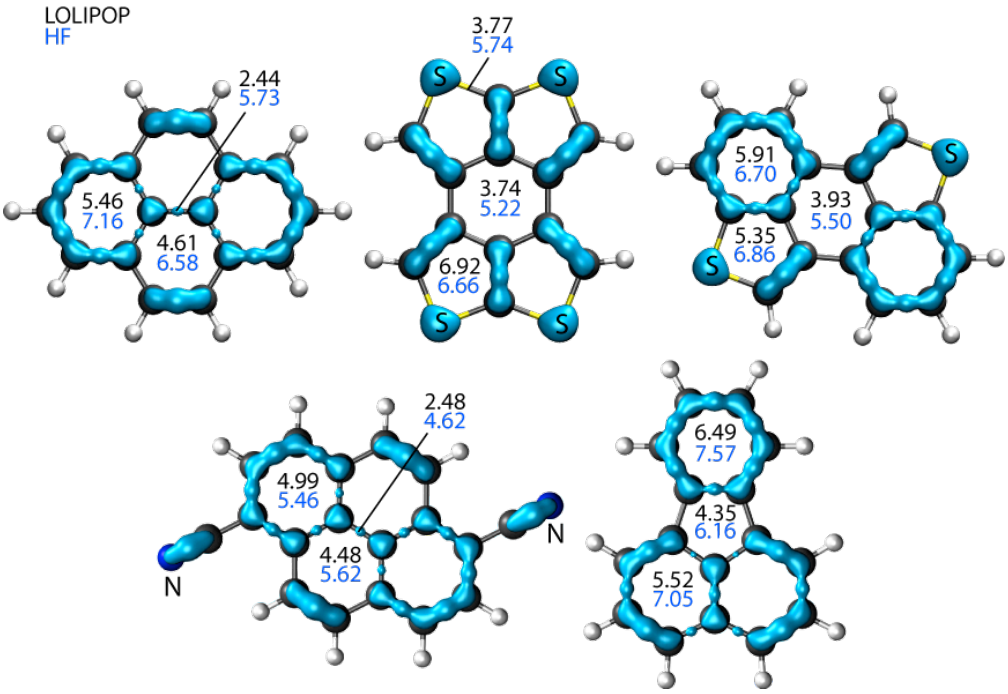

Fig. S11 LOLIPOP index (black), HF interaction energies for benzene (blue) and LOL isovalues of 0.55 obtained from the π-density. Nitrogen, sulfur and oxygen atoms are explicitly indicated and values corresponding to stacking on bonds are noted outside molecules.

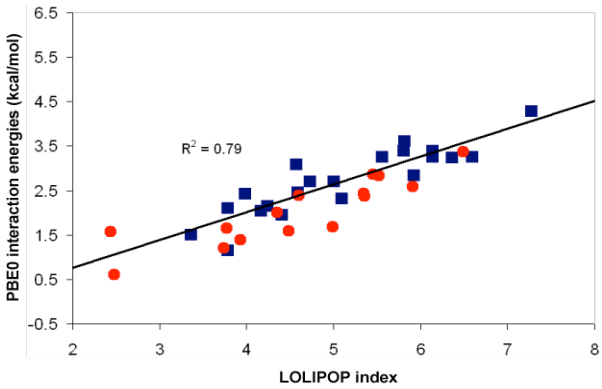

Fig. S12 PBE0 interaction energies for the validation set (blue squares) and candidate chemosensors (red circles) plotted against LOLIPOP index. Linear regression takes only validation set into account.

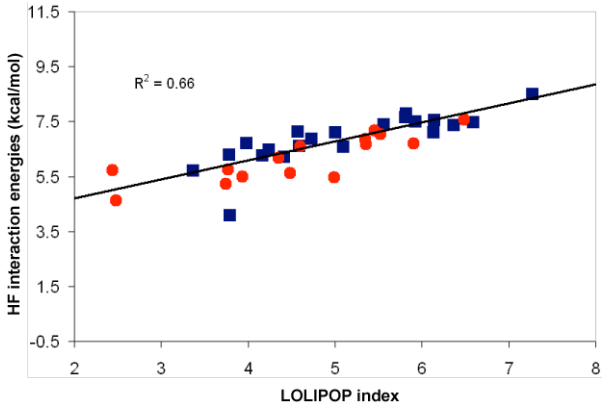

Fig. S13 HF interaction energies for the validation set (blue squares) and candidate chemosensors (red circles) plotted against LOLIPOP index. Linear regression takes only validation set into account.

Experimental section

General: Sodium fluoranthene-8-sulfonate was purchased from Sigma Aldrich and used without further purifications. Buffer solution (100 mM phosphate buffer, pH 7.0) was prepared by dissolving appropriate amounts of K_2HPO_4 and KH_2PO_4 in water. Fluorescence measurements were performed at room temperature on a Varian Cary Eclipse spectrofluorimeter. Absorbance spectra were recorded on a Perkin-Elmer Lambda 40 spectrometer.

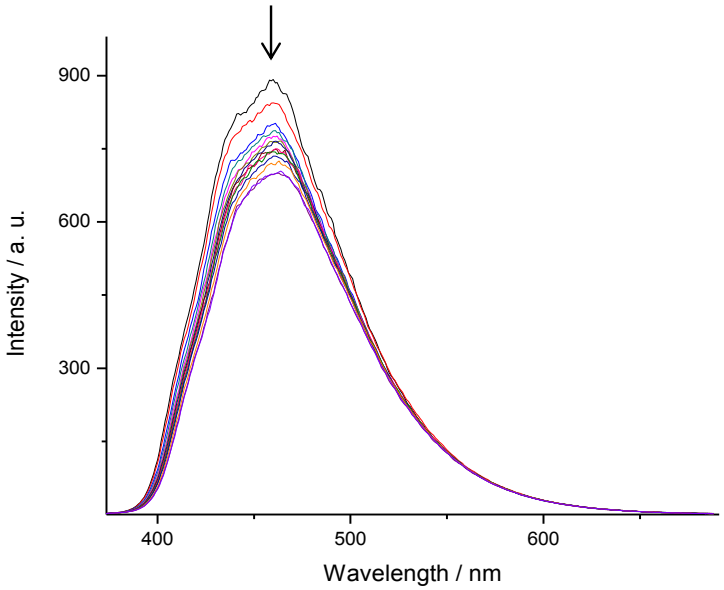

Figure S14. Fluorescence spectra (λ_{ex} = 350 nm) of buffered aqueous solutions (100 mM phosphate buffer, pH 7.0) containing sodium fluoranthene-8-sulfonate (23 µM) and different amounts of caffeine (0 – 4.5 mM).

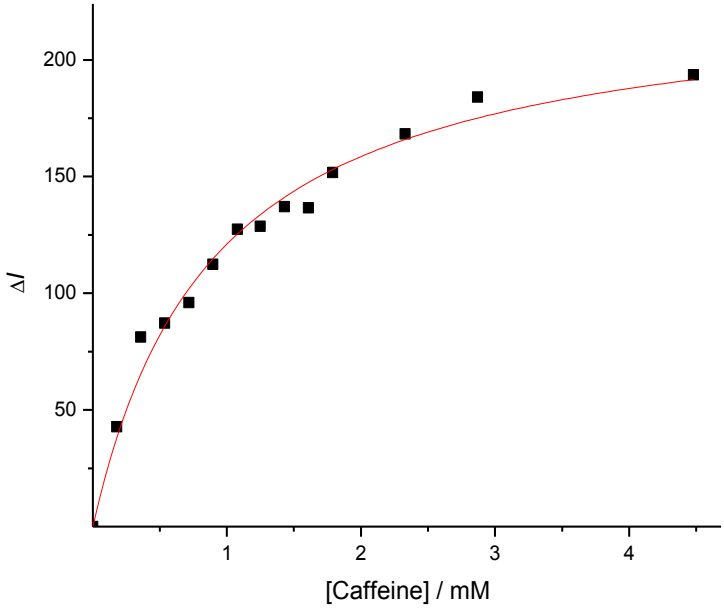

Figure S15. Difference in fluorescence emission intensity at 459 nm (λ_{ex} = 350 nm) of buffered aqueous solutions (100 mM phosphate buffer, pH 7.0) containing sodium fluoranthene-8-sulfonate (23 µM) and different amounts of caffeine (0 – 4.5 mM). The red line shows the curve obtained from fitting the data to a 1:1 binding model (apparent binding constant: K_a = 1.1±0.1 x 10^3 M^{-1}). Data points are the average of three independent measurements.

The binding constant was calculated assuming a negligible self-association of the dye. UV-Vis data suggest that this assumption is a valid approximation: spectra of buffered aqueous solutions (100 mM phosphate buffer, pH 7.0) containing different amounts of sodium fluoranthene-8-sulfonate (0.27 mM – 2.5 µM) showed a linear correlation between absorbance and concentration. Furthermore, variation of the dye concentration did not result in shifts of the position of the maxima/minima in the spectra.

References

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XYZ geometries of all species

Benzene

```
13
Benzene
C    -0.696603   -1.206830    3.500000
C     0.696679   -1.206683    3.500000
C     1.393322    0.000000    3.500000
C     0.696577    1.206833    3.500000
C    -0.696629    1.206713    3.500000
C    -1.393344   -0.000036    3.500000
X     0.000000    0.000000    3.500000
H     1.242820   -2.152980    3.500000
H     2.485925   -0.000280    3.500000
H     1.243168    2.152847    3.500000
H    -1.242938    2.152912    3.500000
H    -2.485923    0.000486    3.500000
H    -1.243041   -2.152961    3.500000
```

s-triazine

```
10
s-triazine
N    -0.687933    1.191776    3.500000
C    -1.293842    0.000001    3.500000
N    -0.687983   -1.191784    3.500000
C     0.647111   -1.120954    3.500000
N     1.375494    0.000000    3.500000
C     0.647152    1.120964    3.500000
```

X	0.000000	0.000000	3.500000
H	-2.382645	0.000002	3.500000
H	1.190790	-2.064182	3.500000
H	1.190858	2.064177	3.500000

Anthracene

24
Anthracene

C	0.000000	0.000000	1.403629
C	0.000000	0.000000	-1.403629
C	0.000000	1.223983	0.722774
C	0.000000	-1.223983	-0.722774
C	0.000000	-1.223983	0.722774
C	0.000000	1.223983	-0.722774
C	0.000000	2.479290	1.407090
C	0.000000	-2.479290	-1.407090
C	0.000000	-2.479290	1.407090
C	0.000000	2.479290	-1.407090
C	0.000000	3.660664	0.712892
C	0.000000	-3.660664	-0.712892
C	0.000000	-3.660664	0.712892
C	0.000000	3.660664	-0.712892
H	0.000000	0.000000	2.492069
H	0.000000	0.000000	-2.492069
H	0.000000	2.477663	2.494766
H	0.000000	-2.477663	-2.494766
H	0.000000	-2.477663	2.494766
H	0.000000	2.477663	-2.494766
H	0.000000	4.606923	1.247530
H	0.000000	-4.606923	-1.247530
H	0.000000	-4.606923	1.247530
H	0.000000	4.606923	-1.247530

Fluoranthene

26
Fluoranthene

C	3.703536	-0.698934	-0.000114
C	2.499775	-1.414437	-0.000312
C	1.297843	-0.713880	-0.000181
C	1.297872	0.713756	0.000113
C	2.499735	1.414424	0.000341
C	3.703535	0.698942	0.000173
C	-0.105234	1.171730	-0.000096
C	-0.903922	0.000012	-0.000038
C	-0.105300	-1.171729	0.000007
C	-0.741033	-2.396876	0.000104
C	-2.163941	-2.429628	0.000134
C	-2.934262	-1.279026	0.000105
C	-2.307444	0.000014	0.000006
C	-0.740961	2.396870	-0.000156
C	-2.163882	2.429646	-0.000103
C	-2.934238	1.279082	-0.000040
H	4.647649	-1.237000	-0.000309
H	-0.185352	-3.331307	0.000082
H	-4.019228	-1.350653	0.000129
H	-0.185308	3.331321	-0.000151
H	-4.019201	1.350732	0.000003
H	2.510113	-2.501595	-0.000303
H	4.647614	1.237083	0.000354
H	2.509988	2.501572	0.000468
H	-2.659320	3.397023	-0.000079
H	-2.659437	-3.396975	0.000151

Coronene

36
Coronene

C	-0.375642	-1.376955	-0.000001
C	1.004679	-1.013807	0.000000
C	1.380350	0.363175	0.000000
C	0.375655	1.376957	0.000000

C	-1.004691	1.013801	0.000000
C	-1.380347	-0.363185	0.000000
C	-2.005646	2.023743	0.000000
C	-1.601209	3.388842	0.000000
C	-0.274034	3.738033	0.000000
C	0.749908	2.748780	0.000000
H	-2.368248	4.159411	0.000000
H	0.014362	4.786355	0.000001
C	-2.755516	-0.724959	0.000000
C	-3.100340	-2.106252	0.000000
C	-2.134322	-3.081015	0.000000
C	-0.749917	-2.748808	0.000000
C	2.755514	0.724962	0.000000
C	3.735480	-0.307727	0.000001
C	3.374304	-1.631718	0.000001
C	2.005667	-2.023762	0.000000
H	4.786329	-0.028742	0.000001
H	4.137907	-2.405692	0.000001
H	-2.418303	-4.130507	0.000000
H	-4.152451	-2.380550	0.000000
C	-3.374301	1.631726	0.000000
C	-3.735480	0.307740	0.000000
C	2.134315	3.081021	0.000000
C	3.100333	2.106262	0.000001
C	1.601214	-3.388826	0.000000
C	0.274023	-3.738022	0.000000
H	-4.137893	2.405708	0.000000
H	-4.786326	0.028742	0.000000
H	2.418284	4.130514	0.000001
H	4.152449	2.380546	0.000001
H	2.368205	-4.159446	0.000000
H	-0.014305	-4.786365	-0.000001

Naphthalene

18
Naphthalene

C	2.433615	-0.708401	0.000000
C	2.433615	0.708401	0.000000
C	1.244732	1.402504	0.000000
C	0.000000	0.717048	0.000000
C	0.000000	-0.717048	0.000000
C	1.244732	-1.402504	0.000000
C	-1.244732	-1.402504	0.000000
C	-1.244732	1.402504	0.000000
C	-2.433615	-0.708401	0.000000
C	-2.433615	0.708401	0.000000
H	3.378094	1.245801	0.000000
H	1.242285	-2.490127	0.000000
H	1.242285	2.490127	0.000000
H	3.378094	-1.245801	0.000000
H	-1.242285	-2.490127	0.000000
H	-3.378094	-1.245801	0.000000
H	-1.242285	2.490127	0.000000
H	-3.378094	1.245802	0.000000

Candidate B

20
Candidate B

S	1.626268	-3.333594	-0.000160
C	0.000073	-2.708216	0.000063
C	0.000010	-1.334698	0.000166
C	1.306345	-0.732885	0.000176
C	2.280404	-1.696172	0.000208
C	1.306370	0.732967	0.000179
C	-0.000010	1.334698	0.000166
C	-1.306345	0.732885	0.000176
C	-1.306370	-0.732967	0.000179
C	-0.000073	2.708216	0.000063
S	1.626136	3.333716	-0.000313
C	2.280404	1.696217	0.000363
S	-1.626268	3.333594	-0.000160
C	-2.280404	1.696172	0.000208

S	-1.626136	-3.333716	-0.000313
C	-2.280404	-1.696217	0.000363
H	-3.355822	1.576066	0.000028
H	3.355822	-1.576066	0.000028
H	3.355836	1.576227	0.000605
H	-3.355836	-1.576227	0.000605

Candidate D

28
Candidate D

C	1.903255	-2.425669	0.000326
C	0.660747	-1.768401	0.000127
C	0.627178	-0.341020	0.000101
C	1.842634	0.406283	0.000275
C	3.071089	-0.301771	0.000473
C	3.089030	-1.706142	0.000496
C	-0.627187	0.341029	-0.000101
C	-1.842628	-0.406277	-0.000275
C	-1.777875	-1.839527	-0.000243
C	-0.579740	-2.487906	-0.000051
C	-0.660760	1.768422	-0.000127
C	-1.903248	2.425676	-0.000326
C	-3.089040	1.706136	-0.000497
C	-3.071108	0.301793	-0.000473
C	0.579745	2.487921	0.000051
C	1.777870	1.839545	0.000243
H	-0.546804	-3.574145	-0.000030
H	-2.706805	-2.401462	-0.000377
H	-1.930030	3.511741	-0.000346
H	-4.043691	2.221885	-0.000651
C	-4.311828	-0.412102	-0.000654
H	1.930001	-3.511735	0.000346
C	4.311832	0.412083	0.000654
H	4.043698	-2.221858	0.000651
H	0.546804	3.574159	0.000030
H	2.706805	2.401473	0.000377
N	-5.319560	-0.995138	-0.000802
N	5.319594	0.995069	0.000802

2-methylene-1,2-dihydronaphthalene

21
2-methylene-1,2-dihydronaphthalene

C	0.000000	0.704993	0.000000
C	0.784918	-0.552898	0.000000
C	0.728910	1.956236	0.000000
C	2.235862	-0.448251	0.000000
C	0.145978	-1.747186	0.000000
C	-1.365632	0.662931	0.000000
C	2.085393	1.984843	0.000000
C	-3.479053	-0.550233	0.000000
C	2.855206	0.756190	0.000000
C	-1.350218	-1.885801	0.000000
C	-2.128508	-0.568416	0.000000
H	0.154016	2.879479	0.000000
H	2.810855	-1.371429	0.000000
H	0.725357	-2.668776	0.000000
H	-1.926029	1.596277	0.000000
H	2.612815	2.934911	0.000000
H	3.940232	0.815784	0.000000
H	-1.648481	-2.491821	0.869883
H	-4.029400	0.386539	0.000000
H	-4.068014	-1.463582	0.000000
H	-1.648481	-2.491821	-0.869883

2-methylnaphthalene

21
2-methylnaphthalene

C	-1.920642	1.240742	0.000069
C	-0.573425	0.792221	0.000006
C	-0.309219	-0.615231	-0.000050

C	-1.407299	-1.516650	-0.000049
C	-2.703490	-1.051093	0.000022
C	-2.963613	0.341196	0.000082
C	1.039894	-1.062734	-0.000113
C	2.100521	-0.181021	-0.000101
C	1.822227	1.215912	-0.000106
C	0.531350	1.686834	-0.000041
C	3.531544	-0.660674	0.000170
H	2.653302	1.917991	-0.000167
H	1.228550	-2.134777	-0.000185
H	0.338534	2.757334	-0.000071
H	-1.206468	-2.585611	-0.000092
H	-3.533565	-1.752485	0.000020
H	-2.115531	2.310841	0.000110
H	-3.990497	0.696583	0.000146
H	4.076083	-0.294249	-0.879602
H	3.588407	-1.753603	-0.002666
H	4.074099	-0.299043	0.883179

2,3,6,7-tetrahydrotriphenylene

34
2,3,6,7-tetrahydrotriphenylene

C	-2.513818	-1.496207	0.000000
C	-1.298300	-0.776916	0.000000
C	-0.086277	-1.510580	0.000000
C	-0.160112	-2.921041	0.000000
C	1.230402	-0.823535	0.000000
C	2.388724	-1.516949	0.000000
C	1.277250	0.668392	0.000000
C	2.478745	1.281571	0.000000
C	0.000000	1.441507	0.000000
C	-0.013970	2.790345	0.000000
C	-1.300086	0.708234	0.000000
C	-2.451608	1.412821	0.000000
H	-3.455992	-0.961805	0.000000
H	0.750163	-3.508096	0.000000
H	2.374164	-2.601607	0.000000
H	2.532142	2.366107	0.000000
H	0.922119	3.340607	0.000000
H	-3.405633	0.896617	0.000000
C	3.771647	-0.933201	0.000000
H	4.314016	-1.333254	0.869475
H	4.314016	-1.333254	-0.869475
C	3.821423	0.610629	0.000000
H	4.389073	0.974244	0.869409
H	4.389073	0.974244	-0.869409
C	-1.231078	3.668757	0.000000
H	-1.172105	4.340281	0.869411
H	-1.172105	4.340281	-0.869411
C	-2.575845	2.908773	0.000000
H	-3.181816	3.203729	0.869454
H	-3.181816	3.203729	-0.869454
C	-1.364260	-3.603345	0.000000
H	-1.372604	-4.689977	0.000000
C	-2.560117	-2.879452	0.000000
H	-3.519022	-3.390665	0.000000

Phenanthrene

24
Phenanthrene

C	-3.562132	-0.296787	0.000008
C	-2.883181	-1.529511	-0.000020
C	-1.500446	-1.566387	-0.000027
C	-0.728950	-0.380771	-0.000004
C	-1.423588	0.866579	0.000012
C	-2.837754	0.878692	0.000022
C	0.728953	-0.380769	0.000000
C	1.500447	-1.566392	0.000022
C	2.883177	-1.529511	0.000021
C	3.562135	-0.296785	-0.000003
C	1.423584	0.866577	-0.000013
C	2.837755	0.878690	-0.000017

C	0.679852	2.093722	-0.000012
C	-0.679849	2.093720	0.000008
H	-3.348681	1.838941	0.000038
H	-1.006739	-2.532407	-0.000055
H	1.006733	-2.532406	0.000054
H	3.446066	-2.459060	0.000042
H	3.348675	1.838944	-0.000028
H	4.648406	-0.271568	-0.000004
H	-1.231620	3.030887	0.000017
H	1.231621	3.030887	-0.000025
H	-4.648406	-0.271560	0.000019
H	-3.446059	-2.459064	-0.000040

2,3,6,7,10,11-hexahydrotriphenylene

36
2,3,6,7,10,11-hexahydrotriphenylene

C	1.796041	2.205084	0.000030
C	0.955471	1.149015	-0.000265
C	-0.516792	1.402353	-0.000361
C	-0.955868	2.678405	-0.000149
C	-0.109178	3.917513	0.000190
C	1.412241	3.655688	0.000289
C	-1.473136	0.252832	-0.000201
C	-0.956417	-1.148920	0.000047
C	0.517503	-1.402494	0.000143
C	1.472687	-0.253897	-0.000010
C	1.012435	-2.658167	0.000167
C	2.461004	-3.050408	0.000056
C	3.447904	-1.863612	-0.000100
C	2.797625	-0.511108	-0.000116
C	-1.842342	-2.167258	0.000215
C	-3.338715	-2.053150	0.000182
C	-3.872618	-0.604927	-0.000070
C	-2.807984	0.452854	-0.000244
H	-1.487045	-3.192761	0.000234
H	-3.203401	1.463626	-0.000921
H	-2.021695	2.883007	-0.000380
H	1.884018	4.138065	-0.868828
H	2.869082	2.041643	0.000637
H	4.120036	-1.924211	0.868896
H	3.507218	0.310072	-0.001110
H	0.335048	-3.506064	0.000333
H	4.118885	-1.923670	-0.870069
H	2.643073	-3.699993	-0.869163
H	2.642898	-3.699700	0.869511
H	-4.525816	-0.437408	-0.869389
H	-4.525666	-0.437494	0.869427
H	-3.726910	-2.605034	-0.868962
H	-3.726921	-2.604707	0.869559
H	-0.392799	4.529817	-0.868767
H	-0.392849	4.528658	0.870132
H	1.883669	4.137336	0.870043

1,2,5,6,9,10-hexahydrotriphenylene

36
1,2,5,6,9,10-hexahydrotriphenylene

C	2.878448	-0.588147	0.000006
C	1.379867	-0.293044	-0.000031
C	0.434482	-1.339820	-0.000031
C	0.910519	-2.731401	0.000000
C	2.204511	-3.072314	0.000028
C	3.323784	-2.075417	0.000033
C	-0.943765	-1.048826	-0.000022
C	-1.377231	0.293266	-0.000008
C	-0.436164	1.341322	-0.000010
C	0.942886	1.045921	-0.000025
C	-0.929505	2.786828	0.000008
C	0.135670	3.916121	0.000004
C	1.558615	3.445109	-0.000013
C	1.910089	2.153950	-0.000027
C	-2.820201	0.577292	0.000008
C	-3.762901	-0.372290	0.000008

C	-3.459804	-1.840240	-0.000008
C	-1.949237	-2.198682	-0.000025
H	-3.134284	1.615032	0.000036
H	-4.813873	-0.087858	0.000022
H	0.169218	-3.522568	0.000066
H	2.484203	-4.124567	0.000184
H	2.330298	4.213206	-0.000125
H	2.965998	1.907587	-0.000041
H	-3.951188	-2.299865	0.869796
H	-3.951203	-2.299843	-0.869815
H	-1.741810	-2.833768	0.870146
H	-1.741798	-2.833762	-0.870193
H	3.967519	-2.271063	0.869860
H	3.967517	-2.270849	-0.869788
H	3.324599	-0.090876	-0.870227
H	3.324755	-0.090643	0.870027
H	-0.016829	4.571608	-0.869649
H	-0.016763	4.571222	0.870021
H	-1.583455	2.924634	-0.869944
H	-1.583284	2.924615	0.870252

Triphenylene

30
Triphenylene

C	-0.327386	1.406662	0.000216
C	-1.389663	0.394429	0.000116
C	-1.054848	-0.987028	0.000116
C	0.353071	-1.400717	0.000214
C	1.381938	-0.419965	-0.000348
C	1.036327	1.005999	-0.000343
C	2.726550	-0.854823	-0.000651
C	3.062064	-2.196760	-0.000253
C	2.048249	-3.163347	0.000566
C	0.723685	-2.764504	0.000792
H	3.529748	-0.127830	-0.001159
H	4.107024	-2.494451	-0.000501
H	2.295885	-4.221283	0.001037
H	-0.040424	-3.532491	0.001536
C	2.032493	2.008426	-0.000650
C	1.716030	3.355022	-0.000248
C	0.372069	3.749907	0.000571
C	-0.622642	2.788659	0.000799
C	-2.104196	-1.933666	-0.000148
C	-3.434012	-1.552829	-0.000308
C	-3.763873	-0.191473	-0.000308
C	-2.755908	0.755861	-0.000145
H	-1.876958	-2.992949	-0.000372
H	-4.214505	-2.308727	-0.000521
H	-4.803792	0.123368	-0.000525
H	-3.038753	1.801738	-0.000374
H	0.107621	4.803768	0.001053
H	-1.653685	3.121240	0.001557
H	3.079559	1.730222	-0.001174
H	2.508582	4.098264	-0.000498

9,10-dimethylene-9,10-dihydroanthracene

28
9,10-dimethylene-9,10-dihydroanthracene

C	0.000000	3.720653	0.698918
C	0.000000	2.514318	1.377723
C	0.000000	1.272413	0.707498
C	0.000000	1.272413	-0.707498
C	0.000000	2.514318	-1.377723
C	0.000000	3.720653	-0.698918
C	0.000000	0.000000	1.476839
C	0.000000	-1.272413	0.707498
C	0.000000	-1.272413	-0.707498
C	0.000000	0.000000	-1.476839
C	0.000000	-2.514318	-1.377723
C	0.000000	-3.720653	-0.698918
C	0.000000	-3.720653	0.698918
C	0.000000	-2.514318	1.377723

C	0.000000	0.000000	-2.827306
C	0.000000	0.000000	2.827306
H	0.000000	2.542033	-2.460354
H	0.000000	-2.542033	2.460354
H	0.000000	-2.542033	-2.460354
H	0.000000	2.542033	2.460354
H	0.000000	4.655213	-1.253155
H	0.000000	-4.655213	1.253155
H	0.000000	-4.655213	-1.253155
H	0.000000	4.655213	1.253155
H	0.000000	-0.909482	3.412946
H	0.000000	0.909482	3.412946
H	0.000000	-0.909482	-3.412946
H	0.000000	0.909482	-3.412946

Pyridine

11
Pyridine

C	1.209288	0.653771	0.000000
C	1.171367	-0.740255	0.000000
C	-0.071442	-1.372805	0.000000
C	-1.220428	-0.579971	0.000000
N	-1.201301	0.759153	0.000000
C	0.000000	1.351215	0.000000
H	2.152468	1.192372	0.000000
H	2.090137	-1.320887	0.000000
H	-0.153078	-2.455860	0.000000
H	-2.206857	-1.041836	0.000000
H	-0.006274	2.440402	0.000000

Pyrene

26
Pyrene

C	-1.428834	-1.235961	-0.000129
C	-0.680832	-2.463854	0.000053
C	0.680675	-2.464020	0.000244
C	1.428860	-1.236201	0.000278
C	0.713435	-0.000080	0.000101
C	-0.713443	-0.000059	-0.000104
C	1.429133	1.236132	0.000129
C	2.832764	1.210565	0.000324
C	3.523827	-0.000243	0.000495
C	2.832901	-1.210701	0.000475
H	-1.231045	-3.401842	0.000038
H	1.230692	-3.402098	0.000385
H	3.379892	2.150618	0.000343
H	4.610502	-0.000048	0.000644
H	3.379709	-2.150935	0.000605
C	0.680799	2.464057	-0.000043
C	-0.680569	2.464199	-0.000237
C	-1.429150	1.236371	-0.000283
C	-2.832600	1.210676	-0.000482
C	-3.523830	-0.000312	-0.000503
C	-2.833124	-1.210613	-0.000324
H	-3.379600	-2.151035	-0.000327
H	-3.380105	2.150522	-0.000621
H	-4.610513	0.000555	-0.000638
H	1.230805	3.402161	-0.000022
H	-1.230411	3.402383	-0.000362

Candidate C

26
Candidate C

S	3.381974	1.564196	0.000003
C	1.748177	2.190985	-0.000059
C	0.790819	1.214670	-0.000015
C	1.381399	-0.106474	-0.000015
C	2.788082	-0.092232	-0.000017
C	-0.670152	1.329016	0.000009
C	-1.381399	0.106474	0.000012

C	-0.790819	-1.214670	0.000015
C	0.670152	-1.329016	0.000002
C	-1.748177	-2.190985	0.000112
S	-3.381974	-1.564196	-0.000107
C	-2.788082	0.092232	0.000026
C	-3.520668	1.283821	0.000054
C	-2.813204	2.484841	0.000051
C	-1.410021	2.513482	0.000021
C	3.520668	-1.283821	-0.000010
C	2.813204	-2.484841	0.000017
C	1.410021	-2.513482	0.000030
H	-3.360856	3.422895	0.000042
H	3.360856	-3.422895	0.000040
H	-4.606149	1.278526	0.000035
H	4.606149	-1.278526	-0.000003
H	-0.900289	3.472648	0.000006
H	0.900289	-3.472648	0.000060
H	-1.602428	-3.262909	0.000179
H	1.602428	3.262909	-0.000083

Radialene

24
Radialene

C	-1.480897	0.256353	-0.000430
C	-0.518373	1.410583	-0.000414
C	0.962451	1.154273	-0.000061
C	1.480933	-0.256409	0.000276
C	0.518359	-1.410618	0.000262
C	-0.962436	-1.154265	-0.000088
C	-0.983369	2.675629	0.003928
C	1.825626	2.189474	-0.003816
C	2.809041	-0.486348	0.003651
C	0.983462	-2.675630	-0.003588
C	-1.825779	-2.189312	0.003497
C	-2.809004	0.486224	-0.003425
H	-3.232493	1.481196	-0.005526
H	-3.542118	-0.308810	-0.004166
H	-0.333479	3.539920	0.007028
H	-2.038313	2.913175	0.005497
H	2.899007	2.058290	-0.004336
H	1.504258	3.221980	-0.007029
H	3.232498	-1.481337	0.005817
H	3.542211	0.308609	0.004638
H	0.333638	-3.539983	-0.006320
H	2.038425	-2.913036	-0.005109
H	-2.899142	-2.057859	0.004156
H	-1.504578	-3.221872	0.006598

S-indacene

20
S-indacene

C	-1.210927	-0.721969	-0.000005
C	1.210925	0.721984	-0.000011
C	-1.193480	0.729656	-0.000003
C	1.193486	-0.729641	-0.000009
C	-0.033451	-1.442555	-0.000008
C	0.033454	1.442581	-0.000007
C	-2.598301	-1.125599	0.000000
C	2.598289	1.125584	-0.000001
C	-2.525432	1.159364	0.000008
C	2.525440	-1.159378	0.000008
C	-3.383236	0.013245	0.000008
C	3.383234	-0.013272	0.000012
H	-0.036773	-2.531429	-0.000006
H	0.036771	2.531456	-0.000004
H	-2.952542	-2.150447	-0.000005
H	2.952559	2.150420	-0.000006
H	-2.859190	2.191979	0.000011
H	2.859164	-2.192006	0.000012
H	-4.465988	0.043964	0.000019
H	4.465987	-0.043944	0.000026

Anthracene-benzene ext. ring complex

36
Anthracene-benzene ext. ring complex
C -1.446398 2.429690 0.000000
C 1.360429 2.478849 0.000000
C -0.787081 3.665408 0.000000
C 0.701112 1.243131 0.000000
C -0.744214 1.217817 0.000000
C 0.658245 3.690722 0.000000
C -1.493275 4.908539 0.000000
C 1.407306 0.000000 0.000000
C -1.406443 -0.049280 0.000000
C 1.320474 4.957820 0.000000
C -0.819871 6.101889 0.000000
C 0.733902 -1.193349 0.000000
C -0.691664 -1.218317 0.000000
C 0.605695 6.126856 0.000000
H -2.534671 2.410630 0.000000
H 2.448702 2.497909 0.000000
H -2.580755 4.887866 0.000000
H 2.494787 0.020674 0.000000
H -2.493980 -0.066701 0.000000
H 2.408011 4.975240 0.000000
H -1.370997 7.038640 0.000000
H 1.285028 -2.130101 0.000000
H -1.209649 -2.173793 0.000000
H 1.123680 7.082332 0.000000
C -0.696603 -1.206830 3.500000
C 0.696679 -1.206683 3.500000
C 1.393322 0.000000 3.500000
C 0.696577 1.206833 3.500000
C -0.696629 1.206713 3.500000
C -1.393344 -0.000036 3.500000
H 1.242820 -2.152980 3.500000
H 2.485925 -0.000280 3.500000
H 1.243168 2.152847 3.500000
H -1.242938 2.152912 3.500000
H -2.485923 0.000486 3.500000
H -1.243041 -2.152961 3.500000

Anthracene-benzene central ring complex

36
Anthracene-benzene central ring complex
C -1.403629 0.000000 0.000000
C 1.403629 0.000000 0.000000
C -0.722774 1.223983 0.000000
C 0.722774 -1.223983 0.000000
C -0.722774 -1.223983 0.000000
C 0.722774 1.223983 0.000000
C -1.407090 2.479290 0.000000
C 1.407090 -2.479290 0.000000
C -1.407090 -2.479290 0.000000
C 1.407090 2.479290 0.000000
C -0.712892 3.660664 0.000000
C 0.712892 -3.660664 0.000000
C -0.712892 -3.660664 0.000000
C 0.712892 3.660664 0.000000
H -2.492069 0.000000 0.000000
H 2.492069 0.000000 0.000000
H -2.494766 2.477663 0.000000
H 2.494766 -2.477663 0.000000
H -2.494766 -2.477663 0.000000
H 2.494766 2.477663 0.000000
H -1.247530 4.606923 0.000000
H 1.247530 -4.606923 0.000000
H -1.247530 -4.606923 0.000000
H 1.247530 4.606923 0.000000
C -0.696603 -1.206830 3.500000
C 0.696679 -1.206683 3.500000
C 1.393322 0.000000 3.500000
C 0.696577 1.206833 3.500000
C -0.696629 1.206713 3.500000

C -1.393344 -0.000036 3.500000
H 1.242820 -2.152980 3.500000
H 2.485925 -0.000280 3.500000
H 1.243168 2.152847 3.500000
H -1.242938 2.152912 3.500000
H -2.485923 0.000486 3.500000
H -1.243041 -2.152961 3.500000

Anthracene-benzene parallel displaced complex

36
Anthracene-benzene parallel displaced complex
C -1.403629 -3.660664 0.000000
C 1.403629 -3.660664 0.000000
C -0.722774 -4.884647 0.000000
C 0.722774 -2.436681 0.000000
C -0.722774 -2.436681 0.000000
C 0.722774 -4.884647 0.000000
C -1.407090 -6.139954 0.000000
C 1.407090 -1.181374 0.000000
C -1.407090 -1.181374 0.000000
C 1.407090 -6.139954 0.000000
C -0.712892 -7.321328 0.000000
C 0.712892 0.000000 0.000000
C -0.712892 0.000000 0.000000
C 0.712892 -7.321328 0.000000
H -2.492069 -3.660664 0.000000
H 2.492069 -3.660664 0.000000
H -2.494766 -6.138327 0.000000
H 2.494766 -1.183001 0.000000
H -2.494766 -1.183001 0.000000
H 2.494766 -6.138327 0.000000
H -1.247530 -8.267587 0.000000
H 1.247530 0.946259 0.000000
H -1.247530 0.946259 0.000000
H 1.247530 -8.267587 0.000000
C -0.696603 -1.206830 3.500000
C 0.696679 -1.206683 3.500000
C 1.393322 0.000000 3.500000
C 0.696577 1.206833 3.500000
C -0.696629 1.206713 3.500000
C -1.393344 -0.000036 3.500000
H 1.242820 -2.152980 3.500000
H 2.485925 -0.000280 3.500000
H 1.243168 2.152847 3.500000
H -1.242938 2.152912 3.500000
H -2.485923 0.000486 3.500000
H -1.243041 -2.152961 3.500000

Fluoranthene-benzene central ring complex

38
Fluoranthene-benzene central ring complex
C -3.407304 0.698815 0.000106
C -2.203563 1.414353 0.000340
C -1.001611 0.713830 0.000176
C -1.001600 -0.713806 -0.000188
C -2.203443 -1.414508 -0.000451
C -3.407263 -0.699061 -0.000249
C 0.401519 -1.171741 0.000000
C 1.200174 0.000000 0.000000
C 0.401519 1.171718 0.000012
C 1.037217 2.396883 -0.000025
C 2.460124 2.429676 -0.000052
C 3.230478 1.279096 -0.000079
C 2.603696 0.000038 -0.000043
C 1.037281 -2.396863 0.000001
C 2.460203 -2.429598 -0.000053
C 3.230526 -1.279012 -0.000059
H -4.351432 1.236855 0.000327
H 0.481510 3.331299 0.000042
H 4.315442 1.350753 -0.000098
H 0.481654 -3.331329 -0.000051
H 4.315491 -1.350632 -0.000104

H -2.213932 2.501510 0.000385
H -4.351327 -1.237228 -0.000457
H -2.213665 -2.501657 -0.000631
H 2.955668 -3.396961 -0.000124
H 2.955593 3.397037 -0.000021
C -0.696603 -1.206830 3.500000
C 0.696679 -1.206683 3.500000
C 1.393322 0.000000 3.500000
C 0.696577 1.206833 3.500000
C -0.696629 1.206713 3.500000
C -1.393344 -0.000036 3.500000
H 1.242820 -2.152980 3.500000
H 2.485925 -0.000280 3.500000
H 1.243168 2.152847 3.500000
H -1.242938 2.152912 3.500000
H -2.485923 0.000486 3.500000
H -1.243041 -2.152961 3.500000

Fluoranthene-benzene ext.ring complex 1

38
Fluoranthene-benzene ext.ring complex 1
C 2.461278 -4.642642 0.000025
C 2.392478 -3.243981 -0.000255
C 1.144442 -2.629305 -0.000116
C -0.045437 -3.418186 0.000268
C 0.034679 -4.807067 0.000577
C 1.296186 -5.415053 0.000401
C -1.202448 -2.501795 0.000045
C -0.667178 -1.188664 0.000005
C 0.750724 -1.206835 0.000000
C 1.420568 0.000000 0.000000
C 0.661622 1.204052 -0.000016
C -0.723022 1.210315 0.000005
C -1.442711 -0.018869 0.000006
C -2.574846 -2.648899 0.000044
C -3.388415 -1.481044 0.000055
C -2.855121 -0.203217 0.000022
H 3.431421 -5.132219 -0.000175
H 2.506438 0.053186 -0.000064
H -1.262834 2.154182 -0.000009
H -3.046653 -3.628362 0.000125
H -3.514348 0.661479 0.000036
H 3.304306 -2.651876 -0.000314
H 1.369322 -6.499273 0.000645
H -0.865764 -5.416329 0.000773
H -4.468457 -1.602646 0.000125
H 1.194087 2.151553 -0.000075
C -0.696603 -1.206830 3.500000
C 0.696679 -1.206683 3.500000
C 1.393322 0.000000 3.500000
C 0.696577 1.206833 3.500000
C -0.696629 1.206713 3.500000
C -1.393344 -0.000036 3.500000
H 1.242820 -2.152980 3.500000
H 2.485925 -0.000280 3.500000
H 1.243168 2.152847 3.500000
H -1.242938 2.152912 3.500000
H -2.485923 0.000486 3.500000
H -1.243041 -2.152961 3.500000

Fluoranthene-benzene ext. ring complex 2

38
Fluoranthene-benzene ext. ring complex 2
C 1.391422 0.000000 0.000000
C 0.709936 1.223340 -0.000025
C -0.681257 1.221305 -0.000011
C -1.398334 -0.013177 -0.000010
C -0.711037 -1.222736 0.000048
C 0.689267 -1.208733 0.000000
C -2.841631 0.295597 -0.000282
C -2.943696 1.709955 0.000034
C -1.664567 2.322003 0.000302

C	-1.598889	3.700708	0.000664
C	-2.812816	4.443756	0.000733
C	-4.056856	3.835771	0.000484
C	-4.157313	2.414943	0.000109
C	-4.006728	-0.444447	-0.000580
C	-5.253581	0.241946	-0.000502
C	-5.341774	1.623781	-0.000186
H	2.478061	-0.008966	-0.000105
H	-0.649030	4.229585	0.000822
H	-4.959040	4.442685	0.000547
H	-3.995634	-1.531565	-0.000779
H	-6.315924	2.106803	-0.000134
H	1.264955	2.158206	0.000207
H	1.235297	-2.148271	0.000050
H	-1.248247	-2.167936	-0.000049
H	-6.167897	-0.345680	-0.000666
H	-2.755370	5.529102	0.000959
C	-0.696603	-1.206830	3.500000
C	0.696679	-1.206683	3.500000
C	1.393322	0.000000	3.500000
C	0.696577	1.206833	3.500000
C	-0.696629	1.206713	3.500000
C	-1.393344	-0.000036	3.500000
H	1.242820	-2.152980	3.500000
H	2.485925	-0.000280	3.500000
H	1.243168	2.152847	3.500000
H	-1.242938	2.152912	3.500000
H	-2.485923	0.000486	3.500000
H	-1.243041	-2.152961	3.500000

Coronene-triazine ext. ring complex

45
Coronene-triazine ext. ring complex

C	-0.725910	3.696418	-0.000001
C	0.701374	3.701188	0.000000
C	1.419157	2.467496	0.000000
C	0.709599	1.229073	0.000000
C	-0.717711	1.224303	0.000000
C	-1.435481	2.458003	0.000000
C	-1.424645	-0.009446	0.000000
C	-0.682129	-1.224245	0.000000
C	0.690207	-1.219682	0.000000
C	1.424682	-0.000000	0.000000
H	-1.224723	-2.166432	0.000000
H	1.238978	-2.158299	0.000001
C	-2.857433	2.453233	0.000000
C	-3.546521	3.699038	0.000000
C	-2.864280	4.889795	0.000000
C	-1.441022	4.925514	0.000000
C	2.841107	2.472253	0.000000
C	3.521900	3.722574	0.000001
C	2.831776	4.908799	0.000001
C	1.408336	4.934959	0.000000
H	4.609151	3.723773	0.000001
H	3.370172	5.853391	0.000001
H	-3.409087	5.830679	0.000000
H	-4.633784	3.692985	0.000000
C	-2.848096	0.016683	0.000000
C	-3.538221	1.202903	0.000000
C	2.847951	0.035687	0.000000
C	3.530193	1.226439	0.000001
C	0.665814	6.149719	0.000000
C	-0.706539	6.145158	0.000000
H	-3.386479	-0.927914	0.000000
H	-4.625472	1.201717	0.000000
H	3.392747	-0.905202	0.000001
H	4.617457	1.232507	0.000001
H	1.208348	7.091944	0.000000
H	-1.255250	7.083812	-0.000001
N	-0.687933	1.191776	3.500000
C	-1.293842	0.000001	3.500000
N	-0.687983	-1.191784	3.500000
C	0.647111	-1.120954	3.500000
N	1.375494	0.000000	3.500000

C	0.647152	1.120964	3.500000
H	-2.382645	0.000002	3.500000
H	1.190790	-2.064182	3.500000
H	1.190858	2.064177	3.500000

Coronene-benzene ext. ring complex

48
Coronene-benzene ext. ring complex

C	-0.725910	3.696418	-0.000001
C	0.701374	3.701188	0.000000
C	1.419157	2.467496	0.000000
C	0.709599	1.229073	0.000000
C	-0.717711	1.224303	0.000000
C	-1.435481	2.458003	0.000000
C	-1.424645	-0.009446	0.000000
C	-0.682129	-1.224245	0.000000
C	0.690207	-1.219682	0.000000
C	1.424682	-0.000000	0.000000
H	-1.224723	-2.166432	0.000000
H	1.238978	-2.158299	0.000001
C	-2.857433	2.453233	0.000000
C	-3.546521	3.699038	0.000000
C	-2.864280	4.889795	0.000000
C	-1.441022	4.925514	0.000000
C	2.841107	2.472253	0.000000
C	3.521900	3.722574	0.000001
C	2.831776	4.908799	0.000001
C	1.408336	4.934959	0.000000
H	4.609151	3.723773	0.000001
H	3.370172	5.853391	0.000001
H	-3.409087	5.830679	0.000000
H	-4.633784	3.692985	0.000000
C	-2.848096	0.016683	0.000000
C	-3.538221	1.202903	0.000000
C	2.847951	0.035687	0.000000
C	3.530193	1.226439	0.000001
C	0.665814	6.149719	0.000000
C	-0.706539	6.145158	0.000000
H	-3.386479	-0.927914	0.000000
H	-4.625472	1.201717	0.000000
H	3.392747	-0.905202	0.000001
H	4.617457	1.232507	0.000001
H	1.208348	7.091944	0.000000
H	-1.255250	7.083812	-0.000001
C	-0.696603	-1.206830	3.500000
C	0.696679	-1.206683	3.500000
C	1.393322	0.000000	3.500000
C	0.696577	1.206833	3.500000
C	-0.696629	1.206713	3.500000
C	-1.393344	-0.000036	3.500000
H	1.242820	-2.152980	3.500000
H	2.485925	-0.000280	3.500000
H	1.243168	2.152847	3.500000
H	-1.242938	2.152912	3.500000
H	-2.485923	0.000486	3.500000
H	-1.243041	-2.152961	3.500000

Coronene-triazine central ring complex

45
Coronene-triazine central ring complex

C	-0.713639	1.236053	-0.000001
C	0.713653	1.236074	0.000000
C	1.427326	0.000000	0.000000
C	0.713651	-1.236056	0.000000
C	-0.713667	-1.236075	0.000000
C	-1.427327	0.000006	0.000000
C	-1.424702	-2.467466	0.000000
C	-0.686233	-3.684728	0.000000
C	0.686111	-3.684732	0.000000
C	1.424641	-2.467501	0.000000
H	-1.231959	-4.625105	0.000000
H	1.231756	-4.625170	0.000001

C	-2.849287	-0.000033	0.000000
C	-3.534226	1.248059	0.000000
C	-2.848027	2.436539	0.000000
C	-1.424658	2.467521	0.000000
C	2.849285	0.000025	0.000000
C	3.534234	1.248073	0.000001
C	2.848062	2.436588	0.000001
C	1.424717	2.467485	0.000000
H	4.621483	1.245654	0.000001
H	3.389598	3.379384	0.000001
H	-3.389700	3.379231	0.000000
H	-4.621503	1.245624	0.000000
C	-2.848058	-2.436599	0.000000
C	-3.534232	-1.248090	0.000000
C	2.848020	-2.436551	0.000000
C	3.534221	-1.248075	0.000001
C	0.686241	3.684710	0.000000
C	-0.686120	3.684715	0.000000
H	-3.389581	-3.379400	0.000000
H	-4.621481	-1.245658	0.000000
H	3.389682	-3.379247	0.000001
H	4.621499	-1.245625	0.000001
H	1.231907	4.625124	0.000000
H	-1.231704	4.625190	-0.000001
N	-0.687933	1.191776	3.500000
C	-1.293842	0.000001	3.500000
N	-0.687983	-1.191784	3.500000
C	0.647111	-1.120954	3.500000
N	1.375494	0.000000	3.500000
C	0.647152	1.120964	3.500000
H	-2.382645	0.000002	3.500000
H	1.190790	-2.064182	3.500000
H	1.190858	2.064177	3.500000

Coronene-benzene central ring complex

48
Coronene-benzene central ring complex

C	-0.713639	1.236053	-0.000001
C	0.713653	1.236074	0.000000
C	1.427326	0.000000	0.000000
C	0.713651	-1.236056	0.000000
C	-0.713667	-1.236075	0.000000
C	-1.427327	0.000006	0.000000
C	-1.424702	-2.467466	0.000000
C	-0.686233	-3.684728	0.000000
C	0.686111	-3.684732	0.000000
C	1.424641	-2.467501	0.000000
H	-1.231959	-4.625105	0.000000
H	1.231756	-4.625170	0.000001
C	-2.849287	-0.000033	0.000000
C	-3.534226	1.248059	0.000000
C	-2.848027	2.436539	0.000000
C	-1.424658	2.467521	0.000000
C	2.849285	0.000025	0.000000
C	3.534234	1.248073	0.000001
C	2.848062	2.436588	0.000001
C	1.424717	2.467485	0.000000
H	4.621483	1.245654	0.000001
H	3.389598	3.379384	0.000001
H	-3.389700	3.379231	0.000000
H	-4.621503	1.245624	0.000000
C	-2.848058	-2.436599	0.000000
C	-3.534232	-1.248090	0.000000
C	2.848020	-2.436551	0.000000
C	3.534221	-1.248075	0.000001
C	0.686241	3.684710	0.000000
C	-0.686120	3.684715	0.000000
H	-3.389581	-3.379400	0.000000
H	-4.621481	-1.245658	0.000000
H	3.389682	-3.379247	0.000001
H	4.621499	-1.245625	0.000001
H	1.231907	4.625124	0.000000
H	-1.231704	4.625190	-0.000001
C	-0.696603	-1.206830	3.500000

C 0.696679 -1.206683 3.500000
C 1.393322 0.000000 3.500000
C 0.696577 1.206833 3.500000
C -0.696629 1.206713 3.500000
C -1.393344 -0.000036 3.500000
H 1.242820 -2.152980 3.500000
H 2.485925 -0.000280 3.500000
H 1.243168 2.152847 3.500000
H -1.242938 2.152912 3.500000
H -2.485923 0.000486 3.500000
H -1.243041 -2.152961 3.500000

Naphthalene-triazine ring complex

27
Naphthalene-triazine ring complex
C 0.683036 -1.222026 0.000000
C 1.399959 0.000000 0.000000
C 0.725745 1.200274 0.000000
C -0.694718 1.238905 0.000000
C -1.420392 0.001962 0.000000
C -0.693632 -1.219114 0.000000
C -2.840855 0.040593 0.000000
C -1.421478 2.459981 0.000000
C -3.515069 1.240867 0.000000
C -2.798145 2.462894 0.000000
H 2.486528 -0.014400 0.000000
H -1.246097 -2.155977 0.000000
H 1.273989 2.139614 0.000000
H 1.225739 -2.163468 0.000000
H -3.389099 -0.898746 0.000000
H -4.601638 1.255268 0.000000
H -0.869013 3.396844 0.000000
H -3.340848 3.404336 0.000000
N -0.687933 1.191776 3.500000
C -1.293842 0.000001 3.500000
N -0.687983 -1.191784 3.500000
C 0.647111 -1.120954 3.500000
N 1.375494 0.000000 3.500000
C 0.647152 1.120964 3.500000
H -2.382645 0.000002 3.500000
H 1.190790 -2.064182 3.500000
H 1.190858 2.064177 3.500000

Naphthalene-benzene ring complex

30
Naphthalene-benzene ring complex
C 0.683036 -1.222026 0.000000
C 1.399959 0.000000 0.000000
C 0.725745 1.200274 0.000000
C -0.694718 1.238905 0.000000
C -1.420392 0.001962 0.000000
C -0.693632 -1.219114 0.000000
C -2.840855 0.040593 0.000000
C -1.421478 2.459981 0.000000
C -3.515069 1.240867 0.000000
C -2.798145 2.462894 0.000000
H 2.486528 -0.014400 0.000000
H -1.246097 -2.155977 0.000000
H 1.273989 2.139614 0.000000
H 1.225739 -2.163468 0.000000
H -3.389099 -0.898746 0.000000
H -4.601638 1.255268 0.000000
H -0.869013 3.396844 0.000000
H -3.340848 3.404336 0.000000
C -0.696603 -1.206830 3.500000
C 0.696679 -1.206683 3.500000
C 1.393322 0.000000 3.500000
C 0.696577 1.206833 3.500000
C -0.696629 1.206713 3.500000
C -1.393344 -0.000036 3.500000
H 1.242820 -2.152980 3.500000
H 2.485925 -0.000280 3.500000

H 1.243168 2.152847 3.500000
H -1.242938 2.152912 3.500000
H -2.485923 0.000486 3.500000
H -1.243041 -2.152961 3.500000

Benzene dimer stacked complex

24
Benzene dimer stacked complex
C 0.000000 0.000000 0.000000
C 1.393282 0.000000 0.000000
C 2.090052 -1.206609 0.000000
C 1.393434 -2.413516 0.000000
C 0.000228 -2.413542 0.000000
C -0.696614 -1.206867 0.000000
H 1.939323 0.946355 0.000000
H 3.182655 -1.206214 0.000000
H 1.940125 -3.359472 0.000000
H -0.545981 -3.359799 0.000000
H -1.789193 -1.207504 0.000000
H -0.546538 0.946074 0.000000
C 0.000000 0.000000 3.500000
C 1.393282 0.000000 3.500000
C 2.090052 -1.206609 3.500000
C 1.393434 -2.413516 3.500000
C 0.000228 -2.413542 3.500000
C -0.696614 -1.206867 3.500000
H 1.939323 0.946355 3.500000
H 3.182655 -1.206214 3.500000
H 1.940125 -3.359472 3.500000
H -0.545981 -3.359799 3.500000
H -1.789193 -1.207504 3.500000
H -0.546538 0.946074 3.500000

Benzene parallel displaced dimer

24
Benzene parallel displaced dimer
C -0.696641 0.000000 0.000000
C 0.696641 0.000000 0.000000
C 1.393411 -1.206609 0.000000
C 0.696793 -2.413516 0.000000
C -0.696413 -2.413542 0.000000
C -1.393255 -1.206867 0.000000
H 1.242682 0.946355 0.000000
H 2.486014 -1.206214 0.000000
H 1.243484 -3.359472 0.000000
H -1.242622 -3.359799 0.000000
H -2.485834 -1.207504 0.000000
H -1.243179 0.946074 0.000000
C -0.696603 -1.206830 3.500000
C 0.696679 -1.206683 3.500000
C 1.393322 0.000000 3.500000
C 0.696577 1.206833 3.500000
C -0.696629 1.206713 3.500000
C -1.393344 -0.000036 3.500000
H 1.242820 -2.152980 3.500000
H 2.485925 -0.000280 3.500000
H 1.243168 2.152847 3.500000
H -1.242938 2.152912 3.500000
H -2.485923 0.000486 3.500000
H -1.243041 -2.152961 3.500000

Benzene-triazine stacked complex

21
Benzene-triazine stacked complex
C -0.696603 -1.206830 0.000000
C 0.696679 -1.206683 0.000000
C 1.393322 0.000000 0.000000
C 0.696577 1.206833 0.000000
C -0.696629 1.206713 0.000000
C -1.393344 -0.000036 0.000000

H	1.242820	-2.152980	0.000000
H	2.485925	-0.000280	0.000000
H	1.243168	2.152847	0.000000
H	-1.242938	2.152912	0.000000
H	-2.485923	0.000486	0.000000
H	-1.243041	-2.152961	0.000000
N	-0.687933	1.191776	3.500000
C	-1.293842	0.000001	3.500000
N	-0.687983	-1.191784	3.500000
C	0.647111	-1.120954	3.500000
N	1.375494	0.000000	3.500000
C	0.647152	1.120964	3.500000
H	-2.382645	0.000002	3.500000
H	1.190790	-2.064182	3.500000
H	1.190858	2.064177	3.500000

Candidate B-benzene displaced complex

32
Candidate B-benzene displaced complex

S	0.871149	-0.000000	-0.000000
C	-0.871150	0.000000	0.000001
C	-1.364218	-1.281965	-0.000229
C	-0.360949	-2.312568	-0.000307
C	0.893961	-1.763101	0.000000
C	-0.887076	-3.680747	-0.000659
C	-2.322385	-3.773469	-0.000875
C	-3.325654	-2.742866	-0.000776
C	-2.799526	-1.374688	-0.000418
C	-2.815452	-5.055435	-0.001310
S	-1.522128	-6.222961	-0.001767
C	-0.323698	-4.929425	-0.000666
S	-4.557752	-5.055434	-0.001755
C	-4.580563	-3.292334	-0.001019
S	-2.164475	1.167527	-0.000294
C	-3.362904	-0.126009	-0.000043
H	-5.541206	-2.794222	-0.001217
H	1.854604	-2.261212	-0.000162
H	0.723137	-5.203445	-0.000349
H	-4.409740	0.148011	0.000123
C	-0.696603	-1.206830	3.500000
C	0.696679	-1.206683	3.500000
C	1.393322	0.000000	3.500000
C	0.696577	1.206833	3.500000
C	-0.696629	1.206713	3.500000
C	-1.393344	-0.000036	3.500000
H	1.242820	-2.152980	3.500000
H	2.485925	-0.000280	3.500000
H	1.243168	2.152847	3.500000
H	-1.242938	2.152912	3.500000
H	-2.485923	0.000486	3.500000
H	-1.243041	-2.152961	3.500000

Candidate B-benzene central ring complex

32
Candidate B-benzene central ring complex

S	-3.333606	-1.626243	0.000366
C	-2.708216	-0.000053	0.000127
C	-1.334698	0.000000	0.000016
C	-0.732895	-1.306340	0.000012
C	-1.696189	-2.280391	-0.000007
C	0.732957	-1.306375	0.000000
C	1.334698	-0.000000	0.000000
C	0.732895	1.306340	-0.000016
C	-0.732957	1.306375	-0.000010
C	2.708216	0.000053	0.000095
S	3.333704	-1.626161	0.000479
C	1.696200	-2.280417	-0.000183
S	3.333606	1.626243	0.000302
C	1.696189	2.280391	-0.000061
S	-3.333704	1.626161	0.000495
C	-1.696200	2.280417	-0.000195
H	1.576091	3.355810	0.000112

H -1.576091 -3.355810 0.000180
H 1.576202 -3.355848 -0.000416
H -1.576202 3.355848 -0.000446
C -0.696603 -1.206830 3.500000
C 0.696679 -1.206683 3.500000
C 1.393322 0.000000 3.500000
C 0.696577 1.206833 3.500000
C -0.696629 1.206713 3.500000
C -1.393344 -0.000036 3.500000
H 1.242820 -2.152980 3.500000
H 2.485925 -0.000280 3.500000
H 1.243168 2.152847 3.500000
H -1.242938 2.152912 3.500000
H -2.485923 0.000486 3.500000
H -1.243041 -2.152961 3.500000

Candidate B-benzene ext. ring complex

32
Candidate B-benzene ext. ring complex
S 1.491425 0.000000 0.000000
C 0.279534 1.251770 0.000178
C -0.984468 0.714321 -0.000000
C -1.027069 -0.723342 -0.000180
C 0.240578 -1.242749 0.000000
C -2.376007 -1.297005 -0.000476
C -3.440982 -0.330290 -0.000546
C -3.398380 1.107373 -0.000347
C -2.049443 1.681036 -0.000044
C -4.704984 -0.867739 -0.000930
S -4.644205 -2.609035 -0.001516
C -2.881261 -2.570312 -0.000539
S -5.916875 0.384031 -0.001198
C -4.666027 1.626780 -0.000462
S 0.218756 2.993066 0.000012
C -1.544188 2.954343 0.000387
H -4.976349 2.663433 -0.000563
H 0.550900 -2.279402 -0.000259
H -2.349986 -3.513020 -0.000327
H -2.075464 3.897051 0.000659
C -0.696603 -1.206830 3.500000
C 0.696679 -1.206683 3.500000
C 1.393322 0.000000 3.500000
C 0.696577 1.206833 3.500000
C -0.696629 1.206713 3.500000
C -1.393344 -0.000036 3.500000
H 1.242820 -2.152980 3.500000
H 2.485925 -0.000280 3.500000
H 1.243168 2.152847 3.500000
H -1.242938 2.152912 3.500000
H -2.485923 0.000486 3.500000
H -1.243041 -2.152961 3.500000

Candidate D-benzene ext. ring complex 1

40
Candidate D-benzene ext. ring complex 1
C 0.716956 1.206427 0.000000
C -0.688319 1.238533 -0.000000
C -1.413703 0.008752 -0.000001
C -0.717000 -1.236399 -0.000001
C 0.700772 -1.217313 0.000000
C 1.401292 -0.000000 -0.000000
C -2.841414 0.025005 -0.000002
C -3.538103 1.270151 -0.000002
C -2.782631 2.489848 -0.000000
C -1.420431 2.471621 -0.000000
C -3.566808 -1.204784 -0.000002
C -4.972059 -1.172676 -0.000003
C -5.656403 0.033771 -0.000004
C -4.955905 1.251064 -0.000003
C -2.834678 -2.437876 -0.000003
C -1.472487 -2.456101 -0.000002
H -0.861960 3.403882 0.000000

H -3.319584 3.433439 -0.000001
H -5.525072 -2.107786 -0.000003
H -6.741355 0.049051 -0.000005
C -5.690956 2.479369 -0.000005
H 1.269938 2.141556 0.000000
C 1.435863 -2.445593 0.000003
H 2.486243 -0.015317 0.000002
H -3.393152 -3.370134 -0.000003
H -0.935526 -3.399688 -0.000002
N -6.286415 3.479810 -0.000008
N 2.031373 -3.446005 0.000006
C -0.696603 -1.206830 3.500000
C 0.696679 -1.206683 3.500000
C 1.393322 0.000000 3.500000
C 0.696577 1.206833 3.500000
C -0.696629 1.206713 3.500000
C -1.393344 -0.000036 3.500000
H 1.242820 -2.152980 3.500000
H 2.485925 -0.000280 3.500000
H 1.243168 2.152847 3.500000
H -1.242938 2.152912 3.500000
H -2.485923 0.000486 3.500000
H -1.243041 -2.152961 3.500000

Candidate D-benzene central bond stacked complex

40
Candidate D-benzene central bond stacked complex
C 2.830788 1.221852 -0.000002
C 1.425239 1.237959 -0.000001
C 0.713901 0.000000 0.000000
C 1.424733 -1.237139 -0.000000
C 2.842196 -1.201915 -0.000000
C 3.528813 0.023294 -0.000002
C -0.713902 -0.000000 0.000000
C -1.424720 1.237134 -0.000000
C -0.683182 2.465352 -0.000000
C 0.679138 2.462633 -0.000001
C -1.425250 -1.237968 0.000001
C -2.830775 -1.221858 0.000002
C -3.528808 -0.023280 0.000001
C -2.842213 1.201908 0.000000
C -0.679130 -2.462646 0.000001
C 0.683180 -2.465362 0.000000
H 1.226959 3.401191 -0.000002
H -1.230842 3.402769 -0.000001
H -3.373107 -2.163203 0.000003
H -4.613865 -0.020352 0.000001
C -3.591199 2.421766 -0.000002
H 3.373089 2.163215 -0.000003
C 3.591222 -2.421748 0.000002
H 4.613869 0.020328 -0.000001
H -1.226955 -3.401200 0.000002
H 1.230848 -3.402776 0.000001
N -4.198009 3.415364 -0.000005
N 4.198082 -3.415316 0.000005
C -0.696603 -1.206830 3.500000
C 0.696679 -1.206683 3.500000
C 1.393322 0.000000 3.500000
C 0.696577 1.206833 3.500000
C -0.696629 1.206713 3.500000
C -1.393344 -0.000036 3.500000
H 1.242820 -2.152980 3.500000
H 2.485925 -0.000280 3.500000
H 1.243168 2.152847 3.500000
H -1.242938 2.152912 3.500000
H -2.485923 0.000486 3.500000
H -1.243041 -2.152961 3.500000

Candidate D-benzene ext. ring complex 2

40
Candidate D-benzene ext. ring complex 2
C 2.831330 -0.020160 -0.000000

C	1.425833	0.000000	0.000000
C	0.710928	-1.235902	0.000000
C	1.418190	-2.475086	-0.000001
C	2.835748	-2.443950	-0.000001
C	3.525896	-1.220726	-0.000001
C	-0.716869	-1.231785	-0.000000
C	-1.424117	0.007394	0.000000
C	-0.679040	1.233469	0.000001
C	0.683266	1.226821	0.000001
C	-1.431784	-2.467696	-0.000000
C	-2.837256	-2.447533	-0.000000
C	-3.531831	-1.246947	-0.000001
C	-2.841705	-0.023744	0.000000
C	-0.689198	-3.694520	-0.000001
C	0.673098	-3.701166	-0.000002
H	1.233792	2.163796	0.000001
H	-1.223994	2.172461	0.000001
H	-3.382301	-3.387310	-0.000000
H	-4.616874	-1.240890	-0.000001
C	-3.587170	1.198268	-0.000002
H	3.376343	0.919636	-0.000000
C	3.581254	-3.665937	0.000001
H	4.610938	-1.226820	0.000001
H	-1.239728	-4.631491	-0.000001
H	1.218060	-4.640154	-0.000001
N	-4.191112	2.193612	-0.000004
N	4.185246	-4.661251	0.000004
C	-0.696603	-1.206830	3.500000
C	0.696679	-1.206683	3.500000
C	1.393322	0.000000	3.500000
C	0.696577	1.206833	3.500000
C	-0.696629	1.206713	3.500000
C	-1.393344	-0.000036	3.500000
H	1.242820	-2.152980	3.500000
H	2.485925	-0.000280	3.500000
H	1.243168	2.152847	3.500000
H	-1.242938	2.152912	3.500000
H	-2.485923	0.000486	3.500000
H	-1.243041	-2.152961	3.500000

2-methylene-1,2-dihydronaphthalene benzene stacked complex

33
2-methylene-1,2-dihydronaphthalene benzene stacked complex

C	-1.448654	0.005185	0.000000
C	-0.684106	1.275560	0.000000
C	-0.699677	-1.234151	0.000000
C	0.768336	1.194305	0.000000
C	-1.342206	2.459397	0.000000
C	-2.814786	0.025237	0.000000
C	0.657091	-1.240897	0.000000
C	-4.947480	1.204190	0.000000
C	1.407007	0.000000	0.000000
C	-2.840442	2.573886	0.000000
C	-3.597404	1.244132	0.000000
H	-1.259620	-2.166537	0.000000
H	1.328379	2.126628	0.000000
H	-0.777752	3.390203	0.000000
H	-3.360071	-0.917018	0.000000
H	1.199753	-2.182344	0.000000
H	2.492852	-0.042103	0.000000
H	-3.148431	3.175022	0.869883
H	-5.482662	0.258672	0.000000
H	-5.551082	2.107930	0.000000
H	-3.148431	3.175022	-0.869883
C	-0.696603	-1.206830	3.500000
C	0.696679	-1.206683	3.500000
C	1.393322	0.000000	3.500000
C	0.696577	1.206833	3.500000
C	-0.696629	1.206713	3.500000
C	-1.393344	-0.000036	3.500000
H	1.242820	-2.152980	3.500000
H	2.485925	-0.000280	3.500000
H	1.243168	2.152847	3.500000
H	-1.242938	2.152912	3.500000

H -2.485923 0.000486 3.500000
H -1.243041 -2.152961 3.500000

2-methylnaphthalene benzene stacked complex

33
2-methylnaphthalene benzene stacked complex
C -1.402179 0.035935 -0.000007
C -0.730634 -1.215141 -0.000008
C 0.701255 -1.235632 0.000000
C 1.402360 0.000000 0.000000
C 0.722724 1.197893 0.000010
C -0.693528 1.216946 0.000007
C 1.372120 -2.488750 -0.000001
C 0.684050 -3.684120 0.000012
C -0.739875 -3.647953 -0.000057
C -1.423892 -2.456211 -0.000053
C 1.400554 -5.012471 0.000349
H -1.290057 -4.586516 -0.000118
H 2.460631 -2.491956 -0.000025
H -2.511592 -2.448643 -0.000132
H 2.489909 -0.015727 0.000005
H 1.272399 2.135354 0.000008
H -2.489837 0.045614 -0.000014
H -1.218713 2.168246 0.000023
H 1.132324 -5.611511 -0.879420
H 2.487186 -4.882251 -0.002443
H 1.136632 -5.608694 0.883361
C -0.696603 -1.206830 3.500000
C 0.696679 -1.206683 3.500000
C 1.393322 0.000000 3.500000
C 0.696577 1.206833 3.500000
C -0.696629 1.206713 3.500000
C -1.393344 -0.000036 3.500000
H 1.242820 -2.152980 3.500000
H 2.485925 -0.000280 3.500000
H 1.243168 2.152847 3.500000
H -1.242938 2.152912 3.500000
H -2.485923 0.000486 3.500000
H -1.243041 -2.152961 3.500000

2-methylnaphthalene triazine stacked complex

30
2-methylnaphthalene triazine stacked complex
C -1.402179 0.035935 -0.000007
C -0.730634 -1.215141 -0.000008
C 0.701255 -1.235632 0.000000
C 1.402360 0.000000 0.000000
C 0.722724 1.197893 0.000010
C -0.693528 1.216946 0.000007
C 1.372120 -2.488750 -0.000001
C 0.684050 -3.684120 0.000012
C -0.739875 -3.647953 -0.000057
C -1.423892 -2.456211 -0.000053
C 1.400554 -5.012471 0.000349
H -1.290057 -4.586516 -0.000118
H 2.460631 -2.491956 -0.000025
H -2.511592 -2.448643 -0.000132
H 2.489909 -0.015727 0.000005
H 1.272399 2.135354 0.000008
H -2.489837 0.045614 -0.000014
H -1.218713 2.168246 0.000023
H 1.132324 -5.611511 -0.879420
H 2.487186 -4.882251 -0.002443
H 1.136632 -5.608694 0.883361
N -0.687933 1.191776 3.500000
C -1.293842 0.000001 3.500000
N -0.687983 -1.191784 3.500000
C 0.647111 -1.120954 3.500000
N 1.375494 0.000000 3.500000
C 0.647152 1.120964 3.500000
H -2.382645 0.000002 3.500000
H 1.190790 -2.064182 3.500000

H 1.190858 2.064177 3.500000

2-methylene-1,2-dihydronaphthalene triazine stacked complex

30
2-methylene-1,2-dihydronaphthalene triazine stacked complex
C -1.448654 0.005185 0.000000
C -0.684106 1.275560 0.000000
C -0.699677 -1.234151 0.000000
C 0.768336 1.194305 0.000000
C -1.342206 2.459397 0.000000
C -2.814786 0.025237 0.000000
C 0.657091 -1.240897 0.000000
C -4.947480 1.204190 0.000000
C 1.407007 0.000000 0.000000
C -2.840442 2.573886 0.000000
C -3.597404 1.244132 0.000000
H -1.259620 -2.166537 0.000000
H 1.328379 2.126628 0.000000
H -0.777752 3.390203 0.000000
H -3.360071 -0.917018 0.000000
H 1.199753 -2.182344 0.000000
H 2.492852 -0.042103 0.000000
H -3.148431 3.175022 0.869883
H -5.482662 0.258672 0.000000
H -5.551082 2.107930 0.000000
H -3.148431 3.175022 -0.869883
N -0.687933 1.191776 3.500000
C -1.293842 0.000001 3.500000
N -0.687983 -1.191784 3.500000
C 0.647111 -1.120954 3.500000
N 1.375494 0.000000 3.500000
C 0.647152 1.120964 3.500000
H -2.382645 0.000002 3.500000
H 1.190790 -2.064182 3.500000
H 1.190858 2.064177 3.500000

2,3,6,7-tetrahydrotriphenylene benzene central ring complex

46
2,3,6,7-tetrahydrotriphenylene benzene central ring complex
C -2.874258 0.073532 0.000000
C -1.462602 0.027810 0.000000
C -0.753089 1.254127 0.000000
C -1.496449 2.455071 0.000000
C 0.731734 1.285345 0.000000
C 1.413537 2.450540 0.000000
C 1.490633 0.000000 0.000000
C 2.838941 0.040553 0.000000
C 0.742921 -1.292285 0.000000
C 1.379659 -2.481455 0.000000
C -0.749598 -1.274995 0.000000
C -1.420063 -2.446712 0.000000
H -3.443084 -0.848267 0.000000
H -0.980922 3.407681 0.000000
H 0.878897 3.394391 0.000000
H 3.407568 -0.884506 0.000000
H 2.465028 -2.513445 0.000000
H -2.504770 -2.453208 0.000000
C 2.906731 2.604186 0.000000
H 3.189712 3.215846 0.869475
H 3.189712 3.215846 -0.869475
C 3.693170 1.274749 0.000000
H 4.365747 1.229109 0.869409
H 4.365747 1.229109 -0.869409
C 0.735333 -3.837111 0.000000
H 1.110130 -4.397423 0.869411
H 1.110130 -4.397423 -0.869411
C -0.809208 -3.817902 0.000000
H -1.198511 -4.368032 0.869454
H -1.198511 -4.368032 -0.869454
C -2.880342 2.473840 0.000000
H -3.410482 3.422413 0.000000
C -3.580385 1.263867 0.000000

H -4.666968 1.250647 0.000000
C -0.696603 -1.206830 3.500000
C 0.696679 -1.206683 3.500000
C 1.393322 0.000000 3.500000
C 0.696577 1.206833 3.500000
C -0.696629 1.206713 3.500000
C -1.393344 -0.000036 3.500000
H 1.242820 -2.152980 3.500000
H 2.485925 -0.000280 3.500000
H 1.243168 2.152847 3.500000
H -1.242938 2.152912 3.500000
H -2.485923 0.000486 3.500000
H -1.243041 -2.152961 3.500000

Phenanthrene-triazine central ring complex

33
Phenanthrene-triazine central ring complex
C -2.732058 2.561725 0.000022
C -3.484090 1.372174 0.000049
C -2.849104 0.143310 0.000046
C -1.438371 0.039752 0.000012
C -0.681099 1.250101 -0.000003
C -1.352942 2.494544 -0.000002
C -0.734810 -1.237152 -0.000003
C -1.400929 -2.485026 -0.000026
C -0.701345 -3.678293 -0.000036
C 0.705992 -3.678066 -0.000022
C 0.692895 -1.243597 -0.000000
C 1.385959 -2.476354 -0.000007
C 1.408778 -0.000000 0.000000
C 0.752608 1.190894 -0.000010
H -0.758472 3.405439 -0.000018
H -3.456938 -0.755288 0.000074
H -2.485271 -2.518788 -0.000051
H -1.243851 -4.619883 -0.000058
H 2.473559 -2.460441 -0.000004
H 1.252294 -4.617308 -0.000029
H 1.307151 2.126423 -0.000018
H 2.495869 -0.031007 0.000005
H -3.234180 3.525313 0.000019
H -4.569874 1.416585 0.000077
N -0.687933 1.191776 3.500000
C -1.293842 0.000001 3.500000
N -0.687983 -1.191784 3.500000
C 0.647111 -1.120954 3.500000
N 1.375494 0.000000 3.500000
C 0.647152 1.120964 3.500000
H -2.382645 0.000002 3.500000
H 1.190790 -2.064182 3.500000
H 1.190858 2.064177 3.500000

Phenanthrene-triazine ext.ring complex

33
Phenanthrene-triazine ext.ring complex
C 0.697317 1.221733 0.000003
C 1.395852 0.000000 0.000000
C 0.706991 -1.199494 0.000000
C -0.706947 -1.240383 0.000005
C -1.409794 0.002360 -0.000004
C -0.683421 1.215782 -0.000001
C -1.466446 -2.484828 0.000016
C -0.856326 -3.761017 0.000063
C -1.608143 -4.922082 0.000067
C -3.014085 -4.859440 0.000024
C -2.893033 -2.427948 -0.000016
C -3.640087 -3.628754 -0.000014
C -3.553058 -1.153825 -0.000041
C -2.844717 0.006796 -0.000027
H -1.236908 2.152146 -0.000004
H 1.274374 -2.124165 -0.000008
H 0.225451 -3.842836 0.000110
H -1.107931 -5.886807 0.000108

H	-4.725911	-3.564622	-0.000040
H	-3.601505	-5.773529	0.000028
H	-3.357223	0.965999	-0.000037
H	-4.640454	-1.136589	-0.000068
H	1.241680	2.162103	0.000008
H	2.482538	-0.003788	-0.000006
N	-0.687933	1.191776	3.500000
C	-1.293842	0.000001	3.500000
N	-0.687983	-1.191784	3.500000
C	0.647111	-1.120954	3.500000
N	1.375494	0.000000	3.500000
C	0.647152	1.120964	3.500000
H	-2.382645	0.000002	3.500000
H	1.190790	-2.064182	3.500000
H	1.190858	2.064177	3.500000

Phenanthrene-benzene central ring complex

36
Phenanthrene-benzene central ring complex

C	-2.732058	2.561725	0.000022
C	-3.484090	1.372174	0.000049
C	-2.849104	0.143310	0.000046
C	-1.438371	0.039752	0.000012
C	-0.681099	1.250101	-0.000003
C	-1.352942	2.494544	-0.000002
C	-0.734810	-1.237152	-0.000003
C	-1.400929	-2.485026	-0.000026
C	-0.701345	-3.678293	-0.000036
C	0.705992	-3.678066	-0.000022
C	0.692895	-1.243597	-0.000000
C	1.385959	-2.476354	-0.000007
C	1.408778	-0.000000	0.000000
C	0.752608	1.190894	-0.000010
H	-0.758472	3.405439	-0.000018
H	-3.456938	-0.755288	0.000074
H	-2.485271	-2.518788	-0.000051
H	-1.243851	-4.619883	-0.000058
H	2.473559	-2.460441	-0.000004
H	1.252294	-4.617308	-0.000029
H	1.307151	2.126423	-0.000018
H	2.495869	-0.031007	0.000005
H	-3.234180	3.525313	0.000019
H	-4.569874	1.416585	0.000077
C	-0.696603	-1.206830	3.500000
C	0.696679	-1.206683	3.500000
C	1.393322	0.000000	3.500000
C	0.696577	1.206833	3.500000
C	-0.696629	1.206713	3.500000
C	-1.393344	-0.000036	3.500000
H	1.242820	-2.152980	3.500000
H	2.485925	-0.000280	3.500000
H	1.243168	2.152847	3.500000
H	-1.242938	2.152912	3.500000
H	-2.485923	0.000486	3.500000
H	-1.243041	-2.152961	3.500000

Phenanthrene-benzene parallel displaced complex

36
Phenanthrene-benzene parallel displaced complex

C	-3.562138	-2.390503	0.000062
C	-2.883188	-3.623228	0.000090
C	-1.500453	-3.660106	0.000077
C	-0.728956	-2.474491	0.000033
C	-1.423592	-1.227140	0.000017
C	-2.837758	-1.215025	0.000028
C	0.728947	-2.474491	0.000007
C	1.500440	-3.660115	-0.000016
C	2.883170	-3.623236	-0.000036
C	3.562129	-2.390511	-0.000032
C	1.423580	-1.227146	-0.000000
C	2.837751	-1.215035	-0.000017
C	0.679850	-0.000000	0.000000

C	-0.679851	0.000000	0.000000
H	-3.348683	-0.254775	0.000011
H	-1.006748	-4.626127	0.000105
H	1.006724	-4.626128	-0.000033
H	3.446057	-4.552786	-0.000058
H	3.348673	-0.254782	-0.000021
H	4.648401	-2.365296	-0.000047
H	-1.231621	0.937168	-0.000008
H	1.231620	0.937164	-0.000003
H	-4.648411	-2.365274	0.000067
H	-3.446068	-4.552780	0.000126
C	-0.696603	-1.206830	3.500000
C	0.696679	-1.206683	3.500000
C	1.393322	0.000000	3.500000
C	0.696577	1.206833	3.500000
C	-0.696629	1.206713	3.500000
C	-1.393344	-0.000036	3.500000
H	1.242820	-2.152980	3.500000
H	2.485925	-0.000280	3.500000
H	1.243168	2.152847	3.500000
H	-1.242938	2.152912	3.500000
H	-2.485923	0.000486	3.500000
H	-1.243041	-2.152961	3.500000

Phenanthrene-benzene ext. ring complex

36
Phenanthrene-benzene ext. ring complex

C	0.697317	1.221733	0.000003
C	1.395852	0.000000	0.000000
C	0.706991	-1.199494	0.000000
C	-0.706947	-1.240383	0.000005
C	-1.409794	0.002360	-0.000004
C	-0.683421	1.215782	-0.000001
C	-1.466446	-2.484828	0.000016
C	-0.856326	-3.761017	0.000063
C	-1.608143	-4.922082	0.000067
C	-3.014085	-4.859440	0.000024
C	-2.893033	-2.427948	-0.000016
C	-3.640087	-3.628754	-0.000014
C	-3.553058	-1.153825	-0.000041
C	-2.844717	0.006796	-0.000027
H	-1.236908	2.152146	-0.000004
H	1.274374	-2.124165	-0.000008
H	0.225451	-3.842836	0.000110
H	-1.107931	-5.886807	0.000108
H	-4.725911	-3.564622	-0.000040
H	-3.601505	-5.773529	0.000028
H	-3.357223	0.965999	-0.000037
H	-4.640454	-1.136589	-0.000068
H	1.241680	2.162103	0.000008
H	2.482538	-0.003788	-0.000006
C	-0.696603	-1.206830	3.500000
C	0.696679	-1.206683	3.500000
C	1.393322	0.000000	3.500000
C	0.696577	1.206833	3.500000
C	-0.696629	1.206713	3.500000
C	-1.393344	-0.000036	3.500000
H	1.242820	-2.152980	3.500000
H	2.485925	-0.000280	3.500000
H	1.243168	2.152847	3.500000
H	-1.242938	2.152912	3.500000
H	-2.485923	0.000486	3.500000
H	-1.243041	-2.152961	3.500000

2,3,6,7,10,11-hexahydrotriphenylene benzene central ring complex

48
2,3,6,7,10,11-hexahydrotriphenylene benzene central ring complex

C	-1.446857	2.448671	-0.000437
C	-0.747199	1.294410	0.000002
C	-1.494680	0.000960	0.000002
C	-2.843827	0.030922	-0.000437
C	-3.713080	1.254307	-0.000950

C	-2.940616	2.590932	-0.000950
C	-0.747442	-1.294273	-0.000003
C	0.746515	-1.294922	0.000000
C	1.494790	0.000000	0.000000
C	0.748018	1.293825	-0.000002
C	2.844161	0.029496	0.000202
C	3.713746	1.252618	0.000431
C	2.942121	2.589424	0.000427
C	1.448116	2.447723	0.000195
C	1.395070	-2.478667	-0.000032
C	0.769857	-3.842947	-0.000073
C	-0.773646	-3.842326	-0.000080
C	-1.397321	-2.477271	-0.000042
H	2.480159	-2.500463	0.000132
H	-2.482483	-2.498213	0.000453
H	-3.404846	-0.898114	-0.000279
H	-3.229928	3.200578	0.868104
H	-0.921955	3.398727	-0.000978
H	3.231863	3.198967	-0.868535
H	0.923459	3.397773	0.001079
H	3.405034	-0.899592	0.000151
H	3.230665	3.198115	0.870430
H	4.386043	1.198503	0.869764
H	4.386000	1.198401	-0.868910
H	-1.157137	-4.397083	0.869187
H	-1.156712	-4.397012	-0.869629
H	1.153026	-4.398212	0.869148
H	1.153007	-4.398149	-0.869373
H	-4.385860	1.200282	0.867895
H	-4.384498	1.199794	-0.871004
H	-3.229073	3.199959	-0.870766
C	-0.696603	-1.206830	3.500000
C	0.696679	-1.206683	3.500000
C	1.393322	0.000000	3.500000
C	0.696577	1.206833	3.500000
C	-0.696629	1.206713	3.500000
C	-1.393344	-0.000036	3.500000
H	1.242820	-2.152980	3.500000
H	2.485925	-0.000280	3.500000
H	1.243168	2.152847	3.500000
H	-1.242938	2.152912	3.500000
H	-2.485923	0.000486	3.500000
H	-1.243041	-2.152961	3.500000

1,2,5,6,9,10-hexahydrotriphenylene benzene central ring complex

48
1,2,5,6,9,10-hexahydrotriphenylene benzene central ring complex

C	2.937784	0.022441	-0.000048
C	1.410588	-0.000000	0.000000
C	0.703118	-1.220237	0.000000
C	1.457684	-2.482671	-0.000042
C	2.794259	-2.547515	-0.000079
C	3.682184	-1.339970	-0.000086
C	-0.705512	-1.221716	0.000001
C	-1.408161	0.001145	-0.000003
C	-0.705181	1.221738	-0.000001
C	0.705150	1.219072	0.000004
C	-1.487869	2.533329	-0.000008
C	-0.680350	3.859155	-0.000004
C	0.809378	3.693817	0.000001
C	1.421247	2.503757	0.000006
C	-2.878658	-0.020587	-0.000009
C	-3.603680	-1.145190	-0.000008
C	-3.002431	-2.518233	-0.000002
C	-1.450360	-2.555262	0.000004
H	-3.401339	0.929338	-0.000029
H	-4.690803	-1.085144	-0.000014
H	0.896786	-3.410499	-0.000107
H	3.286312	-3.518776	-0.000243
H	1.404786	4.605385	0.000113
H	2.505297	2.481975	0.000012
H	-3.387694	-3.069854	-0.869806
H	-3.387701	-3.069843	0.869805
H	-1.115611	-3.133444	-0.870172

H -1.115588 -3.133443 0.870167
H 4.352505 -1.397706 -0.869918
H 4.352471 -1.397505 0.869730
H 3.270984 0.601498 0.870185
H 3.271076 0.601766 -0.870069
H -0.965603 4.468697 0.869653
H -0.965471 4.468340 -0.870017
H -2.156174 2.532365 0.869949
H -2.156015 2.532389 -0.870247
C -0.696603 -1.206830 3.500000
C 0.696679 -1.206683 3.500000
C 1.393322 0.000000 3.500000
C 0.696577 1.206833 3.500000
C -0.696629 1.206713 3.500000
C -1.393344 -0.000036 3.500000
H 1.242820 -2.152980 3.500000
H 2.485925 -0.000280 3.500000
H 1.243168 2.152847 3.500000
H -1.242938 2.152912 3.500000
H -2.485923 0.000486 3.500000
H -1.243041 -2.152961 3.500000

Triphenylene-benzene ext.ring complex

42
Triphenylene-benzene ext.ring complex
C -1.420053 -0.002290 -0.000153
C -2.887378 -0.003934 -0.000574
C -3.599363 1.226351 -0.000053
C -2.866903 2.497915 0.000903
C -1.445481 2.499252 0.000651
C -0.710564 1.229323 0.000119
C -0.773423 3.742401 0.001177
C -1.457607 4.944589 0.002086
C -2.858361 4.943404 0.002599
C -3.540794 3.740146 0.002016
H 0.309539 3.771391 0.000922
H -0.907516 5.881585 0.002473
H -3.409949 5.879514 0.003464
H -4.623801 3.767800 0.002539
C 0.702179 1.192400 0.000100
C 1.403359 0.000000 -0.000000
C 0.704164 -1.213793 0.000000
C -0.679087 -1.205644 -0.000069
C -5.012035 1.186199 -0.000647
C -5.710703 -0.007665 -0.001615
C -5.009018 -1.219992 -0.002128
C -3.625793 -1.208924 -0.001657
H -5.579305 2.109195 -0.000488
H -6.797208 -0.000069 -0.002061
H -5.543619 -2.165908 -0.002981
H -3.107996 -2.160631 -0.002296
H 1.240779 -2.158568 0.000080
H -1.195016 -2.158260 0.000053
H 1.267252 2.116757 0.000207
H 2.489844 0.009886 -0.000008
C -0.696603 -1.206830 3.500000
C 0.696679 -1.206683 3.500000
C 1.393322 0.000000 3.500000
C 0.696577 1.206833 3.500000
C -0.696629 1.206713 3.500000
C -1.393344 -0.000036 3.500000
H 1.242820 -2.152980 3.500000
H 2.485925 -0.000280 3.500000
H 1.243168 2.152847 3.500000
H -1.242938 2.152912 3.500000
H -2.485923 0.000486 3.500000
H -1.243041 -2.152961 3.500000

Triphenylene-benzene central ring complex

42
Triphenylene-benzene central ring complex
C -0.722081 -1.250882 0.000220

C	-1.444250	0.026427	-0.000226
C	-0.722328	1.250907	-0.000221
C	0.745049	1.237476	0.000228
C	1.444402	0.000000	0.000000
C	0.699212	-1.263927	-0.000000
C	2.857359	0.025226	0.000029
C	3.568462	1.211690	0.000435
C	2.879394	2.431237	0.000924
C	1.496088	2.434644	0.000821
H	3.414550	-0.903851	-0.000220
H	4.654834	1.192775	0.000447
H	3.423860	3.371508	0.001396
H	0.988214	3.391582	0.001314
C	1.360975	-2.512637	0.000020
C	0.666746	-3.709096	0.000420
C	-0.733969	-3.696264	0.000905
C	-1.406310	-2.487378	0.000808
C	-1.451194	2.461696	-0.000823
C	-2.834290	2.483858	-0.001314
C	-3.545630	1.277170	-0.001319
C	-2.856562	0.077745	-0.000829
H	-0.925853	3.409185	-0.001051
H	-3.361355	3.433991	-0.001781
H	-4.632163	1.278210	-0.001794
H	-3.431212	-0.840753	-0.001069
H	-1.293337	-4.627749	0.001380
H	-2.489508	-2.505893	0.001312
H	2.443698	-2.550810	-0.000242
H	1.209028	-4.650626	0.000427
C	-0.696603	-1.206830	3.500000
C	0.696679	-1.206683	3.500000
C	1.393322	0.000000	3.500000
C	0.696577	1.206833	3.500000
C	-0.696629	1.206713	3.500000
C	-1.393344	-0.000036	3.500000
H	1.242820	-2.152980	3.500000
H	2.485925	-0.000280	3.500000
H	1.243168	2.152847	3.500000
H	-1.242938	2.152912	3.500000
H	-2.485923	0.000486	3.500000
H	-1.243041	-2.152961	3.500000

9,10-dimethylene-9,10-dihydroanthracene triazine central ring complex

37
9,10-dimethylene-9,10-dihydroanthracene triazine central ring complex

C	-0.698918	-3.720653	0.000000
C	-1.377723	-2.514318	0.000000
C	-0.707498	-1.272413	0.000000
C	0.707498	-1.272413	0.000000
C	1.377723	-2.514318	0.000000
C	0.698918	-3.720653	0.000000
C	-1.476839	0.000000	0.000000
C	-0.707498	1.272413	0.000000
C	0.707498	1.272413	0.000000
C	1.476839	0.000000	0.000000
C	1.377723	2.514318	0.000000
C	0.698918	3.720653	0.000000
C	-0.698918	3.720653	0.000000
C	-1.377723	2.514318	0.000000
C	2.827306	0.000000	0.000000
C	-2.827306	0.000000	0.000000
H	2.460354	-2.542033	0.000000
H	-2.460354	2.542033	0.000000
H	2.460354	2.542033	0.000000
H	-2.460354	-2.542033	0.000000
H	1.253155	-4.655213	0.000000
H	-1.253155	4.655213	0.000000
H	1.253155	4.655213	0.000000
H	-1.253155	-4.655213	0.000000
H	-3.412946	0.909482	0.000000
H	-3.412946	-0.909482	0.000000
H	3.412946	0.909482	0.000000
H	3.412946	-0.909482	0.000000
N	-0.687933	1.191776	3.500000

C	-1.293842	0.000001	3.500000
N	-0.687983	-1.191784	3.500000
C	0.647111	-1.120954	3.500000
N	1.375494	0.000000	3.500000
C	0.647152	1.120964	3.500000
H	-2.382645	0.000002	3.500000
H	1.190790	-2.064182	3.500000
H	1.190858	2.064177	3.500000

9,10-dimethylene-9,10-dihydroanthracene triazine ext. ring complex

37
9,10-dimethylene-9,10-dihydroanthracene triazine ext. ring complex

C	-0.752448	6.216869	0.000000
C	-1.420846	5.004737	0.000000
C	-0.739958	3.768646	0.000000
C	0.674986	3.780823	0.000000
C	1.334498	5.028450	0.000000
C	0.645337	6.228898	0.000000
C	-1.498320	2.489659	0.000000
C	-0.718057	1.223914	0.000000
C	0.696886	1.236091	0.000000
C	1.455248	2.515078	0.000000
C	1.377774	0.000000	0.000000
C	0.709376	-1.212132	0.000000
C	-0.688408	-1.224162	0.000000
C	-1.377570	-0.023713	0.000000
C	2.805665	2.526700	0.000000
C	-2.848737	2.478037	0.000000
H	2.416850	5.065481	0.000000
H	-2.459922	-0.060744	0.000000
H	2.460603	-0.018397	0.000000
H	-2.503675	5.023134	0.000000
H	1.191510	7.168193	0.000000
H	-1.234582	-2.163457	0.000000
H	1.271635	-2.141888	0.000000
H	-1.314707	7.146624	0.000000
H	-3.426529	1.563549	0.000000
H	-3.442182	3.382445	0.000000
H	3.399111	1.622292	0.000000
H	3.383457	3.441188	0.000000
N	-0.687933	1.191776	3.500000
C	-1.293842	0.000001	3.500000
N	-0.687983	-1.191784	3.500000
C	0.647111	-1.120954	3.500000
N	1.375494	0.000000	3.500000
C	0.647152	1.120964	3.500000
H	-2.382645	0.000002	3.500000
H	1.190790	-2.064182	3.500000
H	1.190858	2.064177	3.500000

9,10-dimethylene-9,10-dihydroanthracene benzene central ring complex

40
9,10-dimethylene-9,10-dihydroanthracene benzene central ring complex

C	-0.698918	-3.720653	0.000000
C	-1.377723	-2.514318	0.000000
C	-0.707498	-1.272413	0.000000
C	0.707498	-1.272413	0.000000
C	1.377723	-2.514318	0.000000
C	0.698918	-3.720653	0.000000
C	-1.476839	0.000000	0.000000
C	-0.707498	1.272413	0.000000
C	0.707498	1.272413	0.000000
C	1.476839	0.000000	0.000000
C	1.377723	2.514318	0.000000
C	0.698918	3.720653	0.000000
C	-0.698918	3.720653	0.000000
C	-1.377723	2.514318	0.000000
C	2.827306	0.000000	0.000000
C	-2.827306	0.000000	0.000000
H	2.460354	-2.542033	0.000000
H	-2.460354	2.542033	0.000000
H	2.460354	2.542033	0.000000

H -2.460354 -2.542033 0.000000
H 1.253155 -4.655213 0.000000
H -1.253155 4.655213 0.000000
H 1.253155 4.655213 0.000000
H -1.253155 -4.655213 0.000000
H -3.412946 0.909482 0.000000
H -3.412946 -0.909482 0.000000
H 3.412946 0.909482 0.000000
H 3.412946 -0.909482 0.000000
C -0.696603 -1.206830 3.500000
C 0.696679 -1.206683 3.500000
C 1.393322 0.000000 3.500000
C 0.696577 1.206833 3.500000
C -0.696629 1.206713 3.500000
C -1.393344 -0.000036 3.500000
H 1.242820 -2.152980 3.500000
H 2.485925 -0.000280 3.500000
H 1.243168 2.152847 3.500000
H -1.242938 2.152912 3.500000
H -2.485923 0.000486 3.500000
H -1.243041 -2.152961 3.500000

9,10-dimethylene-9,10-dihydroanthracene benzene ext. ring complex

40
9,10-dimethylene-9,10-dihydroanthracene benzene ext. ring complex
C -0.752448 6.216869 0.000000
C -1.420846 5.004737 0.000000
C -0.739958 3.768646 0.000000
C 0.674986 3.780823 0.000000
C 1.334498 5.028450 0.000000
C 0.645337 6.228898 0.000000
C -1.498320 2.489659 0.000000
C -0.718057 1.223914 0.000000
C 0.696886 1.236091 0.000000
C 1.455248 2.515078 0.000000
C 1.377774 0.000000 0.000000
C 0.709376 -1.212132 0.000000
C -0.688408 -1.224162 0.000000
C -1.377570 -0.023713 0.000000
C 2.805665 2.526700 0.000000
C -2.848737 2.478037 0.000000
H 2.416850 5.065481 0.000000
H -2.459922 -0.060744 0.000000
H 2.460603 -0.018397 0.000000
H -2.503675 5.023134 0.000000
H 1.191510 7.168193 0.000000
H -1.234582 -2.163457 0.000000
H 1.271635 -2.141888 0.000000
H -1.314707 7.146624 0.000000
H -3.426529 1.563549 0.000000
H -3.442182 3.382445 0.000000
H 3.399111 1.622292 0.000000
H 3.383457 3.441188 0.000000
C -0.696603 -1.206830 3.500000
C 0.696679 -1.206683 3.500000
C 1.393322 0.000000 3.500000
C 0.696577 1.206833 3.500000
C -0.696629 1.206713 3.500000
C -1.393344 -0.000036 3.500000
H 1.242820 -2.152980 3.500000
H 2.485925 -0.000280 3.500000
H 1.243168 2.152847 3.500000
H -1.242938 2.152912 3.500000
H -2.485923 0.000486 3.500000
H -1.243041 -2.152961 3.500000

Pyridine-triazine stacked complex

20
Pyridine-triazine stacked complex
C 1.385693 0.000000 0.000000
C 0.706307 1.217859 0.000000
C -0.688134 1.202714 0.000000

C	-1.339119	-0.032184	0.000000
N	-0.701821	-1.210094	0.000000
C	0.637077	-1.178295	0.000000
H	2.471072	-0.040397	0.000000
H	1.251570	2.158050	0.000000
H	-1.262205	2.124730	0.000000
H	-2.427279	-0.079828	0.000000
H	1.136081	-2.146470	0.000000
N	-0.687933	1.191776	3.500000
C	-1.293842	0.000001	3.500000
N	-0.687983	-1.191784	3.500000
C	0.647111	-1.120954	3.500000
N	1.375494	0.000000	3.500000
C	0.647152	1.120964	3.500000
H	-2.382645	0.000002	3.500000
H	1.190790	-2.064182	3.500000
H	1.190858	2.064177	3.500000

Pyridine-benzene central ring complex

23
Pyridine-benzene central ring complex

C	1.385693	0.000000	0.000000
C	0.706307	1.217859	0.000000
C	-0.688134	1.202714	0.000000
C	-1.339119	-0.032184	0.000000
N	-0.701821	-1.210094	0.000000
C	0.637077	-1.178295	0.000000
H	2.471072	-0.040397	0.000000
H	1.251570	2.158050	0.000000
H	-1.262205	2.124730	0.000000
H	-2.427279	-0.079828	0.000000
H	1.136081	-2.146470	0.000000
C	-0.696603	-1.206830	3.500000
C	0.696679	-1.206683	3.500000
C	1.393322	0.000000	3.500000
C	0.696577	1.206833	3.500000
C	-0.696629	1.206713	3.500000
C	-1.393344	-0.000036	3.500000
H	1.242820	-2.152980	3.500000
H	2.485925	-0.000280	3.500000
H	1.243168	2.152847	3.500000
H	-1.242938	2.152912	3.500000
H	-2.485923	0.000486	3.500000
H	-1.243041	-2.152961	3.500000

Pyrene-benzene ext. ring complex 1

38
Pyrene-benzene ext. ring complex 1

C	-0.689288	-1.251555	0.000003
C	0.747236	-1.191322	-0.000000
C	1.406366	0.000000	0.000000
C	0.694080	1.248987	-0.000003
C	-0.733876	1.221243	-0.000002
C	-1.424521	-0.027353	0.000003
C	-1.469231	2.445864	-0.000004
C	-0.767485	3.661753	-0.000001
C	0.626529	3.680430	-0.000001
C	1.351338	2.489951	-0.000005
H	1.301723	-2.126789	-0.000005
H	2.493457	0.027258	-0.000007
H	-1.325272	4.595520	0.000000
H	1.152322	4.631432	0.000002
H	2.438762	2.513357	-0.000001
C	-2.905944	2.385356	-0.000011
C	-3.564986	1.194144	-0.000008
C	-2.852883	-0.055193	0.000007
C	-3.509685	-1.295735	0.000011
C	-2.784560	-2.486736	0.000008
C	-1.391162	-2.468126	-0.000001
H	-0.832736	-3.401502	-0.000018
H	-4.597107	-1.319939	0.000016
H	-3.311286	-3.437231	-0.000009

H -3.460633 3.320699 -0.000012
H -4.652085 1.167091 -0.000017
C -0.696603 -1.206830 3.500000
C 0.696679 -1.206683 3.500000
C 1.393322 0.000000 3.500000
C 0.696577 1.206833 3.500000
C -0.696629 1.206713 3.500000
C -1.393344 -0.000036 3.500000
H 1.242820 -2.152980 3.500000
H 2.485925 -0.000280 3.500000
H 1.243168 2.152847 3.500000
H -1.242938 2.152912 3.500000
H -2.485923 0.000486 3.500000
H -1.243041 -2.152961 3.500000

Pyrene-benzene ext. ring complex 2

38
Pyrene-benzene ext. ring complex 2
C -3.555517 1.236267 -0.000009
C -2.807379 2.464078 -0.000007
C -1.445872 2.464092 -0.000006
C -0.697823 1.236190 -0.000001
C -1.413385 0.000149 -0.000002
C -2.840263 0.000286 -0.000008
C -0.697824 -1.236143 0.000002
C 0.705810 -1.210731 0.000000
C 1.397007 0.000000 -0.000000
C 0.706215 1.210535 0.000002
H -3.357488 3.402127 -0.000003
H -0.895751 3.402109 0.000001
H 1.252833 -2.150845 0.000001
H 2.483682 -0.000316 -0.000003
H 1.253128 2.150708 -0.000002
C -1.446294 -2.463985 0.000011
C -2.807662 -2.463976 0.000007
C -3.556107 -1.236064 -0.000011
C -4.959554 -1.210214 -0.000015
C -5.650650 0.000851 -0.000014
C -4.959810 1.211075 -0.000006
H -5.506181 2.151558 0.000009
H -5.507164 -2.149999 -0.000020
H -6.737333 0.000105 0.000002
H -0.896393 -3.402150 0.000013
H -3.357609 -3.402098 0.000016
C -0.696603 -1.206830 3.500000
C 0.696679 -1.206683 3.500000
C 1.393322 0.000000 3.500000
C 0.696577 1.206833 3.500000
C -0.696629 1.206713 3.500000
C -1.393344 -0.000036 3.500000
H 1.242820 -2.152980 3.500000
H 2.485925 -0.000280 3.500000
H 1.243168 2.152847 3.500000
H -1.242938 2.152912 3.500000
H -2.485923 0.000486 3.500000
H -1.243041 -2.152961 3.500000

Pyrene-benzene central bond stacked complex

38
Pyrene-benzene central bond stacked complex
C -1.428721 1.236179 -0.000002
C -0.680605 2.464002 -0.000000
C 0.680902 2.464042 -0.000001
C 1.428973 1.236153 0.000003
C 0.713433 0.000099 0.000002
C -0.713445 0.000210 -0.000003
C 1.429016 -1.236180 0.000004
C 2.832649 -1.210744 0.000000
C 3.523825 -0.000000 0.000000
C 2.833012 1.210522 0.000004
H -1.230730 3.402042 0.000005
H 1.231007 3.402068 0.000006

H 3.379690 -2.150848 -0.000001
H 4.610500 -0.000296 -0.000004
H 3.379907 2.150705 -0.000001
C 0.680568 -2.464035 0.000012
C -0.680800 -2.464051 0.000010
C -1.429267 -1.236153 -0.000006
C -2.832715 -1.210327 -0.000009
C -3.523832 0.000725 -0.000006
C -2.833013 1.210962 0.000002
H -3.379402 2.151435 0.000019
H -3.380307 -2.150122 -0.000013
H -4.610515 -0.000041 0.000012
H 1.230486 -3.402191 0.000013
H -1.230730 -3.402183 0.000019
C -0.696603 -1.206830 3.500000
C 0.696679 -1.206683 3.500000
C 1.393322 0.000000 3.500000
C 0.696577 1.206833 3.500000
C -0.696629 1.206713 3.500000
C -1.393344 -0.000036 3.500000
H 1.242820 -2.152980 3.500000
H 2.485925 -0.000280 3.500000
H 1.243168 2.152847 3.500000
H -1.242938 2.152912 3.500000
H -2.485923 0.000486 3.500000
H -1.243041 -2.152961 3.500000

Candidate C-benzene ext. ring complex 1

38
Candidate C-benzene ext. ring complex 1
S -5.957705 -0.094359 0.000486
C -4.722160 -1.333546 0.000485
C -3.449631 -0.833151 0.000325
C -3.449382 0.613986 0.000284
C -4.739309 1.175276 0.000373
C -2.162643 -1.533989 0.000219
C -1.014255 -0.708345 0.000101
C -1.014007 0.738792 0.000057
C -2.300995 1.439630 0.000152
C 0.258523 1.239187 -0.000156
S 1.494068 0.000000 0.000000
C 0.275672 -1.269635 0.000000
C 0.457948 -2.656481 -0.000003
C -0.678199 -3.464023 0.000113
C -1.970810 -2.917306 0.000231
C -4.921585 2.562122 0.000341
C -3.785438 3.369664 0.000201
C -2.492827 2.822947 0.000101
H -0.561236 -4.543924 0.000143
H -3.902402 4.449566 0.000157
H 1.451008 -3.094805 -0.000051
H -5.914646 3.000446 0.000401
H -2.827716 -3.584793 0.000333
H -1.635921 3.490434 -0.000017
H 0.563096 2.277213 -0.000276
H -5.026733 -2.371572 0.000563
C -0.696603 -1.206830 3.500000
C 0.696679 -1.206683 3.500000
C 1.393322 0.000000 3.500000
C 0.696577 1.206833 3.500000
C -0.696629 1.206713 3.500000
C -1.393344 -0.000036 3.500000
H 1.242820 -2.152980 3.500000
H 2.485925 -0.000280 3.500000
H 1.243168 2.152847 3.500000
H -1.242938 2.152912 3.500000
H -2.485923 0.000486 3.500000
H -1.243041 -2.152961 3.500000

Candidate C-benzene central ring complex

38
Candidate C-benzene central ring complex

S	0.126037	3.724053	-0.000042
C	-1.169235	2.547436	0.000032
C	-0.728523	1.253025	0.000002
C	0.717039	1.185519	0.000004
C	1.337673	2.447966	-0.000007
C	-1.488418	-0.000000	-0.000009
C	-0.717039	-1.185519	0.000001
C	0.728523	-1.253025	0.000000
C	1.488418	-0.000000	-0.000000
C	1.169235	-2.547436	-0.000083
S	-0.126037	-3.724053	0.000148
C	-1.337673	-2.447966	0.000000
C	-2.731492	-2.565590	-0.000027
C	-3.485357	-1.393138	-0.000037
C	-2.879156	-0.127334	-0.000021
C	2.731492	2.565590	-0.000015
C	3.485357	1.393138	-0.000029
C	2.879156	0.127334	-0.000028
H	-4.569528	-1.459786	-0.000028
H	4.569528	1.459786	-0.000052
H	-3.215496	-3.537205	0.000002
H	3.215496	3.537205	-0.000032
H	-3.506096	0.759668	-0.000016
H	3.506096	-0.759668	-0.000048
H	2.191984	-2.899923	-0.000145
H	-2.191984	2.899923	0.000051
C	-0.696603	-1.206830	3.500000
C	0.696679	-1.206683	3.500000
C	1.393322	0.000000	3.500000
C	0.696577	1.206833	3.500000
C	-0.696629	1.206713	3.500000
C	-1.393344	-0.000036	3.500000
H	1.242820	-2.152980	3.500000
H	2.485925	-0.000280	3.500000
H	1.243168	2.152847	3.500000
H	-1.242938	2.152912	3.500000
H	-2.485923	0.000486	3.500000
H	-1.243041	-2.152961	3.500000

Candidate C-benzene ext. ring complex 2

38
Candidate C-benzene ext. ring complex 2

S	5.483255	-0.157431	0.000051
C	3.861778	-0.815435	-0.000035
C	2.885874	0.142341	-0.000003
C	3.451010	1.474568	0.000007
C	4.857708	1.487304	0.000024
C	1.427364	-0.000000	0.000000
C	0.692804	1.208678	-0.000005
C	1.257940	2.540904	0.000008
C	2.716450	2.683246	0.000015
C	0.282036	3.498681	0.000093
S	-1.339441	2.840676	-0.000150
C	-0.713893	1.195942	-0.000011
C	-1.423494	-0.009477	0.000005
C	-0.693129	-1.196709	0.000010
C	0.710346	-1.198436	0.000000
C	5.567308	2.692722	0.000043
C	4.836943	3.879955	0.000062
C	3.433469	3.881682	0.000055
H	-1.222691	-2.145093	-0.000008
H	5.366506	4.828338	0.000094
H	-2.508877	-0.024998	-0.000029
H	6.652691	2.708244	0.000066
H	1.238377	-2.147651	-0.000009
H	2.905437	4.830897	0.000080
H	0.407202	4.573203	0.000163
H	3.736612	-1.889957	-0.000063
C	-0.696603	-1.206830	3.500000
C	0.696679	-1.206683	3.500000
C	1.393322	0.000000	3.500000
C	0.696577	1.206833	3.500000
C	-0.696629	1.206713	3.500000
C	-1.393344	-0.000036	3.500000

H 1.242820 -2.152980 3.500000
H 2.485925 -0.000280 3.500000
H 1.243168 2.152847 3.500000
H -1.242938 2.152912 3.500000
H -2.485923 0.000486 3.500000
H -1.243041 -2.152961 3.500000

Radialene-benzene stacked complex

36
Radialene-benzene stacked complex
C -1.502930 -0.000023 0.000002
C -0.751419 1.301488 -0.000000
C 0.751423 1.301554 -0.000001
C 1.502958 0.000000 0.000000
C 0.751395 -1.301499 -0.000000
C -0.751426 -1.301518 -0.000002
C -1.425407 2.468664 -0.004645
C 1.425346 2.468833 0.003766
C 2.850825 -0.000002 -0.003059
C 1.425482 -2.468624 0.004153
C -1.425541 -2.468674 -0.003600
C -2.850784 -0.000088 0.002681
H -3.437801 0.908055 0.004532
H -3.437524 -0.908533 0.003398
H -0.932485 3.431152 -0.007750
H -2.505410 2.522761 -0.006474
H 2.505371 2.522684 0.004533
H 0.932549 3.431381 0.006744
H 3.437814 -0.908167 -0.004975
H 3.437633 0.908376 -0.004022
H 0.932636 -3.431162 0.006890
H 2.505480 -2.522580 0.005934
H -2.505595 -2.522257 -0.004505
H -0.932899 -3.431304 -0.006465
C -0.696603 1.206830 3.500000
C 0.696679 1.206683 3.500000
C 1.393322 0.000000 3.500000
C 0.696577 -1.206833 3.500000
C -0.696629 -1.206713 3.500000
C -1.393344 0.000036 3.500000
H 1.242820 2.152980 3.500000
H 2.485925 0.000280 3.500000
H 1.243168 -2.152847 3.500000
H -1.242938 -2.152912 3.500000
H -2.485923 -0.000486 3.500000
H -1.243041 2.152961 3.500000

Radialene-triazine stacked complex

33
Radialene-triazine stacked complex
C -1.502930 0.000023 -0.000002
C -0.751419 -1.301488 -0.000001
C 0.751423 -1.301554 0.000000
C 1.502958 0.000000 0.000000
C 0.751395 1.301499 0.000001
C -0.751426 1.301518 0.000003
C -1.425407 -2.468664 0.004643
C 1.425346 -2.468833 -0.003768
C 2.850825 0.000002 0.003059
C 1.425482 2.468624 -0.004151
C -1.425541 2.468674 0.003602
C -2.850784 0.000088 -0.002681
H -3.437801 -0.908055 -0.004533
H -3.437524 0.908533 -0.003397
H -0.932485 -3.431152 0.007747
H -2.505410 -2.522761 0.006472
H 2.505371 -2.522684 -0.004535
H 0.932549 -3.431381 -0.006747
H 3.437814 0.908167 0.004976
H 3.437633 -0.908376 0.004021
H 0.932636 3.431162 -0.006887
H 2.505480 2.522580 -0.005932

H -2.505595 2.522257 0.004507
H -0.932899 3.431304 0.006468
N -0.687933 1.191776 3.500000
C -1.293842 0.000001 3.500000
N -0.687983 -1.191784 3.500000
C 0.647111 -1.120954 3.500000
N 1.375494 0.000000 3.500000
C 0.647152 1.120964 3.500000
H -2.382645 0.000002 3.500000
H 1.190790 -2.064182 3.500000
H 1.190858 2.064177 3.500000

S-indacene-benzene central ring complex

34
S-indacene-benzene central ring complex
C -0.749858 1.193864 0.000002
C 0.749855 -1.193861 -0.000000
C 0.701782 1.210076 0.000000
C -0.701785 -1.210080 -0.000002
C -1.442952 -0.000001 0.000001
C 1.442960 0.000000 0.000000
X 0.000000 0.000000 0.000000
C -1.185543 2.571508 0.000002
C 1.185510 -2.571495 -0.000015
C 1.100495 2.551632 -0.000006
C -1.100527 -2.551639 -0.000024
C -0.065203 3.382635 -0.000004
C 0.065158 -3.382632 -0.000030
H -2.531610 -0.021924 -0.000001
H 2.531619 0.021928 -0.000003
H -2.218329 2.901894 0.000008
H 2.218284 -2.901910 -0.000011
H 2.125095 2.909240 -0.000008
H -2.125140 -2.909213 -0.000029
H -0.059595 4.465808 -0.000011
H 0.059596 -4.465805 -0.000048
C -0.696603 -1.206830 3.500000
C 0.696679 -1.206683 3.500000
C 1.393322 0.000000 3.500000
C 0.696577 1.206833 3.500000
C -0.696629 1.206713 3.500000
C -1.393344 -0.000036 3.500000
X 0.000000 0.000000 3.500000
H 1.242820 -2.152980 3.500000
H 2.485925 -0.000280 3.500000
H 1.243168 2.152847 3.500000
H -1.242938 2.152912 3.500000
H -2.485923 0.000486 3.500000
H -1.243041 -2.152961 3.500000

S-indacene-benzene above double bond stacked complex

32
S-indacene-benzene above double bond stacked complex
C -1.332088 -4.184894 -0.000025
C -1.146597 -1.371362 -0.000001
C -2.517416 -3.346730 -0.000032
C 0.038735 -2.209519 0.000002
C -0.070559 -3.624325 -0.000008
C -2.408133 -1.931920 -0.000019
C -1.787086 -5.556280 -0.000042
C -0.691580 -0.000001 0.000001
C -3.627109 -4.199564 -0.000058
C 1.148454 -1.356700 0.000000
C -3.170230 -5.556280 -0.000062
C 0.691580 0.000000 0.000000
H 0.824105 -4.244997 -0.000006
H -3.302801 -1.311252 -0.000026
H -1.144286 -6.429555 -0.000037
H -1.334354 0.873291 0.000006
H -4.666744 -3.888361 -0.000068
H 2.188080 -1.667938 0.000003
H -3.809986 -6.430355 -0.000084

H	1.331297	0.874103	-0.000003
C	-0.696603	-1.206830	3.500000
C	0.696679	-1.206683	3.500000
C	1.393322	0.000000	3.500000
C	0.696577	1.206833	3.500000
C	-0.696629	1.206713	3.500000
C	-1.393344	-0.000036	3.500000
H	1.242820	-2.152980	3.500000
H	2.485925	-0.000280	3.500000
H	1.243168	2.152847	3.500000
H	-1.242938	2.152912	3.500000
H	-2.485923	0.000486	3.500000
H	-1.243041	-2.152961	3.500000

S-indacene-benzene above single bond stacked complex

32
S-indacene-benzene above single bond stacked complex

C	-2.604429	-3.253425	0.000028
C	0.002775	-2.179713	0.000003
C	-1.431806	-4.109273	0.000036
C	-1.169843	-1.323859	-0.000001
C	-2.475783	-1.878964	0.000009
C	-0.125859	-3.554177	0.000022
C	-3.758891	-4.122299	0.000045
C	1.157207	-1.310830	0.000000
C	-1.885890	-5.433113	0.000062
C	-0.715781	-0.000000	0.000000
C	-3.317468	-5.433113	0.000066
C	0.715781	0.000000	0.000000
H	-3.349524	-1.229168	0.000007
H	0.747880	-4.203977	0.000030
H	-4.791644	-3.791813	0.000040
H	2.189968	-1.641285	-0.000004
H	-1.259169	-6.319064	0.000073
H	-1.342533	0.885931	-0.000004
H	-3.941661	-6.318369	0.000089
H	1.340012	0.885229	0.000003
C	-0.696603	-1.206830	3.500000
C	0.696679	-1.206683	3.500000
C	1.393322	0.000000	3.500000
C	0.696577	1.206833	3.500000
C	-0.696629	1.206713	3.500000
C	-1.393344	-0.000036	3.500000
H	1.242820	-2.152980	3.500000
H	2.485925	-0.000280	3.500000
H	1.243168	2.152847	3.500000
H	-1.242938	2.152912	3.500000
H	-2.485923	0.000486	3.500000
H	-1.243041	-2.152961	3.500000

Candidate B caffeine optimized complex

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Candidate B caffeine optimized complex

N	1.470050	2.132049	-1.119023
C	2.134727	2.201049	0.108776
N	1.361025	2.096642	1.249219
C	0.091265	1.961610	-1.333289
C	-0.612305	1.893052	-0.091459
C	0.007794	1.947986	1.139089
N	-1.945940	1.713248	0.188186
C	-2.038412	1.678375	1.531193
N	-0.875584	1.820129	2.147522
C	1.989113	2.224995	2.542621
O	3.336278	2.354641	0.161134
O	-0.394360	1.892880	-2.448377
C	-3.009684	1.619409	-0.777806
C	2.316254	2.300374	-2.283186
H	-2.996873	1.534100	2.028139
H	3.010907	1.837007	2.475127
H	1.398864	1.653822	3.268452
H	2.026683	3.279058	2.860836
H	-2.741917	0.887800	-1.548460

H	-3.176956	2.591340	-1.263529
H	-3.923484	1.295986	-0.264953
H	3.162852	1.605853	-2.231778
H	2.714534	3.324883	-2.321643
H	1.698822	2.102514	-3.165202
C	-1.002801	-1.535805	-1.384460
C	-1.664736	-1.570868	-0.117457
C	-1.141501	-1.491942	1.210954
C	0.307564	-1.363113	1.286552
C	0.968972	-1.337033	0.020565
C	0.446316	-1.401720	-1.307674
C	-3.031507	-1.698651	-0.189764
C	-2.158110	-1.551743	2.126770
C	1.219892	-1.253166	2.302959
C	2.335328	-1.199868	0.092292
C	1.462173	-1.313273	-2.222999
C	-1.914815	-1.640006	-2.401549
S	-3.729696	-1.708598	1.388350
S	-3.555058	-1.796280	-1.830591
S	2.859155	-1.118249	1.732095
S	3.029697	-1.159561	-1.483347
H	-2.095783	-1.503095	3.212806
H	-1.736486	-1.632962	-3.475692
H	1.038113	-1.233438	3.376438
H	1.396010	-1.313978	-3.309858

Candidate E-caffeine optimized complex

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Candidate E-caffeine optimized complex

N	-0.992365	-1.819475	-1.438332
C	-2.051903	-1.868405	-0.529811
N	-1.733176	-1.844637	0.812549
C	0.377586	-1.719191	-1.142822
C	0.593030	-1.700940	0.270111
C	-0.425165	-1.763880	1.198437
N	1.746607	-1.605755	1.008721
C	1.358774	-1.613087	2.298252
N	0.048405	-1.713437	2.457828
C	-2.806891	-1.924672	1.774173
O	-3.202922	-1.936895	-0.907586
O	1.233058	-1.662749	-2.007825
C	3.084342	-1.498040	0.485159
C	-1.378484	-1.908649	-2.831357
H	2.083753	-1.546899	3.109146
H	-3.580661	-1.189175	1.523053
H	-2.385054	-1.714402	2.763127
H	-3.263551	-2.925650	1.765291
H	3.169570	-0.605479	-0.146437
H	3.326357	-2.380940	-0.121068
H	3.784303	-1.417795	1.325499
H	-2.090701	-1.111313	-3.074772
H	-1.864130	-2.874794	-3.029689
H	-0.466623	-1.810315	-3.429241
C	-0.631553	1.646158	-0.095175
C	0.087420	1.696033	1.119773
C	-0.616606	1.646169	2.301599
C	-2.030634	1.549973	2.244853
C	-2.724438	1.503432	1.050531
C	-2.023068	1.543943	-0.182779
C	1.505150	1.784581	0.752496
H	-0.115116	1.666113	3.271296
H	-3.814483	1.427595	1.050406
C	0.234798	1.687294	-1.209506
C	-0.316472	1.631148	-2.470046
C	-1.726494	1.532644	-2.589668
C	-2.565832	1.484172	-1.492545
C	1.595059	1.774309	-0.666420
H	0.304151	1.647121	-3.368372
H	-3.644398	1.383119	-1.629285
C	2.654488	1.872031	1.527210
C	2.832568	1.849348	-1.292167
C	3.981855	1.946948	-0.504684
C	3.893989	1.958286	0.888834
H	2.590250	1.881509	2.617784

H	4.961226	2.012407	-0.983706
H	2.906353	1.830372	-2.381310
H	4.805439	2.036898	1.485880
H	-2.161271	1.484672	-3.590665
H	-2.587955	1.506548	3.183306

Candidate A-caffeine optimized complex

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Candidate A-caffeine optimized complex

N	-2.005607	-2.090440	-0.430604
C	-2.926256	-1.148211	0.035279
N	-2.529208	-0.347065	1.083037
C	-0.690825	-2.290853	0.020573
C	-0.368304	-1.382750	1.076450
C	-1.257408	-0.451373	1.572428
N	0.800873	-1.161684	1.765261
C	0.544779	-0.142054	2.607058
N	-0.695889	0.312366	2.527268
C	-3.460809	0.626048	1.600557
O	-4.026357	-1.045267	-0.467754
O	0.042647	-3.133031	-0.470065
C	2.044894	-1.874712	1.590699
C	-2.476610	-2.909283	-1.527460
H	1.310018	0.251383	3.275291
H	-3.923594	1.167912	0.767173
H	-2.900820	1.314482	2.242932
H	-4.256349	0.135287	2.181272
H	1.942916	-2.514525	0.707445
H	2.259590	-2.500760	2.469080
H	2.862934	-1.161475	1.427699
H	-2.782181	-2.273953	-2.370287
H	-3.352943	-3.495646	-1.218539
H	-1.654825	-3.571221	-1.818723
C	2.860962	1.380196	0.067663
C	2.604119	2.509517	0.911607
C	1.379902	3.099476	0.944979
C	0.302475	2.624950	0.129509
C	0.529873	1.508273	-0.718712
C	1.804186	0.879180	-0.742258
C	-0.524471	1.009953	-1.532040
C	-1.777923	1.631445	-1.480789
C	-1.989962	2.728288	-0.652022
C	-0.964773	3.218767	0.148668
H	3.419100	2.888385	1.533341
H	1.195760	3.955359	1.598478
H	-2.596378	1.231741	-2.083902
H	-2.972949	3.203502	-0.625273
H	-1.138931	4.074064	0.805594
C	-0.275329	-0.135744	-2.355130
C	0.937726	-0.747028	-2.366836
C	2.022202	-0.257050	-1.568762
C	3.286629	-0.858937	-1.580959
C	4.322193	-0.351474	-0.803472
C	4.113653	0.753827	0.015872
H	4.928578	1.146727	0.628750
H	3.448754	-1.734344	-2.213959
H	5.304611	-0.828040	-0.831498
H	-1.092776	-0.518370	-2.970363
H	1.104702	-1.635686	-2.978033

Candidate C-caffeine optimized complex

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Candidate C-caffeine optimized complex

N	1.577597	2.126711	-1.022553
C	2.184887	2.188284	0.234483
N	1.363268	2.066495	1.337041
C	0.211249	1.944629	-1.299468
C	-0.546874	1.861229	-0.091047
C	0.017041	1.909565	1.166860
N	-1.890919	1.668216	0.126823
C	-2.043135	1.621695	1.463907
N	-0.910104	1.766106	2.132757

C	1.952036	2.168970	2.651415
O	3.381832	2.348438	0.348197
O	-0.222494	1.877842	-2.436153
C	-2.910748	1.577186	-0.886550
C	2.475274	2.311301	-2.144873
H	-3.021548	1.465807	1.916692
H	2.867321	1.567580	2.685517
H	1.218516	1.799463	3.376365
H	2.210113	3.213468	2.884971
H	-2.597881	0.865267	-1.658653
H	-3.073307	2.556606	-1.358822
H	-3.839347	1.227389	-0.420247
H	3.320364	1.617770	-2.063125
H	2.870203	3.337769	-2.153250
H	1.900218	2.120935	-3.056698
S	3.031774	-1.193399	-1.596237
C	1.432091	-1.324035	-2.237281
C	0.469015	-1.419138	-1.271547
C	1.043803	-1.379183	0.045017
C	2.440010	-1.249028	0.037271
C	-0.976835	-1.535122	-1.399561
C	-1.692166	-1.592189	-0.187093
C	-1.117803	-1.542353	1.130375
C	0.328817	-1.427395	1.257368
C	-2.082874	-1.604142	2.095507
S	-3.687361	-1.725933	1.453150
C	-3.090416	-1.704032	-0.181460
C	-3.810328	-1.774781	-1.375876
C	-3.097013	-1.712367	-2.567971
C	-1.701573	-1.587881	-2.587156
C	3.160897	-1.176371	1.230756
C	2.447789	-1.236467	2.422399
C	1.052184	-1.358963	2.443565
H	-3.638890	-1.759304	-3.514999
H	2.990134	-1.178907	3.368592
H	-4.897424	-1.870918	-1.378444
H	4.245384	-1.060018	1.230291
H	-1.180451	-1.527868	-3.543831
H	0.529812	-1.388835	3.401367
H	-1.944493	-1.568862	3.174906
H	1.288299	-1.307753	-3.316389

Candidate D-caffeine optimized complex

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Candidate D-caffeine optimized complex

N	-1.327023	1.552543	-0.842241
C	-1.245936	0.619281	-1.878518
N	-0.003836	0.412789	-2.442684
C	-0.273678	2.288035	-0.276972
C	0.967151	1.990412	-0.923846
C	1.081438	1.093290	-1.966149
N	2.247644	2.435633	-0.692401
C	3.026913	1.795798	-1.587213
N	2.357392	0.973840	-2.379684
C	0.108375	-0.546934	-3.515614
O	-2.225489	0.014700	-2.259621
O	-0.441566	3.053613	0.657151
C	2.656547	3.415608	0.288643
C	-2.654026	1.728868	-0.287826
H	4.104132	1.956126	-1.617906
H	-0.291243	-1.516865	-3.190454
H	1.169386	-0.634345	-3.773875
H	-0.468243	-0.215271	-4.390893
H	1.851121	3.510619	1.025819
H	2.816625	4.395093	-0.185731
H	3.582337	3.079240	0.773861
H	-3.025725	0.775673	0.109614
H	-3.348667	2.065037	-1.069037
H	-2.578730	2.473307	0.510638
C	0.597514	-2.190874	-0.288650
C	-0.518532	-2.942540	-0.770328
C	-1.762043	-2.776062	-0.247319
C	-1.991443	-1.850896	0.816941
C	-0.903655	-1.091501	1.322194

C	0.393339	-1.260158	0.765354
C	-1.108315	-0.156469	2.372149
C	-2.392734	-0.002078	2.911065
C	-3.457036	-0.747179	2.432043
C	-3.267987	-1.663499	1.390429
H	-0.354690	-3.654533	-1.582072
H	-2.609592	-3.345339	-0.633093
H	-2.547948	0.717481	3.717322
H	-4.454562	-0.624027	2.855782
C	-4.381182	-2.411776	0.901406
C	0.004791	0.606105	2.843790
C	1.245174	0.448152	2.310821
C	1.477127	-0.482895	1.252115
C	2.745689	-0.648377	0.653247
C	2.936039	-1.569791	-0.383102
C	1.877918	-2.334066	-0.840914
H	2.029745	-3.046368	-1.654146
C	3.831051	0.175053	1.073216
H	3.922465	-1.665152	-0.837760
H	-0.164124	1.333924	3.639271
H	2.085128	1.042562	2.675374
N	-5.282616	-3.023331	0.503445
N	4.694618	0.877346	1.402803