Supplementary Data for:

Metal-Free Hydrogenation Catalysis of Polycyclic Aromatic Hydrocarbons

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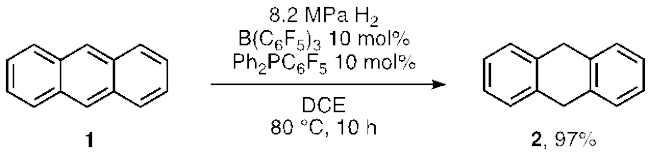
General Procedure

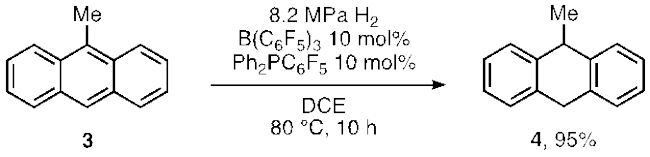
Unless otherwise noted, all materials were obtained from commercial suppliers and used without further purification. 1,2-Dichloroethane (DCE) was degassed through a freeze-pump-thaw and dried by molecular sieves (4Å) prior to use. All reactions were performed using pressure vessel (Parr Instrument Company). Work-up and purification procedures were carried out with reagent-grade solvents under air.

Hydrogenation of Anthracene (1)



In a N_2-filled glove box, a 6 mL glass vial equipped with a stir bar was charged with a yellow solution of $B(C_6F_5)_3$ (10 mg, 20 μmol), $Ph_2PC_6F_5$ (7 mg, 20 μmol), and anthracene (**1**, 35 mg, 200 μmol) in DCE (2 mL). The vial was put into power reactor. The reactor was filled by dihydrogen (8.2 MPa) out of the glove box and the reactor was left to stir at 80 °C for 10 hrs. The reaction mixture was concentrated under reduced pressure. The crude product was purified by silica gel column chromatography with hexane to obtain 9,10-dihydroanthracene (**2**, 34 mg, 97%). NMR data are consistent with those reported.[S1]

Hydrogenation of 9-Methylanthracene (3)



In a N_2-filled glove box, a 6 mL glass vial equipped with a stir bar was charged with a yellow solution of $B(C_6F_5)_3$ (10 mg, 20 μmol), $Ph_2PC_6F_5$ (7 mg, 20 μmol), and 9-methylanthracene (**3**, 38 mg, 200 μmol) in DCE (2 mL). The vial was put into power reactor. The reactor was filled by

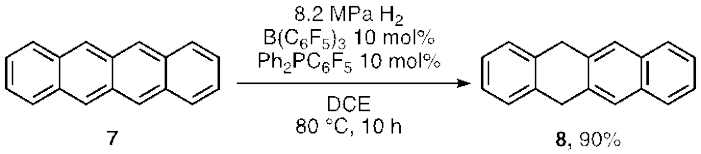
S1) Nandi, P.; Dye, J. L.; Jackson, J. E. *J. Org. Chem.* **2009**, *74*, 5790-5792.

dihydrogen (8.2 MPa) out of the glove box and the reactor was left to stir at 80 °C for 10 hrs. The reaction mixture was concentrated under reduced pressure. The crude product was purified by silica gel column chromatography with hexane to obtain 9-methyl-9,10-dihydroanthracene (**4**, 36 mg, 95%). NMR data are consistent with those reported.[S1]

Hydrogenation of 9-Phenylanthracene (5)

In a N_2-filled glove box, a 6 mL glass vial equipped with a stir bar was charged with a yellow solution of $B(C_6F_5)_3$ (10 mg, 20 μmol), $Ph_2PC_6F_5$ (7 mg, 20 μmol), and 9,10-dimethylanthracene (**5**, 41 mg, 200 μmol) in DCE (2 mL). The vial was put into power reactor. The reactor was filled by dihydrogen (8.2 MPa) out of the glove box and the reactor was left to stir at 80 °C for 48 hrs. The reaction mixture was concentrated under reduced pressure. The crude product was purified by silica gel column chromatography with hexane/CH_2Cl_2 to obtain the 75:25 mixture of *cis*- and *trans*-9,10-dimethyl-9,10-dihydroanthracene (**6**, 33 mg, 80%). NMR data are consistent with those reported.[S2]

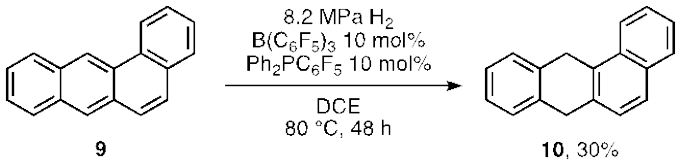
Hydrogenation of Tetracene (7)



In a N_2-filled glove box, a 6 mL glass vial equipped with a stir bar was charged with a yellow solution of $B(C_6F_5)_3$ (10 mg, 20 μmol), $Ph_2PC_6F_5$ (7 mg, 20 μmol), and tetracene (**7**, 45 mg, 200 μmol) in DCE (2 mL). The vial was put into power reactor. The reactor was filled by dihydrogen (8.2 MPa) out of the glove box and the reactor was left to stir at 80 °C for 10 hrs. The reaction mixture was concentrated under reduced pressure. The crude product was purified by silica gel column chromatography with hexane/CH_2Cl_2 to obtain 5,12-dihydrotetracene (**8**, 41 mg, 90%). NMR data are consistent with those reported.[S3]

S2) Prakash, G. K. S.; Mathew, T.; Marinez, E. R.; Esteves, P. M.; Rasul, G. Olah, G. A. *J. Org. Chem.* **2006**, *71*, 3952–3958.
S3) Luo, J.; Hart, H. *J. Org. Chem.* **1987**, *52*, 4833−4836.

Hydrogenation of Tetraphene (9)



9 **10**, 30%

In a N_2-filled glove box, a 6 mL glass vial equipped with a stir bar was charged with a yellow solution of $B(C_6F_5)_3$ (10 mg, 20 μmol), $Ph_2PC_6F_5$ (7 mg, 20 μmol), and tetraphene (**9**, 45 mg, 200 μmol) in DCE (2 mL). The vial was put into power reactor. The reactor was filled by dihydrogen (8.2 MPa) out of the glove box and the reactor was left to stir at 80 °C for 48 hrs. The reaction mixture was concentrated under reduced pressure. The crude product was purified by silica gel column chromatography with hexane/CH_2Cl_2 to obtain 7,12-dihydrotetraphene (**10**, 14 mg, 30%). NMR data are consistent with those reported.[S2]

X-ray Crystallography of 8

Single crystals were coated in Paratone-N oil, mounted on a MiTegen Micromount and placed under an N_2 stream. The data were collected on a Bruker Apex II diffractometer. The data were collected at 150(2) K for all crystals. Data reduction was performed using the SAINT software package, and an absorption correction was applied using SADABS. The structures were solved by direct methods using XS and refined by full-matrix least squares on F^2 using XL as implemented in the SHELXTL suite of programs.[S4] All non-hydrogen atoms were refined anisotropically. Carbon-bound hydrogen atoms were placed in calculated positions using an appropriate riding model and coupled isotropic temperature factors.

Table S1. Crystallographic data and refinement details for **8**.

	8
formula	$C_{18}H_{14}$
fw	230.29
T (K)	150(2)
λ (Å)	0.71073
cryst syst	Orthorhombic
space group	$P2_12_12_1$
a, (Å)	6.0792(3)
b, (Å)	7.5470(3)
c, (Å)	25.7083(12)
α, (deg)	90
β, (deg)	90
γ, (deg)	90
V, (Å^3)	1179.49(9)
Z	4
D_{calc}, (g / cm^3)	1.297
μ (mm^{-1})	0.073
F(000)	488
cryst size (mm)	0.36 × 0.20 × 0.20
2θ range, (deg)	1.58–27.61
reflns collected	10527
indep reflns/R_{int}	2713/0.0215
params	163
GOF on F^2	0.920
R_1, wR_2 [I>2σ(I)]	0.0344, 0.1053
R_1, wR_2 (all data)	0.0388, 0.1105

S4) (a) Sheldrick, G. M. *Acta Crystallogr*. **1990**, *A46*, 467. (b) Sheldrick, G. M. SHELXTL; Bruker AXS Inc., Madison, WI, 2000. (c) Sheldrick, G. M. *Acta Crystallogr*. **2008**, *A64*, 112.

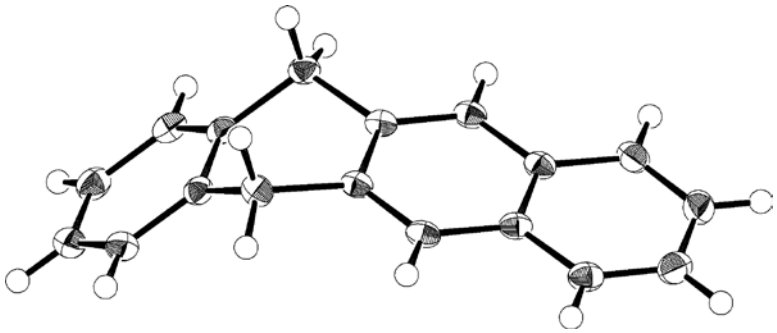


Figure S1. ORTEP drawing of **8** with 50% thermal ellipsoids.

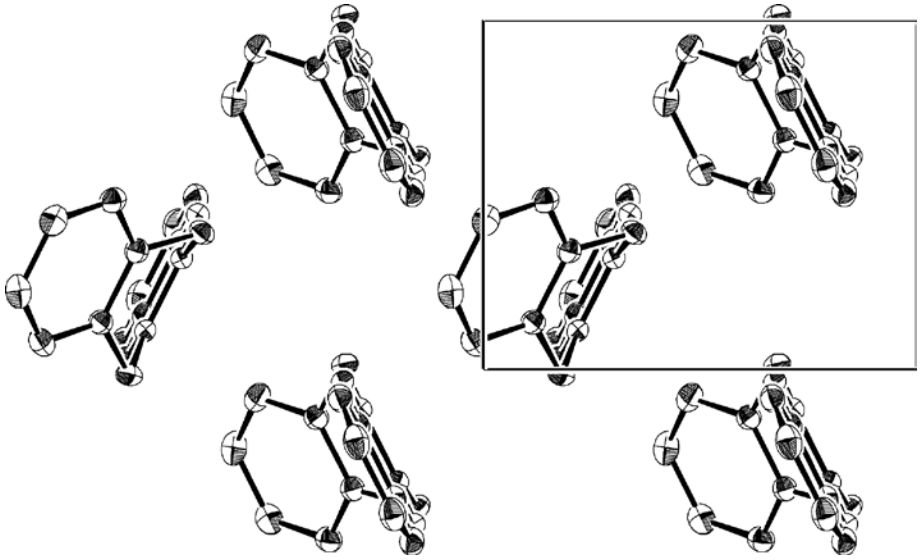


Figure S2. Packing mode of **8**.

Theoretical Methods and Technical Details of the Computations

The Gaussian 09 program[S5] running on a SGI Altix4700 system was used for optimization (B3LYP/6-31G(d)).[S6] All structures were optimized without any symmetry assumptions. Zero-point energy, enthalpy, and Gibbs free energy at 298.15 K and 1 atm were estimated from the gas-phase studies. Harmonic vibration frequency calculation at the same level was performed to verify all stationary points as local minima (with no imaginary frequency).

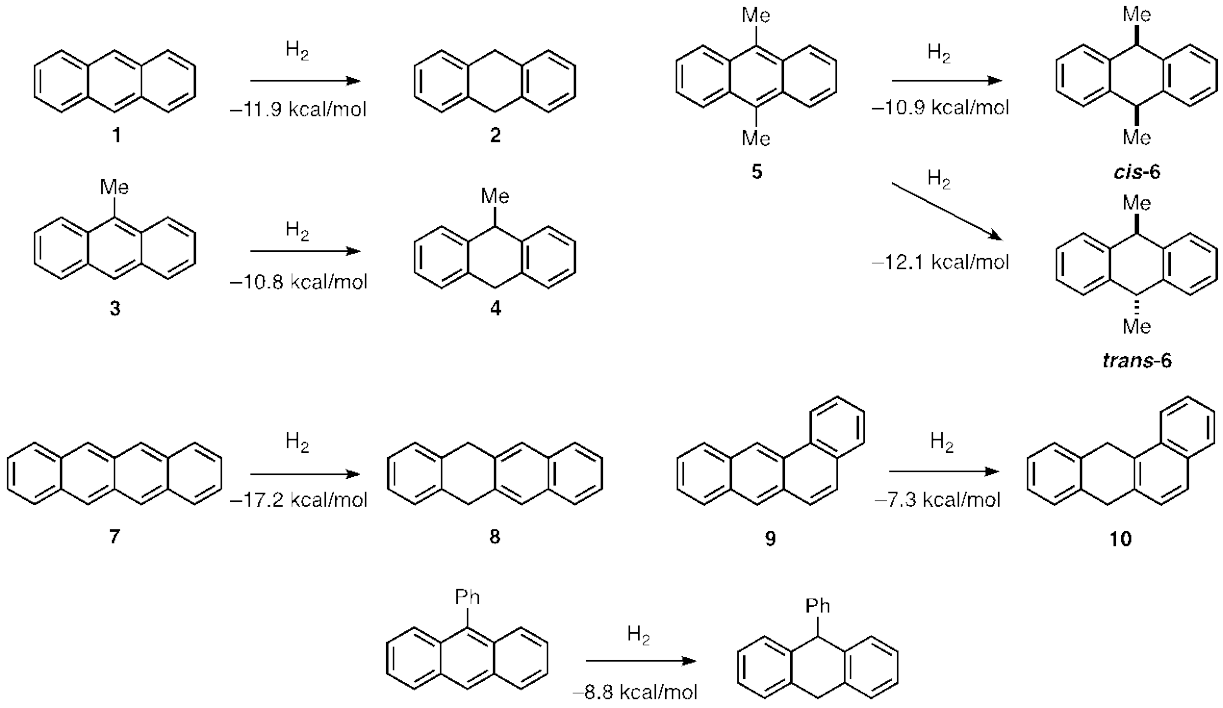


Figure S3. Heats of hydrogenation (ΔH).

S5) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09, Revision C.01*, Gaussian, Inc., Wallingford CT, 2010.

S6) (a) Becke, A. D. *J. Chem. Phys.*, 1993, **98**, 5648–5652. (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B*, 1988, **37**, 785–789.

Table S2. Cartesian coordinates of optimized species.

1 (*H* = -539.325606 Hartree)

C	3.660679	0.713146	-0.000017	C	-1.223922	-0.722626	0.000024	H	4.607360	1.246657	-0.000044
C	2.479530	1.407036	0.000046	C	-1.223924	0.722624	0.000006	H	2.476862	2.494579	0.000097
C	1.223923	0.722624	0.000030	C	-2.479530	1.407037	-0.000027	H	2.476866	-2.494578	-0.000027
C	1.223924	-0.722625	0.000022	H	-2.476865	2.494579	-0.000067	H	4.607356	-1.246662	-0.000119
C	2.479532	-1.407036	-0.000025	C	-3.660680	0.713145	-0.000055	H	-0.000004	-2.491749	0.000047
C	3.660681	-0.713142	-0.000061	C	-3.660680	-0.713143	-0.000007	H	-4.607357	1.246662	-0.000091
C	0.000000	1.403377	0.000024	C	-2.479531	-1.407037	0.000029	H	-4.607357	-1.246660	-0.000023
C	0.000001	-1.403378	0.000028	H	-0.000006	2.491747	0.000046	H	-2.476869	-2.494580	0.000074

2 (*H* = -540.506554 Hartree)

C	-3.564255	-0.697807	-0.500688	C	0.000001	-1.431560	0.689461	H	0.000003	1.530489	1.788424
C	-3.564278	0.697780	-0.500639	C	2.412768	1.390084	-0.124469	H	-0.000002	-1.530160	1.788569
C	-2.412773	1.390082	-0.124457	C	3.564276	0.697782	-0.500645	H	2.407482	2.478098	-0.133677
C	-1.258781	0.702180	0.262142	C	3.564258	-0.697805	-0.500681	H	4.453771	1.245723	-0.800205
C	-1.258784	-0.702185	0.262153	C	2.412750	-1.390097	-0.124485	H	4.453732	-1.245758	-0.800283
C	-2.412745	-1.390099	-0.124496	H	-4.453725	-1.245761	-0.800300	H	2.407443	-2.478110	-0.133699
C	0.000000	1.431617	0.689338	H	-4.453776	1.245721	-0.800191	H	-0.000002	2.455701	0.298709
C	1.258779	0.702180	0.262138	H	-2.407490	2.478096	-0.133656	H	0.000002	-2.455735	0.299076
C	1.258786	-0.702184	0.262155	H	-2.407435	-2.478111	-0.133718				

3 (*H* = -578.607429 Hartree)

C	3.67925	0.442133	0.011522	C	-1.22151	0.487557	-0.002138	H	4.60273	-1.530859	0.005527
C	2.50971	1.155961	0.008425	C	-2.49945	1.135582	0.007025	H	0.02210	-2.718814	-0.011099
C	1.22807	0.510270	-0.002102	H	-2.54632	2.218827	0.014412	H	-4.62217	0.939263	0.018762
C	1.22645	-0.939435	-0.004864	C	-3.66841	0.418245	0.010815	H	-4.58315	-1.557488	0.007097
C	2.47041	-1.646148	-0.003611	C	-3.64773	-1.004574	0.005045	H	-2.41849	-2.755018	-0.005166
C	3.66537	-0.981342	0.003990	C	-2.45014	-1.667902	-0.002049	C	-0.06255	2.723501	-0.014386
C	-0.00272	1.210514	-0.007236	H	4.63054	0.967578	0.020692	H	-0.53061	3.108114	0.900781
C	0.01355	-1.630711	-0.007972	H	2.56597	2.238029	0.018837	H	0.91863	3.189737	-0.094279
C	-1.21034	-0.956425	-0.004167	H	2.44044	-2.733294	-0.007463	H	-0.65930	3.090570	-0.857884

4 (*H* = -579.786723 Hartree)

C	3.495903	0.381037	-0.697659	C	-2.361692	-1.643442	-0.046241	H	-2.344824	-2.727178	0.048431
C	3.489935	-1.006200	-0.565946	C	-3.489956	-1.006172	-0.565942	H	-4.353154	-1.591155	-0.872240
C	2.361670	-1.643465	-0.046237	C	-3.495918	0.381065	-0.697649	H	-4.364939	0.888270	-1.108603
C	1.246081	-0.904000	0.349103	C	-2.380302	1.126181	-0.306270	H	-2.401622	2.205069	-0.421698
C	1.249368	0.497671	0.222707	H	4.364922	0.888238	-1.108623	C	0.000064	2.744622	0.374767
C	2.380294	1.126160	-0.306274	H	4.353128	-1.591190	-0.872244	H	0.000001	2.928474	-0.705604
C	-0.000013	-1.561990	0.904021	H	2.344798	-2.727200	0.048440	H	-0.880114	3.233054	0.803955
C	-1.246099	-0.903983	0.349102	H	2.401610	2.205052	-0.421699	H	0.880348	3.232975	0.803832
C	-1.249371	0.497690	0.222706	H	-0.000012	-1.464822	2.003730	H	-0.000018	-2.637009	0.693824
C	0.000012	1.247065	0.695011	H	0.000023	1.163994	1.797295				

5 (*H* = -617.887873 Hartree)

C	-3.672767	0.688744	-0.085529	C	2.479151	1.412532	-0.041921	H	4.616128	-1.226125	-0.132905
C	-2.491322	1.378365	-0.029736	H	2.502822	2.495207	-0.071410	H	2.516459	-2.461636	-0.046168
C	-1.223020	0.711213	0.021373	C	3.665580	0.730945	-0.093336	C	-0.054197	2.951520	0.134532
C	-1.214468	-0.738275	0.018496	C	3.672709	-0.688734	-0.086323	H	-0.277060	3.404133	-0.841425
C	-2.479217	-1.412526	-0.041253	C	2.491277	-1.378365	-0.030231	H	-0.825339	3.292119	0.831958

C	-3.665650	-0.730938	-0.092419	H	-4.616190	1.226140	-0.131973	H	0.886316	3.377504	0.484634
C	-0.012305	1.438788	0.063085	H	-2.516512	2.461633	-0.045797	C	0.054404	-2.951525	0.134410
C	0.012288	-1.438796	0.063048	H	-2.502936	-2.495200	-0.070641	H	0.278513	-3.403959	-0.841340
C	1.222994	-0.711208	0.021087	H	-4.603893	-1.276754	-0.145340	H	0.824884	-3.291978	0.832663
C	1.214438	0.738258	0.018199	H	4.603807	1.276762	-0.146544	H	-0.886369	-3.377834	0.483381

***cis*-6** (*H* = -619.067225 Hartree)

C	-3.443080	-0.695884	-0.782591	C	3.443088	0.695948	-0.782525	H	4.292880	-1.245243	-1.179278
C	-3.443074	0.695922	-0.782541	C	3.443102	-0.695855	-0.782587	H	2.352271	-2.476177	-0.285146
C	-2.342320	1.390984	-0.273908	C	2.342351	-1.390960	-0.274001	C	0.000001	-2.921228	0.677907
C	-1.239067	0.704985	0.237329	H	-4.292856	-1.245280	-1.179276	H	0.000219	-3.242219	-0.369916
C	-1.239067	-0.705016	0.237285	H	-4.292851	1.245364	-1.179161	H	0.880970	-3.350527	1.165139
C	-2.342328	-1.390980	-0.273996	H	-2.352254	2.476209	-0.284973	H	-0.881206	-3.350476	1.164756
C	-0.000009	1.395947	0.806992	H	-2.352243	-2.476198	-0.285110	C	-0.000056	2.921153	0.677830
C	1.239067	0.704995	0.237335	H	-0.000025	1.173395	1.890151	H	-0.000052	3.242037	-0.370025
C	1.239090	-0.705009	0.237299	H	-0.000007	-1.173419	1.890081	H	-0.881160	3.350443	1.164830
C	0.000009	-1.396005	0.806931	H	2.352253	2.476221	-0.284965	H	0.881013	3.350486	1.164853
C	2.342324	1.390999	-0.273896	H	4.292864	1.245397	-1.179140				

***trans*-6** (*H* = -619.069169 Hartree)

C	3.541332	0.671688	-0.675902	C	-3.531483	-0.710685	-0.850813	H	-4.424883	1.250873	-0.931380
C	3.531468	-0.710701	-0.850818	C	-3.541346	0.671703	-0.675885	H	-2.436611	2.397786	-0.056917
C	2.382106	-1.432446	-0.529065	C	-2.409522	1.319920	-0.176954	C	0.000042	2.796766	0.652077
C	1.246657	-0.791481	-0.026117	H	4.424863	1.250858	-0.931414	H	0.000025	3.146248	-0.386591
C	1.254568	0.604087	0.158606	H	4.405958	-1.223080	-1.243104	H	-0.877910	3.213994	1.153939
C	2.409518	1.319908	-0.176951	H	2.360866	-2.510554	-0.676293	H	0.878048	3.213945	1.153898
C	-0.000018	-1.587536	0.318118	H	2.436604	2.397776	-0.056934	C	0.000011	-2.040213	1.800566
C	-1.246667	-0.791469	-0.026107	H	-0.000035	-2.500341	-0.291733	H	-0.889326	-2.642596	2.016749
C	-1.254570	0.604103	0.158593	H	0.000016	1.025033	1.815598	H	0.889321	-2.642654	2.016680
C	0.000008	1.265596	0.738540	H	-2.360888	-2.510538	-0.676285	H	0.000054	-1.184552	2.483911
C	-2.382125	-1.432429	-0.529058	H	-4.405977	-1.223060	-1.243095				

7 (*H* = -692.911636 Hartree)

C	-4.888989	0.715459	-0.000049	C	1.235456	-1.406340	0.000037	H	-3.708352	-2.496775	-0.000006
C	-4.888989	-0.715459	-0.000032	C	2.450564	-0.725916	0.000002	H	-3.708353	2.496775	-0.000038
C	-3.711316	-1.409284	-0.000016	C	2.450564	0.725916	-0.000005	H	-1.235034	-2.494521	0.000015
C	-2.450564	-0.725916	0.000019	C	1.235456	1.406341	0.000000	H	-1.235035	2.494521	0.000055
C	-2.450564	0.725916	0.000023	C	3.711316	-1.409284	-0.000033	H	1.235035	-2.494521	0.000058
C	-3.711317	1.409283	-0.000016	C	4.888989	-0.715459	-0.000042	H	1.235035	2.494522	-0.000037
C	-1.235456	-1.406340	0.000039	C	4.888989	0.715459	-0.000003	H	3.708351	-2.496775	-0.000071
C	0.000000	-0.726067	0.000037	C	3.711317	1.409284	-0.000013	H	5.836721	-1.246990	-0.000040
C	0.000000	0.726068	0.000028	H	-5.836722	1.246989	-0.000061	H	5.836722	1.246989	0.000006
C	-1.235456	1.406341	0.000048	H	-5.836721	-1.246991	-0.000042	H	3.708353	2.496775	0.000016

8 (*H* = -694.101121 Hartree)

C	-4.632537	-0.697704	-0.832223	C	2.419273	0.716071	0.004681	H	-1.399298	1.477256	1.940879
C	-4.632541	0.697724	-0.832197	C	2.419282	-0.716067	0.004697	H	-1.227448	2.462176	0.498277
C	-3.544893	1.390913	-0.298936	C	1.202901	-1.396844	0.275698	H	-1.227436	-2.462187	0.498176
C	-2.457241	0.702433	0.244867	C	3.631915	1.402531	-0.272327	H	-1.399310	-1.477343	1.940829
C	-2.457238	-0.702443	0.244843	C	4.791695	0.708400	-0.535100	H	1.201838	2.485452	0.264471
C	-3.544887	-1.390908	-0.298985	C	4.791706	-0.708379	-0.535073	H	1.201862	-2.485458	0.264487
C	-1.266952	1.424113	0.846547	C	3.631935	-1.402519	-0.272281	H	3.628690	2.490262	-0.272753
C	0.038077	0.713355	0.545762	H	-5.471641	-1.245376	-1.253014	H	5.712807	1.245706	-0.744547

C	0.038080	-0.713370	0.545756	H	-5.471647	1.245409	-1.252969	H	5.712826	-1.245679	-0.744501
C	-1.266952	-1.424144	0.846501	H	-3.538526	2.478879	-0.307043	H	3.628728	-2.490250	-0.272667
C	1.202887	1.396838	0.275687	H	-3.538512	-2.478873	-0.307137				

9 (*H* = -692.924370 Hartree)

C	-4.366745	-1.378886	-0.000206	C	0.942969	2.354570	0.000013	H	-4.107783	2.028667	0.000446
C	-4.758610	-0.011390	0.000074	C	2.264464	2.051349	-0.000221	H	-2.735136	-2.764919	-0.000514
C	-3.811484	0.982241	0.000235	C	2.721649	0.684501	-0.000180	H	-1.706785	2.697966	0.000300
C	-2.420981	0.665562	0.000132	C	1.774136	-0.379681	0.000064	H	-0.387959	-2.089135	-0.000512
C	-2.023819	-0.716215	-0.000126	C	4.102093	0.390921	-0.000274	H	0.612715	3.390571	0.000074
C	-3.036909	-1.719974	-0.000309	C	4.555617	-0.916156	-0.000062	H	3.012009	2.841041	-0.000392
C	-1.417489	1.648794	0.000212	C	3.626619	-1.969158	0.000318	H	4.809829	1.216801	-0.000487
C	-0.062290	1.323025	0.000121	C	2.266598	-1.702173	0.000391	H	5.621532	-1.126759	-0.000145
C	0.343346	-0.062010	0.000013	H	-5.128536	-2.153767	-0.000334	H	3.972361	-2.999337	0.000583
C	-0.652741	-1.036279	-0.000194	H	-5.815280	0.242166	0.000160	H	1.574495	-2.537535	0.000806

10 (*H* = -694.098009 Hartree)

C	4.267494	-1.398271	-0.483962	C	-2.251853	2.040159	-0.268048	H	1.693563	2.632778	0.035327
C	4.662705	-0.059691	-0.527631	C	-2.712150	0.699449	-0.193067	H	1.540553	1.921580	1.626467
C	3.747927	0.940398	-0.202166	C	-1.775640	-0.344568	0.112104	H	0.610676	-1.293952	1.720549
C	2.439699	0.620474	0.178008	C	-4.077583	0.374692	-0.408528	H	0.357445	-2.026477	0.153925
C	2.041863	-0.722198	0.222079	C	-4.522410	-0.924274	-0.317441	H	-0.586763	3.365638	-0.095526
C	2.962471	-1.721191	-0.115904	C	-3.609016	-1.956268	-0.002569	H	-2.962670	2.828316	-0.504885
C	1.444983	1.696787	0.550340	C	-2.276142	-1.673849	0.205258	H	-4.770229	1.179568	-0.644293
C	0.007231	1.314655	0.260886	H	4.969424	-2.186123	-0.744163	H	-5.570475	-1.158929	-0.482383
C	-0.396065	-0.008952	0.321511	H	5.675072	0.204011	-0.822055	H	-3.961572	-2.981203	0.077667
C	0.629553	-1.082993	0.637656	H	4.049067	1.985140	-0.245203	H	-1.602289	-2.485708	0.456681
C	-0.931636	2.335404	-0.041753	H	2.649610	-2.763213	-0.092746				

9-phenylanthracene (*H* = -770.290274 Hartree)

C	-0.639818	3.668673	0.000204	C	-0.639124	-3.668740	-0.000253	C	1.608532	0.000153	-0.000051
C	0.069462	2.496214	0.000077	C	-2.063762	-3.658125	-0.000199	C	2.325430	-0.000636	1.206237
C	-0.593943	1.226200	0.000004	C	-2.739547	-2.467814	-0.000103	C	2.325522	0.000994	-1.206243
C	-2.039580	1.220305	0.000057	H	-0.113394	4.619446	0.000284	C	3.721331	-0.000539	1.206800
C	-2.740011	2.467347	0.000161	H	1.153860	2.517504	0.000066	H	1.781062	-0.001325	2.146834
C	-2.064453	3.657786	0.000237	H	-3.827339	2.446316	0.000178	C	3.721448	0.001083	-1.206693
C	0.110509	0.000032	-0.000048	H	-2.608867	4.598202	0.000304	H	1.781271	0.001577	-2.146910
C	-2.721108	-0.000230	0.000029	H	-3.809355	-0.000335	0.000070	C	4.423221	0.000327	0.000074
C	-2.039354	-1.220639	-0.000045	H	-0.112515	-4.619410	-0.000376	H	4.259922	-0.001138	2.150906
C	-0.593717	-1.226263	-0.000070	H	-2.607996	-4.598645	-0.000232	H	4.260081	0.001744	-2.150774
C	0.069933	-2.496146	-0.000201	H	-3.826879	-2.446995	-0.000091	H	5.509987	0.000392	0.000140
H	1.154337	-2.517226	-0.000247								

9,10-dihydro-9-phenylanthracene (*H* = -771.466332 Hartree)

C	0.619745	-3.596040	0.449540	C	0.619668	3.596049	0.449530	H	3.738859	0.000036	-0.268484
C	2.013536	-3.574044	0.482159	C	-0.087857	2.450248	0.083535	C	-1.639001	-0.000018	-0.334261
C	2.688377	-2.404003	0.136561	H	0.079053	-4.501487	0.712396	C	-2.622735	-0.000032	-1.328738
C	1.986510	-1.255599	-0.241507	H	2.571936	-4.459278	0.775002	C	-2.048721	-0.000012	1.008636
C	0.581244	-1.268262	-0.256358	H	3.775912	-2.378183	0.157578	C	-3.981078	-0.000039	-0.999233
C	-0.087805	-2.450254	0.083546	H	-1.172197	-2.476564	0.066572	H	-2.323241	-0.000037	-2.374702
C	2.716114	0.000026	-0.662381	H	2.819233	0.000027	-1.761450	C	-3.401819	-0.000019	1.342243
C	1.986483	1.255635	-0.241507	H	-0.120447	-0.000008	-1.808722	H	-1.297779	0.000001	1.794228
C	0.581216	1.268269	-0.256361	H	3.775861	2.378254	0.157588	C	-4.374482	-0.000032	0.338106

C	-0.162820	-0.000006	-0.705831	H	2.571840	4.459324	0.775006	H	-4.727638	-0.000050	-1.789159
C	2.688326	2.404052	0.136565	H	0.078956	4.501486	0.712379	H	-3.698756	-0.000013	2.387892
C	2.013459	3.574080	0.482159	H	-1.172250	2.476538	0.066553	H	-5.429501	-0.000037	0.598906