Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Exploiting the "Lego brick" approach to predict accurate molecular structures of PAHs and PANHs
Supporting Information

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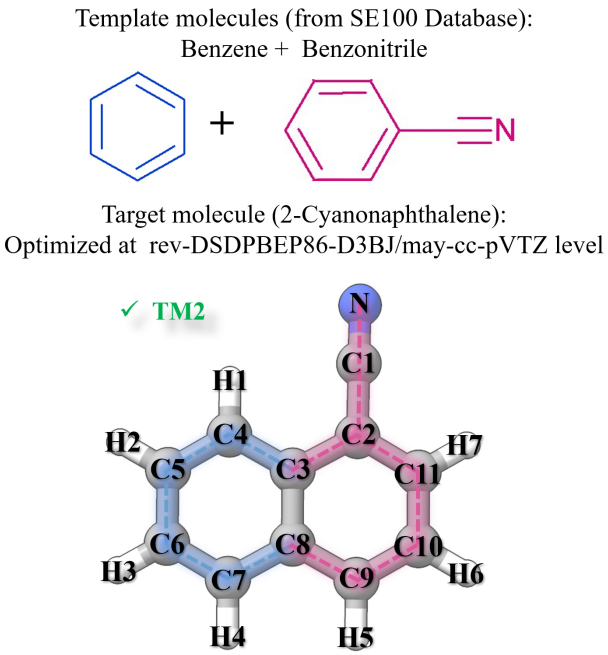

Figure S1: Graphical description of the TM approach for 2-cyanonaphtalene (TM2): benzene and benzonitrile as fragments

Table S1: Rotational constants (MHz) of 1- and 2-cyanonaphthalene from the TM2 approach (see Figure S1). The relative error with respect to the experimental value is reported in square brackets.

Parameter	B_e TM2	$B_e + \Delta B_{vib}$ TM2
1-Cyanonaphthalene		
A	1488.188 [0.63]	1480.361 [0.10]
B	961.488 [0.49]	955.677 [-0.12]
C	584.108 [0.54]	580.788 [-0.03]
MAE	0.55	0.08
2-Cyanonaphthalene		
A_0	2722.999 [0.59]	2704.594 [-0.09]
B_0	609.386 [0.54]	606.363 [0.04]
C_0	497.949 [0.54]	495.372 [0.02]
MAE	0.56	0.05

Table S2: Vibrational corrections (in MHz) for the molecules of the benchmark study and their contribution with respect to the experimental rotational constant (in percent).

	ΔB_{vib}^{B3}	$\Delta B_{vib}^{B3}/B_0^{Exp}$ (%)		ΔB_{vib}^{B3}	$\Delta B_{vib}^{B3}/B_0^{Exp}$(%)
	Naphthalene			*cis*-1-Naphthol	
ΔA	-23.486	0.75	ΔA	-14.879	0.76
ΔB	-7.832	0.64	ΔB	-6.300	0.56
ΔC	-5.751	0.65	ΔC	-4.212	0.59
	Anthracene			Quinoline	
ΔA	-16.475	0.77	ΔA	-22.978	0.73
ΔB	-2.757	0.61	ΔB	-8.015	0.63
ΔC	-2.277	0.61	ΔC	-5.808	0.64
	Phenanthrene			Isoquinoline	
ΔA	-11.197	0.70	ΔA	-24.308	0.76
ΔB	-3.679	0.67	ΔB	-7.581	0.61
ΔC	-2.635	0.64	ΔC	-5.675	0.64
	Pyrene			Phenanthridine	
ΔA	-7.095	0.70	ΔA	-11.003	0.67
ΔB	-3.440	0.62	ΔB	-3.689	0.66
ΔC	-2.231	0.62	ΔC	-2.629	0.63
	1-Cyanonaphthalene			3-Cyanopyridine	
ΔA	-7.827	0.53	ΔA	-41.122	0.71
ΔB	-5.811	0.61	ΔB	-6.037	0.38
ΔC	-3.320	0.57	ΔC	-5.888	0.48
	2-Cyanonaphthalene			2-Ethynylpyridine	
ΔA	-18.405	0.68	ΔA	-42.266	0.72
ΔB	-3.023	0.50	ΔB	-6.097	0.39
ΔC	-2.577	0.52	ΔC	-5.947	0.48
	9-Cyanoanthracene			*cis*-3-Hydroxy-pyridine	
ΔA	-5.205	0.53	ΔA	-42.203	0.73
ΔB	-2.776	0.62	ΔB	-17.719	0.66
ΔC	-1.756	0.57	ΔC	-12.492	0.68
	9-Cyanophenantrene			4-Hydroxy-pyridine	
ΔA	-5.115	0.60	ΔA	-47.701	0.80
ΔB	-2.861	0.59	ΔB	-15.979	0.61
ΔC	-1.761	0.57	ΔC	-12.160	0.66
	trans-2-Naphthol			Benzoic acid	
ΔA	-22.428	0.79	ΔA	-29.123	0.75
ΔB	-4.937	0.60	ΔB	-7.856	0.64
ΔC	-3.930	0.61	ΔC	-5.700	0.61

Table S3: Comparison of computed equilibrium rotational constants with the experimental counterparts for naphthalene, anthracene, phenanthrene, pyrene, 9-cyanoanthracene, 9-cyanophenantrene, *trans*-2-naphthol, *cis*-1-naphthol, phenanthridine, 3-cyanopyridine, 2-ethynylpyridine, *cis*-3-hydroxypyridine, 4-hydroxypyridine, and benzoic acid. All values in MHz.

	B_e revDSD	B_e TM	B_e TM+LR	ΔB_{vib}
		Naphthalene		
A	3130.862 [0.37]	3141.652 [0.71]		-23.486
B	1236.581 [0.29]	1240.611 [0.62]		-7.832
C	886.460 [0.29]	889.396 [0.62]		-7.832
MAE	0.32	0.65		
		Anthracene		
A	2153.234 [0.33]	2160.276 [0.65]		-16.457
B	453.659 [0.25]	455.133 [0.57]		-2.757
C	374.712 [0.18]	375.931 [0.51]		-2.277
MAE	0.25	0.58		
		Phenanthrene		
A	1620.349 [0.29]	1625.745 [0.62]		-11.197
B	553.912 [0.30]	555.676 [0.62]		-3.679
C	412.798 [0.24]	414.128 [0.57]		-2.635
MAE	0.28	0.60		
		Pyrene		
A	1014.425 [0.33]	1017.6849 [0.65]		-7.095
B	558.034 [0.31]	559.827 [0.63]		-3.440
C	359.999 [0.29]	361.156 [0.61]		-2.231
MAE	0.31	0.63		
		9-Cyanoanthracene		
A	986.795 [0.10]	989.752 [0.40]	990.547 [0.48]	-5.205
B	452.515 [0.29]	453.950 [0.61]	453.950 [0.61]	-2.776
C	310.246 [0.20]	311.213 [0.52]	311.291 [0.54]	-1.756
MAE	0.20	0.51	0.54	
		9-Cyanophenantrene		
A	847.626 [0.18]	850.289 [0.49]	850.621 [0.53]	-5.114
B	487.474 [0.22]	488.977 [0.53]	489.109 [0.56]	-2.861
C	309.487 [0.18]	310.448 [0.49]	310.545 [0.52]	-1.761
MAE	0.19	0.50	0.54	
		***cis* 1-Naphthol**		
A	1953.905 [0.33]	1959.411 [0.61]	1961.468 [0.72]	-14.879

B	1127.056 [0.24]	1130.586 [0.56]	1130.796 [0.58]	-6.300
C	714.764 [0.23]	716.921 [0.54]	717.280 [0.59]	-4.212
MAE	0.27	0.57	0.63	
		***trans* 2-Naphthol**		
A	2857.094 [0.41]	2866.643 [0.75]	2867.191 [0.77]	-22.428
B	827.321 [0.22]	829.667 [0.50]	830.266 [0.57]	-4.937
C	641.549 [0.23]	643.442 [0.52]	643.830 [0.58]	-3.930
MAE	0.29	0.59	0.64	
		Quinoline		
A	3156.993 [0.36]	3167.722 [0.71]		-22.978
B	1275.015 [0.27]	1279.635 [0.63]		-8.015
C	908.215 [0.27]	911.447 [0.63]		-5.808
MAE	0.30	0.66		
		Isoquinoline		
A	3211.062 [0.38]	3222.231 [0.73]		-24.308
B	1241.346 [0.28]	1245.540 [0.61]		-7.581
C	895.254 [0.28]	898.304 [0.62]		-5.675
MAE	0.31	0.65		
		Phenanthridine		
A	1648.171 [0.35]	1653.563 [0.68]		-11.003
B	559.106 [0.25]	561.008 [0.59]		-3.689
C	417.484 [0.23]	418.890 [0.57]		-2.629
MAE	0.28	0.61		
		3-Cyanopyridine		
A	5847.865 [0.43]	5869.468 [0.80]	5869.471 [0.80]	-41.122
B	1570.988 [-0.02]	1575.581 [0.27]	1577.336 [0.38]	-6.037
C	1238.322 [0.09]	1242.144 [0.40]	1243.235 [0.49]	-5.888
MAE	0.17	0.49	0.56	
		2-Ethynylpyridine		
A	5882.858 [0.43]	5903.948 [0.79]	5903.949 [0.79]	-42.266
B	1581.417 [-0.01]	1585.529 [0.25]	1587.260 [0.36]	-6.097
C	1246.370 [0.10]	1249.871 [0.38]	1250.946 [0.47]	-5.947
MAE	0.17	0.47	0.54	
		***cis* 3-Hydroxy-pyridine**		
A	5841.587 [0.42]	5861.085 [0.76]	5861.083 [0.76]	-42.203
B	2695.546 [0.22]	2702.079 [0.46]	2706.594 [0.63]	-17.719
C	1844.444 [0.27]	1849.447 [0.55]	1851.561 [0.66]	-12.492
MAE	0.30	0.59	0.68	
		4-Hydroxy-pyridine		
A	6017.179 [0.45]	6038.088 [0.79]	6038.090 [0.79]	-47.701
B	2637.092 [0.20]	2643.375 [0.44]	2647.835 [0.61]	-15.979

C	1833.529 [0.27]	1838.507 [0.54]	1840.664 [0.66]	-12.160
MAE	0.30	0.59	0.69	
		***cis* Benzoic acid**		
A	3884.367 [0.31]	3901.433 [0.75]	3901.435 [0.75]	-29.123
B	1229.556 [0.18]	1232.632 [0.43]	1234.188 [0.56]	-7.856
C	933.930 [0.15]	936.691 [0.44]	937.589 [0.54]	-5.700
MAE	0.21	0.54	0.62	

Table S4: Cartesian coordinates (revDSD/mayTZ and TM) of naphthalene, anthracene, phenanthrene, pyrene, 1-cyanonaphthalene, 2-cyanonaphthalene, 9-cyanoanthracene, 9-cyanophenantrene, *trans* 2-naphthol, *cis* 1-naphthol, quinoline, isoquinoline, phenanthridine, 3-cyanopyridine, 2-ehynylpyridine, *cis* 3-hydroxy-pyridine, 4-hydroxy-pyridine, benzoic acid, 1-ethynylnaphthalene, 2-ethynylnaphthalene, 9-ethynylanthracene, 9-ethynylphenanthrene, 1-pyrenecarbonitrile, 2-pyrenecarbonitrile, 4-pyrenecarbonitrile, 1-ethynylpyrene, 2-ethynylpyrene, and 4-ethynylpyrene.

revDSD/mayTZ				**TM**			
				Naphthalene			
C	0.000000	0.000000	0.712073	C	0.0000000	0.000000	0.7109500
C	0.000000	0.000000	-0.712073	C	0.0000000	0.000000	-0.710950
C	0.000000	1.241127	1.400008	C	0.0000000	1.239172	1.397809
C	0.000000	-1.241127	1.400008	C	0.0000000	-1.239172	1.397809
C	0.000000	1.241127	-1.400008	C	0.0000000	1.239172	-1.397809
C	0.000000	-1.241127	-1.400008	C	0.0000000	-1.239172	-1.397809
C	0.000000	2.427364	0.707757	C	0.0000000	2.423552	0.706645
C	0.000000	-2.427364	0.707757	C	0.0000000	-2.423552	0.706645
C	0.000000	2.427364	-0.707757	C	0.0000000	2.423552	-0.706645
C	0.000000	-2.427364	-0.707757	C	0.0000000	-2.423552	-0.706645
H	0.000000	1.237638	2.484723	H	0.0000000	1.235696	2.478903
H	0.000000	-1.237638	2.484723	H	0.0000000	-1.235696	2.478903
H	0.000000	1.237638	-2.484723	H	0.0000000	1.235696	-2.478903
H	0.000000	-1.237638	-2.484723	H	0.0000000	-1.235696	-2.478903
H	0.000000	3.369004	1.243693	H	0.0000000	3.362082	1.240821
H	0.000000	-3.369004	1.243693	H	0.0000000	-3.362082	1.240821
H	0.000000	3.369004	-1.243693	H	0.0000000	3.362082	-1.240821
H	0.000000	-3.369004	-1.243693	H	0.0000000	-3.362082	-1.240821
				Anthracene			
C	0.000000	0.000000	1.401095	C	0.000000	0.000000	1.398900
C	0.000000	0.000000	-1.401095	C	0.000000	0.000000	-1.398900
H	0.000000	0.000000	2.487026	H	0.000000	0.000000	2.483400
H	0.000000	0.000000	-2.487026	H	0.000000	0.000000	-2.483400
C	0.000000	1.219468	0.718019	C	0.000000	1.217507	0.716921
C	0.000000	-1.219468	00.718019	C	0.000000	-1.217507	0.716921
C	0.000000	1.219468	-0.718019	C	0.000000	1.217507	-0.716921
C	0.000000	-1.219468	0-0.718019	C	0.000000	-1.217507	-0.716921
C	0.000000	2.472096	1.404943	C	0.000000	2.468194	1.402778
C	0.000000	2.472096	-1.404943	C	0.000000	2.468194	-1.402778
C	0.000000	-2.472096	01.404943	C	0.000000	-2.468194	1.402778
C	0.000000	-2.472096	0-1.404943	C	0.000000	-2.468194	-1.402778
C	0.000000	3.650422	0.712855	C	0.000000	3.644585	0.711823
C	0.000000	3.650422	-0.712855	C	0.000000	3.644585	-0.711823
C	0.000000	-3.650422	00.712855	C	0.000000	-3.644585	0.711823
C	0.000000	-3.650422	0-0.712855	C	0.000000	-3.644585	-0.711823
H	0.000000	2.469376	2.489625	H	0.000000	2.465484	2.483875
H	0.000000	2.469376	-2.489625	H	0.000000	2.465484	-2.483875
H	0.000000	-2.469376	02.489625	H	0.000000	-2.465484	2.483875

H	0.000000	-2.469376	0-2.489625	H	0.000000	-2.465484	-2.483875
H	0.000000	4.593846	1.245662	H	0.000000	4.584891	1.242868
H	0.000000	4.593846	-1.245662	H	0.000000	4.584891	-1.242868
H	0.000000	-4.593846	01.245662	H	0.000000	-4.584891	1.242868
H	0.000000	-4.593846	0-1.245662	H	0.000000	-4.584891	-1.242868
			Phenanthrene				
C	0.000000	0.678585	2.087008	C	0.000000	0.725550	-0.375579
C	0.000000	-0.678585	2.087008	C	0.000000	-0.725550	-0.375579
C	0.000000	1.417347	0.858066	C	0.000000	1.415203	0.861124
C	0.000000	-1.417347	0.858066	C	0.000000	-1.415203	0.861124
H	0.000000	1.230540	3.0206700	C	0.000000	0.677555	2.088170
H	0.000000	-1.230540	3.020670	C	0.000000	-0.677555	2.088170
C	0.000000	0.726640	-0.380583	H	0.000000	1.227661	3.018731
C	0.000000	-0.726640	-0.380583	H	0.000000	-1.227661	3.018731
C	0.000000	2.829346	0.872510	C	0.000000	1.489058	-1.561329
C	0.000000	-2.829346	0.872510	C	0.000000	-1.489058	-1.561329
C	0.000000	3.550597	-0.301469	C	0.000000	2.825029	0.875537
C	0.000000	-3.550597	-0.301469	C	0.000000	-2.825029	0.875537
C	0.000000	2.871011	-1.532284	C	0.000000	2.866492	-1.525500
C	0.000000	-2.871011	-1.532284	C	0.000000	-2.866492	-1.525500
C	0.000000	1.491346	-1.568186	C	0.000000	3.545041	-0.296588
C	0.000000	-1.491346	-1.568186	C	0.000000	-3.545041	-0.296588
H	0.000000	3.339327	1.829859	H	0.000000	0.996357	-2.520371
H	0.000000	-3.339327	1.829859	H	0.000000	-0.996357	-2.520371
H	0.000000	4.633661	-0.278396	H	0.000000	3.333334	1.829687
H	0.000000	-4.633661	-0.278396	H	0.000000	-3.333334	1.829687
H	0.000000	3.431971	-2.459245	H	0.000000	3.425566	-2.449416
H	0.000000	-3.431971	-2.459245	H	0.000000	-3.425566	-2.449416
H	0.000000	0.997015	-2.530381	H	0.000000	4.624498	-0.273638
H	0.000000	-0.997015	-2.530381	H	0.000000	-4.624498	-0.273638
			Pyrene				
C	0.000000	0.000000	0.712350	C	0.000000	0.711250	0.000005
C	0.000000	0.000000	-0.712350	C	0.000000	-0.711250	0.000005
C	0.000000	1.231000	1.424155	C	0.000000	1.421963	-1.229108
C	0.000000	1.231000	-1.424155	C	0.000000	-1.421963	-1.229108
C	0.000000	-1.231000	1.424155	C	0.000000	1.421963	1.229118
C	0.000000	-1.231000	-1.424155	C	0.000000	-1.421963	1.229118
C	0.000000	2.459233	0.679620	C	0.000000	0.678555	-2.455480
C	0.000000	2.459233	-0.679620	C	0.000000	-0.678555	-2.455480
C	0.000000	-2.459233	0.679620	C	0.000000	0.678555	2.455490
C	0.000000	-2.459233	-0.679620	C	0.000000	-0.678555	2.455490
C	0.000000	1.208589	2.824612	C	0.000000	2.820184	-1.206733
C	0.000000	1.208589	-2.824612	C	0.000000	-2.820184	-1.206733
C	0.000000	-1.208589	2.824612	C	0.000000	2.820184	1.206743
C	0.000000	-1.208589	-2.824612	C	0.000000	-2.820184	1.206743
C	0.000000	0.000000	3.514996	C	0.000000	3.509490	-0.000033
C	0.000000	0.000000	-3.514996	C	0.000000	-3.509490	-0.000033
H	0.000000	3.394957	1.228280	H	0.000000	1.225388	-3.388085
H	0.000000	3.394957	-1.228280	H	0.000000	-1.225388	-3.388085
H	0.000000	-3.394957	1.228280	H	0.000000	1.225388	3.388095

H	0.000000	-3.394957	-1.228280	H	0.000000	-1.225388	3.388095
H	0.000000	2.147000	3.368484	H	0.000000	3.362239	-2.142007
H	0.000000	2.147000	-3.368484	H	0.000000	-3.362239	-2.142007
H	0.000000	-2.147000	3.368484	H	0.000000	3.362239	2.142017
H	0.000000	-2.147000	-3.368484	H	0.000000	-3.362239	2.142017
H	0.000000	0.000000	4.598615	H	0.000000	4.589490	-0.000033
H	0.000000	0.000000	-4.598615	H	0.000000	-4.589490	-0.000033
			1-Cyanonaphthalene				
C	-0.062509	-0.253560	0.000000	C	0.0000000	0.2725870	0.0000000
C	-0.520322	-1.594742	0.000000	C	-0.3414350	1.6457750	0.0000000
C	-1.866914	-1.867527	0.000000	C	-1.6577580	2.0315930	0.0000000
C	-2.813441	-0.816458	0.000000	C	-2.6886990	1.0664670	0.0000000
C	-2.394386	0.491000	0.000000	C	-2.3829710	-0.2698050	0.0000000
C	-1.011483	0.807081	0.000000	C	-1.0340640	-0.7018220	0.0000000
C	-0.555504	2.150054	0.000000	C	-0.6945470	-2.0766190	0.0000000
C	0.787254	2.441331	0.000000	C	0.6164630	-2.4804620	0.0000000
C	1.738374	1.400655	0.000000	C	1.6510500	-1.5260160	0.0000000
C	1.325127	0.083304	0.000000	C	1.3518950	-0.1804710	0.0000000
H	0.204502	-2.400361	0.000000	H	0.4467280	2.3842980	0.0000000
H	-2.207938	-2.895617	0.000000	H	-1.9091750	3.0815100	0.0000000
H	-3.871654	-1.047812	0.000000	H	-3.7199250	1.3860140	0.0000000
H	-3.114706	1.301472	0.000000	H	-3.1670640	-1.0135190	0.0000000
H	-1.289110	2.948710	0.000000	H	-1.4907690	-2.8074810	0.0000000
H	1.124099	3.470311	0.000000	H	0.8636940	-3.5308590	0.0000000
H	2.797096	1.627364	0.000000	H	2.6831740	-1.8409410	0.0000000
C	2.303749	-0.965064	0.000000	C	2.4161470	0.7807840	0.0000000
N	3.088474	-1.823919	0.000000	N	3.2681220	1.5669860	0.0000000
			2-Cyanonaphthalene				
C	-0.564940	-0.588821	0.000000	C	0.7064340	-0.3379940	0.0000000
C	-1.589949	-1.570216	0.000000	C	1.9185100	-1.0718030	0.0000000
C	-2.911340	-1.197471	0.000000	C	1.9018040	-2.4425010	0.0000000
C	-3.267154	0.172524	0.000000	C	0.6732000	-3.1408340	0.0000000
C	-2.295288	1.143370	0.000000	C	-0.5148490	-2.4555950	0.0000000
C	-0.922385	0.789881	0.000000	C	-0.5300840	-1.0401770	0.0000000
C	0.105449	1.769137	0.000000	C	-1.7407360	-0.3032500	0.0000000
C	1.426695	1.406078	0.000000	C	-1.7333580	1.0646300	0.0000000
C	1.779837	0.029401	0.000000	C	-0.4975540	1.7622210	0.0000000
C	0.804410	-0.945794	0.000000	C	0.6948700	1.0751610	0.0000000
H	-1.312172	-2.618321	0.000000	H	2.8553880	-0.5331250	0.0000000
H	-3.688111	-1.952391	0.000000	H	2.8294910	-2.9947090	0.0000000
H	-4.313458	0.453181	0.000000	H	0.6739480	-4.2205330	0.0000000
H	-2.566036	2.193343	0.000000	H	-1.4553060	-2.9879990	0.0000000
H	-0.169738	2.817778	0.000000	H	-2.6796860	-0.8401220	0.0000000
H	2.209804	2.153332	0.000000	H	-2.6562260	1.6254330	0.0000000
H	1.084663	-1.992744	0.000000	H	1.6311760	1.6166310	0.0000000
C	3.165478	-0.343364	0.000000	C	-0.4975540	3.1971310	0.0000000
N	4.288615	-0.645510	0.000000	N	-0.4975540	4.3560710	0.0000000
			9-Cyanoanthracene				
C	-1.788793	-0.000001	0.000000	C	0.0000000	0.0000000	-1.7860680
C	1.009133	0.000000	0.000000	C	0.0000000	0.0000000	1.0074320

C	-1.109737	-1.221125	0.000000	C	0.0000000	1.2191730	-1.1080980
C	-1.109737	1.221123	0.000000	C	0.0000000	-1.2191730	-1.1080980
C	0.323687	-1.231384	0.000000	C	0.0000000	1.2294560	0.3230580
C	0.323686	1.231382	0.000000	C	0.0000000	-1.2294560	0.3230580
C	-1.808613	-2.466243	0.000000	C	0.0000000	2.4623990	-1.8059580
C	-1.808613	2.466242	0.000000	C	0.0000000	-2.4623990	-1.8059580
C	1.003438	-2.485241	0.000000	C	0.0000000	2.4814340	1.0017430
C	1.003438	2.485239	0.000000	C	0.0000000	-2.4814340	1.0017430
C	-1.126164	-3.649733	0.000000	C	0.0000000	3.6440400	-1.1246200
C	-1.126164	3.649732	0.000000	C	0.0000000	-3.6440400	-1.1246200
C	0.297689	-3.656741	0.000000	C	0.0000000	3.6510630	0.2970740
C	0.297689	3.656740	0.000000	C	0.0000000	-3.6510630	0.2970740
H	-2.892835	-2.451333	0.000000	H	0.0000000	2.4475080	-2.8865560
H	-2.892835	2.451332	0.000000	H	0.0000000	-2.4475080	-2.8865560
H	2.086973	-2.495180	0.000000	H	0.0000000	2.4913710	2.0816970
H	2.086973	2.495179	0.000000	H	0.0000000	-2.4913710	2.0816970
H	-1.664888	-4.589448	0.000000	H	0.0000000	4.5806300	-1.6615880
H	-1.664888	4.589447	0.000000	H	0.0000000	-4.5806300	-1.6615880
H	0.825622	-4.602663	0.000000	H	0.0000000	4.5938800	0.8232370
H	0.825622	4.602662	0.000000	H	0.0000000	-4.5938800	0.8232370
H	-2.874568	-0.000001	0.000000	H	0.0000000	0.0000000	-2.8682680
C	2.440752	0.000001	0.000000	C	0.0000000	0.0000000	2.4390320
N	3.604952	0.000006	0.000000	N	0.0000000	0.0000000	3.5991320

9-Cyanophenantrene

N	-3.603860	-2.315029	0.000000	N	-3.5975020	-2.3121500	0.0000000
C	-2.568573	-1.784213	0.000000	C	-2.5662130	-1.7826040	0.0000000
C	-1.299006	-1.117299	0.000000	C	-1.2967210	-1.1154960	0.0000000
C	-0.152575	-1.857132	0.000000	C	-0.1521320	-1.8540780	0.0000000
C	1.128785	-1.227494	0.000000	C	1.1272220	-1.2253460	0.0000000
C	1.219812	0.187470	0.000000	C	1.2180240	0.1874390	0.0000000
C	2.303121	-2.012701	0.000000	C	2.2997990	-2.0092940	0.0000000
C	3.545879	-1.419799	0.000000	C	3.5405850	-1.4172420	0.0000000
C	3.643687	-0.016954	0.000000	C	3.6381660	-0.0166370	0.0000000
C	2.507369	0.766558	0.000000	C	2.5035760	0.7655800	0.0000000
C	0.000000	0.977640	0.000000	C	0.0000000	0.9763610	0.0000000
C	-1.258793	0.325467	0.000000	C	-1.2566740	0.3250480	0.0000000
C	-2.448359	1.084202	0.000000	C	-2.4444950	1.0823570	0.0000000
C	-2.402153	2.461433	0.000000	C	-2.3985670	2.4573900	0.0000000
C	-1.159666	3.117022	0.000000	C	-1.1581620	3.1121280	0.0000000
C	0.012688	2.389695	0.000000	C	0.0124040	2.3861760	0.0000000
H	-0.207403	-2.939630	0.000000	H	-0.2066820	-2.9330000	0.0000000
H	2.207786	-3.092881	0.000000	H	2.2048600	-3.0859160	0.0000000
H	4.442436	-2.027319	0.000000	H	4.4341770	-2.0227140	0.0000000
H	4.618821	0.455082	0.000000	H	4.6100550	0.4538950	0.0000000
H	2.618885	1.842114	0.000000	H	2.6146630	1.8375400	0.0000000
H	0.954258	2.921360	0.000000	H	0.9507110	2.9162870	0.0000000
H	-1.119321	4.199561	0.000000	H	-1.1181460	4.1910860	0.0000000
H	-3.320514	3.035420	0.000000	H	-3.3139600	3.0293690	0.0000000
H	-3.401226	0.568130	0.000000	H	-3.3940400	0.5678040	0.0000000

***cis*-1-Naphthol**

C	0.023977	0.434573	0.000000	C	0.0000000	0.4419110	0.0000000
C	1.034924	1.431004	0.000000	C	0.9909970	1.4551550	0.0000000
C	2.366284	1.090639	0.000000	C	2.3262520	1.1397520	0.0000000
C	2.753160	-0.268611	0.000000	C	2.7373270	-0.2100400	0.0000000
C	1.797398	-1.254091	0.000000	C	1.8013090	-1.2112470	0.0000000
C	0.413913	-0.937825	0.000000	C	0.4143870	-0.9208410	0.0000000
C	-0.574753	-1.952911	0.000000	C	-0.5539730	-1.9523150	0.0000000
C	-1.906015	-1.615568	0.000000	C	-1.8890250	-1.6399850	0.0000000
C	-2.309229	-0.264579	0.000000	C	-2.3163200	-0.2987030	0.0000000
C	-1.369289	0.739384	0.000000	C	-1.3964450	0.7207240	0.0000000
H	0.779348	2.486018	0.000000	H	0.7170460	2.5017970	0.0000000
H	3.121804	1.866824	0.000000	H	3.0649700	1.9270460	0.0000000
H	3.804739	-0.528618	0.000000	H	3.7899400	-0.4499170	0.0000000
H	2.087586	-2.299064	0.000000	H	2.1095720	-2.2472580	0.0000000
H	-0.263697	-2.990949	0.000000	H	-0.2250170	-2.9809970	0.0000000
H	-2.663552	-2.390107	0.000000	H	-2.6297360	-2.4256800	0.0000000
H	-3.358041	0.003851	0.000000	H	-3.3663640	-0.0504100	0.0000000
O	-1.826268	2.025987	0.000000	O	-1.8757610	1.9954900	0.0000000
H	-1.080637	2.631927	0.000000	H	-1.1413810	2.6150250	0.0000000
				***trans*-2-Naphthol**			
C	-0.300635	-0.617142	0.000000	C	0.0000000	0.6859080	0.0000000
C	-1.409644	-1.504310	0.000000	C	-0.6414490	1.9505290	0.0000000
C	-2.695455	-1.021551	0.000000	C	-2.0096290	2.0429820	0.0000000
C	-2.940004	0.372817	0.000000	C	-2.8080310	0.8766830	0.0000000
C	-1.887424	1.254896	0.000000	C	-2.2157990	-0.3599160	0.0000000
C	-0.548994	0.785792	0.000000	C	-0.8053710	-0.4865420	0.0000000
C	0.558678	1.669880	0.000000	C	-0.1638950	-1.7477850	0.0000000
C	1.844715	1.190528	0.000000	C	1.2030600	-1.8434790	0.0000000
C	2.082677	-0.205225	0.000000	C	1.9960860	-0.6731560	0.0000000
C	1.033210	-1.091615	0.000000	C	1.4084810	0.5660910	0.0000000
H	-1.224463	-2.572895	0.000000	H	-0.0327360	2.8437330	0.0000000
H	-3.531259	-1.711230	0.000000	H	-2.4834710	3.0134840	0.0000000
H	-3.959129	0.740013	0.000000	H	-3.8842050	0.9638630	0.0000000
H	-2.066054	2.324928	0.000000	H	-2.8191690	-1.2570990	0.0000000
H	0.379595	2.739466	0.000000	H	-0.7675620	-2.6444060	0.0000000
H	2.685833	1.877010	0.000000	H	1.6830760	-2.8132860	0.0000000
H	1.233907	-2.156447	0.000000	H	2.0297950	1.4494760	0.0000000
O	3.355817	-0.705603	0.000000	O	3.3587280	-0.7443420	0.0000000
H	3.979656	0.026451	0.000000	H	3.6237200	-1.6689170	0.0000000
				Quinoline			
N	-1.192516	-1.396835	0.000000	N	-1.132978	1.441459	0.000000
C	-2.319464	-0.717778	0.000000	C	-2.284439	0.809461	0.000000
C	-2.399956	0.696123	0.000000	C	-2.421669	-0.597965	0.000000
C	-1.237347	1.422632	0.000000	C	-1.291561	-1.369214	0.000000
C	0.002498	0.739110	0.000000	C	-0.027558	-0.737432	0.000000
C	1.252562	1.408598	0.000000	C	1.192641	-1.455685	0.000000
C	2.423534	0.691416	0.000000	C	2.389617	-0.787392	0.000000
C	2.393848	-0.724343	0.000000	C	2.416995	0.626243	0.000000
C	1.196741	-1.397888	0.000000	C	1.249874	1.346360	0.000000
C	-0.027241	-0.683153	0.000000	C	0.000000	0.682579	0.000000

H	-3.233204	-1.305070	0.000000	H	-3.171299	1.431394	0.000000
H	-3.368806	1.179455	0.000000	H	-3.406648	-1.040685	0.000000
H	-1.250961	2.507300	0.000000	H	-1.348750	-2.449701	0.000000
H	1.267580	2.493202	0.000000	H	1.164011	-2.536406	0.000000
H	3.376227	1.207175	0.000000	H	3.317610	-1.339281	0.000000
H	3.325669	-1.277105	0.000000	H	3.367144	1.139258	0.000000
H	1.150362	-2.479781	0.000000	H	1.247160	2.425656	0.000000
			Isoquinoline				
N	-2.414706	-0.700222	0.000000	N	-2.416106	0.680115	0.000000
C	-2.380146	0.662903	0.000000	C	-2.370780	-0.680530	0.000000
C	-1.223277	1.399944	0.000000	C	-1.209875	-1.407237	0.000000
C	0.026447	0.732889	0.000000	C	0.032129	-0.731560	0.000000
C	1.276159	1.402432	0.000000	C	1.285204	-1.390141	0.000000
C	2.445656	0.681145	0.000000	C	2.447019	-0.660743	0.000000
C	2.422554	-0.735188	0.000000	C	2.412730	0.753141	0.000000
C	1.224738	-1.407225	0.000000	C	1.211495	1.414578	0.000000
C	0.005586	-0.685447	0.000000	C	0.000000	0.684255	0.000000
C	-1.260530	-1.329023	0.000000	C	-1.269225	1.316770	0.000000
H	-1.295788	-2.416194	0.000000	H	-1.312960	2.400588	0.000000
H	-3.347246	1.152613	0.000000	H	-3.331449	-1.176624	0.000000
H	-1.262696	2.483163	0.000000	H	-1.240590	-2.487100	0.000000
H	1.295596	2.486519	0.000000	H	1.313149	-2.470479	0.000000
H	3.398374	1.197276	0.000000	H	3.400615	-1.167535	0.000000
H	3.356006	-1.284715	0.000000	H	3.338720	1.308189	0.000000
H	1.196682	-2.491383	0.000000	H	1.174898	2.495459	0.000000
			Phenanthridine				
N	-0.713313	2.050451	0.000000	N	-2.156707	-0.369919	0.000000
C	0.585033	2.026675	0.000000	C	-1.509269	-1.493073	0.000000
C	1.386942	0.835625	0.000000	C	-0.081111	-1.619015	0.000000
C	2.794775	0.908496	0.000000	C	0.534768	-2.884617	0.000000
C	3.549843	-0.244427	0.000000	C	1.906878	-2.988015	0.000000
C	2.906765	-1.496510	0.000000	C	2.690787	-1.821552	0.000000
C	1.528892	-1.583827	0.000000	C	2.102023	-0.575220	0.000000
C	0.735528	-0.416969	0.000000	C	0.699247	-0.445079	0.000000
C	-0.711698	-0.415961	0.000000	C	0.000000	0.818896	0.000000
C	-1.490727	-1.592738	0.000000	C	0.652466	2.067836	0.000000
C	-2.869233	-1.530453	0.000000	C	-0.067362	3.242529	0.000000
C	-3.524608	-0.285787	0.000000	C	-1.471583	3.214507	0.000000
C	-2.786158	0.878009	0.000000	C	-2.132249	2.007374	0.000000
C	-1.377065	0.834386	0.000000	C	-1.413917	0.796863	0.000000
H	1.095105	2.988394	0.000000	H	-2.102874	-2.402007	0.000000
H	3.271316	1.882854	0.000000	H	-0.085721	-3.769926	0.000000
H	4.631603	-0.191704	0.000000	H	2.382115	-3.957166	0.000000
H	3.500020	-2.403232	0.000000	H	3.767769	-1.902232	0.000000
H	1.061816	-2.559842	0.000000	H	2.728474	0.302565	0.000000
H	-1.006638	-2.560896	0.000000	H	1.730361	2.112005	0.000000
H	-3.448537	-2.445975	0.000000	H	0.452240	4.189092	0.000000
H	-4.607068	-0.244211	0.000000	H	-2.029473	4.138905	0.000000
H	-3.258213	1.852591	0.000000	H	-3.210002	1.949604	0.000000
			3-Cyanopyridine				

N	3.141555	-0.024762	0.000000	N	-0.0242040	3.1791660	0.0000000
C	1.979303	0.000002	0.000000	C	-0.0242040	2.0207660	0.0000000
C	0.545888	0.030543	0.000000	C	-0.0242040	0.5870660	0.0000000
C	-0.182092	-1.165321	0.000000	C	1.1850910	-0.1141690	0.0000000
N	-1.513814	-1.209113	0.000000	N	1.2571350	-1.4424170	0.0000000
C	-2.167851	-0.041826	0.000000	C	0.1059730	-2.1200510	0.0000000
C	-1.535829	1.200176	0.000000	C	-1.1468360	-1.5158400	0.0000000
C	-0.149014	1.242333	0.000000	C	-1.2184110	-0.1328910	0.0000000
H	0.339903	-2.115833	0.000000	H	2.1216140	0.4265240	0.0000000
H	-3.250537	-0.104955	0.000000	H	0.1919050	-3.1981320	0.0000000
H	-2.120899	2.110406	0.000000	H	-2.0419920	-2.1186420	0.0000000
H	0.389630	2.181347	0.000000	H	-2.1664940	0.3837240	0.0000000
			2-Ethynylpyridine				
H	4.237816	0.023002	0.000000	H	0.0105600	4.2562540	0.0000000
C	3.174260	0.019201	0.000000	C	0.0105600	3.1945540	0.0000000
C	1.964525	0.014878	0.000000	C	0.0105600	1.9878540	0.0000000
C	0.527718	0.009743	0.000000	C	0.0105600	0.5510540	0.0000000
N	-0.080767	-1.189276	0.000000	N	1.2054760	-0.0606760	0.0000000
C	-1.415715	-1.194804	0.000000	C	1.2061970	-1.3933760	0.0000000
C	-2.200151	-0.043201	0.000000	C	0.0535340	-2.1725320	0.0000000
C	-1.560010	1.191668	0.000000	C	-1.1766570	-1.5293140	0.0000000
C	-0.171447	1.222428	0.000000	C	-1.2023810	-0.1433520	0.0000000
H	-1.881721	-2.174603	0.000000	H	2.1815930	-1.8616980	0.0000000
H	-3.279912	-0.118971	0.000000	H	0.1252220	-3.2497490	0.0000000
H	-2.129383	2.113118	0.000000	H	-2.0977190	-2.0940330	0.0000000
H	0.375003	2.156387	0.000000	H	-2.1322200	0.4046320	0.0000000
			***cis*-3-Hydroxy-pyridine**				
H	2.601159	-0.883748	0.000000	H	-0.892080	2.600597	0.000000
O	2.278443	0.023415	0.000000	O	0.011874	2.278872	0.000000
C	0.914566	0.011772	0.000000	C	0.000000	0.918424	0.000000
C	0.167978	-1.167343	0.000000	C	-1.177483	0.173189	0.000000
N	-1.166375	-1.192847	0.000000	N	-1.203180	-1.158963	0.000000
C	-1.807957	-0.020627	0.000000	C	-0.033013	-1.799692	0.000000
C	-1.147368	1.206439	0.000000	C	1.192344	-1.140321	0.000000
C	0.241165	1.229351	0.000000	C	1.215448	0.245587	0.000000
H	0.674053	-2.130676	0.000000	H	-2.138118	0.678006	0.000000
H	-2.891010	-0.066089	0.000000	H	-0.078565	-2.879732	0.000000
H	-1.713323	2.129490	0.000000	H	2.112959	-1.705006	0.000000
H	0.801967	2.155479	0.000000	H	2.139293	0.804777	0.000000
			4-Hydroxy-pyridine				
H	2.650271	0.838734	0.000000	H	-0.844613	2.632095	0.000000
O	2.294952	-0.056153	0.000000	O	0.049366	2.283885	0.000000
C	0.938039	0.002139	0.000000	C	0.000000	0.929985	0.000000
C	0.224207	1.198418	0.000000	C	-1.189351	0.209808	0.000000
C	-1.165866	1.135939	0.000000	C	-1.117973	-1.177758	0.000000
N	-1.869011	-0.000235	0.000000	N	0.020892	-1.872411	0.000000
C	-1.158465	-1.136303	0.000000	C	1.150499	-1.155684	0.000000
C	0.228744	-1.196637	0.000000	C	1.201766	0.229767	0.000000
H	0.731625	2.156874	0.000000	H	-2.148611	0.709703	0.000000
H	-1.742337	2.055270	0.000000	H	-2.031004	-1.758545	0.000000

H	-1.733841	-2.056071	0.000000	H	2.071416	-1.723504	0.000000
H	0.753549	-2.142684	0.000000	H	2.141987	0.759334	0.000000
			***cis* Benzoic acid**				
C	-2.605297	0.025106	0.000000	C	0.2617890	-2.5887200	0.0000000
C	-1.929109	-1.194933	0.000000	C	1.3980960	-1.7834750	0.0000000
C	-1.890237	1.221404	0.000000	C	-1.0040060	-2.0107620	0.0000000
C	-0.539539	-1.218709	0.000000	C	1.2688060	-0.4019110	0.0000000
C	-0.498687	1.202931	0.000000	C	-1.1387770	-0.6278140	0.0000000
C	0.177902	-0.019662	0.000000	C	0.0000000	0.1781200	0.0000000
C	1.661054	-0.097189	0.000000	C	-0.0863820	1.6608050	0.0000000
O	2.300734	-1.124242	0.000000	O	0.8605720	2.4071230	0.0000000
O	2.253444	1.121334	0.000000	O	-1.3590990	2.1140090	0.0000000
H	3.205826	0.950077	0.000000	H	-1.2940800	3.0758140	0.0000000
H	0.006773	-2.153131	0.000000	H	2.1344440	0.2418900	0.0000000
H	0.062884	2.127204	0.000000	H	-2.1160470	-0.1730460	0.0000000
H	-2.485588	-2.124050	0.000000	H	2.3795860	-2.2326760	0.0000000
H	-2.416410	2.168063	0.000000	H	-1.8840150	-2.6359860	0.0000000
H	-3.688620	0.043076	0.000000	H	0.3629710	-3.6638690	0.0000000
			1-Ethynylnaphthalene				
C	-0.0470670	-0.2562760	0.0000000	C	0.2017980	0.1634480	0.0000000
C	-0.4966010	-1.6006390	0.0000000	C	1.4554400	0.8203010	0.0000000
C	-1.8402620	-1.8888830	0.0000000	C	2.6221150	0.0983230	0.0000000
C	-2.7973110	-0.8476720	0.0000000	C	2.5908190	-1.3133300	0.0000000
C	-2.3886920	0.4631920	0.0000000	C	1.3898180	-1.9743630	0.0000000
C	-1.0087980	0.7936360	0.0000000	C	0.1677870	-1.2576500	0.0000000
C	-0.5705350	2.1423620	0.0000000	C	-1.0807790	-1.9253750	0.0000000
C	0.7698250	2.4427510	0.0000000	C	-2.2534640	-1.2143570	0.0000000
C	1.7305520	1.4106510	0.0000000	C	-2.2310520	0.1932640	0.0000000
C	1.3434690	0.0830090	0.0000000	C	-1.0339430	0.8812050	0.0000000
H	0.2383440	-2.3961370	0.0000000	H	1.4766140	1.8994940	0.0000000
H	-2.1707650	-2.9206880	0.0000000	H	3.5721330	0.6115810	0.0000000
H	-3.8536810	-1.0881970	0.0000000	H	3.5160840	-1.8699740	0.0000000
H	-3.1164930	1.2672930	0.0000000	H	1.3575640	-3.0548820	0.0000000
H	-1.3125610	2.9332890	0.0000000	H	-1.0937600	-3.0061970	0.0000000
H	1.0982220	3.4749770	0.0000000	H	-3.2023180	-1.7293450	0.0000000
H	2.7863540	1.6517420	0.0000000	H	-3.1562960	0.7491670	0.0000000
C	2.3346020	-0.9483340	0.0000000	C	-1.0339430	2.3116050	0.0000000
C	3.1740250	-1.8218120	0.0000000	C	-1.0339430	3.5200050	0.0000000
H	3.9110220	-2.5887080	0.0000000	H	-1.0339430	4.5817050	0.0000000
			2-Ethynylnaphthalene				
C	-0.5482090	-0.5892230	0.0000000	C	0.7039260	-0.3597450	0.0000000
C	-1.5735570	-1.5706980	0.0000000	C	1.9126010	-1.0997200	0.0000000
C	-2.8962140	-1.2008340	0.0000000	C	1.8923450	-2.4707700	0.0000000
C	-3.2550340	0.1682710	0.0000000	C	0.6619920	-3.1658110	0.0000000
C	-2.2831400	1.1395240	0.0000000	C	-0.5231110	-2.4748930	0.0000000
C	-0.9097940	0.7880420	0.0000000	C	-0.5335110	-1.0595310	0.0000000
C	0.1192920	1.7657670	0.0000000	C	-1.7395240	-0.3150370	0.0000000
C	1.4399110	1.4000710	0.0000000	C	-1.7228140	1.0529610	0.0000000
C	1.8068890	0.0242630	0.0000000	C	-0.4880460	1.7576430	0.0000000
C	0.8222040	-0.9442120	0.0000000	C	0.6976380	1.0537110	0.0000000

H	-1.2946410	-2.6187410	0.0000000	H	2.8516980	-0.5645180	0.0000000
H	-3.6713340	-1.9577480	0.0000000	H	2.8188430	-3.0253600	0.0000000
H	-4.3017790	0.4477220	0.0000000	H	0.6587670	-4.2456060	0.0000000
H	-2.5547850	2.1895430	0.0000000	H	-1.4659900	-3.0036080	0.0000000
H	-0.1548980	2.8150520	0.0000000	H	-2.6810070	-0.8460310	0.0000000
H	2.2213700	2.1496180	0.0000000	H	-2.6438110	1.6154880	0.0000000
H	1.0995580	-1.9922530	0.0000000	H	1.6371160	1.5874350	0.0000000
C	3.1905030	-0.3407410	0.0000000	C	-0.4880460	3.1885430	0.0000000
C	4.3615010	-0.6496560	0.0000000	C	-0.4880460	4.3966430	0.0000000
H	5.3898530	-0.9209410	0.0000000	H	-0.4880460	5.4582430	0.0000000
			2-Quinolinecarbonitrile				
N	0.801391	-0.914744	0.000000	N	0.6511790	1.0244080	0.0000000
C	1.699929	0.051151	0.000000	C	-0.5266920	1.6135680	0.0000000
C	1.398450	1.436639	0.000000	C	-1.7693470	0.9351160	0.0000000
C	0.080182	1.811497	0.000000	C	-1.7578030	-0.4326350	0.0000000
C	-0.925236	0.816409	0.000000	C	-0.5221970	-1.1158180	0.0000000
C	-2.309940	1.119056	0.000000	C	-0.4227850	-2.5275220	0.0000000
C	-3.238131	0.107421	0.000000	C	0.8073000	-3.1322610	0.0000000
C	-2.823606	-1.247454	0.000000	C	1.9887860	-2.3541430	0.0000000
C	-1.489508	-1.570612	0.000000	C	1.9232570	-0.9852110	0.0000000
C	-0.509643	-0.545806	0.000000	C	0.6659070	-0.3346120	0.0000000
H	2.202156	2.160917	0.000000	H	-2.6882620	1.5008480	0.0000000
H	-0.200252	2.858827	0.000000	H	-2.6813530	-0.9952010	0.0000000
H	-2.621631	2.157605	0.000000	H	-1.3284910	-3.1171050	0.0000000
H	-4.295534	0.342338	0.000000	H	0.8794420	-4.2094480	0.0000000
H	-3.569961	-2.032456	0.000000	H	2.9490240	-2.8475810	0.0000000
H	-1.148350	-2.598049	0.000000	H	2.8100750	-0.3705600	0.0000000
C	3.087470	-0.356097	0.000000	C	-0.5266920	3.0596680	0.0000000
N	4.202464	-0.683351	0.000000	N	-0.5266920	4.2175680	0.0000000
			3-Quinolinecarbonitrile				
N	0.088163	1.732503	0.000000	N	-1.7063540	-0.2968190	0.0000000
C	1.342644	1.353973	0.000000	C	-1.6144380	1.0081480	0.0000000
C	1.756980	-0.008926	0.000000	C	-0.3785520	1.7122840	0.0000000
C	0.799045	-0.997978	0.000000	C	0.7953710	0.9979100	0.0000000
C	-0.562919	-0.627546	0.000000	C	0.7350740	-0.4095990	0.0000000
C	-1.614238	-1.579437	0.000000	C	1.8938730	-1.2233820	0.0000000
C	-2.921702	-1.161304	0.000000	C	1.7750930	-2.5887250	0.0000000
C	-3.231005	0.220649	0.000000	C	0.4976340	-3.1947060	0.0000000
C	-2.231353	1.163284	0.000000	C	-0.6407230	-2.4292130	0.0000000
C	-0.874167	0.761260	0.000000	C	-0.5485840	-1.0189200	0.0000000
H	2.096765	2.134661	0.000000	H	-2.5399200	1.5696550	0.0000000
H	1.082282	-2.044308	0.000000	H	1.7508190	1.5039860	0.0000000
H	-1.368465	-2.635496	0.000000	H	2.8663210	-0.7519410	0.0000000
H	-3.723897	-1.888989	0.000000	H	2.6590860	-3.2083020	0.0000000
H	-4.268071	0.533618	0.000000	H	0.4217540	-4.2717360	0.0000000
H	-2.445945	2.224417	0.000000	H	-1.6249390	-2.8714340	0.0000000
C	3.154207	-0.325405	0.000000	C	-0.3785520	3.1448840	0.0000000
N	4.288371	-0.582299	0.000000	N	-0.3785520	4.3036840	0.0000000
			4-Quinolinecarbonitrile				
N	-0.667313	2.091185	0.000000	N	-0.9420630	-1.9787400	0.0000000

C	0.611918	2.399115	0.000000	C	0.2819350	-2.4555770	0.0000000
C	1.657831	1.449323	0.000000	C	1.4446350	-1.6567010	0.0000000
C	1.331593	0.111386	0.000000	C	1.3020720	-0.2896140	0.0000000
C	-0.037779	-0.277128	0.000000	C	0.0000000	0.2789650	0.0000000
C	-0.464215	-1.627519	0.000000	C	-0.2400620	1.6723360	0.0000000
C	-1.805824	-1.922052	0.000000	C	-1.5276680	2.1443620	0.0000000
C	-2.770098	-0.885817	0.000000	C	-2.6211890	1.2490250	0.0000000
C	-2.379788	0.430673	0.000000	C	-2.4123250	-0.1058710	0.0000000
C	-1.003643	0.767892	0.000000	C	-1.0962400	-0.6248090	0.0000000
H	0.854787	3.457000	0.000000	H	0.3796490	-3.5335570	0.0000000
H	2.691364	1.769776	0.000000	H	2.4230000	-2.1124320	0.0000000
H	0.277527	-2.417764	0.000000	H	0.5986580	2.3530570	0.0000000
H	-2.130434	-2.955341	0.000000	H	-1.7093560	3.2084630	0.0000000
H	-3.823556	-1.137885	0.000000	H	-3.6276810	1.6395500	0.0000000
H	-3.097347	1.241290	0.000000	H	-3.2299290	-0.8099770	0.0000000
C	2.360509	-0.888933	0.000000	C	2.4564630	0.5627980	0.0000000
N	3.185511	-1.708412	0.000000	N	3.3811430	1.2610480	0.0000000

9-Ethynylanthracene

C	0.000012	-1.813481	0.000000	C	1.8012600	0.0000050	0.0000000
C	0.000000	1.002111	0.000000	C	-1.0099400	0.0000050	0.0000000
C	-1.218687	-1.131042	0.000000	C	1.1198710	-1.2168020	0.0000000
C	1.218705	-1.131032	0.000000	C	1.1198710	1.2168120	0.0000000
C	-1.227524	0.302810	0.000000	C	-0.3106690	-1.2274890	0.0000000
C	1.227530	0.302820	0.000000	C	-0.3106690	1.2274990	0.0000000
C	-2.463908	-1.830486	0.000000	C	1.8198580	-2.4591760	0.0000000
C	2.463932	-1.830465	0.000000	C	1.8198580	2.4591860	0.0000000
C	-2.484764	0.977302	0.000000	C	-0.9824580	-2.4836340	0.0000000
C	2.484764	0.977323	0.000000	C	-0.9824580	2.4836440	0.0000000
C	-3.649212	-1.151101	0.000000	C	1.1431230	-3.6434590	0.0000000
C	3.649230	-1.151070	0.000000	C	1.1431230	3.6434690	0.0000000
C	-3.657127	0.272534	0.000000	C	-0.2772930	-3.6531980	0.0000000
C	3.657133	0.272565	0.000000	C	-0.2772930	3.6532080	0.0000000
H	-2.447254	-2.914910	0.000000	H	2.9007080	-2.4411580	0.0000000
H	2.447287	-2.914889	0.000000	H	2.9007080	2.4411680	0.0000000
H	-2.492220	2.060062	0.000000	H	-2.0616220	-2.4924880	0.0000000
H	2.492211	2.060084	0.000000	H	-2.0616220	2.4924980	0.0000000
H	-4.587922	-1.691991	0.000000	H	1.6834480	-4.5783480	0.0000000
H	4.587945	-1.691952	0.000000	H	1.6834480	4.5783580	0.0000000
H	-4.603421	0.800283	0.000000	H	-0.8020570	-4.5970230	0.0000000
H	4.603422	0.800322	0.000000	H	-0.8020570	4.5970330	0.0000000
H	-0.000023	-2.899271	0.000000	H	2.8834600	-0.0000330	0.0000000
C	-0.000028	2.430234	0.000000	C	-2.4380400	-0.0000200	0.0000000
C	-0.000052	3.642569	0.000000	C	-3.6473400	-0.0000410	0.0000000
H	-0.000072	4.706359	0.000000	H	-4.7092400	-0.0000600	0.0000000

9-Ethynylphenanthrene

H	-3.893430	3.704398	0.000000	H	0.3793340	5.3684560	0.0000000
C	-3.073445	3.026877	0.000000	C	0.3793340	4.3066560	0.0000000
C	-2.139518	2.255211	0.000000	C	0.3793340	3.0981560	0.0000000
C	-1.036948	1.344201	0.000000	C	0.3793340	1.6679560	0.0000000
C	0.242523	1.823811	0.000000	C	1.5621210	0.9882080	0.0000000

C	1.370864	0.948653	0.000000	C	1.6061100	-0.4369130	0.0000000
C	1.176880	-0.455302	0.000000	C	0.4021150	-1.1804870	0.0000000
C	2.680691	1.478592	0.000000	C	2.8470370	-1.1080750	0.0000000
C	3.778780	0.647242	0.000000	C	2.9054830	-2.4819330	0.0000000
C	3.592574	-0.746599	0.000000	C	1.7142530	-3.2250250	0.0000000
C	2.320659	-1.283067	0.000000	C	0.4925080	-2.5872350	0.0000000
C	-0.178572	-0.978701	0.000000	C	-0.8628230	-0.4700270	0.0000000
C	-1.278127	-0.082740	0.000000	C	-0.8724250	0.9460680	0.0000000
C	-2.594662	-0.590852	0.000000	C	-2.1007680	1.6363260	0.0000000
C	-2.828907	-1.949099	0.000000	C	-3.2951680	0.9529090	0.0000000
C	-1.745136	-2.842654	0.000000	C	-3.2937610	-0.4494900	0.0000000
C	-0.450995	-2.364588	0.000000	C	-2.1028550	-1.1415710	0.0000000
H	0.412338	2.894556	0.000000	H	2.4925940	1.5374810	0.0000000
H	2.805931	2.555890	0.000000	H	3.7543170	-0.5203650	0.0000000
H	4.779407	1.062092	0.000000	H	3.8594470	-2.9873930	0.0000000
H	4.452240	-1.406027	0.000000	H	1.7533340	-4.3042170	0.0000000
H	2.212011	-2.359112	0.000000	H	-0.4032210	-3.1868500	0.0000000
H	0.364865	-3.074472	0.000000	H	-2.1304710	-2.2191170	0.0000000
H	-1.923200	-3.911368	0.000000	H	-4.2279180	-0.9910790	0.0000000
H	-3.844650	-2.325583	0.000000	H	-4.2292670	1.4943980	0.0000000
H	-3.420688	0.109336	0.000000	H	-2.0871210	2.7155400	0.0000000

1-Pyrenecarbonitrile

C	1.029776	-1.886346	0.000000	C	0.8763140	1.9860410	0.0000000
C	-0.233074	-2.390592	0.000000	C	2.0350330	1.2786170	0.0000000
C	-1.381645	-1.531323	0.000000	C	2.0357330	-0.1535830	0.0000000
C	-2.688510	-2.035537	0.000000	C	3.2208550	-0.8962590	0.0000000
C	-3.781201	-1.173803	0.000000	C	3.1861330	-2.2852250	0.0000000
C	-3.593213	0.205230	0.000000	C	1.9715380	-2.9603160	0.0000000
C	-2.302932	0.750106	0.000000	C	0.7638830	-2.2552700	0.0000000
C	-2.074721	2.166896	0.000000	C	-0.5050420	-2.9208770	0.0000000
C	-0.814638	2.677491	0.000000	C	-1.6671800	-2.2194710	0.0000000
C	0.333910	1.817978	0.000000	C	-1.6676800	-0.7871710	0.0000000
C	1.639840	2.328430	0.000000	C	-2.8571610	-0.0490290	0.0000000
C	2.733572	1.477311	0.000000	C	-2.8315630	1.3344340	0.0000000
C	2.549631	0.089756	0.000000	C	-1.6125840	2.0178780	0.0000000
C	1.255633	-0.469913	0.000000	C	-0.3908980	1.3187220	0.0000000
C	-1.182247	-0.124450	0.000000	C	0.7920640	-0.8362220	0.0000000
C	0.138486	0.409134	0.000000	C	-0.4248160	-0.1001670	0.0000000
H	1.886613	-2.549855	0.000000	H	0.8937510	3.0660000	0.0000000
H	-0.390357	-3.463600	0.000000	H	2.9850360	1.7942120	0.0000000
H	-2.840696	-3.109236	0.000000	H	4.1683210	-0.3762250	0.0000000
H	-4.785801	-1.579424	0.000000	H	4.1099110	-2.8443330	0.0000000
H	-4.448509	0.871971	0.000000	H	1.9506180	-4.0410140	0.0000000
H	-2.934202	2.828395	0.000000	H	-0.5192860	-4.0017830	0.0000000
H	-0.656040	3.750186	0.000000	H	-2.6177330	-2.7338410	0.0000000
H	1.790513	3.401884	0.000000	H	-3.8035680	-0.5701600	0.0000000
H	3.740196	1.876279	0.000000	H	-3.7512400	1.8991180	0.0000000
C	3.696383	-0.769052	0.000000	C	-1.6125840	3.4505780	0.0000000
N	4.627933	-1.466695	0.000000	N	-1.6125840	4.6102780	0.0000000

2-Pyrenecarbonitrile

C	2.891554	0.000001	0.000000	C	2.9294240	0.0000110	0.0000000
C	2.202537	1.215873	0.000000	C	2.2415060	1.2139430	0.0000000
C	2.202537	-1.215872	0.000000	C	2.2415060	-1.2139220	0.0000000
C	0.805187	1.232416	0.000000	C	0.8464040	1.2304570	0.0000000
C	0.805187	-1.232415	0.000000	C	0.8464040	-1.2304360	0.0000000
C	0.062791	2.462143	0.000000	C	0.1051680	2.4582590	0.0000000
C	0.062792	-2.462143	0.000000	C	0.1051680	-2.4582380	0.0000000
C	-1.296020	2.459927	0.000000	C	-1.2514310	2.4560450	0.0000000
C	-1.296019	-2.459927	0.000000	C	-1.2514310	-2.4560240	0.0000000
C	-2.039721	1.231290	0.000000	C	-1.9939970	1.2292810	0.0000000
C	-2.039721	-1.231290	0.000000	C	-1.9939970	-1.2292600	0.0000000
C	-3.439806	1.208837	0.000000	C	-3.3919170	1.2068620	0.0000000
C	-3.439805	-1.208838	0.000000	C	-3.3919170	-1.2068410	0.0000000
C	-4.129779	-0.000001	0.000000	C	-4.0808060	-0.0000760	0.0000000
C	0.094517	0.000000	0.000000	C	0.1368550	-0.0000210	0.0000000
C	-1.328886	0.000000	0.000000	C	-1.2842830	-0.0000640	0.0000000
H	2.755820	2.147571	0.000000	H	2.7929530	2.1425470	0.0000000
H	2.755820	-2.147570	0.000000	H	2.7929530	-2.1425260	0.0000000
H	0.611977	3.397055	0.000000	H	0.6525390	3.3900840	0.0000000
H	0.611978	-3.397054	0.000000	H	0.6525390	-3.3900630	0.0000000
H	-1.845104	3.395159	0.000000	H	-1.7986910	3.3881670	0.0000000
H	-1.845103	-3.395159	0.000000	H	-1.7986910	-3.3881460	0.0000000
H	-3.983986	2.146848	0.000000	H	-3.9342740	2.1417290	0.0000000
H	-3.983986	-2.146849	0.000000	H	-3.9342740	-2.1417080	0.0000000
H	-5.213219	0.000000	0.000000	H	-5.1606060	-0.0000760	0.0000000
C	4.327205	0.000000	0.000000	C	4.3651240	0.0000110	0.0000000
N	5.490259	-0.000001	0.000000	N	5.5241240	0.0000110	0.0000000

4-Pyrenecarbonitrile

C	1.642847	-1.219931	0.000000	C	1.8790120	-0.8853750	0.0000000
C	0.588237	-2.088835	0.000000	C	1.0155410	-1.9416570	0.0000000
C	-0.760715	-1.614052	0.000000	C	-0.3979700	-1.7394610	0.0000000
C	-1.851353	-2.493735	0.000000	C	-1.2946400	-2.8133250	0.0000000
C	-3.152483	-2.002194	0.000000	C	-2.6645120	-2.5854220	0.0000000
C	-3.388883	-0.630261	0.000000	C	-3.1632390	-1.2879740	0.0000000
C	-2.326037	0.282280	0.000000	C	-2.3002210	-0.1873920	0.0000000
C	-2.538431	1.702345	0.000000	C	-2.7848410	1.1619180	0.0000000
C	-1.491370	2.568382	0.000000	C	-1.9282440	2.2138710	0.0000000
C	-0.134596	2.097775	0.000000	C	-0.5078820	2.0172930	0.0000000
C	0.956129	2.976012	0.000000	C	0.3891740	3.0897920	0.0000000
C	2.259165	2.489745	0.000000	C	1.7598540	2.8674300	0.0000000
C	2.505608	1.119721	0.000000	C	2.2680290	1.5738680	0.0000000
C	1.441416	0.211370	0.000000	C	1.4028780	0.4771250	0.0000000
C	-0.993048	-0.211246	0.000000	C	-0.8987170	-0.4110030	0.0000000
C	0.105213	0.696031	0.000000	C	0.0000000	0.6913320	0.0000000
H	0.770936	-3.157339	0.000000	H	1.4018830	-2.9506190	0.0000000
H	-1.669894	-3.562754	0.000000	H	-0.9094070	-3.8230320	0.0000000
H	-3.988002	-2.691743	0.000000	H	-3.3471720	-3.4219190	0.0000000
H	-4.406200	-0.254392	0.000000	H	-4.2307470	-1.1183500	0.0000000
H	-3.557834	2.072220	0.000000	H	-3.8532260	1.3252640	0.0000000
H	-1.664582	3.638943	0.000000	H	-2.3057280	3.2267140	0.0000000

H	0.773370	4.044946	0.000000	H	0.0026890	4.0991280	0.0000000
H	3.092311	3.182071	0.000000	H	2.4396930	3.7062220	0.0000000
H	3.523781	0.748495	0.000000	H	3.3354640	1.4089510	0.0000000
C	2.981968	-1.732826	0.000000	C	3.2924860	-1.1271290	0.0000000
N	4.074668	-2.132309	0.000000	N	4.4380440	-1.3051000	0.0000000
			1-Ethynylpyrene				
C	1.687439	-1.358507	0.000000	C	0.8895790	1.9645240	0.0000000
C	0.703223	-2.304440	0.000000	C	2.0445260	1.2507680	0.0000000
C	-0.686796	-1.940425	0.000000	C	2.0363520	-0.1814080	0.0000000
C	-1.715130	-2.900107	0.000000	C	3.2164890	-0.9321670	0.0000000
C	-3.055197	-2.509187	0.000000	C	3.1726560	-2.3207760	0.0000000
C	-3.398206	-1.155778	0.000000	C	1.9533200	-2.9872640	0.0000000
C	-2.403304	-0.161744	0.000000	C	0.7501450	-2.2742060	0.0000000
C	-2.722376	1.240180	0.000000	C	-0.5227040	-2.9324950	0.0000000
C	-1.741080	2.188867	0.000000	C	-1.6796690	-2.2225890	0.0000000
C	-0.351474	1.824161	0.000000	C	-1.6709210	-0.7905160	0.0000000
C	0.674935	2.786981	0.000000	C	-2.8534090	-0.0423420	0.0000000
C	2.011093	2.406103	0.000000	C	-2.8167740	1.3409730	0.0000000
C	2.379401	1.046399	0.000000	C	-1.5978370	2.0291820	0.0000000
C	1.372880	0.043080	0.000000	C	-0.3844630	1.3099930	0.0000000
C	-1.028371	-0.553303	0.000000	C	0.7870370	-0.8547140	0.0000000
C	0.000000	0.438764	0.000000	C	-0.4253510	-0.1092640	0.0000000
H	2.737819	-1.651457	0.000000	H	0.9108850	3.0437130	0.0000000
H	0.962039	-3.365862	0.000000	H	2.9982560	1.7598630	0.0000000
H	-1.451962	-3.960282	0.000000	H	4.1674790	-0.4181840	0.0000000
H	-3.841022	-3.267301	0.000000	H	4.0927280	-2.8863430	0.0000000
H	-4.448482	-0.855525	0.000000	H	1.9247580	-4.0678870	0.0000000
H	-3.774852	1.533207	0.000000	H	-0.5434750	-4.0132950	0.0000000
H	-1.997926	3.250690	0.000000	H	-2.6339400	-2.7304540	0.0000000
H	0.411201	3.846779	0.000000	H	-3.8041510	-0.5563640	0.0000000
H	2.797771	3.161686	0.000000	H	-3.7345020	1.9093890	0.0000000
C	3.763525	0.694293	0.000000	C	-1.5978370	3.4582820	0.0000000
C	4.945630	0.406597	0.000000	C	-1.5978370	4.6659820	0.0000000
H	5.988274	0.156462	0.000000	H	-1.5978370	5.7277820	0.0000000
			2-Ethynylpyrene				
C	2.920119	-0.000121	0.000000	C	-2.9295540	0.0000360	0.0000000
C	2.219002	1.211430	0.000000	C	-2.2294970	-1.2095950	0.0000000
C	2.218926	-1.211627	0.000000	C	-2.2294970	1.2096670	0.0000000
C	0.821587	1.230166	0.000000	C	-0.8343220	-1.2282600	0.0000000
C	0.821510	-1.230276	0.000000	C	-0.8343220	1.2283320	0.0000000
C	0.078386	2.459767	0.000000	C	-0.0922000	-2.4559950	0.0000000
C	0.078231	-2.459830	0.000000	C	-0.0922000	2.4560670	0.0000000
C	-1.280724	2.459346	0.000000	C	1.2647000	-2.4555330	0.0000000
C	-1.280878	-2.459324	0.000000	C	1.2647000	2.4556050	0.0000000
C	-2.025957	1.231388	0.000000	C	2.0087570	-1.2294380	0.0000000
C	-2.026035	-1.231319	0.000000	C	2.0087570	1.2295100	0.0000000
C	-3.426187	1.208925	0.000000	C	3.4067770	-1.2069760	0.0000000
C	-3.426263	-1.208769	0.000000	C	3.4067770	1.2070480	0.0000000
C	-4.116414	0.000099	0.000000	C	4.0958810	-0.0000460	0.0000000
C	0.108511	-0.000035	0.000000	C	-0.1224020	0.0000380	0.0000000

C	-1.314832	0.000011	0.000000	C	1.2986750	0.0000400	0.0000000
H	2.769738	2.145072	0.000000	H	-2.7783860	-2.1401780	0.0000000
H	2.769603	-2.145304	0.000000	H	-2.7783860	2.1402500	0.0000000
H	0.627849	3.394791	0.000000	H	-0.6397980	-3.3879180	0.0000000
H	0.627636	-3.394889	0.000000	H	-0.6397980	3.3879900	0.0000000
H	-1.828968	3.395245	0.000000	H	1.8111790	-3.3883450	0.0000000
H	-1.829181	-3.395189	0.000000	H	1.8111790	3.3884170	0.0000000
H	-3.970313	2.147126	0.000000	H	3.9491300	-2.1420770	0.0000000
H	-3.970447	-2.146936	0.000000	H	3.9491300	2.1421480	0.0000000
H	-5.199975	0.000150	0.000000	H	5.1758810	-0.0000740	0.0000000
C	4.351852	0.000015	0.000000	C	-4.3612540	-0.0001510	0.0000000
C	5.562839	0.000129	0.000000	C	-5.5681540	-0.0003090	0.0000000
H	6.626419	0.000230	0.000000	H	-6.6298540	-0.0004480	0.0000000

4-Ethynylpyrene

C	1.668048	-1.228273	0.000000	C	0.5503060	2.0039180	0.0000000
C	0.604471	-2.089297	0.000000	C	1.7335400	1.3209390	0.0000000
C	-0.745861	-1.617823	0.000000	C	1.7775730	-0.1064820	0.0000000
C	-1.836180	-2.498466	0.000000	C	2.9886790	-0.8073820	0.0000000
C	-3.139006	-2.010424	0.000000	C	3.0002400	-2.1963340	0.0000000
C	-3.379921	-0.639343	0.000000	C	1.8085990	-2.9117460	0.0000000
C	-2.317887	0.274306	0.000000	C	0.5767810	-2.2489760	0.0000000
C	-2.531794	1.694041	0.000000	C	-0.6699640	-2.9566750	0.0000000
C	-1.485314	2.560920	0.000000	C	-1.8525190	-2.2916940	0.0000000
C	-0.127821	2.092070	0.000000	C	-1.9015360	-0.8585320	0.0000000
C	0.960085	2.973739	0.000000	C	-3.1127510	-0.1602200	0.0000000
C	2.263382	2.488783	0.000000	C	-3.1273600	1.2281040	0.0000000
C	2.510699	1.118728	0.000000	C	-1.9389800	1.9491130	0.0000000
C	1.451161	0.204503	0.000000	C	-0.7075900	1.2889270	0.0000000
C	-0.983938	-0.216520	0.000000	C	0.5567130	-0.8301040	0.0000000
C	0.114584	0.690250	0.000000	C	-0.6817720	-0.1307190	0.0000000
H	0.784751	-3.158444	0.000000	H	2.6638030	1.8707640	0.0000000
H	-1.652779	-3.567323	0.000000	H	3.9176230	-0.2547440	0.0000000
H	-3.972522	-2.702730	0.000000	H	3.9422260	-2.7243930	0.0000000
H	-4.398026	-0.265409	0.000000	H	1.8245580	-3.9926280	0.0000000
H	-3.551634	2.063189	0.000000	H	-0.6489490	-4.0374700	0.0000000
H	-1.659563	3.631489	0.000000	H	-2.7863460	-2.8364370	0.0000000
H	0.774528	4.042338	0.000000	H	-4.0406690	-0.7147730	0.0000000
H	3.095802	3.182436	0.000000	H	-4.0701930	1.7546490	0.0000000
H	3.527625	0.746167	0.000000	H	-1.9558000	3.0283820	0.0000000
C	3.002999	-1.740888	0.000000	C	0.5503060	3.4339180	0.0000000
C	4.133954	-2.175168	0.000000	C	0.5503060	4.6412180	0.0000000
H	5.126957	-2.556476	0.000000	H	0.5503060	5.7030180	0.0000000

Table S5: Cartesian coordinates (TM+LR) of 1-cyanonaphthalene, 2-cyanonaphthalene, 9-cyanoanthracene, 9-cyanophenantrene, 3-cyanopyridine, 2-ehynylpyridine, *cis*-Benzoic acid, 1-ethynylnaphthalene, 2-ethynylnaphthalene, 2-quinolinecarbonitrile, 3-quinolinecarbonitrile, 4-quinolinecarbonitrile, 9-ethynylanthracene, 9-ethynylphenanthrene, 1-pyrenecarbonitrile, 2-pyrenecarbonitrile, 4-pyrenecarbonitrile, 1-ethynylpyrene, 2-ethynylpyrene, and 4-ethynylpyrene.

	TM+LR		
	1-Cyanonaphthalene		
C	0.0000000	0.2728740	0.0000000
C	-0.3430370	1.6456640	0.0000000
C	-1.6598090	2.0299460	0.0000000
C	-2.6896240	1.0636170	0.0000000
C	-2.3823370	-0.2722970	0.0000000
C	-1.0329270	-0.7027400	0.0000000
C	-0.6918050	-2.0771400	0.0000000
C	0.6196740	-2.4794530	0.0000000
C	1.6531480	-1.5238010	0.0000000
C	1.3524220	-0.1786050	0.0000000
H	0.4442640	2.3851060	0.0000000
H	-1.9124510	3.0795690	0.0000000
H	-3.7212210	1.3819610	0.0000000
H	-3.1655610	-1.0169260	0.0000000
H	-1.4871740	-2.8089300	0.0000000
H	0.8681310	-3.5295610	0.0000000
H	2.6856380	-1.8375220	0.0000000
C	2.4135950	0.7821190	0.0000000
N	3.2646530	1.5693140	0.0000000
	2-Cyanonaphthalene		
C	0.7064530	-0.3376030	0.0000000
C	1.9185300	-1.0713720	0.0000000
C	1.9018570	-2.4420300	0.0000000
C	0.6732270	-3.1404170	0.0000000
C	-0.5148380	-2.4552070	0.0000000
C	-0.5301070	-1.0398100	0.0000000
C	-1.7408790	-0.3028100	0.0000000
C	-1.7335010	1.0652010	0.0000000
C	-0.4977400	1.7627670	0.0000000
C	0.6954640	1.0752580	0.0000000
H	2.8553860	-0.5326760	0.0000000
H	2.8295410	-2.9942050	0.0000000
H	0.6740010	-4.2201060	0.0000000
H	-1.4553000	-2.9876430	0.0000000
H	-2.6789170	-0.8391600	0.0000000
H	-2.6554540	1.6254480	0.0000000
H	1.6305660	1.6160320	0.0000000
C	-0.4977400	3.1950670	0.0000000
N	-0.4977400	4.3540070	0.0000000
	9-Cyanoanthracene		

C	0.0000000	0.0000000	-1.7857490
C	0.0000000	0.0000000	1.0077510
C	0.0000000	1.2191730	-1.1077790
C	0.0000000	-1.2191730	-1.1077790
C	0.0000000	1.2294560	0.3233770
C	0.0000000	-1.2294560	0.3233770
C	0.0000000	2.4623990	-1.8056390
C	0.0000000	-2.4623990	-1.8056390
C	0.0000000	2.4814340	1.0020620
C	0.0000000	-2.4814340	1.0020620
C	0.0000000	3.6440400	-1.1243010
C	0.0000000	-3.6440400	-1.1243010
C	0.0000000	3.6510630	0.2973930
C	0.0000000	-3.6510630	0.2973930
H	0.0000000	2.4475080	-2.8862370
H	0.0000000	-2.4475080	-2.8862370
H	0.0000000	2.4913710	2.0820160
H	0.0000000	-2.4913710	2.0820160
H	0.0000000	4.5806300	-1.6612690
H	0.0000000	-4.5806300	-1.6612690
H	0.0000000	4.5938800	0.8235560
H	0.0000000	-4.5938800	0.8235560
H	0.0000000	0.0000000	-2.8679490
C	0.0000000	0.0000000	2.4367510
N	0.0000000	0.0000000	3.5968510

9-Cyanophenantrene

N	-3.5961200	-2.3100000	0.0000000
C	-2.5646740	-1.7807600	0.0000000
C	-1.2973400	-1.1152640	0.0000000
C	-0.1529690	-1.8541850	0.0000000
C	1.1265710	-1.2258320	0.0000000
C	1.2177900	0.1869270	0.0000000
C	2.2989160	-2.0101260	0.0000000
C	3.5398760	-1.4184410	0.0000000
C	3.6378730	-0.0178650	0.0000000
C	2.5035130	0.7646880	0.0000000
C	0.0000000	0.9762100	0.0000000
C	-1.2568660	0.3252680	0.0000000
C	-2.4444630	1.0829280	0.0000000
C	-2.3981290	2.4579480	0.0000000
C	-1.1575300	3.1123190	0.0000000
C	0.0128210	2.3860210	0.0000000
H	-0.2078390	-2.9330910	0.0000000
H	2.2036580	-3.0867200	0.0000000
H	4.4332900	-2.0241770	0.0000000
H	4.6099000	0.4523800	0.0000000
H	2.6149170	1.8366150	0.0000000
H	0.9512850	2.9158540	0.0000000
H	-1.1171950	4.1912650	0.0000000
H	-3.3133530	3.0301980	0.0000000

H	-3.3941600	0.5686570	0.0000000
	***trans* 2-Naphthol**		
C	0.0000000	0.6858600	0.0000000
C	-0.6416240	1.9503930	0.0000000
C	-2.0098170	2.0426560	0.0000000
C	-2.8080570	0.8762460	0.0000000
C	-2.2156540	-0.3602700	0.0000000
C	-0.8052090	-0.4867010	0.0000000
C	-0.1635570	-1.7478550	0.0000000
C	1.2034110	-1.8433600	0.0000000
C	1.9962750	-0.6729260	0.0000000
C	1.4084970	0.5662390	0.0000000
H	-0.0330350	2.8436810	0.0000000
H	-2.4837940	3.0130920	0.0000000
H	-3.8842440	0.9632770	0.0000000
H	-2.8189000	-1.2575370	0.0000000
H	-0.7671010	-2.6445600	0.0000000
H	1.6835620	-2.8131000	0.0000000
H	2.0296890	1.4497100	0.0000000
O	3.3582280	-0.7438870	0.0000000
H	3.6224110	-1.6651570	0.0000000
	***cis* 1-Naphthol**		
C	0.0000000	0.4420180	0.0000000
C	0.9909860	1.4552730	0.0000000
C	2.3262440	1.1398850	0.0000000
C	2.7373340	-0.2099020	0.0000000
C	1.8013280	-1.2111200	0.0000000
C	0.4144030	-0.9207300	0.0000000
C	-0.5539450	-1.9522140	0.0000000
C	-1.8890020	-1.6399000	0.0000000
C	-2.3163120	-0.2986230	0.0000000
C	-1.3964480	0.7208150	0.0000000
H	0.7170220	2.5019110	0.0000000
H	3.0649530	1.9271880	0.0000000
H	3.7899500	-0.4497680	0.0000000
H	2.1096030	-2.2471280	0.0000000
H	-0.2249780	-2.9808930	0.0000000
H	-2.6297040	-2.4256030	0.0000000
H	-3.3663590	-0.0503420	0.0000000
O	-1.8755320	1.9949200	0.0000000
H	-1.1437580	2.6122710	0.0000000
	3-Cyanopyridine		
N	-0.0242040	3.1771610	0.0000000
C	-0.0242040	2.0187610	0.0000000
C	-0.0242040	0.5877010	0.0000000
C	1.1850910	-0.1135340	0.0000000
N	1.2571350	-1.4417810	0.0000000
C	0.1059730	-2.1194150	0.0000000
C	-1.1468360	-1.5152050	0.0000000
C	-1.2184110	-0.1322550	0.0000000

H	2.1216140	0.4271600	0.0000000
H	0.1919050	-3.1974960	0.0000000
H	-2.0419920	-2.1180060	0.0000000
H	-2.1664940	0.3843600	0.0000000

2-Ethynylpyridine

H	0.0105600	4.2542490	0.0000000
C	0.0105600	3.1925490	0.0000000
C	0.0105600	1.9858490	0.0000000
C	0.0105600	0.5516890	0.0000000
N	1.2054760	-0.0600400	0.0000000
C	1.2061970	-1.3927400	0.0000000
C	0.0535340	-2.1718970	0.0000000
C	-1.1766570	-1.5286780	0.0000000
C	-1.2023810	-0.1427170	0.0000000
H	2.1815930	-1.8610620	0.0000000
H	0.1252220	-3.2491140	0.0000000
H	-2.0977190	-2.0933980	0.0000000
H	-2.1322200	0.4052680	0.0000000

***cis* 3-Hydroxy-pyridine**

H	-0.8920870	2.6001040	0.0000000
O	0.0118670	2.2783800	0.0000000
C	0.0000000	0.9185320	0.0000000
C	-1.1774820	0.1732960	0.0000000
N	-1.2031780	-1.1588570	0.0000000
C	-0.0330110	-1.7995840	0.0000000
C	1.1923460	-1.1402110	0.0000000
C	1.2154490	0.2456960	0.0000000
H	-2.1381180	0.6781110	0.0000000
H	-0.0785610	-2.8796240	0.0000000
H	2.1129610	-1.7048960	0.0000000
H	2.1392940	0.8048880	0.0000000

4-Hydroxy-pyridine

H	-0.8446470	2.6315180	0.0000000
O	0.0493340	2.2833120	0.0000000
C	0.0000000	0.9301110	0.0000000
C	-1.1893480	0.2099280	0.0000000
C	-1.1179620	-1.1776370	0.0000000
N	0.0209060	-1.8722850	0.0000000
C	1.1505090	-1.1555530	0.0000000
C	1.2017700	0.2298990	0.0000000
H	-2.1486100	0.7098180	0.0000000
H	-2.0309910	-1.7584290	0.0000000
H	2.0714290	-1.7233680	0.0000000
H	2.1419880	0.7594710	0.0000000

***cis* Benzoic acid**

C	0.2608950	-2.5878110	0.0000000
C	1.3974620	-1.7829330	0.0000000
C	-1.0047130	-2.0094440	0.0000000
C	1.2686180	-0.4013280	0.0000000
C	-1.1390380	-0.6264520	0.0000000

C	0.0000000	0.1791130	0.0000000
C	-0.0857470	1.6591320	0.0000000
O	0.8614480	2.4051430	0.0000000
O	-1.3583170	2.1127460	0.0000000
H	-1.2929870	3.0745300	0.0000000
H	2.1344640	0.2421940	0.0000000
H	-2.1161600	-0.1713680	0.0000000
H	2.3788070	-2.2324510	0.0000000
H	-1.8849240	-2.6343830	0.0000000
H	0.3617290	-3.6629930	0.0000000

1-Ethynylnaphthalene

C	0.2017980	0.1638750	0.0000000
C	1.4554400	0.8207290	0.0000000
C	2.6221150	0.0987500	0.0000000
C	2.5908190	-1.3129030	0.0000000
C	1.3898180	-1.9739360	0.0000000
C	0.1677870	-1.2572230	0.0000000
C	-1.0807790	-1.9249480	0.0000000
C	-2.2534640	-1.2139300	0.0000000
C	-2.2310520	0.1936920	0.0000000
C	-1.0339430	0.8816320	0.0000000
H	1.4766140	1.8999210	0.0000000
H	3.5721330	0.6120090	0.0000000
H	3.5160840	-1.8695470	0.0000000
H	1.3575640	-3.0544540	0.0000000
H	-1.0937600	-3.0057700	0.0000000
H	-3.2023180	-1.7289180	0.0000000
H	-3.1562960	0.7495950	0.0000000
C	-1.0339430	2.3094020	0.0000000
C	-1.0339430	3.5178020	0.0000000
H	-1.0339430	4.5795020	0.0000000

2-Ethynylnaphthalene

C	0.7039260	-0.3593180	0.0000000
C	1.9126010	-1.0992930	0.0000000
C	1.8923450	-2.4703430	0.0000000
C	0.6619920	-3.1653840	0.0000000
C	-0.5231110	-2.4744660	0.0000000
C	-0.5335110	-1.0591040	0.0000000
C	-1.7395240	-0.3146100	0.0000000
C	-1.7228140	1.0533880	0.0000000
C	-0.4880460	1.7580700	0.0000000
C	0.6976380	1.0541390	0.0000000
H	2.8516980	-0.5640900	0.0000000
H	2.8188430	-3.0249330	0.0000000
H	0.6587670	-4.2451790	0.0000000
H	-1.4659900	-3.0031810	0.0000000
H	-2.6810070	-0.8456040	0.0000000
H	-2.6438110	1.6159160	0.0000000
H	1.6371160	1.5878630	0.0000000
C	-0.4880460	3.1863400	0.0000000

C	-0.4880460	4.3944400	0.0000000
H	-0.4880460	5.4560400	0.0000000

2-Quinolinecarbonitrile

N	0.6511790	1.0248640	0.0000000
C	-0.5266920	1.6140240	0.0000000
C	-1.7693470	0.9355720	0.0000000
C	-1.7578030	-0.4321790	0.0000000
C	-0.5221970	-1.1153630	0.0000000
C	-0.4227850	-2.5270670	0.0000000
C	0.8073000	-3.1318050	0.0000000
C	1.9887860	-2.3536870	0.0000000
C	1.9232570	-0.9847550	0.0000000
C	0.6659070	-0.3341560	0.0000000
H	-2.6882620	1.5013040	0.0000000
H	-2.6813530	-0.9947450	0.0000000
H	-1.3284910	-3.1166490	0.0000000
H	0.8794420	-4.2089920	0.0000000
H	2.9490240	-2.8471250	0.0000000
H	2.8100750	-0.3701040	0.0000000
C	-0.5266920	3.0574240	0.0000000
N	-0.5266920	4.2153240	0.0000000

3-Quinolinecarbonitrile

N	-1.7063540	-0.2963800	0.0000000
C	-1.6144380	1.0085860	0.0000000
C	-0.3785520	1.7127230	0.0000000
C	0.7953710	0.9983490	0.0000000
C	0.7350740	-0.4091600	0.0000000
C	1.8938730	-1.2229430	0.0000000
C	1.7750930	-2.5882860	0.0000000
C	0.4976340	-3.1942670	0.0000000
C	-0.6407230	-2.4287750	0.0000000
C	-0.5485840	-1.0184810	0.0000000
H	-2.5399200	1.5700940	0.0000000
H	1.7508190	1.5044250	0.0000000
H	2.8663210	-0.7515020	0.0000000
H	2.6590860	-3.2078630	0.0000000
H	0.4217540	-4.2712970	0.0000000
H	-1.6249390	-2.8709960	0.0000000
C	-0.3785520	3.1427230	0.0000000
N	-0.3785520	4.3015230	0.0000000

4-Quinolinecarbonitrile

N	-0.9392080	-1.9796680	0.0000000
C	0.2853930	-2.4549570	0.0000000
C	1.4470820	-1.6546120	0.0000000
C	1.3027900	-0.2877060	0.0000000
C	0.0000000	0.2792250	0.0000000
C	-0.2418240	1.6722920	0.0000000
C	-1.5300250	2.1426900	0.0000000
C	-2.6224130	1.2459710	0.0000000
C	-2.4118360	-0.1086600	0.0000000

C	-1.0950970	-0.6259340	0.0000000
H	0.3844690	-3.5328130	0.0000000
H	2.4260220	-2.1091060	0.0000000
H	0.5960350	2.3540730	0.0000000
H	-1.7130590	3.2065600	0.0000000
H	-3.6293980	1.6352230	0.0000000
H	-3.2285490	-0.8137990	0.0000000
C	2.4540130	0.5646170	0.0000000
N	3.3778090	1.2640360	0.0000000

9-Ethynylanthracene

C	1.8027010	0.0000050	0.0000000
C	-1.0084990	0.0000050	0.0000000
C	1.1213130	-1.2168020	0.0000000
C	1.1213130	1.2168120	0.0000000
C	-0.3103170	-1.2255780	0.0000000
C	-0.3103170	1.2255880	0.0000000
C	1.8196330	-2.4601140	0.0000000
C	1.8196330	2.4601240	0.0000000
C	-0.9837900	-2.4808210	0.0000000
C	-0.9837900	2.4808310	0.0000000
C	1.1413100	-3.6434880	0.0000000
C	1.1413100	3.6434980	0.0000000
C	-0.2801930	-3.6513290	0.0000000
C	-0.2801930	3.6513390	0.0000000
H	2.9005060	-2.4435450	0.0000000
H	2.9005060	2.4435550	0.0000000
H	-2.0629640	-2.4882270	0.0000000
H	-2.0629640	2.4882370	0.0000000
H	1.6803810	-4.5791010	0.0000000
H	1.6803810	4.5791110	0.0000000
H	-0.8062230	-4.5944490	0.0000000
H	-0.8062230	4.5944590	0.0000000
H	2.8849010	-0.0000330	0.0000000
C	-2.4339990	-0.0000200	0.0000000
C	-3.6432990	-0.0000410	0.0000000
H	-4.7051990	-0.0000600	0.0000000

9-Ethynylphenanthrene

H	0.3793340	5.3661750	0.0000000
C	0.3793340	4.3043750	0.0000000
C	0.3793340	3.0958750	0.0000000
C	0.3793340	1.6682750	0.0000000
C	1.5621210	0.9885270	0.0000000
C	1.6061100	-0.4365940	0.0000000
C	0.4021150	-1.1801680	0.0000000
C	2.8470370	-1.1077560	0.0000000
C	2.9054830	-2.4816140	0.0000000
C	1.7142530	-3.2247060	0.0000000
C	0.4925080	-2.5869160	0.0000000
C	-0.8628230	-0.4697080	0.0000000
C	-0.8724250	0.9463870	0.0000000

C	-2.1007680	1.6366450	0.0000000
C	-3.2951680	0.9532280	0.0000000
C	-3.2937610	-0.4491710	0.0000000
C	-2.1028550	-1.1412520	0.0000000
H	2.4925940	1.5378000	0.0000000
H	3.7543170	-0.5200460	0.0000000
H	3.8594470	-2.9870740	0.0000000
H	1.7533340	-4.3038980	0.0000000
H	-0.4032210	-3.1865310	0.0000000
H	-2.1304710	-2.2187980	0.0000000
H	-4.2279180	-0.9907600	0.0000000
H	-4.2292670	1.4947170	0.0000000
H	-2.0871210	2.7158590	0.0000000

1-Pyrenecarbonitrile

C	0.8763140	1.9863330	0.0000000
C	2.0350330	1.2789090	0.0000000
C	2.0357330	-0.1532910	0.0000000
C	3.2208550	-0.8959670	0.0000000
C	3.1861330	-2.2849330	0.0000000
C	1.9715380	-2.9600250	0.0000000
C	0.7638830	-2.2549780	0.0000000
C	-0.5050420	-2.9205850	0.0000000
C	-1.6671800	-2.2191790	0.0000000
C	-1.6676800	-0.7868790	0.0000000
C	-2.8571610	-0.0487370	0.0000000
C	-2.8315630	1.3347260	0.0000000
C	-1.6125840	2.0181700	0.0000000
C	-0.3908980	1.3190140	0.0000000
C	0.7920640	-0.8359300	0.0000000
C	-0.4248160	-0.0998750	0.0000000
H	0.8937510	3.0662920	0.0000000
H	2.9850360	1.7945040	0.0000000
H	4.1683210	-0.3759330	0.0000000
H	4.1099110	-2.8440410	0.0000000
H	1.9506180	-4.0407220	0.0000000
H	-0.5192860	-4.0014910	0.0000000
H	-2.6177330	-2.7335490	0.0000000
H	-3.8035680	-0.5698680	0.0000000
H	-3.7512400	1.8994100	0.0000000
C	-1.6125840	3.4482200	0.0000000
N	-1.6125840	4.6079200	0.0000000

2-Pyrenecarbonitrile

C	2.9297100	0.0000110	0.0000000
C	2.2417930	1.2139430	0.0000000
C	2.2417930	-1.2139220	0.0000000
C	0.8466900	1.2304570	0.0000000
C	0.8466900	-1.2304360	0.0000000
C	0.1054540	2.4582590	0.0000000
C	0.1054540	-2.4582380	0.0000000
C	-1.2511440	2.4560450	0.0000000

C	-1.2511440	-2.4560240	0.0000000
C	-1.9937100	1.2292810	0.0000000
C	-1.9937100	-1.2292600	0.0000000
C	-3.3916300	1.2068620	0.0000000
C	-3.3916300	-1.2068410	0.0000000
C	-4.0805190	-0.0000760	0.0000000
C	0.1371410	-0.0000210	0.0000000
C	-1.2839970	-0.0000640	0.0000000
H	2.7932390	2.1425470	0.0000000
H	2.7932390	-2.1425260	0.0000000
H	0.6528260	3.3900840	0.0000000
H	0.6528260	-3.3900630	0.0000000
H	-1.7984040	3.3881670	0.0000000
H	-1.7984040	-3.3881460	0.0000000
H	-3.9339880	2.1417290	0.0000000
H	-3.9339880	-2.1417080	0.0000000
H	-5.1603190	-0.0000760	0.0000000
C	4.3628100	0.0000110	0.0000000
N	5.5218100	0.0000110	0.0000000

4-Pyrenecarbonitrile

C	1.8796700	-0.8846390	0.0000000
C	1.0166410	-1.9412820	0.0000000
C	-0.3969550	-1.7396760	0.0000000
C	-1.2931760	-2.8139150	0.0000000
C	-2.6631420	-2.5865850	0.0000000
C	-3.1624120	-1.2893450	0.0000000
C	-2.2998540	-0.1884030	0.0000000
C	-2.7850370	1.1607050	0.0000000
C	-1.9288800	2.2130160	0.0000000
C	-0.5084360	2.0170310	0.0000000
C	0.3881710	3.0899050	0.0000000
C	1.7589450	2.8681160	0.0000000
C	2.2676600	1.5747660	0.0000000
C	1.4029670	0.4776620	0.0000000
C	-0.8982560	-0.4114270	0.0000000
C	0.0000000	0.6912830	0.0000000
H	1.4034040	-2.9500830	0.0000000
H	-0.9075210	-3.8234610	0.0000000
H	-3.3454530	-3.4233670	0.0000000
H	-4.2299900	-1.1201670	0.0000000
H	-3.8534910	1.3236050	0.0000000
H	-2.3067870	3.2257010	0.0000000
H	0.0012650	4.0990790	0.0000000
H	2.4384330	3.7071920	0.0000000
H	3.3351640	1.4102950	0.0000000
C	3.2906240	-1.1253560	0.0000000
N	4.4362560	-1.3028480	0.0000000

1-Ethynylpyrene

C	0.8895790	1.9648100	0.0000000
C	2.0445260	1.2510550	0.0000000

C	2.0363520	-0.1811220	0.0000000
C	3.2164890	-0.9318810	0.0000000
C	3.1726560	-2.3204890	0.0000000
C	1.9533200	-2.9869780	0.0000000
C	0.7501450	-2.2739190	0.0000000
C	-0.5227040	-2.9322090	0.0000000
C	-1.6796690	-2.2223030	0.0000000
C	-1.6709210	-0.7902290	0.0000000
C	-2.8534090	-0.0420560	0.0000000
C	-2.8167740	1.3412590	0.0000000
C	-1.5978370	2.0294690	0.0000000
C	-0.3844630	1.3102800	0.0000000
C	0.7870370	-0.8544280	0.0000000
C	-0.4253510	-0.1089780	0.0000000
H	0.9108850	3.0440000	0.0000000
H	2.9982560	1.7601490	0.0000000
H	4.1674790	-0.4178970	0.0000000
H	4.0927280	-2.8860570	0.0000000
H	1.9247580	-4.0676010	0.0000000
H	-0.5434750	-4.0130090	0.0000000
H	-2.6339400	-2.7301680	0.0000000
H	-3.8041510	-0.5560770	0.0000000
H	-3.7345020	1.9096750	0.0000000
C	-1.5978370	3.4559690	0.0000000
C	-1.5978370	4.6636690	0.0000000
H	-1.5978370	5.7254690	0.0000000

2-Ethynylpyrene

C	-2.9298400	0.0000360	0.0000000
C	-2.2297840	-1.2095950	0.0000000
C	-2.2297840	1.2096670	0.0000000
C	-0.8346090	-1.2282610	0.0000000
C	-0.8346090	1.2283320	0.0000000
C	-0.0924860	-2.4559950	0.0000000
C	-0.0924860	2.4560670	0.0000000
C	1.2644140	-2.4555330	0.0000000
C	1.2644140	2.4556050	0.0000000
C	2.0084710	-1.2294380	0.0000000
C	2.0084710	1.2295100	0.0000000
C	3.4064900	-1.2069760	0.0000000
C	3.4064900	1.2070480	0.0000000
C	4.0955950	-0.0000460	0.0000000
C	-0.1226890	0.0000380	0.0000000
C	1.2983880	0.0000400	0.0000000
H	-2.7786720	-2.1401780	0.0000000
H	-2.7786720	2.1402500	0.0000000
H	-0.6400840	-3.3879180	0.0000000
H	-0.6400840	3.3879900	0.0000000
H	1.8108930	-3.3883450	0.0000000
H	1.8108930	3.3884170	0.0000000
H	3.9488440	-2.1420770	0.0000000

H	3.9488440	2.1421480	0.0000000
H	5.1755950	-0.0000740	0.0000000
C	-4.3589400	-0.0001510	0.0000000
C	-5.5658400	-0.0003090	0.0000000
H	-6.6275400	-0.0004480	0.0000000
	4-Ethynylpyrene		
C	0.5503060	2.0042040	0.0000000
C	1.7335400	1.3212260	0.0000000
C	1.7775730	-0.1061950	0.0000000
C	2.9886790	-0.8070960	0.0000000
C	3.0002400	-2.1960480	0.0000000
C	1.8085990	-2.9114600	0.0000000
C	0.5767810	-2.2486890	0.0000000
C	-0.6699640	-2.9563880	0.0000000
C	-1.8525190	-2.2914080	0.0000000
C	-1.9015360	-0.8582460	0.0000000
C	-3.1127510	-0.1599330	0.0000000
C	-3.1273600	1.2283900	0.0000000
C	-1.9389800	1.9493990	0.0000000
C	-0.7075900	1.2892130	0.0000000
C	0.5567130	-0.8298180	0.0000000
C	-0.6817720	-0.1304320	0.0000000
H	2.6638030	1.8710500	0.0000000
H	3.9176230	-0.2544570	0.0000000
H	3.9422260	-2.7241060	0.0000000
H	1.8245580	-3.9923420	0.0000000
H	-0.6489490	-4.0371840	0.0000000
H	-2.7863460	-2.8361500	0.0000000
H	-4.0406690	-0.7144860	0.0000000
H	-4.0701930	1.7549360	0.0000000
H	-1.9558000	3.0286680	0.0000000
C	0.5503060	3.4316040	0.0000000
C	0.5503060	4.6389040	0.0000000
H	0.5503060	5.7007040	0.0000000

Simulations of rotational spectra

Simulations of rotational spectra for the 13 systems of the "application" dataset (see main text) are provided as separate files in the PGOPHER format: 1-ethynylnaphthalene.pgo, 2-ethynylnaphthalene.pgo, 2-quinolinecarbonitrile.pgo, 3-quinolinecarbonitrile.pgo, 4-quinolinecarbonitrile.pgo, 9-ethynylanthracene.pgo, 9-ethynylphenanthrene.pgo, 1-pyrenecarbonitrile.pgo, 2-pyrenecarbonitrile.pgo, 4-pyrenecarbonitrile.pgo, 1-ethynylpyrene.pgo, 2-ethynylpyrene.pgo, and 4-ethynylpyrene.pgo.