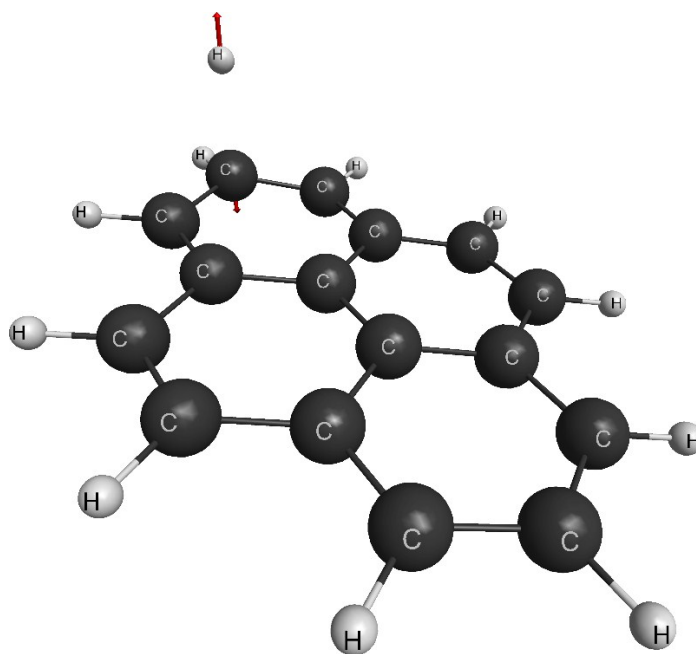


Transition state Cartesian coordinates and imaginary normal mode visualization

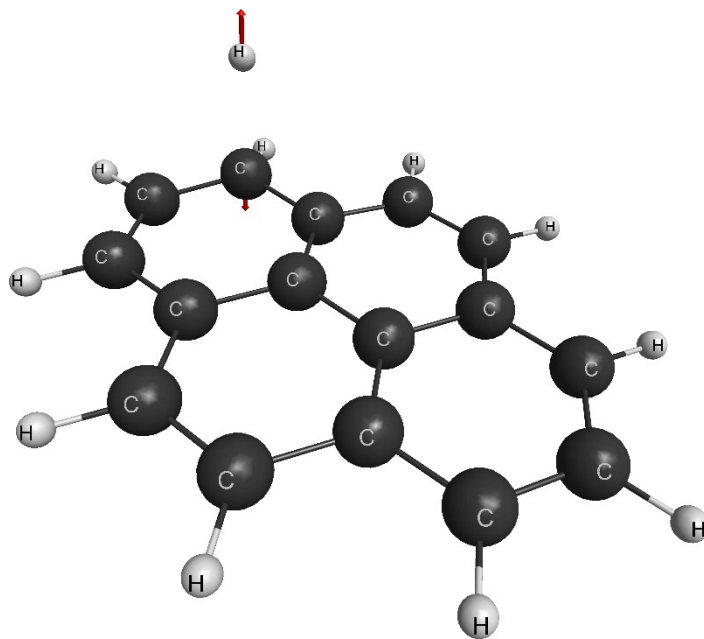
Pyrene e1-ts; Img freq = 1967i

6	-0.715218862	0.146558703	0.000000000
6	0.678207207	-0.132573657	0.000000000
6	-3.498011720	0.544249916	0.000000000
6	3.491856565	-0.443491114	0.000000000
6	-2.812831270	0.448364200	-1.210844081
6	-2.812831270	0.448364200	1.210844081
6	2.766891646	-0.460268261	-1.217364427
6	2.766891646	-0.460268261	1.217364427
6	-1.431159690	0.200826837	-1.234356352
6	-1.431159690	0.200826837	1.234356352
6	1.391554618	-0.213267243	-1.236294075
6	1.391554618	-0.213267243	1.236294075
6	0.648035396	-0.146915887	-2.461808667
6	0.648035396	-0.146915887	2.461808667
6	-0.696454014	0.094947110	-2.460850722
6	-0.696454014	0.094947110	2.460850722
1	-1.242355282	0.155402747	-3.401593880
1	-1.242355282	0.155402747	3.401593880
1	1.189525362	-0.229652865	-3.403309284
1	1.189525362	-0.229652865	3.403309284
1	-4.570115364	0.729003740	0.000000000
1	4.139898688	1.051120623	0.000000000
1	-3.356543661	0.513813029	-2.152365698
1	-3.356543661	0.513813029	2.152365698
1	3.305563311	-0.552084219	-2.159349457
1	3.305563311	-0.552084219	2.159349457
1	4.503980651	-0.846559106	0.000000000



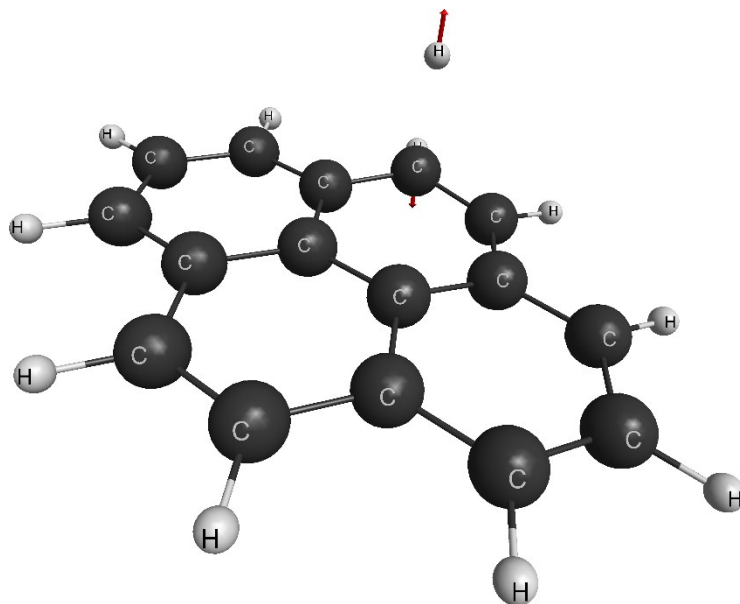
Pyrene e2-ts; img freq = 1941i

6	-4.382179998	-3.476479998	-0.009500000
6	-2.988469999	-3.476029998	-0.031730000
6	-2.272049999	-2.267869999	0.005350000
6	-2.990749999	-1.034620000	-0.028090000
6	-4.417929998	-1.044730000	0.025300000
6	-5.092129998	-2.275789999	-0.010750000
6	-0.841460000	-2.229379999	-0.027670000
6	-2.286209999	0.198720000	0.046010000
6	-0.863420000	0.206250000	0.003290000
6	-0.165880000	-1.039620000	0.009270000
6	-0.175460000	1.447689999	0.114590000
1	0.893480000	1.454209999	-0.098350000
6	-0.904580000	2.651739999	-0.037350000
6	-2.290059999	2.643059999	-0.029160000
6	-3.007109999	1.431269999	-0.008180000
6	-4.436769998	1.394309999	0.019200000
6	-5.115019998	0.206640000	0.004090000
1	-6.204079997	0.197270000	0.023870000
1	-4.983079998	2.336579999	0.000390000
1	-0.293570000	-3.170839999	-0.027170000
1	-4.921349998	-4.421129998	-0.030910000
1	-2.441539999	-4.417899998	-0.029430000
1	-6.181109997	-2.285509999	0.007460000
1	0.923360000	-1.028600000	-0.000960000
1	-0.367780000	3.597369998	-0.064760000
1	-2.840929999	3.579989998	-0.100870000
1	0.206430000	1.484919999	1.754359999



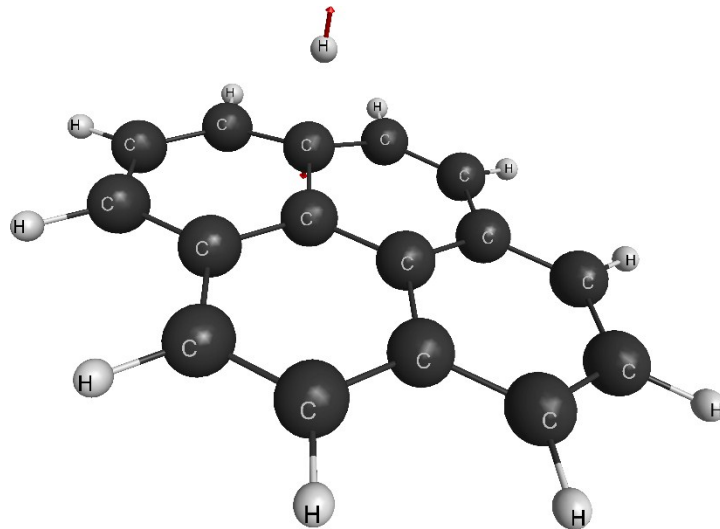
Pyrene e3-ts; img freq = 1997

6	0.718421752	-0.017659971	-0.022321172
6	-0.705205685	-0.018572275	0.043472709
6	3.527295879	-0.010564848	-0.062443380
6	-3.515468959	-0.015453983	-0.022130659
6	2.835726917	1.197576905	-0.047079956
6	-2.824366773	1.192413548	0.040454918
6	2.834702392	-1.223899930	-0.053514923
6	-2.824309670	-1.227538956	-0.045213836
6	1.431927002	1.217905808	0.021004670
6	-1.418822259	1.215759471	0.018432743
6	1.436882163	-1.246422048	-0.005128339
6	-1.420931766	-1.251667613	-0.044755625
6	-0.677759242	2.440990128	0.070491533
6	0.688334062	2.442475982	0.023587921
6	-0.683487110	-2.475334694	-0.095865091
6	0.692900642	-2.492266188	0.065857098
1	1.234771185	-3.412166274	-0.152707469
1	-1.231270916	-3.414504827	-0.158856691
1	1.236007659	3.383776053	0.048263299
1	-1.226541877	3.381908697	0.076659457
1	4.614184147	-0.010722933	-0.107496253
1	-4.603320838	-0.015794175	-0.016667416
1	3.381437663	2.140080264	-0.037608750
1	-3.370623564	2.134607745	0.047916307
1	3.383875243	-2.164471867	-0.044264985
1	-3.371713637	-2.167538035	-0.099725096
1	0.887088938	-2.833855432	1.723241239



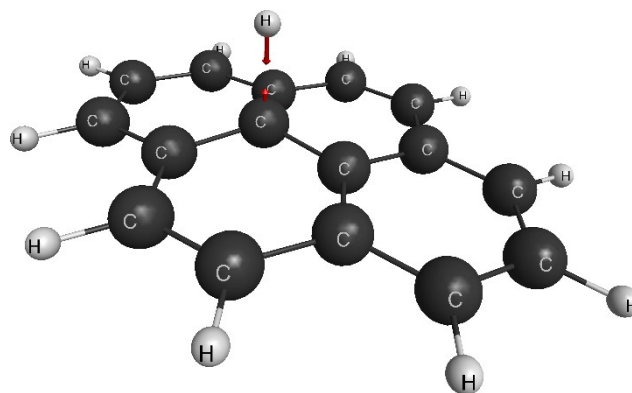
Pyrene i1-ts; img freq = 2235i

6	0.704380000	0.006470000	0.073970000
6	-0.714290000	0.004280000	0.088230000
6	3.516779998	-0.006850000	-0.029550000
6	-3.522569998	0.003700000	-0.020340000
6	2.827169999	1.205659999	0.012780000
6	-2.834579999	1.213449999	-0.001840000
6	2.833169999	-1.215359999	0.023400000
6	-2.828169999	-1.208889999	0.010440000
6	1.419519999	1.233569999	0.064250000
6	-1.428359999	1.238239999	0.001820000
6	1.426169999	-1.237589999	0.260600000
6	-1.428189999	-1.231349999	0.024540000
6	-0.686690000	2.461939999	0.020500000
6	0.681350000	2.459419999	0.006450000
6	-0.683900000	-2.463369999	0.012000000
6	0.673850000	-2.471489999	0.073350000
1	1.225519999	-3.410169998	0.061270000
1	-1.232119999	-3.397779998	-0.102250000
1	1.231169999	3.399779998	0.001350000
1	-1.232809999	3.403759998	-0.016770000
1	4.598799998	-0.004840000	-0.143460000
1	-4.610359998	0.001200000	-0.032470000
1	3.374699998	2.146529999	-0.015070000
1	-3.381689998	2.154389999	-0.042410000
1	3.374759998	-2.159469999	0.000970000
1	-3.374929998	-2.150289999	-0.023070000
1	1.437539999	-1.244829999	1.846649999



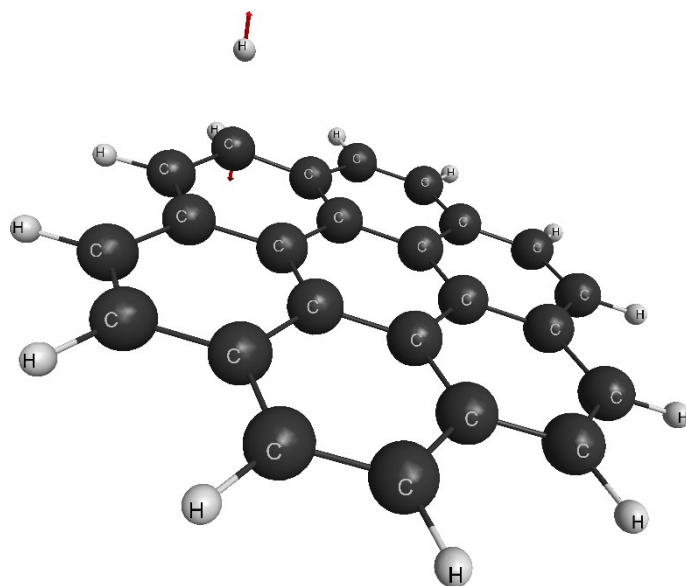
Pyrene i2-ts; img freq = 2025

6	0.727384788	-0.178367160	0.002630942
6	-0.716349415	-0.104926561	0.001393336
6	3.500202580	0.320116262	-0.009022154
6	-3.519058961	-0.199941811	0.004205202
6	2.813784594	0.222941665	-1.221163176
6	2.814411450	0.276204266	1.206567793
6	-2.828719175	-0.193661916	-1.207401454
6	-2.828071192	-0.140195056	1.214001554
6	1.425256769	0.056612866	-1.248146039
6	1.425911276	0.111252974	1.241528807
6	-1.424111191	-0.180673356	-1.229734901
6	-1.423473818	-0.126377348	1.235032803
6	-0.681676407	-0.146946850	-2.457953397
6	-0.680413908	-0.038755852	2.460189753
6	0.680926305	-0.028148999	-2.464246402
6	0.682205450	0.080018988	2.460547305
1	1.218235417	0.042006305	-3.409408795
1	1.220006294	0.191548169	3.401443962
1	-1.229400360	-0.206866582	-3.397601025
1	-1.227668574	-0.057288036	3.401858920
1	4.579639595	0.454886419	-0.012256173
1	-4.606824208	-0.215980817	0.004829417
1	3.354045983	0.324322664	-2.161642746
1	3.355141429	0.418755256	2.141413996
1	-3.375438097	-0.236322481	-2.148458090
1	-3.374273043	-0.141166781	2.156301401
1	0.866046414	-1.745126286	0.036909418



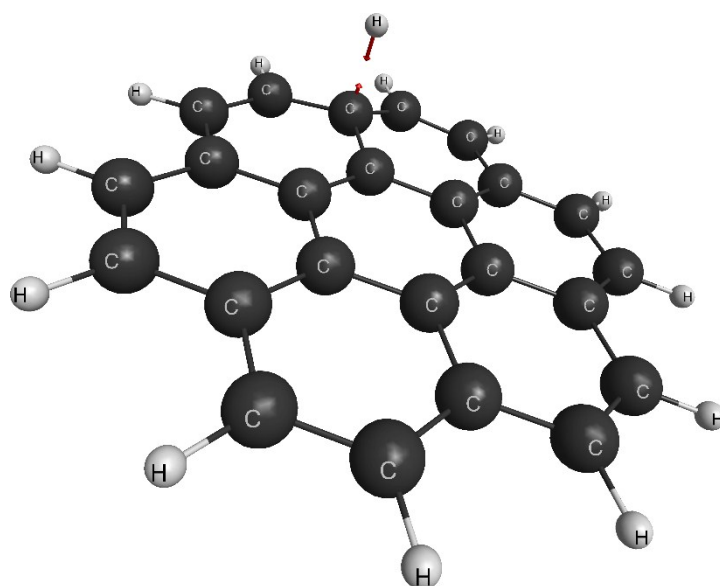
Coronene e-ts; img freq = 1967i

6	-0.095116424	-1.087925392	0.476563366
6	1.238348490	-1.578224621	0.532389474
6	2.309251887	-0.688596000	0.238210124
6	2.044038394	0.693261318	0.017989520
6	0.698103557	1.150951421	-0.063414562
6	-0.354205126	0.238766922	0.221703572
6	3.653971038	-1.152875638	0.296735508
6	3.114703094	1.583923894	-0.271711508
6	4.463676050	1.120722883	-0.206518515
6	4.725398817	-0.264199498	-0.003024199
6	5.535183903	2.007490102	-0.479108657
6	5.251188903	3.412233239	-0.641080696
6	3.929372575	3.827666656	-0.809268890
6	2.846510094	2.957977571	-0.526229580
6	1.494498459	3.389221919	-0.597447774
6	0.457018686	2.523967624	-0.332320155
1	-0.572538518	2.877125088	-0.379113820
1	1.289421303	4.437991737	-0.809060090
1	-0.915237048	-1.773262133	0.687770608
1	-1.382750682	0.595651861	0.181340643
1	5.637604076	3.969483117	0.892060348
1	3.720371912	4.870674211	-1.043612281
6	1.530717541	-2.948435910	0.765192647
6	2.829631637	-3.404189791	0.789511303
6	3.917440268	-2.534919377	0.510251367
1	0.708983683	-3.632170390	0.975404951
1	3.033978980	-4.458457260	0.973023464
6	5.267850096	-2.979558748	0.536684687
6	6.305562989	-2.116061793	0.274639080
6	6.069125261	-0.732388063	0.045401543
1	5.468825415	-4.035063533	0.716743391
1	7.333589701	-2.476095694	0.294239635
6	6.862124874	1.515640781	-0.446951514
1	7.683774067	2.205040626	-0.637935824
6	7.120292764	0.178510664	-0.232044762
1	8.147866789	-0.182974434	-0.216800279
1	6.048662497	4.042216642	-1.035992126



Coronene i1-ts; img freq = 2229i

6	-3.512407343	0.439874340	-1.244491670
6	-3.512407343	0.439874340	1.244491670
6	-2.829338818	0.380041291	0.000000000
6	-1.423530569	0.157229227	0.000000000
6	-0.710605350	0.125754185	-1.231753713
6	-0.710605350	0.125754185	1.231753713
6	-1.419856322	0.178147641	-2.464719994
6	-1.419856322	0.178147641	2.464719994
6	-2.826408264	0.379696468	-2.436224553
6	-2.826408264	0.379696468	2.436224553
6	0.694385878	-0.107841926	-1.231194168
6	0.694385878	-0.107841926	1.231194168
6	1.397082728	-0.187346672	0.000000000
6	2.798716440	-0.534625001	0.000000000
6	3.507289058	-0.397244473	-1.252807079
6	3.507289058	-0.397244473	1.252807079
6	2.829033312	-0.257860589	-2.433132129
6	2.829033312	-0.257860589	2.433132129
6	1.409336477	-0.122288343	-2.461766930
6	1.409336477	-0.122288343	2.461766930
6	0.682612456	-0.036072929	-3.676838565
6	0.682612456	-0.036072929	3.676838565
6	-0.684387129	0.135354254	-3.679005425
6	-0.684387129	0.135354254	3.679005425
1	-1.224801925	0.195279020	-4.623009772
1	-1.224801925	0.195279020	4.623009772
1	1.229229100	-0.062134660	-4.618916710
1	1.229229100	-0.062134660	4.618916710
1	-4.591401764	0.590413302	-1.244009323
1	-4.591401764	0.590413302	1.244009323
1	-3.367580458	0.435284340	-3.380090652
1	-3.367580458	0.435284340	3.380090652
1	4.591078139	-0.503526846	-1.246781154
1	4.591078139	-0.503526846	1.246781154
1	3.377387058	-0.199017151	-3.372742300
1	3.377387058	-0.199017151	3.372742300
1	2.657714373	-2.108172110	0.000000000



Coronene i2-ts; img freq = 2325i

6	0.697882216	-0.040588288	3.682040696
6	0.697882216	-0.040588288	-3.682040696
6	3.536393263	0.052145295	1.243702689
6	3.536393263	0.052145295	-1.243702689
6	2.850582950	0.034252172	2.436388855
6	2.850582950	0.034252172	-2.436388855
6	-0.677880648	-0.095508608	3.682088238
6	-0.677880648	-0.095508608	-3.682088238
6	-3.523317952	-0.188286611	1.244172059
6	-3.523317952	-0.188286611	-1.244172059
6	-2.833816070	-0.134134792	2.435357375
6	-2.833816070	-0.134134792	-2.435357375
6	1.431072306	-0.025344426	2.465826258
6	1.431072306	-0.025344426	-2.465826258
6	2.848384544	0.086808008	0.000000000
6	-1.412493791	-0.050580269	2.466577408
6	-1.412493791	-0.050580269	-2.466577408
6	-2.848661721	-0.138209280	0.000000000
6	0.716319473	0.042828472	1.235426477
6	0.716319473	0.042828472	-1.235426477
6	1.427848271	0.025969942	0.000000000
6	-0.700954797	-0.011897755	1.241462496
6	-0.700954797	-0.011897755	-1.241462496
6	-1.428869700	0.137173526	0.000000000
1	1.244418309	-0.066156613	4.624113524
1	1.244418309	-0.066156613	-4.624113524
1	4.625225792	0.087359471	1.241472733
1	4.625225792	0.087359471	-1.241472733
1	3.396522550	0.005129414	3.378721116
1	3.396522550	0.005129414	-3.378721116
1	-1.222892987	-0.122612190	4.624983510
1	-1.222892987	-0.122612190	-4.624983510
1	-4.606620539	-0.305194449	1.248894040
1	-4.606620539	-0.305194449	-1.248894040
1	-3.376128635	-0.170603303	3.379440618
1	-3.376128635	-0.170603303	-3.379440618
1	-1.527384275	1.711232763	0.000000000

