

## **Supporting Information**

# **Exploration of Minimum Energy Conical Intersection Structures of Small Polycyclic Aromatic Hydrocarbons: Toward an Understanding of the Size Dependence of Fluorescence Quantum Yields**

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Cartesian coordinates (in Å) of the ground state equilibrium structure and the optimized MECI structures at the SF-BHLYP/6-31G\* level for 5 PAHs, benzene, naphthalene, phenanthrene, anthracene, and pyrene. Relative energies in eV and the  $\langle S^2 \rangle$  values for each state are also shown.

**benzene**

benzene s0min	0.00 [0.05]	4.90 [2.00]	4.94 [1.09]	6.44 [1.02]	7.19 [0.06]
C	1.386178999438		0.000049818026		0.000119021570
H	2.464191047764		0.000092500596		0.000295711505
C	0.693037935296		1.202593432959		0.000380959392
C	0.693112101456		-1.202535623668		-0.000261021654
C	-0.693020790606		-1.202577696024		-0.000468275290
C	-0.693096631481		1.202547598656		0.000150062273
C	-1.386149913327		-0.000036839137		-0.000317712204
H	1.233279855195		-2.135592887381		-0.000375686358
H	-1.233099184865		-2.135685968496		-0.000851490119
H	1.233135284486		2.135691682542		0.000659305709
H	-1.233242037863		2.135616977340		0.000359124509
H	-2.464162665494		-0.000073995413		-0.000482999334

benzene-01	5.24 [1.37]	5.57 [0.27]	5.57 [0.65]	8.18 [0.27]	8.71 [0.67]
C	1.35308262678200		-0.05536604793600		-0.07301809407600
H	2.41564839600600		0.08908353165500		0.02677864807200
C	0.44381907339700		1.07425390514200		0.00371361220200
C	0.74385804150900		-1.28792673715500		-0.20496538810100
C	-0.62840852888400		-1.19921160739400		-0.07601253918300
C	-0.69874083591500		1.21295658879900		-0.85680411862300
C	-1.15172635042900		0.15309385094700		0.00174994958500
H	1.27815621525100		-2.21299674839000		-0.33638863272300
H	-1.28545556843000		-2.04698849392700		0.02163513201700
H	0.72397336898900		1.90612681545200		0.63998994513000
H	-1.23741148547900		2.14559134484300		-0.87953858632600
H	-2.01374706114900		0.32526865713700		0.63621623659100

benzene-02	5.00 [1.09]	5.68 [0.83]	5.68 [0.15]	7.49 [1.02]	8.82 [1.01]
C	1.01253255873200		0.04551094635500		-0.31365313323300
H	2.00302980192000		0.04978084545000		-0.74281995548500
C	0.42872737011000		1.28315270766300		0.01154366488200
C	0.45220600219800		-1.19170028844500		0.03973220951900
C	-0.77802017612900		-1.19371582531600		0.67149223702500
C	-0.80487473439800		1.28177305211900		0.62994132953800
C	-1.54929835815400		0.03269545599900		0.56580063630900
H	1.05939671966000		-2.08266346114800		-0.03061304784400
H	-1.13160762229300		-2.08164331067500		1.17888856426500
H	1.02105934604600		2.18238556078200		-0.07638514754600

H	-1.18810568195100	2.18206982140000	1.09178671500700
H	-1.52663680124400	0.01662841000500	-0.55402683893500

benzene-03 5.24 [1.06] 5.70 [0.42] 5.70 [0.80] 7.35 [0.88] 8.35 [0.22]

C	1.44024232164000	-0.02919579433500	-0.28237751695000
H	2.07716884476500	-0.13607771920200	-1.15354318333000
C	0.80427367245700	1.19589471660200	-0.06953315418300
C	0.64079930316500	-1.13371766389200	0.16199599999800
C	-0.56343165467100	-1.27557231659500	-0.59753578569000
C	-0.57123586814800	1.11440052395200	0.11827553527400
C	-1.22748740327800	-0.10047413795200	-0.26690503840700
H	0.68490858699400	-1.46724068686800	1.19886648137200
H	-1.08004094341000	-2.18144048759100	-0.86224588401700
H	1.28158148693800	2.13988339954900	-0.28990579434900
H	-1.17145021827800	1.98942428112200	0.30296590861600
H	-2.31058403586800	-0.11271175109600	-0.26432119964400

benzene-04 5.23 [1.29] 5.80 [0.53] 5.80 [0.33] 8.68 [0.95] 9.27 [1.02]

C	1.03655645089500	-0.14963296963600	0.12972522998900
H	1.99989388974600	-0.25144493655100	0.60416526518900
C	0.60496536700800	1.09977184578300	-0.46384506268800
C	0.48297713874800	-1.38138127779500	-0.63446898257800
C	-0.20810736032900	-0.79893001836700	0.62709102097500
C	-0.76912133974400	1.22761098707800	-0.36156488079100
C	-1.27830274161700	0.11713907567100	0.28903143618600
H	1.03942789973000	-2.29236514232000	-0.42590475291000
H	-0.25135719759800	-1.42656692117500	1.50323143693600
H	1.25838664377100	1.78356771552500	-0.97759625893200
H	-1.35503393690600	2.01967391933500	-0.79326108378800
H	-2.32258211036200	-0.08408837961700	0.45432867794600

benzene-05 6.02 [2.00] 6.74 [0.01] 6.75 [0.01] 7.50 [0.01] 8.70 [1.89]

C	1.17731926645500	0.23683925803400	0.12264923939200
H	2.21680500578400	0.01130457549700	0.27611382750700
C	0.63956097769500	1.36704813773800	-0.33331675169500
C	0.22759286828900	-2.09140859884600	-0.10374361560100
C	0.07256612328700	-0.76301991463700	0.42679798439500
C	-0.82081751129900	1.22670983410500	-0.39787160005500
C	-1.17125819918000	0.01075931897000	0.01833774488600
H	0.33569807142500	-3.12292450120700	-0.31903564958200
H	0.03323090548700	-0.86292055798600	1.52622775259100
H	1.17452470264500	2.25808291142500	-0.61476767723600
H	-1.48895072009100	2.00200183333500	-0.73243946803100
H	-2.15856878717000	-0.40911839851600	0.08198025898400

benzene-06 8.73 [1.35] 9.33 [0.74] 9.33 [0.60] 10.26 [0.80] 11.56 [0.52]

C	1.74702541393600	-0.45088149937100	-0.34804774147000
H	2.80188867534800	-0.32165209174700	-0.47258583732000
C	0.26698117040500	2.16123640310800	0.07983450658600
C	0.78784895320900	-1.33479176318000	-0.44445618237600
C	-0.61886204471900	-1.20632626697500	-0.14758845027200
C	-0.65224899078700	1.19489102469100	0.24589842164000
C	-1.25502854462200	-0.01561718982200	0.21837792605600
H	1.09071128767200	-2.32171035986400	-0.80721847185200
H	-1.21913927402200	-2.09569824016100	-0.22071195384200
H	0.83046394191300	2.39724690575600	0.99255638811200
H	-1.23426952225000	2.18677081754200	0.43375935637200
H	-2.30363376409600	-0.05436450289200	0.46124291834500

## naphthalene

naphthalene s0min	0.00 [0.03]	3.65 [2.00]	4.48 [1.05]	5.10 [0.04]	5.59 [1.00]
C	2.414163382103	0.715606022427	-0.000000000000		
C	1.230934646281	1.398288646210	0.000000000000		
C	2.420669654952	-0.693210945865	-0.000000000000		
C	-0.003296782981	0.709762162491	-0.000000000000		
C	1.243826858438	-1.386870413315	-0.000000000000		
C	0.003297328328	-0.709762938349	-0.000000000000		
C	-1.243826370259	1.386871347150	0.000000000000		
C	-1.230934795940	-1.398288119702	-0.000000000000		
C	-2.420669208905	0.693211156305	-0.000000000000		
C	-2.414163285743	-0.715605114360	0.000000000000		
H	3.348714959493	1.252677742543	-0.000000000000		
H	1.223244111981	2.477131143279	-0.000000000000		
H	3.360177224930	-1.221563913229	-0.000000000000		
H	1.245982357979	-2.465725929624	0.000000000000		
H	-1.245984210904	2.465726801835	0.000000000000		
H	-1.223244086505	-2.477130201044	-0.000000000000		
H	-3.360178321769	1.221561710717	-0.000000000000		
H	-3.348713461480	-1.252679157465	0.000000000000		

naphthalene-01	4.78 [1.08]	5.35 [0.68]	5.35 [0.34]	7.32 [1.13]	8.25 [1.11]
C	2.46866381823900	0.73944769035600	-0.25300310998700		
C	1.27415890222800	1.38244189894400	-0.02599905130900		
C	2.49562588118500	-0.65408111709100	-0.33331942498800		
C	0.09209065799100	0.64121298334800	0.11772478556300		
C	1.34190891498800	-1.40311642841900	-0.18595700810200		
C	0.11841335686600	-0.77905203996100	0.02183405746800		
C	-1.16731992210900	1.28600874438200	0.32718598603500		
C	-1.16261038543600	-1.48443050177700	0.30551773636300		
C	-2.38041222817300	0.63677866533100	0.30719558296700		
C	-2.33655236123200	-0.73497174732100	-0.01134309283700		
H	3.37902501685000	1.30482891712800	-0.36408217070700		
H	1.24246595942400	2.45734412459700	0.06923567335400		
H	3.43222982197300	-1.15454902957500	-0.52193792576400		
H	1.36321521998600	-2.47746287196500	-0.24683679110700		
H	-1.15985208344900	2.36290945795600	0.41747370817700		
H	-1.13803117512100	-1.18556050268100	1.38306481590400		
H	-3.29627181394200	1.20909245670800	0.31792133135200		
H	-3.19411495355900	-1.17061275320800	-0.51496817863500		

naphthalene-02	5.13 [1.37]	5.45 [0.30]	5.45 [0.66]	7.95 [0.78]	8.27 [0.89]
C	2.34364915401000	0.42735702838800	-0.04256225347100		
C	1.21837945211400	1.36782050751900	0.05159822644700		
C	2.44579566051700	-0.64891695204900	0.85925805505000		

C	-0.04418630235200	0.78439086026700	0.14770564212900
C	1.35642700626000	-1.16900723895800	0.03846413503800
C	0.02440500141700	-0.63142023286100	0.01409357048000
C	-1.30054663252700	1.41607824907300	0.23149401873300
C	-1.14836929219100	-1.36241241721700	-0.16397096616900
C	-2.44305883796500	0.66575618081000	0.10686577050700
C	-2.36832081631100	-0.72036739630200	-0.10704861804200
H	3.16027139339500	0.68488604582800	-0.71064575971300
H	1.39854347118400	2.42930626557300	0.02746349822200
H	3.36065647777500	-1.21255673495400	0.93531287662200
H	1.54849695271600	-2.08497983467200	-0.50383662581100
H	-1.35582474567700	2.48550242192900	0.35895060507500
H	-1.10190021550700	-2.43071773862100	-0.30553244443700
H	-3.40830991301300	1.14309054187100	0.15362124025300
H	-3.27694853821100	-1.29010665998600	-0.21480775667400

naphthalene-03 5.18 [1.11] 5.57 [0.75] 5.57 [0.32] 7.51 [1.27] 8.17 [1.08]

C	2.17166527515200	0.68679161627600	0.66219783396000
C	1.03042699092600	1.33520667306400	0.24906343983600
C	2.19402343181700	-0.70383206267000	0.82621300797800
C	-0.15532585963500	0.62917495794500	0.00393426496300
C	1.05809053698000	-1.42934685292700	0.57334485546800
C	-0.13227832611000	-0.78862771436300	0.18637427257700
C	-1.34888453904400	1.30461513196600	-0.45961204460800
C	-1.30662176889400	-1.46018799543900	-0.26948611999400
C	-2.52494333978000	0.64615119836900	-0.52889163053700
C	-2.55026160109100	-0.79370561107700	-0.15856398718500
H	3.06795911198400	1.25675699799000	0.84747301904300
H	1.04145214199700	2.40431027530000	0.11037012041800
H	3.10208388891700	-1.19599254504000	1.13255825929200
H	1.05895297147500	-2.50273188202300	0.67900673069900
H	-1.27161501020800	2.34738525851000	-0.72716030996600
H	-1.19414212817100	-2.43185185469200	-0.74133455646100
H	-3.44540500587100	1.17428829459300	-0.72857341604000
H	-2.45713443618300	-0.53983815276700	0.93207250781000

naphthalene-04 5.11 [1.27] 5.63 [0.29] 5.63 [0.60] 7.53 [1.02] 8.31 [1.13]

C	2.24757039763400	0.88768584458700	0.72800277945500
C	1.31465130052700	1.15717031100300	-0.32075203324300
C	2.33321328266000	-0.45878299195400	0.44112998787000
C	-0.05176463972800	0.71147137894900	-0.07754258577600
C	1.26178454797400	-1.25076296395700	-0.11561571029500
C	-0.04944895492600	-0.70054720485500	-0.16294509917300
C	-1.19760662154000	1.41075835097200	0.25842452520900
C	-1.27670500032100	-1.37625824812400	-0.09823345781800
C	-2.39369196868000	0.71841246502800	0.35392830146300

C	-2.42952506833000	-0.66307918052300	0.14884816858300
H	3.09251107508600	1.47172459851600	1.03743991585400
H	1.63334747958300	1.24648082683500	-1.36072998974700
H	3.28958073956100	-0.95710204595500	0.56408966018500
H	1.42477301981900	-2.30690684129300	-0.24938655107300
H	-1.17134377314900	2.48152038152400	0.37791820434400
H	-1.30813306556400	-2.44735120588700	-0.22201883372900
H	-3.30693995899900	1.25496298304000	0.55153618714100
H	-3.37414536625900	-1.18016943835800	0.20172201922700

naphthalene-05 5.11 [1.28] 5.65 [0.69] 5.65 [0.21] 8.27 [1.15] 8.37 [1.18]

C	2.23487259156700	1.00675190765400	-0.59950608086100
C	1.15206783098600	1.59210992477700	0.01690118798400
C	2.18535560618800	-0.33029869576000	-1.00914429319300
C	0.00975479749900	0.81324008647000	0.24446967122500
C	1.04990472425000	-1.10250743790200	-0.81695224430600
C	-0.03991494324400	-0.53387854404000	-0.18528995172700
C	-1.21913535932100	1.13711171325700	0.85957857200600
C	-1.38914084190200	-1.06893180565300	0.09314174582300
C	-2.09018122640100	0.00897942593600	0.85443647417300
C	-2.47045256513700	-0.33999031562100	-0.66178665613900
H	3.13173616363000	1.57921205510600	-0.77047421253600
H	1.18644599874000	2.62181615089300	0.33447323350200
H	3.04775682768300	-0.76491244580000	-1.48828885442700
H	1.02212985573300	-2.12608324548200	-1.15374786223000
H	-1.47354998191300	2.10581968094000	1.25498824219900
H	-1.52371131106800	-2.11254584817100	0.34027943954200
H	-2.85588774025000	-0.14950970224600	1.59365734530900
H	-3.44180179652600	-0.82739033761300	-0.69125630105800

naphthalene-06 5.54 [1.08] 5.67 [0.39] 5.67 [0.95] 7.44 [1.08] 7.89 [1.12]

C	2.37430312861200	0.69398542986300	-0.09878213200300
C	1.24910385916700	1.43321351476500	0.15789063068100
C	2.30026639261200	-0.67344549545600	-0.43246096771400
C	-0.02494896969500	0.84510704468200	0.02637275938000
C	1.08299490559900	-1.30063088543600	-0.45065596073200
C	-0.08709117129000	-0.56989768624600	-0.17280789840700
C	-1.28661306569900	1.45997526803000	0.22046236290200
C	-1.31134516208600	-1.20690956362800	0.18808957067300
C	-2.40736058916600	0.62593283628200	-0.13279266537600
C	-2.47741010470100	-0.56409796933400	0.62129575270700
H	3.33986245397800	1.17406065499900	-0.06947277557500
H	1.32325214328900	2.48554430552500	0.38015269679200
H	3.20247096023500	-1.22286901313200	-0.64365750851100
H	1.01861842955500	-2.36187532478600	-0.63719399393400
H	-1.39343226779200	1.95023784735500	1.18569996030800

H	-1.35492363726700	-2.28548962089100	0.08565461649700
H	-2.96374842742700	0.74781615565600	-1.06185160692100
H	-3.35673605407000	-1.12158069093700	0.89839284435700

naphthalene-07 5.26 [1.10] 5.69 [0.83] 5.69 [0.28] 7.58 [0.97] 8.16 [0.50]

C	2.55764079182400	0.60708084275300	-0.54334165928900
C	1.38117082724000	1.23273794645600	-0.12437107912700
C	2.47415092205600	-0.75710300936600	-0.70380361421600
C	0.15555190076600	0.54141199063200	-0.30998992453700
C	1.24559754787800	-1.27270012854600	-0.14548970994500
C	0.06007929137300	-0.85569616909300	-0.76504658077400
C	-1.11219779414800	1.13468025424100	-0.02404869446400
C	-1.17318208389000	-1.47299085308200	-1.01348335936100
C	-2.28889470416000	0.52853845024900	-0.34720573767300
C	-2.34276510463900	-0.78032373062000	-0.88213080560400
H	3.40589389979700	1.17501669401400	-0.89602644326300
H	1.34010193774100	2.27881289532100	0.12766718775800
H	2.86020912614300	-1.22821834913600	-1.59927933252500
H	1.22111360231200	-1.76056497305300	0.82920192114500
H	-1.11444944076500	2.12626886302200	0.39911445651500
H	-1.17359895260000	-2.50359703549600	-1.33110068706700
H	-3.21172072350400	1.06018965451500	-0.17486713735800
H	-3.28877294700900	-1.23534724165800	-1.11877773110400

naphthalene-08 5.75 [1.83] 5.94 [0.18] 5.94 [0.13] 7.65 [0.95] 8.10 [0.17]

C	2.27685745394500	0.54197195497300	0.26855291604400
C	1.06857278462600	1.08358777257300	0.56342608767800
C	2.41941070930100	-0.68558661359600	-0.43969343497000
C	-0.15110158435300	0.50076799484000	0.00964327157900
C	1.28075689560300	-1.42136788270600	-0.71332312909100
C	0.04494080742100	-0.83542571540000	-0.55295286205500
C	-1.28928988274800	1.34147433050600	-0.30906664662900
C	-1.06282602949000	-1.05417521359800	0.31859333795500
C	-2.50804445666600	0.68857260074600	-0.42287203984700
C	-2.41739153073600	-0.63556442693500	-0.07687095166800
H	3.16967763975000	1.04098460086600	0.61382177311500
H	1.00045946919900	2.00229450477100	1.12440398060100
H	3.40058716586300	-1.08278717204500	-0.63498533319600
H	1.34591713591400	-2.46159101089200	-0.99691669065000
H	-1.15712499451900	2.40389168302300	-0.41888070192800
H	-0.92630300963800	-1.65482447968700	1.20930298879900
H	-3.41073532129000	1.16277292421700	-0.76788329268900
H	-3.23031834015200	-1.34163785608600	-0.10424876107700

naphthalene-09 5.45 [1.08] 6.06 [1.03] 6.06 [0.95] 7.58 [0.12] 8.02 [0.14]

C	2.20677058354000	0.78707747851700	-0.14206051118300
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C	1.22069227817300	1.34282453461300	0.79258930697900
C	2.39663610791400	-0.59428193303700	-0.11279076184700
C	0.13320220790700	0.70180076528200	0.09437951937700
C	1.33262905537500	-1.40207211602100	0.35016182871600
C	0.10607908924300	-0.76726925590800	0.30444264537900
C	-0.95776299972600	1.32425485340400	-0.57706165459500
C	-1.18265767884800	-1.38111736131300	0.29327202449600
C	-2.10935755062500	0.63327076256900	-0.74949230417200
C	-2.23093681142200	-0.71579575130700	-0.25093727763300
H	2.69187415798600	1.42094278154700	-0.86722636960800
H	1.34749068290800	1.36673868651500	1.86971844876100
H	3.27493541578900	-1.04373331356300	-0.55294723438100
H	1.42697002993800	-2.46339633122700	0.49635680598200
H	-0.88440574830500	2.36539063194900	-0.84558092445800
H	-1.28419864661200	-2.40572704136700	0.61327138379700
H	-2.96992939132400	1.10561568283100	-1.19247261530800
H	-3.18629566655600	-1.20818130720900	-0.33807469190100

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naphthalene-10 5.68 [1.28] 6.09 [0.40] 6.09 [0.72] 7.61 [0.38] 8.33 [0.65]

C	1.96248022441500	0.74437687727500	0.35238570380500
C	1.14985932890300	1.23557801432700	1.48356838618900
C	2.28908831698000	-0.62950099616100	0.14361122557100
C	0.19861776606000	0.63125484598200	0.63112634340300
C	1.28391608848400	-1.52189803602000	0.46820699981800
C	0.08200482577300	-0.86650402393200	0.68245588038600
C	-0.95894803076400	1.33846843170400	0.07302126226700
C	-1.22191299205900	-1.41732589052200	0.78893490721900
C	-2.15170824288700	0.72599496486100	0.06206526675800
C	-2.30024672712200	-0.65257893637900	0.49134727439700
H	2.45466196317500	1.49648144516000	-0.24788647206100
H	1.09353920441800	2.29749480028800	1.66822542608300
H	3.22602753496000	-0.91790409202700	-0.30297615155800
H	1.39060581326100	-2.59283461679500	0.47167269533500
H	-0.85176338250600	2.37474166145500	-0.20253797189200
H	-1.33512661867400	-2.46635315074100	1.01302036067100
H	-3.03234241839400	1.26058106200200	-0.25589228824600
H	-3.28934951848400	-1.07941699302300	0.51495246035500

naphthalene-11 6.28 [1.69] 6.70 [0.31] 6.70 [0.30] 8.38 [0.20] 9.07 [1.14]

C	1.92989367494500	0.71739668155000	-0.48856390411300
C	0.83886918765700	1.40596354911600	0.21056091025400
C	2.16976959896000	-0.59436260759300	-0.26858779154000
C	-0.00266484676700	0.64127571567000	1.11455519252200
C	1.17376412084100	-1.41134817270700	0.36407322601600
C	0.00373744938000	-0.81177347308600	0.79472016373200
C	-0.85066297368100	1.39586373157500	0.21156233467500

C	-1.16291990136900	-1.42362023508600	0.36882382757000
C	-1.93541728979500	0.69710794626700	-0.49056292813400
C	-2.16448525769500	-0.61555526865800	-0.26706131581600
H	2.62507907236300	1.30744908161500	-1.06471776429600
H	1.07324486627200	2.43232773589300	0.45913799828500
H	3.03776243742000	-1.06971667257700	-0.69557420798100
H	1.21976984841900	-2.48225995221500	0.23578780000600
H	-1.09434335791100	2.42030786303900	0.45949344196600
H	-1.20110704009000	-2.49525397334800	0.24483301123400
H	-2.63306356175400	1.28013984212400	-1.07077414544000
H	-3.02929507867600	-1.09859772360700	-0.69197194439300

naphthalene-12 8.37 [1.16] 8.96 [0.69] 8.96 [0.91] 10.07 [0.74] 11.12 [1.09]

C	2.36500700613900	0.65076810171000	-0.18900971065300
C	1.20323029446600	1.23589662752200	0.32978219173400
C	2.54705128540600	-0.67218265563300	-0.39980311067000
C	-0.02310970434800	0.55583806740200	0.63804881677000
C	2.32895684198700	-2.00029675199500	-0.41832075894900
C	-0.29324086476100	-0.78162904910000	0.41871929000000
C	-1.11908069470500	1.23946524277100	1.20867050804300
C	-1.43276262447400	-1.47368331711700	0.65752423816700
C	-2.31084361655700	0.59859941295100	1.50098936815500
C	-2.48438631857300	-0.75135179295200	1.23680837653600
H	3.19763381578400	1.30029935359600	-0.40088195309200
H	1.22723402223800	2.29539413917200	0.51981319778700
H	3.57407602565700	-1.12221508147200	-0.70736759690400
H	1.93548101182500	-2.36292652429800	-1.37836374921200
H	-1.01260007946400	2.29521774870500	1.40932376328400
H	-1.53503556003500	-2.52414239795400	0.43541759676300
H	-3.11701262969500	1.16394447593700	1.93980385576200
H	-3.41126967047100	-1.24835974590700	1.47418045247400

## phenanthrene

phenanthrene s0min	0.00 [0.02]	3.76 [1.99]	4.47 [1.04]	5.10 [0.09]	5.18 [1.01]
C	-0.728965598636	0.380342918686	0.002390377797		
C	0.724589513606	0.388118105169	0.006427319451		
C	-1.500582783025	1.553909389357	0.008888999373		
C	-1.408541101981	-0.859622705650	-0.008237348442		
C	-2.815391072896	-0.882100662515	-0.011710189852		
C	-2.873389195320	1.509033661274	0.005063383887		
C	-3.540739663934	0.279147492158	-0.005304811539		
C	-0.663166491850	-2.076536347785	-0.015469588624		
H	-3.315476805374	-1.837891196421	-0.019748404166		
H	-1.018051581672	2.515415696724	0.016855053963		
H	-3.438077854893	2.427123934127	0.010150236139		
H	-4.618142070981	0.248764577165	-0.008058003322		
C	1.483486954784	1.569898262307	0.017431564845		
C	1.417473349055	-0.844451869082	-0.000597532276		
C	2.824481642728	-0.851882579142	0.003669305486		
C	2.856721472678	1.539707617671	0.021260956463		
C	3.537272090517	0.317075975065	0.014354926368		
C	0.685266328448	-2.069280243760	-0.011896958635		
H	3.334941531198	-1.802212271751	-0.001766042263		
H	0.990570053573	2.526151715318	0.022987556879		
H	3.411473037875	2.463801744180	0.029746291575		
H	4.614945326173	0.298141001646	0.017660540211		
H	-1.205874288096	-3.008583577968	-0.024011108077		
H	1.238101208024	-2.995374636784	-0.017598525244		

phenanthrene-01	4.89 [1.12]	5.31 [0.88]	5.31 [0.12]	7.40 [1.29]	7.95 [1.05]
C	-0.84429784624500	0.26800639210600	-0.00002488457300		
C	0.60072139132000	0.24481166445500	-0.27096195031000		
C	-1.55210707080000	1.46438701289500	0.15467821697000		
C	-1.53690058536300	-0.95901623052000	0.12153866175700		
C	-2.91175571479800	-0.94537183030600	0.32274421901600		
C	-2.91292139224100	1.45724856831200	0.37951954243000		
C	-3.59546796529800	0.24812006857200	0.45604542223600		
C	-0.77089523269000	-2.23541363114400	-0.08258668463600		
H	-3.41817391194700	-1.89211531678600	0.39646358074500		
H	-1.04282653020500	2.41161890061600	0.09478666929000		
H	-3.44259610985900	2.38838932277100	0.49794460873800		
H	-4.65855661993700	0.24087945037000	0.63739801609800		
C	1.32592021185000	1.39710329540500	-0.59260075978800		
C	1.34107175805300	-0.96802225240900	-0.15014967960000		
C	2.74152449052000	-0.96976491200500	-0.27139795255800		
C	2.69455203170700	1.36224264413800	-0.75820454798100		
C	3.41852099652900	0.17954220675200	-0.58791621428800		

C	0.60074081351100	-2.12089071481400	0.23594546617000
H	3.26944419919700	-1.90065360735500	-0.13701407112100
H	0.81527334262300	2.33448973405700	-0.72327130136300
H	3.21539938167100	2.27115645108800	-1.01310152421600
H	4.48922922038400	0.17615141947600	-0.70504824877100
H	-0.60919028318800	-2.02168487013700	-1.17243324227400
H	1.14320532486700	-2.89149638707900	0.77964339246600

phenanthrene-02 4.74 [1.08] 5.35 [0.11] 5.35 [0.93] 7.00 [1.18] 7.81 [1.14]

C	-0.85091302515000	0.49305731891100	0.02401330594600
C	0.56697084555700	0.50737056761900	0.06373297990700
C	-1.59368985079200	1.69320169278600	0.03695270256500
C	-1.53614686466400	-0.74957377247900	-0.01092202558200
C	-2.94429256079300	-0.74470946902600	-0.03147416029400
C	-2.95989631942100	1.66480158708600	0.01927096427500
C	-3.63986510533900	0.43406773767000	-0.01880034226700
C	-0.79442053115700	-1.96418754944600	-0.02438991853000
H	-3.46828431127300	-1.68717551552600	-0.05781568278000
H	-1.03931643281500	2.61530190212600	0.05958913149300
H	-3.52171278318500	2.58445634816800	0.03388688769800
H	-4.71789259650100	0.42126423002300	-0.03748184797200
C	1.40754680009000	1.72646384922400	-0.00915114712000
C	1.26832702674400	-0.71485059167000	0.04103114976100
C	2.68920326863900	-0.68132679204300	0.13491986584000
C	2.69498182244300	1.63243156966700	0.61618855405300
C	3.42742653413800	0.45705402190500	0.40381754599500
C	0.55984531160000	-1.94918877636300	0.00383801377800
H	3.20603224119900	-1.62958897086200	0.09725053999800
H	1.75680532413000	1.49296317512800	-1.04314006373000
H	3.10758674855700	2.40789173946300	1.25176925631000
H	4.47796631665100	0.36784364867100	0.63902130142800
H	-1.33256127198800	-2.89790012379800	-0.06063333750600
H	1.11805911920400	-2.87251868208700	-0.02166528794400

phenanthrene-03 5.03 [1.28] 5.43 [0.74] 5.43 [0.31] 7.50 [0.88] 7.96 [0.96]

C	-0.75419517168700	0.41204203821300	0.07866844734300
C	0.68345620766300	0.44068128295900	0.05815268808500
C	-1.54299968591100	1.56791024079300	0.18753094694100
C	-1.39578382403500	-0.84471346688100	-0.03573222768700
C	-2.80208587060300	-0.89524529857300	-0.04328624297600
C	-2.91316240430400	1.49078618034600	0.17689030371600
C	-3.55013739761600	0.24825624481700	0.05892900544600
C	-0.61361410486800	-2.03200991752100	-0.15088993118300
H	-3.28559907648800	-1.85571942235500	-0.13023634036400
H	-1.06291605762900	2.52667643831200	0.29557015863900
H	-3.50255594650000	2.38893598116500	0.26600965331200

H	-4.62659581532600	0.19468280649000	0.05347581990600
C	1.52579025702300	1.53332107256600	-0.06868351587600
C	1.41503911828700	-0.77025873470400	0.03691580057400
C	2.84728195490600	-0.61057081407600	0.12040970785000
C	2.95403681568800	1.23066073244700	-0.02700602358300
C	3.50485004067200	0.36953739119000	0.96069341609800
C	0.75010015163000	-1.99628421932200	-0.12108832421000
H	3.46603333527500	-1.34834131981100	-0.37456195112500
H	1.19807071440900	2.54214875961900	-0.25182286565800
H	3.60623058338000	1.80766826571400	-0.67430911817800
H	4.57234170079800	0.31572427248000	1.09434340786600
H	-1.12776005180700	-2.97473295189400	-0.25020956977700
H	1.32045202925200	-2.90898252815400	-0.19106028423300

phenanthrene-04 5.13 [1.32] 5.48 [0.37] 5.48 [0.65] 7.55 [0.89] 8.12 [0.43]

C	-0.78067131115300	0.29188454621800	-0.06657770534600
C	0.63246302792100	0.35707743480800	0.08152066840000
C	-1.68866916872500	1.41219019888400	0.01275327365500
C	-1.41759610284100	-0.95109558808100	-0.26001278912900
C	-2.79985304987400	-0.84703317619100	-0.14853868764100
C	-2.86491547155300	1.57029109645800	-0.82575645749800
C	-3.31221626847200	0.51172166559500	0.00516855025900
C	-0.64540693746100	-2.13767873323200	-0.41583214249400
H	-3.46988972610200	-1.68961201841000	-0.12289007799600
H	-1.42542325636100	2.24469938061700	0.65075815082300
H	-3.38821735525200	2.51203584747000	-0.82517759290200
H	-4.15880860103200	0.65534013927400	0.66932284110700
C	1.33306494083900	1.55953078393900	0.31447551414300
C	1.37610184579500	-0.84809251159100	-0.03593536966600
C	2.77314207794100	-0.80511373499100	0.10593447207500
C	2.69501614061500	1.56776643349500	0.45666334855500
C	3.42510627538300	0.37463921420300	0.35434518066700
C	0.70086139597700	-2.08031003772000	-0.30148707343900
H	3.33065452670000	-1.72450691703700	0.01643536427100
H	0.78647692790400	2.48585794141400	0.37357682648300
H	3.21037943529600	2.49656203064900	0.64037303549300
H	4.49730165814700	0.38938628422800	0.46295885795300
H	-1.14577957680000	-3.07613805082400	-0.59328932189800
H	1.29545909383800	-2.97506088369600	-0.39683168055100

phenanthrene-05 5.11 [1.04] 5.53 [1.02] 5.53 [0.25] 7.20 [0.92] 7.88 [1.20]

C	-0.78974446265200	0.50014327620900	-0.52332506109900
C	0.62879792678100	0.52713458142700	-0.55734250711000
C	-1.56820477384200	1.66420364869000	-0.63930341138500
C	-1.44786580261100	-0.74310297655500	-0.37373294740700
C	-2.84679150628300	-0.79058777305700	-0.37942326642400

C	-2.94117637227400	1.59180436420100	-0.62656333005100
C	-3.59120356469600	0.35891496256500	-0.50804915899200
C	-0.64710421303200	-1.90700291095400	-0.15093161672900
H	-3.33639829025900	-1.74626012355500	-0.27234392130400
H	-1.07387209235200	2.61582031407300	-0.75366563910400
H	-3.52316002061700	2.49556861205400	-0.71132289287400
H	-4.66754588064400	0.31340344218300	-0.50907952461600
C	1.55829351432800	1.47282859758900	-0.05821480416500
C	1.43109414440100	-0.66477139230500	-0.40097342458400
C	2.85749264364400	-0.65965078342800	-0.47675558820600
C	2.71648606630100	1.64341115183600	-0.89163295363500
C	3.48969074120700	0.49598855927000	-0.93599096431400
C	0.70521192862300	-1.86473979843100	-0.11207999714000
H	3.37039344793400	-1.60455559811500	-0.40875561579900
H	1.55727437663400	1.75450354131500	0.99437034710200
H	2.62725942946400	2.24547468542500	-1.78878057019600
H	4.41278292716000	0.44324215183800	-1.49511277385300
H	-1.15382705437700	-2.84505038941300	0.01705207759900
H	1.26832502043400	-2.75951884328100	0.09914658181900

phenanthrene-06 5.17 [1.07] 5.54 [0.98] 5.54 [0.23] 7.28 [1.17] 7.83 [1.33]

C	-0.58783136932100	0.52260893010000	-0.21440623594600
C	0.81233894744300	0.50753450946500	0.08869549044900
C	-1.38350087090600	1.66212440860300	-0.00391119027600
C	-1.19273126802600	-0.63666394799900	-0.74966905550800
C	-2.56632500337600	-0.62930407764200	-1.04579871117800
C	-2.72541988967700	1.64180209586600	-0.28989146755800
C	-3.32461717630100	0.48952551671600	-0.81718680573100
C	-0.38386108055500	-1.78885246010500	-0.96339720442400
H	-3.01614548581900	-1.51907332416400	-1.45779000485200
H	-0.92408704605600	2.56234113738500	0.37041391070300
H	-3.32297182585600	2.52207589850900	-0.11690328985300
H	-4.37727407085800	0.48893841887900	-1.04735551906500
C	1.49055675979400	1.44255947615900	0.91593319524200
C	1.59709791162100	-0.65422777886300	-0.14746757586000
C	3.00356930423900	-0.70465712311400	0.15823532653700
C	2.86667791685300	1.65957228366500	0.65501314309000
C	3.66318480620700	0.43414336405600	0.49073950359100
C	0.94122196024500	-1.80209015034800	-0.67066760828100
H	3.51981564333100	-1.64385837567900	0.03681682639100
H	0.97776321409500	1.86159475738900	1.77746616542900
H	2.84303762085800	1.87962211407600	-0.44081521026100
H	4.74254537567900	0.47665645052600	0.47180799846400
H	-0.85350452275900	-2.67503955060400	-1.36146081537600
H	1.52040478869600	-2.69638138095800	-0.83297480023800

phenanthrene-07					
	5.51 [1.95]	5.64 [0.11]	5.64 [0.12]	7.63 [1.01]	7.98 [0.32]
C	-0.89869128385900	0.27732291974700			0.37077330504300
C	0.51342204904900	0.25803040336900			-0.05558286738100
C	-1.51638513218600	1.51703850188300			0.80587318841700
C	-1.46984343507900	-1.01765741535000			0.71660747908300
C	-2.41311088922200	-0.55837714322900			-0.25393442311700
C	-2.89753134845600	1.57162297552700			0.70073970674400
C	-3.41090549158300	0.46211357999200			0.07555287105800
C	-0.70693054479900	-2.18002473957300			0.79856697853800
H	-2.48847460502800	-1.08127588309300			-1.19974488481500
H	-0.90515859088200	2.32788957003000			1.16163954102000
H	-3.49321812950200	2.39121188975600			1.06360860590700
H	-4.44794349873200	0.32168084051200			-0.17912180501500
C	1.12876869974900	1.38009988968200			-0.59969119348600
C	1.28237998500700	-0.90339798041900			0.19433769239900
C	2.64991612624600	-0.87373331049000			-0.09349467337500
C	2.48441922370000	1.38661252277700			-0.88221207013700
C	3.24601041042500	0.25532833223400			-0.62077930552200
C	0.65190734376000	-2.10821962156100			0.68025336389500
H	3.24180449013800	-1.75478101170100			0.09943350840600
H	0.53321691614100	2.25452749303700			-0.80707839348000
H	2.94293537475400	2.26570918147300			-1.30463646503900
H	4.30266431664200	0.25357900242200			-0.83495176651500
H	-1.20064472465400	-3.13148049716100			0.92861282188900
H	1.26751167043600	-2.98088067516700			0.82606610180800

phenanthrene-08					
	5.17 [1.10]	5.66 [0.68]	5.66 [0.53]	7.21 [0.92]	8.00 [0.80]
C	-0.92847044053300	0.29542595860900			-0.28567122115600
C	0.48473067231900	0.23154193168800			0.04214892284700
C	-1.69550635934000	1.49565666921400			-0.17880051939200
C	-1.51964755179400	-0.96499421388800			-0.70019868666600
C	-2.80224375934400	-0.78106284600100			-0.13325129205200
C	-3.01370645737000	1.49034667333400			-0.63408313008600
C	-3.58111547054500	0.24224747529600			-0.78632554546400
C	-0.74521302325600	-2.10809971157200			-0.96676145397300
H	-3.03538254302700	-1.13494391921900			0.86952849266800
H	-1.18666639317800	2.42382588251600			0.00479132791700
H	-3.46228647673500	2.38253240688300			-1.04540726532900
H	-4.11573982282600	-0.00336579105600			-1.69557177523600
C	1.14532752655700	1.30690127960500			0.66285614998800
C	1.24339471773300	-0.91208862018700			-0.31686063274700
C	2.62882490800500	-0.90470206703800			-0.08587018935200
C	2.49934323514400	1.28305006098400			0.88954114630600
C	3.24944902565900	0.16997219701500			0.50012360446300
C	0.60590182160300	-2.07035461242400			-0.86136013149600
H	3.20278005195400	-1.77286076028500			-0.36908210543700

H	0.57799450508700	2.16410007380700	0.97868764249800
H	2.98002729656200	2.11895621099700	1.37044520553000
H	4.31357740908900	0.15001654425100	0.67204354745900
H	-1.25084679875400	-3.01086010136500	-1.26988823936600
H	1.20846850179600	-2.92839272566600	-1.10832642001800

phenanthrene-09 5.03 [1.23] 5.67 [0.22] 5.67 [0.71] 7.53 [1.17] 8.15 [1.17]

C	-0.73963763845000	0.31988425949700	0.17921507602100
C	0.67110130687800	0.44458072312400	-0.05751660275300
C	-1.52168103978200	1.32310386089700	0.77123586512500
C	-1.36213780701900	-0.88258362894200	-0.23160450246400
C	-2.74876138866600	-1.03583864589700	-0.03836771146000
C	-2.87021850277400	1.14681272403500	0.94999175889800
C	-3.49113004741700	-0.04202794132500	0.54099860468200
C	-0.58413745119800	-1.91839361344700	-0.82770510732300
H	-3.21931196864300	-1.95386839725700	-0.35352486582100
H	-1.05498379973700	2.24037297001900	1.09103473880400
H	-3.45704959618800	1.92587096465300	1.40866486323700
H	-4.55125537781700	-0.17055994006500	0.68543144616500
C	1.55395410593200	1.48105918503200	0.23705001830500
C	1.40076970918100	-0.61380227750400	-0.63837523157800
C	2.82253407194000	-0.26212694385900	-0.66681743760700
C	2.89451998101600	1.13023253876100	-0.14231680304700
C	3.41224076989900	-0.07604872461400	0.72990934525100
C	0.76277574174700	-1.80066994767000	-1.01917189391200
H	3.46292942759500	-0.61812034593200	-1.46019176032600
H	1.29218093070800	2.40377934857200	0.72586941852700
H	3.61645656545200	1.86654446530100	-0.45343764727300
H	4.50016802617200	-0.08963125033900	0.75263432944500
H	-1.09234289589500	-2.82176688008000	-1.12649324990600
H	1.32797888420200	-2.60674665008000	-1.45722442651000

phenanthrene-10 5.19 [1.10] 5.67 [0.23] 5.67 [0.85] 7.27 [1.20] 8.18 [1.15]

C	-0.43070759484900	0.50010961716000	-0.22229943525700
C	0.95173848630900	0.39969296898600	0.16204111016300
C	-1.14763416728600	1.71564184860600	-0.16141119444600
C	-1.11311766346000	-0.65096681964100	-0.69373639670400
C	-2.47020138909500	-0.55276661647200	-1.05296040292000
C	-2.46656253957900	1.78457678985700	-0.51981549739200
C	-3.13895320597500	0.63744134403100	-0.96547360121400
C	-0.42915518430600	-1.89637353213700	-0.79433110528600
H	-2.97627721259500	-1.43803655387600	-1.40392103553900
H	-0.64765621637600	2.61438493668900	0.15051208869000
H	-2.98838871784700	2.72576649565400	-0.46574751537200
H	-4.17773756918700	0.69790825165500	-1.24634533847300
C	1.64878672223000	1.51170259101100	0.77114958600000



C	1.60143755215600	-0.85170117814200	-0.00536244557300
C	2.91241821910100	-0.93172759230700	0.53242684766300
C	2.98702294372100	1.46630025931000	0.96331080274400
C	3.70544797474000	0.24580285746300	0.52985387679600
C	0.87603803906000	-1.98989394583700	-0.46162401695800
H	3.23669125213800	-1.86961476005300	0.97269924774700
H	1.08692757410900	2.36903985831600	1.09912621098700
H	3.52106685927500	2.33840811435400	1.31206979833200
H	3.57130498629900	0.50262468046000	-0.55244183296100
H	-0.97632003505600	-2.75863868708400	-1.14017242691000
H	1.39814282934800	-2.93009936232900	-0.53911325575300

phenanthrene-11 5.11 [1.19] 5.67 [0.83] 5.67 [0.18] 7.10 [1.01] 8.06 [1.20]

C	-0.83637868340300	0.21539979867900	0.23354717384700
C	0.59686774383300	0.24565675122200	0.35510729552400
C	-1.72033085185800	1.30960386623600	0.26923162208100
C	-1.45584759344000	-0.96541110494900	-0.22316801902400
C	-2.89521323528500	-0.81889715270400	-0.11607307131600
C	-2.95477658232500	1.23161823439400	-0.47184445307800
C	-3.45627658537700	0.08832271358400	-1.06913075339600
C	-0.70923436078200	-1.98898772408400	-0.82744066458000
H	-3.35735140961800	-0.97024232312200	0.86105135850400
H	-1.40492518889800	2.28107579331300	0.60770457611500
H	-3.56222869180900	2.13004447156500	-0.49751827032600
H	-4.42453275852600	0.05429456766400	-1.53202264731800
C	1.29060190900300	1.31498096206800	0.94677519840100
C	1.33135270882600	-0.85703623681300	-0.14535213976500
C	2.73606832294400	-0.84409012164700	-0.02959341599600
C	2.65732767578400	1.29810886120700	1.04988630323000
C	3.38793811772800	0.20777863641400	0.55520344924100
C	0.65294957352500	-1.94518723224300	-0.76619776940000
H	3.29382572352200	-1.68517470059900	-0.41097594562600
H	0.73685036435200	2.15478926443200	1.33315961967800
H	3.17300194545500	2.12515611551400	1.51029295467300
H	4.46274404846800	0.20020999793800	0.63727473864200
H	-1.21286683159900	-2.83314178544300	-1.26896043873900
H	1.23909786558600	-2.76048965902600	-1.15829027664900

phenanthrene-12 5.10 [1.25] 5.69 [0.76] 5.69 [0.16] 7.58 [1.17] 8.23 [1.15]

C	-0.79996914980900	0.13403287163900	-0.12629828320300
C	0.60728544762000	0.17610310927000	-0.23826951969000
C	-1.80779154054500	1.13831982520100	-0.48327816887000
C	-1.43953449870600	-0.95993575116700	0.48395899315700
C	-2.81678929930900	-0.73155634448900	0.49157517630300
C	-2.53055812042800	1.71060269548500	0.73474558777100
C	-3.12029478728600	0.52920101245700	-0.12415855017300

C	-0.68119266112900	-2.04323667764500	1.01486449791400
H	-3.54770240777800	-1.38349199505300	0.93955662771100
H	-1.69072901331300	1.76230358586300	-1.35639990776300
H	-3.07153527876300	2.63384285214400	0.53779902235700
H	-4.04175941030800	0.70878010828400	-0.65231174811700
C	1.29959471567000	1.25420628028900	-0.82837199173900
C	1.34537365909800	-0.92814658950900	0.26666631194400
C	2.74563647185700	-0.91459757187800	0.14777140633100
C	2.66398831764200	1.23925903639500	-0.92476112773300
C	3.39324382521300	0.14355383071900	-0.43525829299500
C	0.66527599781800	-2.02193432484300	0.89118824819000
H	3.30847231251700	-1.75282858962400	0.52727625095800
H	0.73880849789700	2.09653091511500	-1.19792357114300
H	3.18327854689600	2.06918509032900	-1.37518132699700
H	4.46794172852300	0.13813714882800	-0.51707406205400
H	-1.18208619106100	-2.86922612936600	1.49307136575800
H	1.26107464056700	-2.83721051860200	1.26968174413000

phenanthrene-13 5.30 [1.29] 5.72 [0.43] 5.72 [0.63] 7.44 [0.60] 8.03 [0.52]

C	-0.49755584763200	0.44543226329600	0.07025939402700
C	0.88185508376600	0.32803879638900	-0.43141831253000
C	-1.11120799246500	1.67143916152500	0.29355107428200
C	-1.24139380982700	-0.74061228817600	0.24247844287700
C	-2.57897057183300	-0.64986441819300	0.62513863882400
C	-2.43567091446300	1.74160643305000	0.69135662756900
C	-3.17394971881200	0.57721281299600	0.85298502251900
C	-0.61011938190800	-2.02635757863700	0.03193291614200
H	-3.14995262091700	-1.55706501684300	0.74777331041200
H	-0.54069203792000	2.57751401679400	0.16911066062300
H	-2.89071765479400	2.70145810253800	0.87352435837400
H	-4.20693008195800	0.62794397544300	1.15599164388300
C	1.44738319148500	1.24167770267400	-1.36293141607800
C	1.54200360290400	-0.99928592017500	-0.26434173151900
C	2.92314094134800	-0.92004672285100	-0.05809453010100
C	2.35667431853400	1.37559272172600	-0.23070409327800
C	3.33853889515800	0.37606070904400	0.09819436801500
C	0.72376236328800	-2.14465364864000	-0.19023162733700
H	3.55233541792600	-1.78487813152800	0.06357075545000
H	0.86838552650200	2.08581073204600	-1.70084027419400
H	2.38529117984100	2.32373683803300	0.29027996522200
H	4.30059406787300	0.65645704828900	0.49396038990000
H	-1.22316169209500	-2.90806391093700	0.12819425318300
H	1.18255819732400	-3.12007418470100	-0.23506656361600

phenanthrene-14 5.57 [1.76] 5.72 [0.20] 5.72 [0.27] 7.45 [1.15] 8.16 [0.25]

C	-0.78985890858200	0.47639865822700	0.33665619693300
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C	0.62631630556500	0.51344804885100	0.45338679108000
C	-1.59230135490000	1.60315934568300	0.57174064354000
C	-1.41943303905200	-0.73930226078700	-0.03152356151600
C	-2.80861232832700	-0.80656384131400	-0.08580737307700
C	-2.96634888282500	1.51510652546300	0.50027370447100
C	-3.58364638327200	0.30527293927500	0.18768566691800
C	-0.58428171598300	-1.84670986457100	-0.45225664478400
H	-3.27868220462000	-1.73563320191100	-0.37032951853100
H	-1.11683198227600	2.53374566802200	0.83629494888400
H	-3.56799679119000	2.38905669520000	0.69265738018000
H	-4.65827504879500	0.24071888128900	0.14281117227500
C	1.55196365903500	1.10491825564100	-0.47158396839000
C	1.45744716927700	-0.62619179810400	0.08694684257900
C	2.82681809707600	-0.76715540205800	0.56882242854700
C	2.92995408803500	1.41777101767100	-0.08906472530500
C	3.59240992471700	0.38662379191700	0.52901911381600
C	0.75609637970400	-1.78678413556200	-0.44844937190400
H	3.19328743430100	-1.72818521616000	0.88744947981200
H	1.18321770793600	1.45874912010700	-1.42735571429000
H	3.36155964328900	2.37860341565000	-0.31496852174200
H	4.59410764794200	0.45649094230500	0.91650780615600
H	-1.07986046873400	-2.73636083047700	-0.81013076146300
H	1.34015839079800	-2.63249961652800	-0.77772526109400

phenanthrene-15 5.44 [1.33] 5.80 [0.61] 5.80 [0.43] 7.63 [0.42] 8.12 [0.89]

C	-0.73419518585300	0.48478626427600	-0.30027698803000
C	0.70198373567100	0.59627720814800	-0.38344078502500
C	-1.58899301508700	1.56999578472000	-0.50304271971100
C	-1.28505574397100	-0.76404974375300	0.06640818367100
C	-2.66272334557000	-0.87895050475700	0.21754922665500
C	-2.95645844996400	1.43236115246600	-0.35777498605700
C	-3.49663444321800	0.20500395224200	0.00502544343400
C	-0.40657294955800	-1.89921114159600	0.30232201450200
H	-3.08057908121000	-1.83100766499600	0.50562284359800
H	-1.17432588101500	2.52073376950100	-0.79561546317300
H	-3.60192062428400	2.27821265866300	-0.52947130077200
H	-4.56247030062400	0.09486297805000	0.12042295354700
C	1.48294682606700	1.72350240134600	-0.18320960771300
C	1.49658387689600	-0.65588148473800	-0.53049073602100
C	2.56971065799100	-0.69248174431300	-1.47365286075900
C	2.81914522009200	1.40534064579300	-0.05402825181800
C	3.16355772192100	0.04390297884500	-0.37194468366900
C	0.90882543928700	-1.85391183022400	0.04675071620400
H	2.98852495296800	-1.64666900463100	-1.75359716712300
H	1.08546514425000	2.71365868650600	-0.04502595592600
H	3.56202986273700	2.08606005543000	0.32650923031500

H	4.00061359766600	-0.40475817671100	0.14756136311600
H	-0.85839692242600	-2.81210216120500	0.65767504243200
H	1.52979766401500	-2.72724821196100	0.16206592998000

phenanthrene-16	5.31 [1.06]	5.90 [0.62]	5.90 [0.75]	7.08 [0.74]	7.91 [0.56]
C	-0.63680984406300	0.41695977138600	-0.05455853923800		
C	0.82703935349700	0.46102357729100	-0.13619144630700		
C	-1.42336868275200	1.55200621191000	-0.27913125785500		
C	-1.28754356775400	-0.80026060526400	0.24759461175700		
C	-2.68366053056300	-0.83832261034100	0.27776209336900		
C	-2.80083538044800	1.49505203808100	-0.24657460289300		
C	-3.43636416343000	0.28961067886200	0.03093457905500		
C	-0.52260758500600	-1.99281381582700	0.51891335846400		
H	-3.17142241317200	-1.77451538790100	0.49932681027400		
H	-0.95024986957800	2.49910620872300	-0.46879094178400		
H	-3.37927878371200	2.38647693213400	-0.42537834124300		
H	-4.51266883710200	0.23851841114600	0.06335503434800		
C	1.52027584989700	1.62248823994000	-0.46438338316600		
C	1.55940757042200	-0.78695072301500	0.17722331384900		
C	2.92326398401100	-0.82966114117900	-0.11161267881600		
C	2.76624782800100	1.48071343962700	0.22738844882900		
C	3.51353905425300	0.41209841928900	-0.35746736912500		
C	0.81971673066600	-1.97290328204600	0.47994493279600		
H	3.38856144880700	-1.76417098312700	-0.39085984675100		
H	1.04414185587200	2.54048715729700	-0.75578626187200		
H	2.87577932253600	1.73105692428500	1.28209968409300		
H	4.05555122629700	0.56558430451200	-1.28384566783900		
H	-1.05802753143700	-2.89952001790800	0.74879807157100		
H	1.38178202232500	-2.87336082566200	0.67373934576600		

phenanthrene-17	5.82 [1.80]	5.90 [0.29]	5.90 [0.11]	7.52 [0.94]	8.21 [0.28]
C	-0.75110593279100	0.28028975395800	0.04128987519600		
C	0.67819162790600	0.12742603212300	0.11940851694300		
C	-1.44971094898100	1.48694864255300	0.07838352465800		
C	-1.47582668844900	-0.95171907982300	-0.09913520103000		
C	-2.87889488447100	-0.90556801871500	-0.35152672958600		
C	-2.81465153000600	1.49659524715400	-0.10681929800400		
C	-3.52341121419500	0.29353392591200	-0.33542499429500		
C	-0.66888382966400	-2.03915987632900	0.06438838629400		
H	-3.42004172832600	-1.82498520904900	-0.50769079656900		
H	-0.91956556074200	2.41860390217100	0.18844443177000		
H	-3.34640003905700	2.43370989926100	-0.11475299577100		
H	-4.58882745793000	0.33382621401600	-0.49591960974200		
C	1.52472998820100	1.21256911482400	0.60378033647200		
C	1.45287232015600	-0.94916366697000	-0.54836003752700		
C	2.81300039791100	-0.82339588214200	-0.84598337635100		

C	2.81382077590600	1.33351239444800	0.22369095612300
C	3.47431379878500	0.33813530577900	-0.57099035982600
C	0.74334643428500	-1.72328723951700	0.37538300002700
H	3.32938338296200	-1.67135345062900	-1.26966152128800
H	1.06751044587800	1.97794419463200	1.20991525247900
H	3.38108551969100	2.18997125271700	0.55278561723700
H	4.50748778206200	0.46800968963000	-0.84368282706100
H	-0.95620850039000	-3.06322811651000	-0.10795167404400
H	1.23659893595600	-2.19129354953600	1.22218211972000

phenanthrene-18 5.79 [1.15] 5.95 [0.90] 5.95 [0.27] 7.73 [1.06] 8.17 [1.14]

C	-0.68420294065900	0.19370214711000	-0.08732484865700
C	0.74217715901400	0.26427896820000	-0.21643081396500
C	-1.53487140484200	1.32583498226600	-0.35392443273100
C	-1.44679827202000	-0.99868713320300	0.34462923261400
C	-2.82661253947700	-0.94045730453400	0.64270629145400
C	-2.84427580086500	1.35653842717400	-0.01002869929300
C	-3.51243981607900	0.22483930409800	0.54307632556200
C	-0.70262385263400	-1.84554178281700	-0.45758139204400
H	-3.31337700935200	-1.84909077610700	0.95843310211400
H	-1.08203696251400	2.21069179987500	-0.76499589508600
H	-3.40410859201200	2.26396222712100	-0.17151295912100
H	-4.55472507731900	0.28486433174800	0.80461568085600
C	1.46381504503300	1.46812781216400	-0.36342132521000
C	1.45412382207100	-0.95514191610300	0.02206768329100
C	2.83633005083600	-0.87271593991900	0.35181508695900
C	2.81372078670100	1.49422789294000	-0.15498193406600
C	3.49156686019000	0.31416485535100	0.23862751487800
C	0.65470205099800	-2.08217662112900	-0.00160103513500
H	3.36621263661400	-1.77358955776100	0.61671168482700
H	0.95433937871700	2.38884064384800	-0.59554276697300
H	3.36031364108000	2.41678631439900	-0.25662397462500
H	4.55157259035200	0.35877733891600	0.43440158432800
H	-1.08863288330000	-2.22404047380600	-1.40535538381200
H	0.73631258535900	-2.81341060570600	0.79301152578000

phenanthrene-19 5.74 [1.25] 6.06 [0.80] 6.06 [0.14] 8.10 [1.19] 8.64 [0.96]

C	-0.88763430889500	0.30385384935500	-0.05363615752800
C	0.56517996313100	0.16731909409600	-0.11665670936300
C	-1.64271658207900	1.47835056460300	-0.04305294852900
C	-1.53729741303500	-0.91167663214500	0.20466205784700
C	-2.86392777934600	-0.97199841246500	0.59659588519300
C	-2.98655016989600	1.41581697910800	0.26680650657400
C	-3.59152956618400	0.20410697720600	0.60360005973600
C	-0.47419727985100	-1.89485163566200	0.05200840344900
H	-3.32890421132400	-1.91335483705200	0.83729982191700

H	-1.17731128956400	2.42831601964200	-0.25004879426400
H	-3.57383731991100	2.31967576370300	0.27223700295800
H	-4.63934616652700	0.18160434592100	0.85434454901000
C	1.38424045001600	1.16959136971200	-0.68026847698000
C	1.19429386869500	-0.96886321411300	0.55568069320900
C	2.63898942284300	-0.97154162538700	0.60341990273500
C	2.74142534355700	1.13052052518100	-0.57677205172100
C	3.36801769528400	0.05171498667100	0.10415472984700
C	0.43177849128200	-2.01186195955900	1.12014293943200
H	3.11698374879000	-1.80090976007700	1.09796836809300
H	0.91102705697900	1.98570499908900	-1.20263227990200
H	3.34477680643000	1.91166144578700	-1.00840522456200
H	4.44268702948200	0.03703357812300	0.19412432902500
H	-0.21936010099800	-2.11480776022500	-0.99666665148900
H	0.91782406350600	-2.87931582460600	1.52011150452300

phenanthrene-20 5.60 [1.19] 6.06 [0.68] 6.06 [0.80] 7.99 [0.24] 8.27 [1.18]

C	-0.40922631395400	0.40866306697800	-0.52149621214500
C	0.93713939467200	0.42674166657000	-0.01081279046600
C	-1.08289876561600	1.58191440952100	-0.89354329304000
C	-1.07977746529900	-0.83166476841800	-0.64894458111100
C	-2.39810448085300	-0.84749775111500	-1.12839687076300
C	-2.37614388973900	1.54112561946400	-1.35671583240400
C	-3.04107164969100	0.31666862515900	-1.47332710762600
C	-0.41137975175000	-2.04268615847500	-0.28055051427800
H	-2.90529696034700	-1.79493073045200	-1.22388953564800
H	-0.56577937184000	2.52510080332100	-0.83206478039800
H	-2.87573399124300	2.45364549725000	-1.63854780451700
H	-4.05384805239600	0.28580514943000	-1.84080080423000
C	1.59975882477700	1.55528762039900	0.49715841734000
C	1.60496357404400	-0.83207189379700	0.24732125620800
C	2.95105268402000	-0.69755097458100	0.69507344691300
C	2.94031322510000	1.26057858323900	0.89868569924900
C	3.63552730289900	0.38582475743100	0.00843880741700
C	0.87584109543600	-2.03805271576000	0.15306775771900
H	3.39610075634600	-1.32709913316800	1.45032038400700
H	1.07243512076000	2.44847555015400	0.78619580609200
H	3.33988508122200	1.55578353142500	1.85828646047600
H	3.48129257935400	0.50741603444900	-1.05643842731500
H	-0.95394385314600	-2.97074345400200	-0.36475531546900
H	1.36510579878800	-2.96357952773600	0.41250956964200

phenanthrene-21 5.69 [1.34] 6.11 [0.33] 6.11 [0.68] 7.68 [0.52] 8.33 [0.62]

C	-0.64043084522300	0.42893361467800	0.19883927435000
C	0.75590644115200	0.48679165336100	0.22146773816400
C	-1.58213681496900	1.48591928516100	0.20853061991100

C	-1.20721897240900	-0.97315190880800	0.06543936756900
C	-2.44204639980500	-1.08366236539400	-0.73864876543900
C	-2.83482731737300	1.28160044260300	-0.26916301442600
C	-3.22823028623800	-0.00835152340700	-0.82784856381200
C	-0.79870927906900	-1.83219857119600	1.06665785442300
H	-2.73233283228000	-2.04320484006400	-1.13250215384400
H	-1.27264243193100	2.47250511136700	0.51533302144300
H	-3.54189580496800	2.09317560858100	-0.30632838803200
H	-4.18565088397400	-0.07783511449100	-1.31954955274200
C	1.58843713802400	1.62781832875900	0.24784036313800
C	1.32858708508300	-0.80586347587300	0.04559218266700
C	2.69459694033100	-0.91063763601000	-0.26466298411700
C	2.92618733331500	1.48823302192800	0.01056346012100
C	3.47564160015300	0.21546757282400	-0.26666819028700
C	0.40133718296500	-1.86607729504200	0.17402847878200
H	3.13052316416600	-1.87977525714700	-0.44835129375400
H	1.16267356928300	2.60463877483500	0.41256682846200
H	3.56905579677200	2.35311970827100	0.01160575669800
H	4.53234218732900	0.13131669756100	-0.46345011570900
H	-1.33855117953000	-2.73517296560300	1.30386554981100
H	0.60795444188100	-2.82553953461500	-0.27479228173300

phenanthrene-22 6.25 [1.86] 6.35 [0.09] 6.35 [0.21] 8.53 [1.00] 8.72 [1.01]

C	-0.64120029195400	0.46936032934300	-0.40043284150400
C	0.80187658400200	0.58151172325300	-0.49223611280000
C	-1.46599611616600	0.97852605710200	0.57955045730600
C	-1.23013302494100	-0.63674469039100	-1.27034844917100
C	-2.66813667930100	-0.52336618847500	-1.51816374566200
C	-2.84646643454600	0.72851440262500	0.53079819269400
C	-3.44479385396300	0.01078564748200	-0.53172742606500
C	-0.80481207260600	-1.57232370036500	-0.36609582007300
H	-3.09287248008500	-0.73691882139400	-2.48854669664400
H	-1.07677573838600	1.71207877792800	1.26964657241500
H	-3.48233799897300	1.19942850301500	1.26274020961800
H	-4.52000964807800	0.05498496570300	-0.63709343118300
C	1.58244108260400	1.48853947312400	-1.18696458012800
C	1.40494278879300	-0.55179642226100	0.13051689137500
C	2.81317648898500	-0.58903832430800	0.27380530414800
C	2.96079780641500	1.41148305470200	-1.07131224493100
C	3.56559039191500	0.39007191178000	-0.31812323767100
C	0.50869905165100	-1.60113368146500	0.29856842226400
H	3.27743640743100	-1.39035053709700	0.82585963126100
H	1.12232154115200	2.29440707944900	-1.73446633575600
H	3.57700797888900	2.16889713670200	-1.52687085362400
H	4.63910271540400	0.37347325679800	-0.22137184096500
H	-1.46943617211900	-2.38405221707200	-0.08897116978500

H 0.83273393670800 -2.54850503283800 0.69820410252600

phenanthrene-23 6.59 [0.05] 6.59 [0.05] 6.74 [1.99] 7.89 [0.04] 9.41 [1.03]

C -0.59055127154800 0.06848516702500 -1.40702952813700  
C 0.72709126399700 0.04964983041700 -1.66598521014200  
C -0.99503144046900 1.46808873251400 -1.21610722546100  
C -1.33880711880700 -1.07664289993100 -0.97391389514000  
C -2.42875844409500 -0.80460318290400 -0.21816169293400  
C -2.14160135646400 1.62094392690700 -0.34752632351300  
C -2.82316794214600 0.54669745204800 0.12379262009600  
C -0.63930301525900 -2.34612810017000 -1.14779857098200  
H -2.99926927299900 -1.61718728457300 0.20899837690700  
H -1.11404029685600 2.03898168912500 -2.13426215740300  
H -2.50633106493300 2.61393023330900 -0.13120638157700  
H -3.68151885338200 0.67683207646800 0.76068254296700  
C 1.04006146667700 1.45572594380700 -1.30155046519400  
C 1.45248629324800 -1.09545155016600 -1.20734928712000  
C 2.58006236751900 -0.88621594961600 -0.47155851740300  
C 1.97448478651100 1.53093988406500 -0.20278552514500  
C 2.75987721995600 0.44200763193100 0.04575169267900  
C 0.69907094314800 -2.35336005934700 -1.29029963848600  
H 3.16238552378100 -1.69581678682000 -0.06756458049300  
H 1.10443841136700 2.23157753330700 -2.05892016785600  
H 2.17893554783600 2.47091207173000 0.28106241675200  
H 3.57353181116100 0.58300207516400 0.74376988335400  
H -1.18685422475400 -3.27306583267100 -1.07938427336100  
H 1.23863249974300 -3.28656481556600 -1.32481231540800

phenanthrene-24 6.54 [1.91] 6.66 [0.13] 6.66 [0.15] 8.19 [0.29] 8.46 [1.05]

C -0.61894844795600 0.35662449023000 -0.86819903233200  
C 0.42601499525100 0.10020233006000 0.03439295391500  
C -1.40121427137000 1.48957062244700 -1.08650738498700  
C -1.09037594387500 -0.78802306014900 0.00755714985400  
C -2.38336870501700 -0.50482434391100 0.65010538690400  
C -2.68749815961200 1.55863259523400 -0.62462706114600  
C -3.13930420527100 0.55294700553600 0.30054224096500  
C -0.59693730241000 -2.11643063682100 -0.11810012680200  
H -2.76786519691500 -1.23761467930800 1.34270244052200  
H -0.95716471197300 2.32110141635200 -1.61381862239700  
H -3.31622978287700 2.40191460551100 -0.85225204122500  
H -4.10993839037000 0.67483306756800 0.75603133815400  
C 0.94815059013700 1.09625196113300 0.98930131874900  
C 1.38118513823800 -1.00322128032700 -0.33593793579400  
C 2.76446704578400 -0.65081293630500 -0.40466473451300  
C 2.27086173314900 1.28280419354900 1.02131515857400  
C 3.19140849022700 0.45554621079700 0.24053198100100



C	0.76057342515800	-2.22185730676700	-0.41972537741300
H	3.46328685204000	-1.31662482233900	-0.88653545773900
H	0.25789291030100	1.71623393594300	1.53612317372300
H	2.69029680547300	2.06671359836600	1.63189305874500
H	4.23737471643000	0.71382730103300	0.24542980270200
H	-1.23053950512400	-2.96262604536600	0.08958775653300
H	1.25778682061200	-3.14363677000000	-0.66844924541900

phenanthrene-25 6.96 [1.56] 7.13 [0.48] 7.13 [0.34] 8.93 [1.03] 9.64 [0.82]

C	-0.71964366788900	0.48003207050100	-0.44315178668200
C	0.69705444419000	0.53771412734300	-0.69452464479100
C	-1.60336853629200	1.55963244384100	-0.58405250452300
C	-1.22389611277400	-0.74827059949600	0.11872069708600
C	-2.59470791089300	-0.81602137352400	0.51299252518300
C	-2.91564034359700	1.44956170062000	-0.20347106704300
C	-3.42046010870200	0.25079283055300	0.35118930664900
C	-0.34064095178700	-1.77705923789400	0.36357577165000
H	-2.96223913629200	-1.73779001598900	0.93547208168200
H	-1.23801031507300	2.47691800687300	-1.01586350207500
H	-3.57976678577500	2.28844385104300	-0.33624519308200
H	-4.45703394271100	0.18965315782400	0.63789460024900
C	1.37934555226800	1.48339330903000	-0.01060925791300
C	1.41352151597700	-0.72116581380200	-1.12101966796400
C	2.62719028364300	-1.12990169806500	-0.12418263809100
C	2.73006801421800	1.29911588079000	0.41684862148800
C	3.23766939486500	0.01986681525100	0.38921135153300
C	0.99040535047500	-1.78263601440800	-0.37507912537900
H	3.29140936417900	-1.91451050656300	-0.44118763654800
H	0.83508532388300	2.33636944136700	0.37011515778700
H	3.26617229864000	2.09659951074900	0.89876284669700
H	4.26331105791400	-0.11735292453900	0.70869046643000
H	-0.62699502630900	-2.63192361892000	0.95348667499900
H	1.34182121970700	-2.77731263909900	-0.61860179699700

phenanthrene-26 7.26 [1.61] 7.45 [0.78] 7.45 [0.08] 9.14 [0.89] 9.34 [0.44]

C	-0.49374049473000	0.51115584421200	-0.33336432524500
C	0.72282689934200	0.31749486805900	-1.21099704455500
C	-1.49660798880400	1.52795191416800	-0.62791497944500
C	-0.98487929411800	-0.67641936959100	0.39211230877500
C	-2.24329409706600	-0.55595060745900	1.09029921157500
C	-2.69900138482200	1.54790490305300	-0.03444177513500
C	-3.05351835071800	0.49705857826600	0.88582425395900
C	-0.36452033039700	-1.88470784854700	0.27411041276800
H	-2.54443024872900	-1.36751866909700	1.73333012609300
H	-1.20868553189300	2.31682293198300	-1.30462816346000
H	-3.40181858028400	2.33962476746000	-0.23194694491200

H	-4.00392202236700	0.54810599027200	1.39355673934700
C	0.98772843486800	1.29770072717500	-0.20541333790500
C	1.46377698618300	-0.90605058041000	-0.97308425394800
C	2.85259501862800	-0.80764071663300	-0.59647026243100
C	2.17075362510300	1.12274632384300	0.69509054160500
C	3.12435654880800	0.23182193513100	0.35073883701500
C	0.89071196665800	-1.99904099795100	-0.40263221615900
H	3.53634941950400	-1.63130113155300	-0.71393016797300
H	0.76047846589400	2.33752028188900	-0.39751789022400
H	2.32078261395600	1.81462240691600	1.50751731135300
H	4.07168586079300	0.22475018413500	0.86665473101300
H	-0.77006738547100	-2.74229822056700	0.78592779795400
H	1.47279528551200	-2.89722441732400	-0.25692731795200

## anthracene

anthracene s0min	0.00 [0.04]	2.56 [1.99]	3.90 [0.13]	3.92 [1.08]	4.75 [1.05]
C	3.525481210113	-1.134297361081			-0.056287399516
H	4.603189966396	-1.124442244919			-0.073947816372
C	2.831679984294	0.034649069448			-0.046085065143
C	2.840829062582	-2.376253497686			-0.043948890918
C	1.408091452768	0.041202249598			-0.022753415811
C	1.482025268308	-2.413541891239			-0.021808835060
C	0.716606724019	-1.213186118742			-0.010373683889
C	0.672322051633	1.219338538161			-0.011692575655
C	-0.672413228278	-1.219530361571			0.012458617001
C	-0.716667204573	1.213007441472			0.011261102309
C	-1.408177997929	-0.041363037016			0.023666953071
H	3.350113223775	0.980498522547			-0.055524499205
H	3.407724519341	-3.292982719848			-0.052379940800
H	0.959504998811	-3.357183662062			-0.012456263019
H	1.193447180583	2.164701561791			-0.021099663015
H	-1.193535854968	-2.164896385722			0.021854261105
C	-1.481997818516	2.413394470558			0.023114611533
C	-2.831776270004	-0.034727866137			0.047351067077
H	-0.959373638498	3.356982767830			0.013770942299
C	-2.840788043118	2.376244327647			0.045768458720
H	-3.350328139898	-0.980508582857			0.056749560763
C	-3.525464191250	1.134297521658			0.058021726524
H	-4.603171938398	1.124527958673			0.076149120913
H	-3.407610317204	3.293007299497			0.054631627090

anthracene-01	4.23 [1.05]	4.94 [0.98]	4.94 [0.11]	6.79 [1.09]	7.40 [1.08]
C	3.43667950410800	-1.13177174872900			0.09627658018000
H	4.47186749713900	-1.22727926887500			0.38388425169700
C	2.80674076108200	0.08466333634700			0.22794654320200
C	2.76659108345000	-2.26122195194100			-0.41691885866100
C	1.47003424066000	0.24346876905200			-0.14746202881400
C	1.44991511281100	-2.16700406786700			-0.75822745304500
C	0.77096439242100	-0.93066829629500			-0.60268280450200
C	0.76775722184400	1.53077869678700			-0.21324519134700
C	-0.61889994832300	-0.84709312233900			-0.70187014534400
C	-0.66621864544200	1.44161354569400			0.08361814394900
C	-1.37915371449300	0.27581931969300			-0.37363942059500
H	3.32943205601800	0.95255807547700			0.59021925357100
H	3.29731639502800	-3.19174566067100			-0.53100882009700
H	0.92146573685400	-3.01691402541900			-1.16278482672300
H	0.57489314164900	1.39678113720000			-1.30903201877700
H	-1.15381634806000	-1.75117219314400			-0.96255779318500
C	-1.41863096600800	2.45166708204100			0.68953835241900

C	-2.79564009671500	0.21546646716500	-0.30515504846400
H	-0.89123405507300	3.31541456698100	1.05491649752100
C	-2.78887513966600	2.35725307428600	0.77272920975300
H	-3.31197531697600	-0.63953744889700	-0.71459352825200
C	-3.48799881815800	1.24643780276000	0.25669923283600
H	-4.56337487822800	1.21794607680200	0.31499410600100
H	-3.34900003524700	3.15376772572100	1.236747444440700

anthracene-02 4.62 [1.08] 5.19 [0.94] 5.19 [0.08] 6.95 [1.26] 7.52 [1.16]

C	3.53374856474700	-1.28749652796400	0.01715351041700
H	4.61151907656700	-1.31034990942000	0.02936086354700
C	2.87897137695100	-0.09116323353900	0.02973972519400
C	2.81509178563400	-2.50386222333900	-0.01464746064800
C	1.46484853631100	-0.03579103852800	0.01006486942400
C	1.45372520737800	-2.48874820907000	-0.03288144416600
C	0.74247667479600	-1.26267820804300	-0.01660234176500
C	0.76650359290700	1.19178623200200	0.02533419610600
C	-0.65770646843600	-1.21360992012000	-0.02663842927400
C	-0.59861761508500	1.24148630172700	0.04219227877600
C	-1.32518300269400	-0.00441747621000	0.00488280678700
H	3.43186069126900	0.83426258478900	0.05219103347700
H	3.34992706315300	-3.43930396588800	-0.02401906877300
H	0.89471790191700	-3.41124567997400	-0.05657971824000
H	1.31491928305300	2.11852842170000	0.04255799400000
H	-1.21628498550700	-2.13606924058400	-0.09041002546200
C	-1.40724609835700	2.49790531803000	-0.05625718223700
C	-2.75578743633000	0.03830315773400	0.02027409311600
H	-1.68799969667800	2.28932324797100	-1.11972834481500
C	-2.73467481298900	2.35237248383400	0.44301235109500
H	-3.27565427586100	-0.90851972041600	-0.01416732617100
C	-3.48842526994900	1.18745035832700	0.18500629108500
H	-4.55561459280500	1.13121801161800	0.33816776196500
H	-3.20653400203700	3.11459050202500	1.05848076373100

anthracene-03 4.81 [1.35] 5.23 [0.33] 5.23 [0.53] 7.33 [0.99] 7.42 [0.69]

C	3.47506306700200	-1.22773400824600	0.35736523266600
H	4.53237330725600	-1.30956272308000	0.55251243748100
C	2.90391018566000	0.02431003631900	0.22875937473600
C	2.70857353370100	-2.38501969314900	0.25155971283800
C	1.53299945367800	0.12984638420600	-0.03012129018600
C	1.34942361585700	-2.29627665600400	-0.03116103766000
C	0.79536688032700	-1.05011048033400	-0.23486703239500
C	0.70188710314800	1.27790492701500	0.01781711729800
C	-0.59043424317400	-0.72357320301000	-0.60029964445200
C	-0.69816132200800	1.13538633560000	0.19415955460500
C	-1.40949600942400	-0.14954114647100	0.38342037579900

H	3.50318134323300	0.91426124934700	0.33631735915300
H	3.17309849259100	-3.35200949309300	0.34860008195500
H	0.75668875618400	-3.18970033245200	-0.14486078887300
H	1.11622251761900	2.27086724002900	0.06972830950600
H	-0.89672060024200	-0.76822899955800	-1.64127068959400
C	-1.58640824384600	2.25841299266600	0.16234255819300
C	-2.76378234647800	-0.20837285890000	0.69216819237900
H	-1.18104065338800	3.21356134315400	-0.13056199141600
C	-2.88426025464500	2.16334326896200	0.57756458123400
H	-3.21942106477400	-1.18302158461600	0.77650134572000
C	-3.49414588981900	0.93447667247200	0.90260458244500
H	-4.51975314300900	0.89405456193200	1.22383725566900
H	-3.47279214223700	3.06674550998500	0.62814619956100

anthracene-04 4.99 [1.37] 5.32 [0.58] 5.32 [0.40] 7.25 [1.15] 7.63 [1.16]

C	3.54739467299700	-0.86483241016600	-0.14036094891400
H	4.62376461392900	-0.86940241086400	-0.08495580183600
C	2.84509063968300	0.23527854854000	0.24675513498000
C	2.86734547279100	-2.00986467490100	-0.61657956292200
C	1.42719177080400	0.25965144183600	0.18481156611300
C	1.50634223497600	-2.02304424680500	-0.69144470760200
C	0.73991577392600	-0.89902765418000	-0.29851180297200
C	0.69055216989800	1.38870213050000	0.55684936807300
C	-0.66674373223400	-0.90861441986500	-0.34790913595800
C	-0.69837274692800	1.38451817831500	0.46477488092900
C	-1.39258519267700	0.17810691842000	0.07869777923900
H	3.35859452929800	1.11180631900800	0.61024437865200
H	3.43332320319000	-2.87503920872200	-0.92182785983300
H	0.98926078469400	-2.89827940851200	-1.05276304267000
H	1.20880837203700	2.28145034909000	0.87079224547400
H	-1.17082892802100	-1.80495201758100	-0.67537021392200
C	-1.56863526677400	2.45958186858500	0.58770604393200
C	-2.81517931534700	0.27418609402500	0.14406207796800
H	-1.26535432373600	3.46091438381700	0.84361374154400
C	-3.00691196592300	2.16298010891900	0.40094297075900
H	-3.40826442749400	-0.34458356052300	-0.51326635686000
C	-3.57480278718500	1.10317297623400	1.09891038896100
H	-4.64462679008800	0.98664486489400	1.15051141287500
H	-3.60020675207200	2.88967150108400	-0.14848139238000

anthracene-05 5.05 [1.12] 5.45 [0.90] 5.45 [0.14] 7.35 [1.28] 7.57 [1.49]

C	3.20252686694700	-1.00897206732300	0.91863811904100
H	4.25320309234500	-0.96833453875300	1.15586391097300
C	2.53054633776300	0.13566211649300	0.61252258571300
C	2.53708025044400	-2.25793127718800	0.93144379689600
C	1.14745667347200	0.10516847094300	0.30454474207700

C	1.21034965637900	-2.32606326701700	0.63888581024900
C	0.47761472078300	-1.15299784897800	0.32120073899800
C	0.43510558492900	1.27034679902100	-0.02815389165500
C	-0.88428632674300	-1.18597474404600	0.00933909389200
C	-0.91184012359400	1.24917937399300	-0.31187559278900
C	-1.58906495164700	-0.02867516116800	-0.27263434466600
H	3.04240055009400	1.08455954883100	0.60157511596800
H	3.08775655301400	-3.15174577463100	1.17378428163600
H	0.69328731773400	-3.27259994481400	0.64644101921700
H	0.96902242559000	2.20727428553800	-0.06196920951700
H	-1.40239997182200	-2.13288963177800	0.00432254616100
C	-1.64040771366500	2.44899529499400	-0.68547511131200
C	-2.93854193680700	-0.00221517655500	-0.74737120290400
H	-1.07204749890600	3.35121347946200	-0.85351557293100
C	-2.98163437770400	2.43784720855500	-0.79029336419600
H	-3.29862198178300	-0.87754074126000	-1.28147951895000
C	-3.72325663202500	1.15790272115700	-0.56897924162100
H	-3.52905312905000	1.22419865697500	0.53812140585200
H	-3.53315323037600	3.35482312690600	-0.93300609812300

anthracene-06 4.93 [1.33] 5.46 [0.45] 5.46 [0.38] 7.33 [1.17] 7.62 [1.07]

C	3.44941705451900	-0.88165694059000	-0.85338754063200
H	4.46527481076300	-0.75728846416900	-1.17326360541900
C	2.78966063242800	-0.24739856792800	0.24835590662500
C	2.90335570543300	-2.10860011018400	-0.57104802031500
C	1.36548361006300	0.04985786209800	0.09250031688800
C	1.58810388193300	-2.31214050700500	0.00923028655900
C	0.68744572114200	-1.21350215607100	0.12054711519600
C	0.69681591405500	1.21945799487900	-0.06867172151900
C	-0.69064386349700	-1.22499092633700	0.15370343075900
C	-0.72134597847800	1.21380554637800	-0.09224122369600
C	-1.41480501756400	-0.02161114160700	0.05068810457200
H	3.16220460240100	-0.33293495237600	1.26912900004100
H	3.50226672002600	-3.00419531078500	-0.71047284391000
H	1.24128096569000	-3.32363109333100	0.13661758838300
H	1.22082598840700	2.16050012058800	-0.12110322884300
H	-1.22569897091600	-2.15710809413600	0.25150435346400
C	-1.46399355070300	2.40894730093400	-0.20055459116800
C	-2.83157434662500	0.00024487345000	0.07167456226700
H	-0.93100297074400	3.34162755668800	-0.30247847979500
C	-2.82946086538100	2.39344928854400	-0.18379591062000
H	-3.36005149886500	-0.93399725435100	0.18004700263500
C	-3.51963986159700	1.17181698351300	-0.04570420823400
H	-4.59763482762900	1.16817626223600	-0.03150704211100
H	-3.38369397201100	3.31308922419500	-0.27696774955100

anthracene-07	5.42 [1.13]	5.61 [0.43]	5.61 [0.92]	6.86 [0.96]	7.88 [1.28]
C	3.51268320853400	-1.29276967069600			-0.12488497815900
H	4.58649606220600	-1.32489390729500			-0.21643166943100
C	2.86121105143300	-0.10208189103200			-0.18740026206700
C	2.79394882985100	-2.50243345719600			0.05818133713600
C	1.44389910350500	-0.03102525396800			-0.07358254754400
C	1.44045665923000	-2.47758130152100			0.17397564353500
C	0.72141624715700	-1.25356401998400			0.11687877957300
C	0.76333823260800	1.18787243944200			-0.10615861652700
C	-0.67104624770200	-1.20792030736200			0.20740894208300
C	-0.61017210723100	1.24424989043400			0.09096918484500
C	-1.34049769354700	0.00179886375300			0.14290369899600
H	3.41203236324900	0.81517506890100			-0.32532239103200
H	3.32812476750600	-3.43726160747400			0.10438846250900
H	0.88573732534700	-3.39276633624900			0.31307237996800
H	1.32709364513900	2.10247940969100			-0.20432070795400
H	-1.22595510083800	-2.13181567451700			0.27547647236100
C	-1.44774059068600	2.38302389321000			0.14756359668400
C	-2.74940511461300	0.08476778675300			-0.08019211301700
H	-1.32348021712200	3.14025971247800			-0.61765487073300
C	-2.82009726620900	2.11210334009100			0.54796785203800
H	-3.31316101883200	-0.83867838237900			-0.00238871889300
C	-3.48137073284700	1.25729906409900			-0.35234771728100
H	-4.53411987673300	1.22330190564700			-0.57885394927100
H	-3.21081003371400	2.34443171054000			1.53723938878300

anthracene-08	5.33 [1.34]	5.70 [0.60]	5.70 [0.24]	7.46 [0.80]	7.85 [1.10]
C	3.40143598425300	-1.09241433545300			-0.31502514470100
H	4.43953471326200	-1.05305857753800			-0.60456592797000
C	2.60206770630900	-0.02272739110800			-0.54009000880400
C	2.90105205898000	-2.27812082552000			0.29949873894100
C	1.22035368274000	-0.04043796192700			-0.16201534319400
C	1.59833112474700	-2.34281937395900			0.66870384293700
C	0.72407670155000	-1.24198276205000			0.45681693701800
C	0.39084161891600	1.03815967446300			-0.38949097686900
C	-0.63431346899300	-1.29900592158500			0.72639474871000
C	-0.94272682688500	1.13840767359000			0.10055543898200
C	-1.44750513944100	-0.19087096285200			0.59679533269400
H	2.99524121426200	0.86762807172400			-1.00412401830300
H	3.56283880461600	-3.11147574620100			0.46607832627300
H	1.20021723487100	-3.23273260554000			1.13144128022600
H	0.80595966504300	1.92244231577600			-0.84716080833900
H	-1.08016991210900	-2.22230902058300			1.06230515020600
C	-1.68145281008600	2.33781972538500			0.09994768413700
C	-2.68724683788400	0.05877586107200			0.03501411769300
H	-1.16716481508100	3.25204472132700			-0.14030219836900

C	-2.99050751476000	2.30325521960600	0.58760484035700
H	-2.95886511674100	-0.40421367484900	-0.91384581298300
C	-3.54691251907200	1.05724653021000	0.65889122187000
H	-4.16523512072400	0.73270734694900	1.48391752694300
H	-3.46996589992600	3.17533073877500	1.00502317064500

anthracene-09 5.38 [1.96] 5.72 [0.10] 5.72 [0.13] 7.33 [0.61] 7.64 [0.70]

C	3.42047022563700	-1.11156989032100	-0.34180474234700
H	4.46867225762500	-1.06973058911600	-0.59140258355300
C	2.61765521183600	-0.03842695498400	-0.60711025525700
C	2.89587823915900	-2.27285893037400	0.25222085696100
C	1.23191265592000	-0.05674100629000	-0.28667567655600
C	1.55711820597400	-2.33351718321900	0.56256475065600
C	0.70774984888600	-1.25121082734300	0.31839898133200
C	0.40374330687600	1.02826920285900	-0.56382548769100
C	-0.71070335870500	-1.33038227755800	0.48988689881300
C	-0.94946272855800	1.11305453383300	-0.01702880972100
C	-1.45910270333900	-0.21978505314100	0.37749434660100
H	3.02788420437400	0.84861756574900	-1.06315603913800
H	3.54050655998000	-3.11098852073200	0.45869086642400
H	1.14338771734900	-3.22730246369200	1.00358898038300
H	0.83615315704100	1.92478779976400	-0.97877458936700
H	-1.18248836803900	-2.29449286052400	0.60024692276000
C	-1.50756207380400	2.35369261504100	0.39942497115500
C	-2.55777454556000	0.23292573082900	-0.36922041383500
H	-0.87061805403900	3.21290798105300	0.51592251147400
C	-2.89769645056600	2.38322751868200	0.57243140038100
H	-2.77926352879100	-0.25844609549300	-1.31013772942500
C	-3.49719607239100	1.23460274006100	0.16560576520200
H	-4.53914926541500	0.98614087479400	0.27207443800200
H	-3.42006835551700	3.21104137033000	1.02060202766600

anthracene-10 5.63 [1.72] 5.95 [0.27] 5.95 [0.35] 7.86 [0.57] 8.15 [0.84]

C	3.04702407920300	-0.72341107016300	-1.01638884916900
H	3.97037858211400	-0.56496180502100	-1.54862361717900
C	2.28687232918600	0.36595018959000	-0.60075153307500
C	2.61620748340900	-2.00700517052200	-0.72517107071900
C	1.09963781102500	0.19141306986700	0.08472886105100
C	1.42732096182300	-2.20526740923500	-0.04164980688100
C	0.63775515924200	-1.12530268060800	0.36183172956500
C	0.39916700513800	1.32722317827600	0.71576910279800
C	-0.66281366127800	-1.31447643684900	0.93475665713100
C	-0.83773009716800	1.12080264137200	1.41126994665900
C	-1.47363787875100	-0.14560022820600	1.03921410208600
H	2.63440594359200	1.36812335507900	-0.79968027848900
H	3.20270107726200	-2.85716679936400	-1.03425095928800



H	1.09102212531200	-3.20730558762300	0.17397429223800
H	1.04546127998100	2.14149492607500	1.01106544610700
H	-1.09736403174000	-2.30078628929300	0.94076198268600
C	-1.10738416455600	2.21760287886700	0.48887107118300
C	-2.64207597051300	-0.14097920443300	0.33790603258900
H	-0.81151396351000	3.22047639620400	0.75867977658800
C	-2.25122213353400	2.12955187316400	-0.38353871108400
H	-3.12799453246400	-1.07521554625400	0.09911061252300
C	-3.06213129346400	1.04382896531200	-0.35302748141700
H	-3.95290565676100	1.00959802128100	-0.95889323002500
H	-2.52277418427500	2.99297995781400	-0.97068540763100

anthracene-11 5.88 [1.51] 6.07 [0.15] 6.07 [0.66] 7.67 [0.80] 8.18 [1.02]

C	3.16996320289700	-0.96233592699600	-0.35554373353900
H	4.05610607067900	-0.45551583897600	-0.70360327044300
C	2.39746677142500	-0.21042081539900	0.71672331681100
C	2.81828559130300	-2.21814052878300	-0.84716702392300
C	1.42810696415900	-0.17587659759000	-0.24872573271800
C	1.48420291037100	-2.57033894617600	-0.77053014130600
C	0.66366271309300	-1.45922938380500	-0.49677056460400
C	0.75979970415100	1.07865068519600	-0.70617938300400
C	-0.67821430787300	-1.34082886965900	-0.33210062498700
C	-0.61751759920100	1.15941737561600	-0.53221883308700
C	-1.34690680123500	-0.05726545447600	-0.29483263786900
H	2.80919206017600	0.72655106679900	1.06427843169400
H	3.56243109317600	-2.84978297121700	-1.30636083787900
H	1.09244736994700	-3.54908050147700	-0.98143750943800
H	1.34999510021400	1.91752352977600	-1.03094886104400
H	-1.29583193294000	-2.22336263141600	-0.27342084261000
C	-1.32036651258700	2.38042464310000	-0.64759955401900
C	-2.72372290710300	0.03384105690000	-0.13362825206800
H	-0.75928871656100	3.28018284378100	-0.84474173349600
C	-2.68280224613900	2.43043286725700	-0.48549178931900
H	-3.28996758945700	-0.86664411186500	0.04304863746800
C	-3.38279806017100	1.25162366961400	-0.21777799246700
H	-4.45231629769400	1.28404172554300	-0.08725787813500
H	-3.20704197778500	3.36854525769000	-0.55665100887000

anthracene-12 5.68 [1.22] 6.09 [0.73] 6.09 [0.63] 7.00 [0.22] 7.95 [1.20]

C	3.08530458836300	-0.65305790299200	-0.83971832013700
H	4.02641086773200	-0.44751662306200	-1.32284579017900
C	2.24831870130300	0.35683157984900	-0.52041058940800
C	2.74141574643000	-2.01430827110300	-0.54061089425000
C	1.03544117673800	0.07293107136000	0.22520058078400
C	1.52606830388400	-2.34461178089000	-0.02100198787100
C	0.57165391119800	-1.33710025622900	0.23916399778000

C	0.56265371530300	0.98352034195800	1.25206574734900
C	-0.80079258434800	-1.46358835252100	0.39561544893700
C	-0.48476939913700	0.91093704109300	0.24943692816400
C	-1.42936883331300	-0.23356040465700	0.27134683729200
H	2.51228750067400	1.38475982595100	-0.70668941552500
H	3.44631184036600	-2.79214849990100	-0.78520550370600
H	1.25138138316700	-3.37784389646200	0.11983808829600
H	1.08298301699800	1.92455062901800	1.37157509089800
H	-1.31769423511500	-2.40370860627200	0.48061340220400
C	-0.91030656752300	2.09861952450200	-0.46947613627100
C	-2.79682995343000	0.03933834834700	0.04844053112100
H	-0.18648711059900	2.87311171772100	-0.66241244712900
C	-2.21838317094200	2.27174398047300	-0.75397488970400
H	-3.52079719247900	-0.74609453504300	0.19618156913100
C	-3.17844426535700	1.25001897015700	-0.44610099920100
H	-4.21804383806400	1.43432369712800	-0.66293370465300
H	-2.55829098518400	3.18362438760400	-1.21698470746700

anthracene-13 6.48 [1.02] 6.95 [0.30] 6.95 [0.85] 8.60 [1.12] 9.13 [1.16]

C	3.24214965004600	-0.87229891584200	0.28792299044300
H	4.25790234101900	-0.74319929583400	0.63224403030000
C	2.60378367483600	0.24909965944400	-0.34798797112100
C	2.65394170298500	-2.09335454328200	0.46940803195500
C	1.39311757396800	0.09172720066900	-0.94767850108800
C	1.36053902083000	-2.26659571502100	-0.07161179623800
C	0.81760974681200	-1.19151026756800	-0.73359062503300
C	0.36034081735400	0.79470479203600	-1.87620221354400
C	-0.58143795946400	-1.10491460951200	-0.88751116639200
C	-0.61977633735700	1.19883357647400	-0.73701693818900
C	-1.36079883388500	0.00603458565100	-0.50699206948700
H	3.14600360534600	1.17915013220900	-0.40725375020900
H	3.18045003042000	-2.91307121349800	0.92415783653700
H	0.84448375109000	-3.21305113111800	-0.00488695501700
H	0.86409442094600	1.75448877134800	-2.11188093260400
H	-1.11117420328400	-2.05739240578600	-0.94090458816000
C	-1.02348996235300	2.24376248294000	0.03452907839000
C	-2.43917777816400	-0.17766861713500	0.32550359545600
H	-0.53668692059600	3.20444159486900	-0.01742716233800
C	-2.19491570737200	2.11743931158300	0.85967162597000
H	-2.95199182106700	-1.12599312927600	0.39052204188100
C	-2.88228576396400	0.95057002764500	1.05053793896400
H	-3.77090085299500	0.90981083683100	1.65430506544200
H	-2.56172243085800	3.00779338909100	1.34938127767400

anthracene-14 6.43 [1.06] 7.06 [0.97] 7.06 [0.13] 8.82 [1.12] 8.93 [1.05]

C	3.14194769414100	-0.63813802035100	0.62817278982300
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H	4.14827188275700	-0.46711926461900	0.97854224501800
C	2.51681129367500	0.36872324275200	-0.19459364669100
C	2.50325536479000	-1.78018800887400	0.95765277692200
C	1.29383589338900	0.14790574568000	-0.74354049171500
C	1.17066233510600	-1.98983674854900	0.45194478640400
C	0.63943291377500	-1.05248947927000	-0.35846742527600
C	0.39035741485100	0.74198605441200	-1.82826783268600
C	-0.81603785866500	-1.10845471875700	-0.74981619318000
C	-0.70872178650100	1.07768273420700	-0.90451477362900
C	-1.64041696505100	-0.04580403843800	-0.90142694083000
H	3.06699290149400	1.26758766143500	-0.42454043129800
H	2.97685540924500	-2.54081118969600	1.55458900074000
H	0.64475562183600	-2.90397729877400	0.68495378778500
H	0.85924120058700	1.65759121833200	-2.20696305415900
H	-1.29462712100400	-2.05388451287100	-0.50030034542100
C	-0.97558354596600	2.00130483088700	0.11022456777100
C	-2.95635408263100	-0.01241783015700	-0.36476466720400
H	-0.27784192953100	2.79413081570400	0.32192029430400
C	-2.31656792243000	2.13234431418100	0.48534034702000
H	-3.65176715387500	-0.82176978767400	-0.51675384763400
C	-3.29718514681700	1.13486658460000	0.30009851369300
H	-4.29640571579000	1.29253661361400	0.66632610775200
H	-2.63887365022700	3.06544713101200	0.92422772214700

## pyrene

pyrene s0min 0.00 [0.05] 2.89 [2.00] 3.96 [1.04] 4.38 [0.07] 4.71 [1.06]

C	2.733468070185	-2.043409579909	0.772898648218
H	3.575354629522	-2.672673761949	1.012157274513
C	2.947642313719	-0.777875864700	0.253799570221
C	1.446938127837	-2.507648895039	0.987777087119
C	1.873966816264	0.052296756147	-0.061476851075
C	0.344097660981	-1.711276723959	0.686881079072
C	0.554979275534	-0.415179871113	0.156293530588
C	2.055843392781	1.367474900137	-0.599468865684
C	-0.554926955210	0.414768778599	-0.156950208408
C	1.001158202845	2.156235523601	-0.896665982436
C	-0.344035963039	1.711153997980	-0.686845391044
H	3.953116148828	-0.424108250278	0.088990026766
H	1.289436741858	-3.495072426658	1.392220557228
H	3.062707563826	1.717542701271	-0.763951252452
C	-2.055800816766	-1.368080814472	0.598414384243
H	1.155142008700	3.144309031010	-1.300965791685
H	-3.062671314678	-1.718364352628	0.762394357743
C	-1.001094286879	-2.156677919424	0.895955784176

H	-1.155040322704	-3.144751632018	1.300264863069
C	-1.873901954391	-0.052684781230	0.060955824352
C	-1.446873638197	2.508148073302	-0.986120110881
C	-2.733393538825	2.044148644364	-0.770613528015
H	-1.289408283479	3.496054787803	-1.389406240966
C	-2.947558445981	0.778000061263	-0.252992496409
H	-3.575263286209	2.674032803636	-1.008279807231
H	-3.953025146526	0.424351814267	-0.087873461021

pyrene-CH-dissociation 3.54 [1.23] 4.34 [0.68] 4.34 [0.32] 5.88 [1.04] 6.42 [1.09]

C	2.65757778927800	-1.73354295210700	1.21382576662700
H	3.49282758072300	-2.31194784318600	1.57332688573700
C	2.88400231072500	-0.64897761659400	0.36915734933500
C	1.37837342688600	-2.06793449135600	1.58976147201700
C	1.82685978752100	0.11456029221200	-0.10924940911000
C	0.27648118135100	-1.32248513638100	1.12938745243200
C	0.50141056667300	-0.22035914279100	0.27217818223100
C	2.02478838050300	1.23355157105300	-0.97816037499500
C	-0.59661237257000	0.54627667090000	-0.20314177887700
C	0.97830918029100	1.96783462316300	-1.43382376538700
C	-0.35586445621400	1.66250173158600	-1.07195924741100
H	3.89117511062900	-0.39414314473000	0.07980003043700
H	1.20415316014000	-2.90735663401000	2.24388396623300
H	3.03280476125300	1.48525015565600	-1.26750035052800
C	-2.10124663967200	-0.88943700506000	1.02947438624500
H	1.15017485787800	2.80731302912100	-2.08860470620700
H	-3.10987599559900	-1.14228770336300	1.31827938712100
C	-1.05411268636400	-1.63526386497700	1.49393855887800
H	-1.23184425705700	-2.47457571624300	2.14751856398200
C	-1.89462020648200	0.20717451387000	0.17889511809300
C	-1.45321450223200	2.43566880577900	-1.54915401711600
C	-2.72163411505300	2.14554715772200	-1.20558011586100
H	-1.22291295543100	3.26877059081500	-2.20105039564900
C	-3.06914862449000	1.01607735939400	-0.32046789193000
H	-3.64065820339400	1.38904889992700	0.53494848404100
H	-3.77010488278800	0.35392244901700	-0.83794261861400

pyrene-01 4.69 [1.16] 5.21 [0.36] 5.21 [0.83] 7.33 [0.88] 7.35 [1.04]

C	2.97438364526700	-1.85319162068500	0.74057840323900
H	3.83944414842600	-2.45913481787500	0.95665638509500
C	3.14640882897500	-0.51244896146700	0.43199171651300
C	1.71340233478600	-2.42643246748600	0.79992777599000
C	2.03818430967000	0.30009798765100	0.14795608662000
C	0.57009715357900	-1.66042270179000	0.52538087614600
C	0.75719556804000	-0.30392874654800	0.16291334366100
C	2.11370431835500	1.69527485932000	-0.10555341197000

C	-0.36264023900000	0.48120472492500	-0.11450637859900
C	0.98659251055300	2.45931049298200	-0.33354627652000
C	-0.27174458352900	1.85683489360500	-0.37335245397300
H	4.13609658131800	-0.08426934118000	0.42121896275300
H	1.60505378105100	-3.46452632408900	1.07122958126900
H	3.08351756779300	2.16673152317200	-0.10193391555200
C	-1.85423937603400	-1.33324839365300	0.39749081478900
H	1.08778391003500	3.51853625286000	-0.50955129227400
H	-2.84885668100700	-1.73635980415900	0.50472545633400
C	-0.76110927366500	-2.14283253435800	0.63352114400600
H	-0.91406322082200	-3.16928662691600	0.92656008663400
C	-1.67185570774900	-0.01199391853000	-0.01351769452400
C	-1.56098196391200	2.48287363085900	-0.64063754831600
C	-2.55526617892600	1.86285768287800	-1.46996214082600
H	-1.71087186694100	3.50109584624200	-0.30133479646800
C	-2.69090932205500	0.97448380301900	-0.35094039847400
H	-3.40783617353900	2.44132154519500	-1.78426635087500
H	-3.62949646228200	0.93994710892200	0.18981630410700

pyrene-02 4.82 [1.11] 5.26 [0.90] 5.26 [0.10] 7.35 [1.30] 7.50 [1.27]

C	2.80896411719400	-1.84081153282100	1.28205172466900
H	3.62809439680300	-2.39337075048500	1.71411882784600
C	3.05934993050300	-0.60602597691600	0.67681913476000
C	1.53630105078900	-2.35897798202400	1.33324311552500
C	2.03107069715200	0.13451691576600	0.13856006839500
C	0.46275712532900	-1.64778339043000	0.78080122620800
C	0.70910868925500	-0.39198637626500	0.18712181740300
C	2.23608003338500	1.40397043796100	-0.63668146004200
C	-0.38288701674800	0.34803192857500	-0.37469943691800
C	1.09249251110700	2.23459798015200	-0.70165505792800
C	-0.20815244372200	1.67756363918300	-0.87508288896800
H	4.05755015884700	-0.20688389637700	0.62683132857300
H	1.35304283379700	-3.31793928467000	1.79120037451900
H	1.99321952392000	0.89545650900400	-1.60909613171800
C	-1.89110287984900	-1.49528982494800	0.21576288780300
H	1.14973520709900	3.31718062415100	-0.61509418400600
H	-2.88877793807200	-1.90442525460600	0.21352714920900
C	-0.86778664551000	-2.17837889248500	0.76639150140900
H	-1.03510863947700	-3.14764844566800	1.20898782811100
C	-1.68502025542600	-0.19810741167000	-0.35545334703500
C	-1.30864114093700	2.41283278563100	-1.31533515715200
C	-2.57063747181700	1.84565292658800	-1.33304420534700
H	-1.15916885970100	3.42360745188400	-1.66020066333700
C	-2.74888762450500	0.55782683771000	-0.86081753486600
H	-3.41441310120200	2.40725657586200	-1.69786105849600
H	-3.73741287932600	0.12578817313000	-0.85416240064200

pyrene-03	4.52 [1.06]	5.32 [0.43]	5.32 [0.62]	6.69 [1.06]	7.30 [1.06]
C	2.53021732126400	-1.69623213490100		1.47250576965400	
H	3.37234577068500	-2.22877302480400		1.88225296611900	
C	2.64102738994800	-0.34471178592200		1.18963388785500	
C	1.34910292155200	-2.37170644689700		1.21194368578600	
C	1.56248998083600	0.35946761416200		0.65516827845900	
C	0.24415253749200	-1.70603708169500		0.67902839909000	
C	0.34771430083000	-0.31977975553300		0.41427839578200	
C	1.64413115782400	1.73789707337300		0.28980423936600	
C	-0.77074005117900	0.37376237725500		-0.10308406206400	
C	0.60548349211400	2.37925350027700		-0.29770875999600	
C	-0.64353392851900	1.72581669962600		-0.52927008137600	
H	3.57352619701800	0.16839439514400		1.36442533543200	
H	1.27926242251500	-3.42898221712000		1.41366682496500	
H	2.57123905255900	2.26062255465200		0.46631533231100	
C	-2.04401930407500	-1.70333107744900		-0.15796773414500	
H	0.70717694923600	3.40922386319300		-0.59878058773500	
H	-2.97084635188600	-2.20525472826700		-0.37589801882800	
C	-0.97497148381400	-2.37425233489600		0.35668658204500	
H	-1.03549837537600	-3.43699606015800		0.53297185890600	
C	-1.99907350394300	-0.30525890386300		-0.34913108671300	
C	-1.67568173455200	2.37105420189600		-1.27588863223100	
C	-2.85805166860400	1.71793966354700		-1.47249916155900	
H	-1.42584378562500	3.28039730524200		-1.80457886833800	
C	-3.14819608538100	0.55419632589200		-0.62547202393300	
H	-3.55799565435800	2.09141600343700		-2.20915104506900	
H	-2.99373787512300	1.12854297901300		0.31788278095700	

pyrene-04	5.07 [1.10]	5.67 [0.34]	5.67 [0.82]	7.15 [0.96]	7.73 [0.40]
C	2.71558951027900	-2.27074751088400		0.12878859659500	
H	3.04629894885800	-3.23000774205200		-0.24453953386400	
C	3.01360921996700	-1.08681895587900		-0.49062151100700	
C	1.48286519075400	-2.14767409058900		0.86199682418900	
C	1.92948546138800	-0.18517064580600		-0.57641537601200	
C	0.32693270565000	-2.06859211373000		0.05010477700200	
C	0.58802429788900	-0.72648967488200		-0.40566105373900	
C	2.06003123009000	1.16622424706000		-1.01285855355900	
C	-0.54956093442400	0.11448286559200		-0.64108329769400	
C	0.99039713104300	1.95770906071200		-1.21769810293200	
C	-0.35443460078400	1.46077346842700		-1.05732724860800	
H	3.90932766626400	-0.93175184143600		-1.07374371394400	
H	1.47897870898100	-1.77942278507100		1.88779388234900	
H	3.05630966363500	1.55274922393300		-1.16136017120400	
C	-2.05224006074100	-1.76909220149800		-0.12801083965800	
H	1.11619046849600	2.98145133799300		-1.53088105269400	

H	-3.05758758841100	-2.14911143644900	-0.05200218671200
C	-0.99271032234100	-2.54175994628400	0.20687708817500
H	-1.13785014072700	-3.53974291940200	0.58850765496700
C	-1.86320976216900	-0.41103838262400	-0.53755340365400
C	-1.46118695717700	2.24839116520100	-1.33551502817600
C	-2.74599681857500	1.73024582637500	-1.21376950774000
H	-1.31665721331600	3.26528635412100	-1.66313895842200
C	-2.95023702143100	0.42486697811500	-0.82863601392400
H	-3.59363811004900	2.36003753815200	-1.43317622957200
H	-3.95002923043200	0.03021691050200	-0.74645024592000

pyrene-05 5.54 [1.36] 5.80 [0.44] 5.80 [0.67] 7.69 [0.74] 8.04 [1.18]

C	2.33300766306400	-2.07266095986200	0.80303605486200
H	2.77478166755700	-3.00106404946400	0.46286058044100
C	2.89117718851000	-0.83158460265900	0.28357209650500
C	1.39723358986100	-2.08153329364200	1.89954309952600
C	1.94163973936300	0.20349938999200	0.09919750248700
C	0.56265875143900	-1.66818102068700	0.79164185844000
C	0.65979799028500	-0.30459403421100	0.26194849077400
C	2.09835994763100	1.54546420545700	-0.32408943176200
C	-0.46556004142800	0.39459729194300	-0.17461658083600
C	0.99623027519700	2.29399884394600	-0.62543130036700
C	-0.31196870329400	1.73644698601000	-0.59649888700000
H	3.92289429129800	-0.76922506909700	-0.01844346963100
H	1.16955338253700	-3.02449711607900	2.37351412288900
H	3.08555711091500	1.96799743413200	-0.42150948717600
C	-1.73463801721000	-1.70496612435200	-0.00050361285000
H	1.11111095935900	3.31741247919900	-0.94535674823400
H	-2.66366781940800	-2.22967867021200	-0.16034381603600
C	-0.65287855466700	-2.38058096973500	0.43300112808200
H	-0.71695774640500	-3.43443995558200	0.64968274760400
C	-1.71426445626900	-0.27803781318000	-0.27442168180300
C	-1.46854627067900	2.43044613005600	-1.01110751422600
C	-2.68230632087700	1.79400608278800	-1.05077967946300
H	-1.38448200214300	3.46177387343900	-1.31500437112800
C	-2.80731135624700	0.43585843252100	-0.70847984881900
H	-3.55654578634400	2.33373041941400	-1.37711268462400
H	-3.76459912948600	-0.05145164820200	-0.80562451093100

pyrene-06 5.75 [1.65] 6.03 [0.19] 6.03 [0.39] 7.65 [0.54] 8.07 [1.12]

C	2.66741578326800	-1.82281301700000	0.96116389254300
H	3.34676033446000	-2.30643079310500	1.64428861736700
C	3.06768261875400	-0.95969410513000	-0.02254610723800
C	1.24267406078700	-1.93507018283900	1.11214468832500
C	1.98818920767000	-0.20727299736400	-0.50112710661900
C	0.31921457228200	-2.08391871970500	-0.04030161404100

C	0.64506517781700	-0.69585061730100	-0.02222310746400
C	2.09843980372000	1.07694234113800	-1.07211568544800
C	-0.45972678135500	0.27460705176400	-0.05746596436900
C	1.08189537987900	1.96905941041000	-0.97836976168500
C	-0.22341457727200	1.60213462419700	-0.45805948020800
H	4.09141421345800	-0.75145461806700	-0.28090543093600
H	0.81946707379400	-2.09833858578700	2.09062819565900
H	3.05472547236100	1.38706094621500	-1.46348499559400
C	-2.03932905366800	-1.59539869897500	0.17886831833600
H	1.21576481024300	2.98074268157000	-1.32628367904100
H	-3.06408688905700	-1.91800438771700	0.27584692528900
C	-1.02101782866200	-2.49398638765600	0.14052054300400
H	-1.22212375148500	-3.54260463226100	0.30756161218100
C	-1.77696866207000	-0.18217931202300	0.08090149515200
C	-1.28095813984300	2.49838242615300	-0.50673087255600
C	-2.57672786328100	2.07966874756200	-0.21303728642000
H	-1.09962236020500	3.51692816058300	-0.81159016121400
C	-2.82669789388300	0.75263437306400	0.04452433505300
H	-3.38866069767500	2.78793119095800	-0.24090586963100
H	-3.83769747405700	0.40881879872700	0.19546966365300

pyrene-07 5.89 [1.15] 6.08 [0.87] 6.08 [0.25] 7.74 [1.10] 8.28 [1.20]

C	2.70844773009800	-2.14507130276000	0.50828077195800
H	3.57721091564100	-2.78446951652300	0.54308405559800
C	2.90273153910600	-0.75232712259000	0.41207542230600
C	1.46831714524400	-2.71370874749300	0.58445506233900
C	1.80850363626800	0.07811618383500	0.29831768807300
C	0.31604295368400	-1.88138651952300	0.63262078410400
C	0.51117773059000	-0.49309890947600	0.33673994695800
C	1.90231285190100	1.50290095169900	0.09564633555700
C	-0.62995839509100	0.25287190768900	-0.05544295685100
C	0.82407834179200	2.24699872938900	-0.20044682802300
C	-0.48936038569500	1.66913488778600	-0.34096557115600
H	3.89917507256000	-0.34328070361800	0.38501933757500
H	1.35873435686200	-3.78077213334600	0.68883702760500
H	2.87515638477600	1.96413301358200	0.16327737259800
C	-1.87515326861000	-1.04244247912100	0.90020963586300
H	0.92209204849500	3.30528427046100	-0.38381735900600
H	-2.33520012433000	-0.71306899248900	1.83670284248100
C	-1.01167953588100	-2.20036965750100	0.83025437393300
H	-1.45456849729400	-3.05277868260200	0.33162441683600
C	-2.00436315802700	-0.26855160821600	-0.23737581025800
C	-1.53146496031100	2.38712602841000	-0.87115897350500
C	-2.80236475468100	1.82655774548600	-1.10869699905200
H	-1.35930809720300	3.41991155149200	-1.13111769640100
C	-3.04006024824700	0.53633165502100	-0.73468279774700



H	-3.58652319969800	2.43107248127000	-1.53113688651400
H	-4.02341485750300	0.10438945960000	-0.82298649799600

pyrene-08      5.93 [1.37] 6.21 [0.13] 6.21 [0.68] 8.22 [1.22] 8.46 [1.27]

C	2.74929912412500	-2.35949510362900	0.35321716966900
H	3.57118087146800	-3.05025355072300	0.44940800730300
C	3.00735760549700	-1.03888796073500	0.06256134682000
C	1.44336275000800	-2.82785709536100	0.57574060919100
C	1.95256032528200	-0.12166287728000	-0.07337939799000
C	0.40274203482100	-1.94105266657000	0.48762734143200
C	0.65282002558200	-0.60322087197800	0.09789737684200
C	2.10309628644300	1.27891408476800	-0.35062647651900
C	-0.49594250287400	0.20780769070500	-0.14528894482000
C	1.02592765541400	2.08611321774400	-0.47903571748300
C	-0.31786857663300	1.57939742128600	-0.40118556809700
H	4.02435131802800	-0.70198394605600	-0.06080798847500
H	1.27571322287700	-3.85551911751100	0.85030977803900
H	3.09835499236500	1.68330452221400	-0.44693177852300
C	-1.89344924601400	-1.88232134678200	-0.37996854974700
H	1.16067062283300	3.13871260143800	-0.67212075652800
H	-2.90521634243400	-2.23196577761600	-0.47271283489300
C	-1.04508523082800	-1.97428260442700	0.74058157508200
H	-1.27105171504500	-1.52289917115900	1.72312582947400
C	-1.79751153305200	-0.40211989806100	-0.18120643727400
C	-1.45313471993800	2.36920692641100	-0.59671459583900
C	-2.72223762474000	1.81056757442700	-0.53695469608300
H	-1.33889804318000	3.42337373313100	-0.79392803414800
C	-2.90329774654500	0.45916638861900	-0.29648359074400
H	-3.58459552071000	2.44099795063600	-0.68274176386200
H	-3.89578457984000	0.04143435435900	-0.28060652432300

pyrene-09      5.95 [1.53] 6.27 [0.22] 6.27 [0.56] 8.08 [0.87] 8.58 [1.17]

C	2.46173654851100	-1.73036332967500	1.59119581867100
H	3.30411117804100	-2.13641414813900	2.12912107286100
C	2.74168959172400	-0.78568063372300	0.52221673953200
C	1.21814007713900	-2.05049412574700	1.95523958198200
C	1.69011571031000	-0.01761307509900	-0.06475195689400
C	0.09686054223900	-1.62053022057800	1.04074859638400
C	0.39676281379900	-0.33829061328800	0.29396641846200
C	1.86735403932800	1.13479375148000	-0.87937387628300
C	-0.67662552267900	0.43326327932900	-0.06839668089100
C	0.80891211787100	1.93541647276800	-1.21707379715500
C	-0.51091743374600	1.63465117329800	-0.78700500668600
H	3.76753702962100	-0.57681285038400	0.26909913480400
H	1.00742069303200	-2.68830567712400	2.79599133550400
H	2.86286216304300	1.40090357533600	-1.19892143518900

C	-1.81394042749300	-1.34088912683500	1.00353084047000
H	0.98075974275200	2.82914338900200	-1.79582804803400
H	-2.47041644097800	-1.68196546474900	1.78519908244400
C	-0.84913806664800	-2.42056953154000	0.48524618189200
H	-0.97219099626300	-3.43417590779900	0.83536272480300
C	-1.92321991051100	-0.04920079206600	0.43601006733900
C	-1.65551516939500	2.43379198864200	-0.94528159391200
C	-2.84685843289900	2.02664979410500	-0.36898513090600
H	-1.60005433301400	3.36700199185800	-1.48153400088400
C	-3.00272012868900	0.81834058134700	0.32341253023900
H	-3.71234777522800	2.66194511495900	-0.47695712254900
H	-3.97191628307000	0.54849358427500	0.71014669120400

pyrene-10 6.17 [1.85] 6.29 [0.17] 6.29 [0.19] 7.40 [0.95] 8.56 [0.32]

C	2.66657874273900	-2.33250799835500	0.41972469432000
H	3.54211154289200	-2.94483526987600	0.56363486011200
C	2.82278093567900	-0.94805368645900	0.27403955657500
C	1.42177239463800	-2.91324401398300	0.44091015836300
C	1.71915136053500	-0.11889246337800	0.06092268997300
C	0.27916870538500	-2.08719497790700	0.29509048535300
C	0.46516525835900	-0.71419159489200	-0.04100441779800
C	1.79145369808100	1.32745854751200	0.00957129150900
C	-0.74275333876300	0.03577326790700	-0.33046357267100
C	0.69124009822200	2.07403649204500	-0.17706798173800
C	-0.60288760431300	1.49248958910900	-0.45475150834300
H	3.80800088288900	-0.51319696126900	0.32827819271700
H	1.30600735390900	-3.96773072877100	0.63073709371600
H	2.75192404137400	1.79720735147000	0.15092012769000
C	-1.91152725136200	-1.15231375477200	0.37218462485100
H	0.76844057445900	3.14990212480000	-0.21152114299700
H	-2.56544462267100	-0.84345023411700	1.17759339690500
C	-1.05321704342300	-2.34960571810000	0.51144459839700
H	-1.47417825384600	-3.31835081886200	0.72430822259700
C	-1.97698641841700	-0.52695601300700	-0.90815806769100
C	-1.57940864493900	2.22256023924100	-1.07480050408000
C	-2.75340997524400	1.63832084933000	-1.60783560095200
H	-1.41981422327400	3.28170186055200	-1.20856338865100
C	-2.95901286407300	0.28964270760200	-1.46352979504800
H	-3.48333541377300	2.25962840538500	-2.09860676539800
H	-3.89899569884900	-0.15602204559600	-1.75399247397200

pyrene-11 5.91 [1.78] 6.32 [0.21] 6.32 [0.27] 8.18 [1.01] 8.65 [0.65]

C	2.40766877214300	-2.02820160549700	1.10315233866700
H	3.21603942903400	-2.56684326004600	1.57360171972800
C	2.71858680908700	-0.80713580102700	0.41746495166200
C	1.13562473747600	-2.42535040940400	1.25114794869600

C	1.65333469679100	0.10383306180400	-0.00466196036100
C	0.08647409276400	-1.78988389433800	0.35942688390800
C	0.36075584062800	-0.33878955563500	0.06628964504300
C	1.88062506123300	1.42482447413300	-0.44832763067100
C	-0.69888540363400	0.46181927679900	-0.32098430236200
C	0.83495060158300	2.24608604711900	-0.80147543111700
C	-0.49411454967300	1.78074853883600	-0.76186415775100
H	3.74495028358400	-0.49583632753000	0.32127072815700
H	0.85694415669700	-3.26402610641000	1.86470947685800
H	2.89247340630900	1.79482673000100	-0.50351684851000
C	-1.91974857327300	-1.56841093665400	0.13755664752700
H	1.03221625031400	3.25749549677200	-1.11990033489200
H	-2.39401318823800	-1.82046168613400	1.07751492708800
C	-0.81397738341600	-2.47621704975900	-0.37530439781800
H	-0.91138435367800	-3.54136856989500	-0.23754013832700
C	-1.97731904024200	-0.16696543965700	-0.27483539759400
C	-1.65173428668400	2.52996086944900	-1.10736021985800
C	-2.88116562363200	1.94816268751300	-1.01547296186300
H	-1.54983738584100	3.55271656008100	-1.43325487805400
C	-3.05847848748200	0.59407771492500	-0.61316189286400
H	-3.75731969047700	2.52249867554900	-1.27141179709100
H	-4.05066826651900	0.17339698077800	-0.60625430832900

pyrene-12	6.12 [1.29]	6.66 [0.33]	6.66 [0.55]	8.33 [0.79]	8.59 [1.02]
C	2.58495387675800	-1.58264077571900	1.12149515178400		
H	3.41614717243800	-2.07448613207200	1.59882063470800		
C	2.79074760918400	-0.43165883076000	0.37424230806300		
C	1.32300792646800	-2.14360321481700	1.16903267416300		
C	1.72397047428300	0.21207017606400	-0.25134385716100		
C	0.23289667818900	-1.50229579255100	0.57025147633100		
C	0.42109371548900	-0.24748432185700	-0.02635649027100		
C	1.92996923712900	1.17512215520200	-1.31224971571000		
C	-0.71562734982900	0.43728768484900	-0.63526477853700		
C	0.92641019618600	1.52009898123100	-2.15117998058000		
C	-0.47178758385300	1.18199423289500	-1.99551516089300		
H	3.79109780351400	-0.05509203477000	0.22830937921600		
H	1.17283737622800	-3.09969989522700	1.64561303306700		
H	2.94194510923300	1.50035118102900	-1.50544888033000		
C	-2.08018021615300	-1.63729895766100	-0.23990346543900		
H	1.17905568251900	2.11831691487800	-3.01668260343100		
H	-3.00826948776100	-2.17570289944100	-0.34357285903000		
C	-1.03298393922100	-2.18341244554000	0.41697950555900		
H	-1.11374782555800	-3.18072945690800	0.82100442484800		
C	-2.00879330216800	-0.26750531155000	-0.61949557330100		
C	-1.12153010476300	1.88274233521400	-0.71251052198600		
C	-2.55127124523700	1.91990478176400	-0.66826403974700		

H	-0.51480159989600	2.68753831059900	-0.33963948060300
C	-3.06284665653000	0.64281657430600	-0.69902429108800
H	-3.12870669446100	2.82776047367100	-0.65107815062800
H	-4.10467698445500	0.37587972045600	-0.71834497644500

pyrene-13      6.68 [1.50] 6.95 [0.53] 6.95 [0.26] 8.94 [1.09] 9.21 [0.69]

C	2.36765082618400	-1.82523919920700	1.17721848779400
H	3.05959673780800	-2.28184150362000	1.87160633500000
C	2.81722553400600	-0.80947345336500	0.40829976085400
C	1.10180900576100	-2.50792429541900	1.00472280777700
C	1.85447962153200	-0.04842081512100	-0.39914008439200
C	0.36367750514900	-2.04094184964200	-0.25372784589700
C	0.56678619892300	-0.61262531333000	-0.50803793447800
C	2.04542823341400	1.26453914658000	-0.77463521037300
C	-0.49746865031200	0.25599202921500	-0.55845265354100
C	0.95862097970000	2.07753631429000	-1.13359014104000
C	-0.32319312260500	1.60866579583000	-0.93743279294200
H	3.80646993061800	-0.40598357763900	0.55047633511300
H	1.16854854835200	-3.57232627455200	1.17641178515800
H	3.02823942277600	1.70270083243300	-0.69928475953400
C	-1.74984825732700	-1.23696882682600	0.87076697199100
H	1.12407925321100	3.09858344341100	-1.43906629482800
H	-2.59297191163500	-1.49251585577200	1.49211212902300
C	-0.65238024145300	-2.24846044570500	0.66576834121000
H	-0.95557308637500	-3.26174444154300	0.89521792740400
C	-1.74214936288000	-0.13924516348200	0.11206621777500
C	-1.47623059341500	2.46691826886400	-0.98061670268900
C	-2.71671364391800	2.04601025478800	-0.49091522968700
H	-1.36302153568100	3.46749793218200	-1.36557068403800
C	-2.86130011800700	0.80716988191300	0.06157317284900
H	-3.55518069079900	2.72170308378800	-0.52395707234500
H	-3.80308420665600	0.50299837762900	0.48810661065900

pyrene-14      7.31 [1.99] 7.40 [0.21] 7.40 [0.05] 8.94 [1.04] 9.23 [1.15]

C	2.76000461624900	-2.38620734965300	0.13903120668400
H	3.55825714722900	-3.10340328638700	0.06418478397100
C	2.89502434082600	-1.04098905407900	-0.12153782161400
C	1.45363919581900	-2.70325570531200	0.43717939865600
C	1.64432510789700	-0.26021180884100	-0.03975802173600
C	0.51100959064200	-1.56715873091100	0.39905289808300
C	0.47873215944200	-0.71882060326800	-0.78647946282900
C	1.75886304049500	1.20251485544900	0.12484454653000
C	-0.59810536624200	0.18448089783300	-0.87728352068600
C	0.92311609887600	2.02994769132400	-0.52291431507300
C	-0.35566004239000	1.56044144663800	-1.05945020824800
H	3.82028935329600	-0.56793442949500	-0.40464748614600

H	1.10457358859500	-3.70006756853500	0.64825852667300
H	2.61352957556700	1.59774701090400	0.65130439057600
C	-1.90931644709900	-1.23598353857600	0.57521483022300
H	1.09864743614800	3.09517962985600	-0.49971138032000
H	-2.85876469626300	-1.46831296762600	1.03416069017300
C	-0.77557025681900	-1.72029741758200	1.10682719738200
H	-0.81200428941500	-2.35496325113000	1.97842845533300
C	-1.88761332088500	-0.20655376920000	-0.46553608128000
C	-1.43198490186500	2.40039955919500	-1.31283026997700
C	-2.73528129971000	1.91239037442700	-1.24931457875200
H	-1.26421436422100	3.45538975554800	-1.46962381441700
C	-2.95653569821700	0.64197868020000	-0.72230022131100
H	-3.56726396006000	2.56241889501600	-1.46270673489500
H	-3.95402783785700	0.35267280122400	-0.42732225994800

pyrene-15	8.02 [1.53]	8.22 [0.28]	8.22 [0.70]	9.81 [1.05]	10.19 [0.58]
C	2.46018813449400	-2.17079077692700	0.12461664414000		
H	3.27394082804000	-2.87371007863700	0.04279351495400		
C	2.52001653448000	-1.00078022210000	-0.53870127819400		
C	1.31860084159900	-2.52430878544000	0.91622433031200		
C	1.48760502032200	-0.00074777001700	-0.41691641787000		
C	0.26230628868400	-1.68986844723200	0.97434803306700		
C	0.25040455326600	-0.38122565189100	0.30197641633400		
C	1.77049581746800	1.29029110019000	-0.75704230553200		
C	-0.52723316087600	0.82565321394700	0.86209067751600		
C	0.81653120907000	2.32690455587500	-0.54799902243100		
C	-0.33269827871900	2.05650599530700	0.12842977170100		
H	3.38399431470000	-0.75268151080900	-1.13383537011100		
H	1.27084436352200	-3.49599129406700	1.38014060206900		
H	2.71409900375900	1.51566656392200	-1.22651359919100		
C	-1.96002898701600	-1.17959509955700	0.98694471185700		
H	0.93268473844000	3.26634833063200	-1.06717455015900		
H	-3.01728238739000	-1.18585107058800	1.19557854638500		
C	-1.05932776140000	-2.02617016543200	1.47069699135500		
H	-1.25094711063500	-2.85953895683000	2.12398454232100		
C	-1.37835404939700	-0.08395119820000	0.15194891714900		
C	-1.49406424714400	2.69232338206100	-0.44818337212600		
C	-2.40936843891600	1.78745096096400	-1.06283056278000		
H	-1.50155532851000	3.73867482654500	-0.70313977148200		
C	-2.24900960697100	0.45051302477600	-0.94409009648000		
H	-3.16587304476800	2.18458058343400	-1.72142159240100		
H	-2.84995844938300	-0.23649712080900	-1.51748934824600		

pyrene-16	8.96 [1.46]	8.96 [0.58]	9.37 [1.81]	10.24 [0.30]	11.11 [1.34]
C	2.46038957386100	-2.37130023649700	-0.81844178302000		
H	3.17713773188900	-3.12216756542400	-1.10700905455100		

C	2.86344365329900	-1.05012816601300	-0.64022348337200
C	1.16760720685500	-2.72815380051300	-0.51512948046500
C	1.96474482475300	-0.06186621341700	-0.23179714593700
C	0.21688574048200	-1.76201552267400	-0.13983699550400
C	0.57722487327300	-0.40525668376000	-0.17182621962000
C	2.45798297357400	1.09797885400100	0.42803676185700
C	-0.45152047543700	0.58024602771700	0.04954764351500
C	0.32763223676700	2.06621846184700	-1.74322373371300
C	-0.39893184141500	1.88548882300300	-0.51870044124000
H	3.90843365546800	-0.79846809827900	-0.72051916403800
H	0.87605146331400	-3.76644819179700	-0.53845045387900
H	3.52840989082100	1.27650063951700	0.32987679545400
C	-1.88722332945300	-1.20348418447200	0.91336267573800
H	-0.02252202936900	2.90961876139600	-2.34332344646800
H	-2.80524170839700	-1.49142654090400	1.40012037891100
C	-1.06542288386400	-2.13342904263900	0.38734495582100
H	-1.31725069991000	-3.18112108351700	0.43223056422300
C	-1.60444527530300	0.19484107526800	0.75518642380400
C	-1.27757863949800	2.85138866740200	-0.02700854389300
C	-2.28341653932500	2.51600493892500	0.87353491956600
H	-1.23853212984300	3.84611899045000	-0.44149689234500
C	-2.48755287029000	1.19208708947800	1.19734837784700
H	-2.97519075061500	3.26756891151900	1.21548352167800
H	-3.35035177413300	0.90546418682500	1.77760252648100

Cartesian coordinates (in Å) of the S<sub>1</sub>-minimum structure (S<sub>1MIN</sub>) and the TS structures between S<sub>1MIN</sub> and the three lowest MECIs at the SF-BHLYP/6-31G\* level for 5 PAHs, benzene, naphthalene, phenanthrene, anthracene, and pyrene. Relative energies in eV and the <S<sup>2</sup>> values for each state are also shown.

benzene-TS1	5.77 eV	3.04 [0.09]	5.29 [1.93]	5.77 [0.24]	7.10 [0.82]
C	1.376924815535	-0.032109960446			-0.122042756751
H	2.445948838101	0.028892815878			0.016097729708
C	0.587393600542	1.147616534965			-0.042335530830
C	0.733700088495	-1.248627832421			-0.284043275645
C	-0.655817184433	-1.183186419410			-0.092374012898
C	-0.706022084527	1.225834659052			-0.693803237460
C	-1.288596035147	0.077229383229			-0.044139074051
H	1.259021576165	-2.178492857703			-0.409718562493
H	-1.233716501584	-2.075761764377			0.094122349415
H	0.937239794718	1.963171771839			0.578856227598
H	-1.243118896695	2.158500179768			-0.693613368777
H	-2.214647449333	0.168256900670			0.510163102715

benzene-TS2,TS3	5.88 eV	5.16 [0.98]	5.70 [1.16]	5.88 [0.71]	6.93 [0.28]
C	1.360171157940	-0.071660913064			-0.353152876101
H	2.090088735288	-0.200082284839			-1.140680549916
C	0.747653856522	1.175634843878			-0.146471684809
C	0.704673428456	-1.229025172404			0.234869957788
C	-0.538751293109	-1.219703164356			-0.514342054928
C	-0.623430016151	1.150468482688			0.115137581104
C	-1.274718567172	-0.052323059667			-0.219614997182
H	0.775846477868	-1.481364814617			1.291197599311
H	-0.939304780943	-2.044672116728			-1.082590888065
H	1.259758623465	2.101833735857			-0.360286313975
H	-1.183187892785	2.038410926649			0.351291376761
H	-2.354982319779	-0.080573833120			-0.267276668200

benzene-S1min	4.78 eV	0.16 [0.05]	4.74 [2.00]	4.78 [1.10]	6.31 [1.02]
C	1.420604424358	0.000055378981			0.000156214024
H	2.496594769884	0.000089652998			0.000325229003
C	0.708204149696	1.230818139433			0.000368884010
C	0.708285036661	-1.230755837437			-0.000276926022
C	-0.708175692660	-1.230803456457			-0.000498191011
C	-0.708256896655	1.230770911421			0.000144109994
C	-1.420576907353	-0.000040420992			-0.000290371992
H	1.246226146454	-2.162822798015			-0.000438080021
H	-1.246057166452	-2.162905442007			-0.000828851013
H	1.246083260447	2.162921201012			0.000702243980
H	-1.246200290430	2.162836895032			0.000306071993
H	-2.496566832871	-0.000075223022			-0.000463332994

naphthalene-TS1		5.76 eV	3.06 [0.14]	4.14 [1.89]	5.76 [0.31]	6.22 [0.95]
C	2.425257571786		0.703434755192		0.042111423152	
C	1.227681924822		1.366195600861		0.204018088634	
C	2.444043536360		-0.663878072177		-0.210376408224	
C	0.004590225868		0.649468227642		0.097919636158	
C	1.247258423103		-1.408000063820		-0.241406027548	
C	0.044070794426		-0.789969564742		-0.033508189720	
C	-1.231598037672		1.278811376978		-0.007088612018	
C	-1.236016335345		-1.455633374066		0.245961325167	
C	-2.465885155127		0.605697151562		-0.182635804806	
C	-2.458187970758		-0.764090334038		-0.114667327607	
H	3.353155529422		1.247277670784		0.116113268767	
H	1.207853518297		2.419214226237		0.437420974982	
H	3.385904801885		-1.168301062769		-0.350888223852	
H	1.271398318267		-2.477745421786		-0.364912040115	
H	-1.234489485146		2.358970832482		-0.042133741738	
H	-1.278680543999		-1.620710147923		1.330659974806	
H	-3.337152121344		1.157187401309		-0.497435753930	
H	-3.372010674097		-1.312211484200		-0.305591831259	

naphthalene-TS2		5.59 eV	3.18 [0.07]	5.00 [1.95]	5.59 [0.28]	6.82 [0.99]
C	2.362715595473		0.553647373174		-0.089639218433	
C	1.194726951325		1.378970539244		-0.085811357349	
C	2.450455232180		-0.658285415918		0.655272320346	
C	-0.046915585916		0.764650903032		0.095087884114	
C	1.296031234146		-1.275398300189		0.036298464740	
C	0.014139302867		-0.671903829806		0.019537007492	
C	-1.290168490015		1.418514846910		0.154171351167	
C	-1.190778428621		-1.370662739546		-0.112316386838	
C	-2.457634357216		0.693975646950		0.099131576414	
C	-2.398120124207		-0.701779483935		-0.054842869748	
H	3.199244019395		0.885847578792		-0.694691542239	
H	1.283510071291		2.432831505802		-0.297625419620	
H	3.381875946344		-1.199057736093		0.626488917490	
H	1.406760671521		-2.247145227150		-0.426752034865	
H	-1.316280038860		2.495561618083		0.212109080788	
H	-1.174887602822		-2.443759263003		-0.218863462209	
H	-3.412464062495		1.190166782795		0.140336148337	
H	-3.315304184445		-1.263818173596		-0.129256615212	

naphthalene-TS3		5.75 eV	3.86 [0.22]	4.52 [1.83]	5.75 [0.29]	6.56 [0.88]
C	2.371016207474		0.668266793225		0.004864735959	
C	1.185665068688		1.329484767225		-0.225077106645	
C	2.420821010447		-0.708615612150		0.281562746859	
C	-0.055886382998		0.673909092893		-0.102565326156	



C	1.242404144086	-1.420716292743	0.259728010362
C	0.021013507951	-0.774499688410	0.067532499717
C	-1.310071843743	1.344719056027	-0.189101371516
C	-1.203615123326	-1.282074489316	-0.445911259916
C	-2.475685512644	0.646208937417	0.130652965688
C	-2.402600785331	-0.729074171728	0.160239958501
H	3.293349219445	1.226063839680	-0.044054633390
H	1.196401358596	2.379241089487	-0.470902269029
H	3.363720734919	-1.199899435835	0.447243076467
H	1.246851751800	-2.491754447989	0.386792113412
H	-1.304430712078	2.420183216292	-0.247785454679
H	-1.227313697637	-1.849442229151	-1.372029857210
H	-3.336597235440	1.168744593167	0.521908193246
H	-2.889688045415	-1.277297090306	0.958564986125

naphthalene-S1min 4.32 eV 0.15 [0.03] 3.46 [2.00] 4.32 [1.06] 4.98 [0.04]

C	-2.532553968472	-0.209363446019	0.000000000000
C	2.532553968472	0.209363446019	0.000000000000
C	1.486608053537	1.134777761676	0.000000000000
C	-1.486608053537	-1.134777761676	0.000000000000
C	-2.250876468497	1.179185542543	0.000000000000
C	2.250876468497	-1.179185542543	0.000000000000
C	0.147298617145	0.726035120484	0.000000000000
C	-0.147298617145	-0.726035120484	0.000000000000
C	-0.927155033264	1.624012594338	0.000000000000
C	0.927155033264	-1.624012594338	0.000000000000
H	-3.553417650593	-0.550829378540	0.000000000000
H	3.553417650593	0.550829378540	0.000000000000
H	1.706281650508	2.190632262518	0.000000000000
H	-1.706281650508	-2.190632262518	0.000000000000
H	-3.058432383494	1.890980581046	0.000000000000
H	3.058432383494	-1.890980581046	0.000000000000
H	-0.718607147072	2.682126011778	0.000000000000
H	0.718607147072	-2.682126011778	0.000000000000

phenanthrene-TS1 5.72 eV 3.29 [0.08] 4.11 [1.96] 5.72 [0.42] 6.20 [0.94]

C	-0.760584825682	0.321480092970	0.168275141043
C	0.685710199479	0.327033326703	0.040491268162
C	-1.505205374190	1.503506284740	0.313302402687
C	-1.455319610445	-0.915981666152	-0.015639006612
C	-2.838391085815	-0.872114699090	-0.228815483867
C	-2.874047099796	1.505262277359	0.191309460003
C	-3.536446825715	0.309479057379	-0.116924270968
C	-0.672889960285	-2.121528947192	-0.082572258911
H	-3.358985907534	-1.797086591713	-0.418009578164
H	-0.999875602171	2.436083761448	0.504511998038

H	-3.430516889866	2.418980817310	0.316348044889
H	-4.608326561643	0.308129528457	-0.236783440587
C	1.434909826365	1.508846196543	-0.095280627582
C	1.434026802031	-0.908199076777	0.085836306951
C	2.841347029007	-0.893865544148	-0.004034931533
C	2.806517744080	1.486632383495	-0.188866675604
C	3.528083953751	0.283234483305	-0.138811345516
C	0.683746194047	-2.054783673659	0.422124969488
H	3.366147276156	-1.834386933519	0.044844109726
H	0.930187976937	2.456851956716	-0.146861370327
H	3.339353989510	2.417467559219	-0.299515179320
H	4.603617318923	0.293200004262	-0.193637301789
H	-0.681454024873	-2.518047880433	-1.102981802470
H	1.115404956621	-2.820062765590	1.054618259641

phenanthrene-TS2 5.71 eV 3.51 [0.20] 4.36 [1.86] 5.71 [0.53] 6.10 [0.78]

C	-0.758839623245	0.381541160340	0.012848274858
C	0.657829988353	0.418250393320	0.014442076443
C	-1.521096447248	1.568402285094	0.015908365823
C	-1.429844885736	-0.873748585445	0.036387559749
C	-2.831892081776	-0.883849080744	0.032980454780
C	-2.892065381568	1.526140667977	0.013013040759
C	-3.550156888902	0.290263293332	0.014088240163
C	-0.670239954774	-2.081068758874	0.062547016010
H	-3.345471000298	-1.832230560819	0.044780490661
H	-0.991666638309	2.506590530906	0.029123675066
H	-3.463332747880	2.439840306999	0.018932137678
H	-4.627842187514	0.258120091576	0.010960067768
C	1.455899658448	1.634912659454	-0.102432294277
C	1.383060042145	-0.812793861183	-0.009698230461
C	2.797715250397	-0.747682130136	-0.142597035198
C	2.840821795356	1.581047207270	0.364131489449
C	3.532936157838	0.414490024374	0.001322509408
C	0.689108125109	-2.042551101504	0.040400830084
H	3.327718938541	-1.677282039431	-0.290962160821
H	1.455789976364	1.904401387439	-1.167840692547
H	3.300583612406	2.360308711810	0.953145004262
H	4.612313294638	0.367739301436	-0.040678997269
H	-1.194784699961	-3.022338583984	0.083065276271
H	1.257139631106	-2.960156892388	0.018967369724

phenanthrene-TS3 5.52 eV 3.54 [0.13] 5.08 [1.81] 5.52 [0.29] 6.91 [1.01]

C	-0.739263120120	0.404410742488	0.089043589873
C	0.695962559404	0.423210825071	0.079231858234
C	-1.524118048764	1.562280219282	0.203430493422
C	-1.397269942498	-0.845106853481	-0.037724009197

C	-2.799986040480	-0.890574325158	-0.051541883185
C	-2.897094067621	1.491202086303	0.181379952026
C	-3.545163590209	0.258049430103	0.053153273816
C	-0.617069105992	-2.032070102922	-0.166800735537
H	-3.287070115356	-1.848580960174	-0.146585760388
H	-1.042953091887	2.517878740795	0.330896066048
H	-3.479260173291	2.393845251603	0.274561761264
H	-4.621602350324	0.211948583980	0.042855453291
C	1.512298289408	1.533797278196	-0.110556635830
C	1.436055368479	-0.798323224042	0.055342364919
C	2.854405031398	-0.711646246698	0.157088813623
C	2.924868700254	1.355934110314	-0.014971853424
C	3.520133161381	0.370325719760	0.838855013048
C	0.748439784282	-2.009221724653	-0.133124251309
H	3.440390333697	-1.503830283244	-0.292253193364
H	1.120848343836	2.488759921945	-0.422894604106
H	3.550663018073	2.004379752679	-0.617713955231
H	4.594667605354	0.339212085950	0.907111149619
H	-1.134880320075	-2.970754064110	-0.286796556046
H	1.306995296075	-2.927628322124	-0.220317607218

anthracene-TS1 4.92 eV (MECI 4.94 eV) 2.82 [0.34] 3.50 [1.69] 4.92 [0.20] 5.68 [1.13]

C	3.521092219894	-1.159526578214	0.202951313318
H	4.591661431773	-1.154280824309	0.335244214388
C	2.843646509389	0.058230468799	0.103468394516
C	2.852347831194	-2.374664429571	0.126892652094
C	1.478487074711	0.095914508874	-0.111067429016
C	1.480074683277	-2.375488432327	-0.033697964231
C	0.782216970806	-1.159226192905	-0.131187307334
C	0.714255723330	1.308496393274	-0.425947848958
C	-0.619021717439	-1.120624819917	-0.143992769077
C	-0.711380298297	1.301316087279	-0.077400241566
C	-1.400117116795	0.042236490528	-0.100568767264
H	3.381364286337	0.989317634541	0.153619736301
H	3.396258355247	-3.301899805153	0.192360233935
H	0.938828667694	-3.304514115485	-0.129373470324
H	0.739266261045	1.384131127626	-1.518927046033
H	-1.139545981380	-2.067429360763	-0.086276060360
C	-1.466738557895	2.431538660354	0.173570392641
C	-2.798660511252	-0.019270478314	0.028302851757
H	-0.965251856940	3.382449712090	0.226294238847
C	-2.855296129530	2.351856322498	0.305263289796
H	-3.297257150236	-0.971488561606	-0.070163246239
C	-3.526687021715	1.138281027121	0.224860488545
H	-4.599282500492	1.101415386097	0.314686955074

H	-3.419507855314	3.257069266340	0.465994007372
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anthracene-TS2	5.32 eV	3.38 [0.38]	4.05 [1.63]	5.32 [0.25]	6.04 [1.01]
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C	3.531013311176	-1.179829554715	0.061036721848
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H	4.608155284144	-1.178761850009	0.108198212541
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C	2.845811768678	0.014611397474	0.099271579284
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C	2.844515971001	-2.395018944443	-0.046283459152
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C	1.446404436943	0.047125955455	0.040847362807
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C	1.473939264447	-2.396209843284	-0.109086666802
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C	0.747604273128	-1.189578093684	-0.056417560507
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C	0.712044689046	1.274971253536	0.064197232299
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C	-0.659645626083	-1.162759132881	-0.097285245684
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C	-0.644972138776	1.303214109038	0.007205465226
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C	-1.359404592283	0.039887223071	-0.023270820526
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H	3.385315302598	0.945369527850	0.173206896788
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H	3.391709309449	-3.322524640466	-0.081678217611
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H	0.931706385226	-3.325064181615	-0.194681168497
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H	1.253023788309	2.206022990539	0.097809430331
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H	-1.199034593650	-2.087157999596	-0.241701526663
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C	-1.476992758561	2.496891357334	-0.223537905875
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C	-2.762461007849	0.054161165502	0.048648138325
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H	-1.555228476591	2.558571137180	-1.319004505631
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C	-2.857514633030	2.407641136504	0.224114509160
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H	-3.259177464661	-0.903812093500	0.108936948910
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C	-3.537684137078	1.212262023875	0.191395247235
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H	-4.570995760352	1.126814648311	0.490881855167
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H	-3.373568212964	3.275352036814	0.619570568504
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anthracene-S1min	3.63 eV	0.25 [0.04]	2.19 [2.00]	3.63 [0.12]	3.99 [1.09]
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C	3.550358121426	-1.170582246189	-0.056857137629
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H	4.627123073856	-1.141465306659	-0.074749591980
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C	2.824673944689	0.029765947835	-0.045915186642
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C	2.884799529492	-2.377889017993	-0.044891910641
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C	1.426812300205	0.033984334774	-0.022846439824
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C	1.482397757715	-2.404819954442	-0.021778893004
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C	0.732789471890	-1.224989164403	-0.010426333912
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C	0.667200504006	1.210082375639	-0.011286718111
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C	-0.667263566532	-1.210240645613	0.012630109894
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C	-0.732840589451	1.224831778563	0.011772946553
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C	-1.426880964827	-0.034132157752	0.024189732233
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H	3.348816090994	0.972040906743	-0.055446205727
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H	3.434662151283	-3.304238413462	-0.053199480829
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H	0.965817902386	-3.351295305759	-0.012520058569
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H	1.188357689570	2.155643668090	-0.020666222127
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H	-1.188421655267	-2.155804178980	0.022026121593
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C	-1.482379227283	2.404703171002	0.023150755560
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C	-2.824746775435	-0.029833802143	0.047273093229
H	-0.965722683000	3.351135281329	0.013912695983
C	-2.884774885980	2.377837831994	0.046277464435
H	-3.348964486209	-0.972067636210	0.056812184213
C	-3.550375578281	1.170556203359	0.058232623403
H	-4.627140765982	1.141495471991	0.076139259953
H	-3.434586359263	3.304218858299	0.054607191954

pyrene-TS-CH-dissociation 6.61 eV 4.89 [0.10] 5.97 [1.22] 6.61 [0.89] 7.13 [0.90]

C	2.675317292038	-1.689513897545	1.231372257705
H	3.511880896919	-2.253998070658	1.610248178699
C	2.897690293128	-0.604661323343	0.416630664059
C	1.380481088087	-2.073461663652	1.572343424924
C	1.818989342312	0.144410633063	-0.087390788648
C	0.280338949074	-1.367193737267	1.099995252534
C	0.494024172843	-0.235637705391	0.257605330932
C	2.005067105594	1.270636810474	-0.923829635627
C	-0.609542002706	0.506586143934	-0.233167907373
C	0.941764140073	1.982323841005	-1.397947464267
C	-0.384993689748	1.624837501071	-1.079257458945
H	3.903037083414	-0.312139366072	0.158327830008
H	1.221779837620	-2.927305375317	2.211240901479
H	3.010139360998	1.561924617384	-1.184389843869
C	-2.118089091715	-1.005131962694	1.000380039367
H	1.103975341452	2.838445018537	-2.033248717622
H	-3.122599513706	-1.282560453540	1.280411998607
C	-1.060162216258	-1.726356877303	1.448516167143
H	-1.213441336678	-2.582524477640	2.085140623690
C	-1.935237999421	0.103646111418	0.144719165226
C	-1.507212329640	2.322781445610	-1.645748231547
C	-2.739049520441	1.987867073022	-1.134324735936
H	-1.371757114193	3.075648204677	-2.400162212158
C	-3.029554413257	0.897818447749	-0.293941467391
H	-3.006344782510	2.274000983445	0.084659110043
H	-4.043306803741	0.666946906503	-0.011836360287

pyrene-TS1 5.28 eV 3.80 [0.18] 4.80 [1.48] 5.28 [0.57] 6.50 [1.12]

C	2.974686178789	-1.854645842496	0.737430933280
H	3.839053511478	-2.459932452776	0.955439131739
C	3.138709577429	-0.512619221475	0.430140318017
C	1.710267283435	-2.420279167924	0.795701826342
C	2.030836368198	0.297644433907	0.142114670381
C	0.568764774660	-1.654606829930	0.516345888420
C	0.745553937056	-0.299459188749	0.140732473423
C	2.115757379562	1.695390803468	-0.089659915932

C	-0.373318535582	0.482482945270	-0.151748721752
C	0.994755927208	2.463126537108	-0.315365319315
C	-0.271039798615	1.868587351604	-0.395448774083
H	4.126104041001	-0.078540742347	0.424346280250
H	1.596151143052	-3.456619310908	1.072090911242
H	3.086999278567	2.164108562313	-0.066062828366
C	-1.852389326987	-1.336663047548	0.415709161189
H	1.098886804814	3.525529334410	-0.471165625831
H	-2.845314546451	-1.738686176944	0.542248469103
C	-0.758224688511	-2.140827960995	0.646358879944
H	-0.904715580553	-3.163914132405	0.955396093911
C	-1.686585966874	-0.019431517293	-0.031078875806
C	-1.505809556040	2.541735994406	-0.691930819133
C	-2.574520351684	1.891964533258	-1.401087799897
H	-1.596118242245	3.582005991356	-0.401495588063
C	-2.737912391380	0.899192041011	-0.373107876831
H	-3.434024941553	2.486045443081	-1.664092119433
H	-3.686297552398	0.797496075596	0.141282654920

pyrene-TS2	5.66 eV	2.97 [0.09]	3.97 [1.93]	5.66 [0.21]	6.06 [1.11]
C	2.749315581379	-2.056812731789		0.813241436562	
H	3.586424475369	-2.695572398662		1.048348257250	
C	2.992759805588	-0.792132159985		0.277306585359	
C	1.471201854002	-2.494436976804		1.068317444478	
C	1.949352132466	0.075902301795		-0.012670422140	
C	0.376599725678	-1.669406903090		0.748646421224	
C	0.609037362618	-0.385509467483		0.208690161844	
C	2.108059552862	1.355919277603		-0.673037326344	
C	-0.504446157203	0.409752388744		-0.206264900543	
C	0.973243438735	2.247913701030		-0.686381337237	
C	-0.325257773271	1.745170107489		-0.724517737394	
H	4.003220129939	-0.459045404732		0.109405376828	
H	1.293543798291	-3.470032243206		1.490246828357	
H	2.364977833486	1.149104327915		-1.720377778105	
C	-2.022094340642	-1.357560844207		0.549032963777	
H	1.099907854412	3.323325822496		-0.635706250394	
H	-3.031957247134	-1.709119016953		0.688701045043	
C	-0.969146720087	-2.121816491931		0.911057055672	
H	-1.127988223415	-3.099586668790		1.337710964841	
C	-1.821906041845	-0.062122404763		-0.014213751059	
C	-1.452391714775	2.548333514128		-1.003265942569	
C	-2.727010575770	2.057554989433		-0.819729529404	
H	-1.296793594683	3.548614098683		-1.373740279846	
C	-2.904996301674	0.766636919722		-0.346816580539	
H	-3.584099502682	2.672326398960		-1.038754437506	
H	-3.904450791673	0.387929687428		-0.200849597886	

pyrene-TS3	5.37 eV	3.43 [0.43]	4.24 [1.59]	5.37 [0.30]	6.02 [0.92]
C	2.733295529138	-2.012719539013			0.842497027368
H	3.580004193190	-2.632240229463			1.088342681414
C	2.934207029581	-0.732334848882			0.367332170541
C	1.448401066382	-2.522030284569			0.980866246508
C	1.837291109962	0.085234150972			0.042059921724
C	0.325074050580	-1.748024840555			0.658601205573
C	0.530389824814	-0.415578449204			0.214302233647
C	1.985265721758	1.379135328523			-0.523795217613
C	-0.588113350674	0.387395732851			-0.104811313817
C	0.908783066101	2.113037134214			-0.925226942711
C	-0.416107933265	1.648819001818			-0.729044469977
H	3.934604190675	-0.357537923538			0.220706528745
H	1.307340228325	-3.534687623435			1.323963670564
H	2.981727883225	1.767038660047			-0.668189840144
C	-2.084584337488	-1.462274757606			0.375952642077
H	1.056749690635	3.073176618941			-1.392370758035
H	-3.089550668489	-1.839592237659			0.461887499552
C	-0.996997916231	-2.251660130139			0.704959342545
H	-1.146904167650	-3.273259082596			1.016617605860
C	-1.910094213950	-0.120162055041			0.054863372902
C	-1.549723643831	2.403249486248			-1.200167175593
C	-2.804033829682	2.020439255457			-0.856836298440
H	-1.371757789306	3.233624068807			-1.866299346928
C	-2.986566936759	0.883197446028			0.053053162084
H	-3.650838885025	2.608101745696			-1.184213059356
H	-2.837742803353	1.371969445096			1.033267532714

pyrene-S1min	3.82 eV	0.13 [0.05]	2.73 [2.00]	3.82 [1.04]	4.31 [0.07]
C	2.748843479112	-2.054970511730			0.777086972648
H	3.589886501837	-2.683570991635			1.016153665381
C	2.962850701426	-0.779217127166			0.254197252026
C	1.451714526071	-2.521295202750			0.992772815813
C	1.888596537209	0.063919421508			-0.066341188586
C	0.335105114944	-1.727099942202			0.693385593478
C	0.539153636513	-0.403232850668			0.152037658343
C	2.063976818518	1.361696462075			-0.597294804948
C	-0.539094705976	0.403031194917			-0.152099659359
C	0.993336992380	2.162467420205			-0.898877034958
C	-0.335053009948	1.727012544714			-0.693174250600
H	3.968685915493	-0.427275629831			0.090304487139
H	1.296219095719	-3.508782881973			1.396776878818
H	3.067260684838	1.720107477079			-0.765301470043
C	-2.063938786105	-1.362152260295			0.596581274410
H	1.156933497972	3.148969328895			-1.303074896877

H	-3.067227948832	-1.720770552701	0.764119207844
C	-0.993301686309	-2.162849716242	0.898366917999
H	-1.156885121055	-3.149443558281	1.302342690315
C	-1.888539991485	-0.064118071243	0.066261500275
C	-1.451633137369	2.521698906564	-0.991365143175
C	-2.748745375310	2.055559992280	-0.775187587967
H	-1.296123074963	3.509464422645	-1.394680011849
C	-2.962783097730	0.779405978111	-0.253289432432
H	-3.589769686597	2.684630520461	-1.013082069559
H	-3.968610880352	0.427528627266	-0.089226364139



Cartesian coordinates (in Å) and relative energies in eV on the Franck-Condon point and the three stable MECIs for benzene optimized by MS-CASPT2/cc-pVDZ calculations for the lowest two singlet states, where the six electrons in six orbitals active space was adopted.

benzene-s0min (CAS(6,6)PT2/cc-pVDZ) 4.84 eV

C	1.406966846217	0.000053071552	0.000098495410
H	2.501210432722	0.000091382047	0.000335442941
C	0.703437831003	1.218457012535	0.000432726194
C	0.703517027962	-1.218396586935	-0.000282412061
C	-0.703413561966	-1.218468854653	-0.000435630228
C	-0.703492934743	1.218437678040	0.000129295398
C	-1.406911128432	-0.000038472969	-0.000339085958
H	1.250668932489	-2.166031618557	-0.000419859440
H	-1.250518098497	-2.166124703514	-0.000856754189
H	1.250524421815	2.166129747127	0.000675080416
H	-1.250662402934	2.166056153951	0.000324155556
H	-2.501163365637	-0.000075808624	-0.000454454041

benzene-01 (CAS(6,6)PT2/cc-pVDZ) 4.97 eV

C	1.371799844796	-0.052551181369	-0.068114828790
H	2.450358864295	0.092508041143	0.038331279800
C	0.456726263175	1.090325784170	0.006429634625
C	0.754552162795	-1.306287399730	-0.214468727265
C	-0.640330609308	-1.214286468439	-0.071800063931
C	-0.703059260662	1.219972452040	-0.874725749390
C	-1.172443879688	0.149540117959	0.004212448484
H	1.296182773879	-2.244194970696	-0.357331401793
H	-1.305640386201	-2.075772859116	0.032583340002
H	0.731045186197	1.938967303161	0.650236863885
H	-1.251024653481	2.169419035403	-0.889272961383
H	-2.045119435912	0.336243805651	0.647276303883

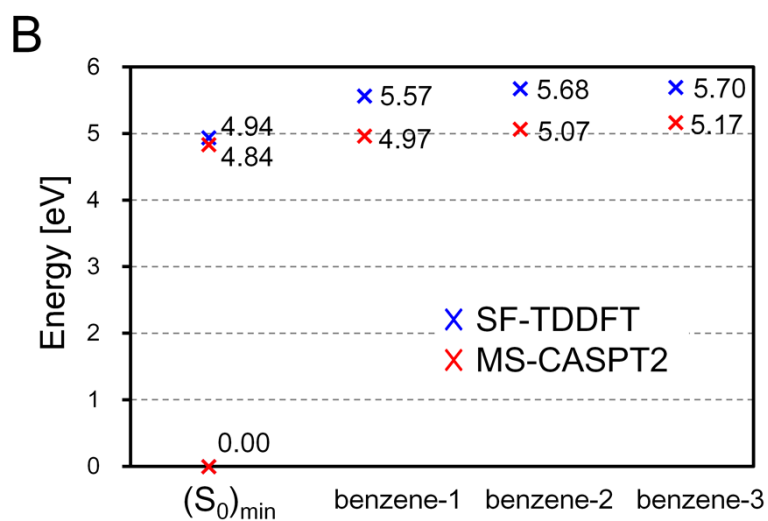
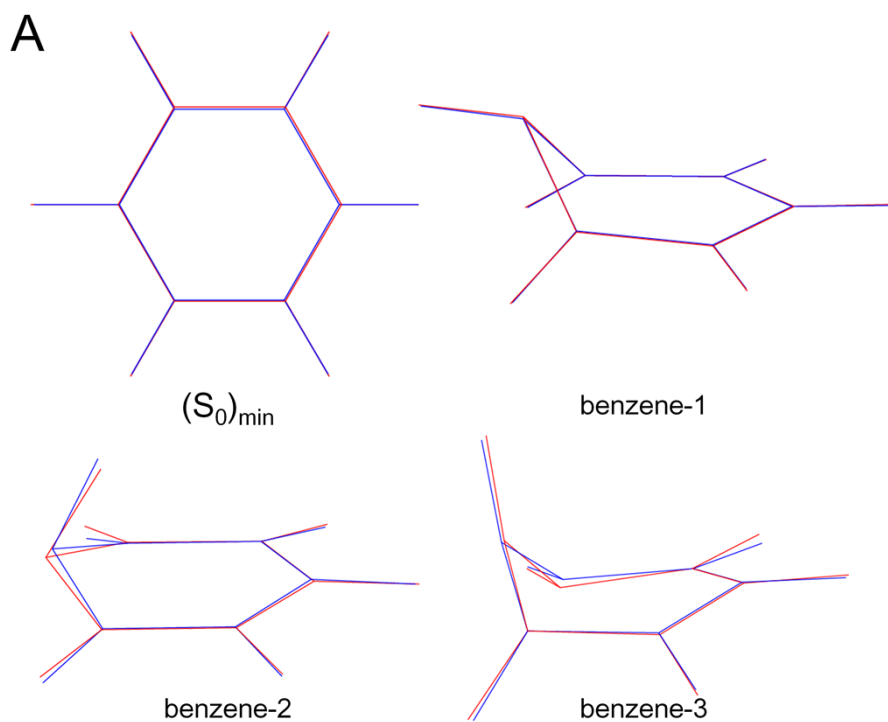
benzene-02 (CAS(6,6)PT2/cc-pVDZ) 5.07 eV

C	1.047118856014	0.047165794885	-0.307158861970
H	2.044973394269	0.050697379484	-0.758754565152
C	0.437619808872	1.293383872210	0.007956797892
C	0.462976625421	-1.200829276909	0.045220932249
C	-0.790734105706	-1.216428765987	0.680489484509
C	-0.817175650347	1.303272720942	0.640381726624
C	-1.573127207614	0.035529685036	0.690697075128
H	1.059249249579	-2.115948910470	-0.052560707103
H	-1.194629832019	-2.152527679831	1.089591331502
H	1.015342208319	2.217131886514	-0.116366216515
H	-1.242449774200	2.243351103164	1.017313651875
H	-1.450755200192	0.019476164163	-0.465123413571

benzene-03 (CAS(6,6)PT2/cc-pVDZ) 5.17 eV

C	1.447363978955	-0.023140529416	-0.280316291057
H	2.116628740242	-0.170129587826	-1.141408458168
C	0.828433678616	1.229161821598	-0.076028158193
C	0.612974692650	-1.129781412621	0.173998330715
C	-0.538063802540	-1.286384544899	-0.685596586335

C	-0.570475953885	1.130378538073	0.122745623485
C	-1.219981076872	-0.102785214235	-0.270495257615
H	0.620285808079	-1.468270563559	1.227095325878
H	-1.086998372866	-2.208861194570	-0.893980158264
H	1.303741197090	2.183327162339	-0.333568918117
H	-1.193807604633	2.005606133604	0.330154384727
H	-2.315352616165	-0.155949993976	-0.176862173725



**Figure.** Comparisons of the  $S_0$ -minimum and three most stable MECIs of benzene between SF-BHHLYP/6-31G\* and MS-CASPT2/cc-pVDZ. (A) The molecular geometries are depicted. Blue lines are for SF-BHHLYP/6-31G\*, while red lines are for MS-CASPT2/cc-pVDZ. (B) The relative energies are shown. Blue cross-marks are for SF-BHHLYP/6-31G\*, while red cross-marks are for MS-CASPT2/cc-pVDZ.