

**Experimental and Computed Absolute Redox Potentials of
Polycyclic Aromatic Hydrocarbons are Highly Linearly
Correlated Over a Wide Range of Structures and Potentials**

*Anthony P. Davis and Albert J. Fry**

Department of Chemistry, Wesleyan University, Middletown, CT 06459

SUPPORTING INFORMATION – Part 2

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Cartesian Coordinates of Optimized PAHs

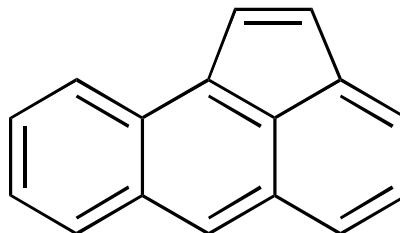
S-14

PAH(01) – aceanthrylene

CAS: 202-03-9

Neutral Structure

C	-3.87109900	-0.65540400	0.00000000
C	-2.76432100	-1.46898300	0.00000000
C	-1.43950600	-0.92305400	0.00000000
C	-1.29340700	0.52955800	0.00000000
C	-2.47150200	1.33661900	0.00000000
C	-3.72149300	0.76285300	0.00000000
C	-0.31478300	-1.77776500	0.00000000
C	0.01832200	1.04946100	0.00000000
C	1.09660100	0.15474200	0.00000000
C	0.99015300	-1.24988200	0.00000000
C	2.22837900	-1.97623200	0.00000000
H	2.21758400	-3.06379000	0.00000000
C	3.42971800	-1.29148200	0.00000000
C	3.50298500	0.14165300	0.00000000
C	2.33143500	0.87071700	0.00000000
H	-0.47405100	-2.85421100	0.00000000
H	-4.86811600	-1.08837800	0.00000000
H	-2.87551800	-2.55110200	0.00000000
H	-2.36406200	2.41838500	0.00000000
H	-4.60786200	1.39255800	0.00000000
H	4.36035600	-1.85342600	0.00000000
H	4.47916200	0.62186900	0.00000000
C	1.97085400	2.29490000	-0.00000100
C	0.60332500	2.39935600	0.00000100
H	2.67637400	3.11897700	-0.00000200
H	0.03898800	3.32574100	0.00000100



Radical Anion

C	-3.89924900	-0.64671600	0.00000000
C	-2.77460200	-1.45832200	0.00000000
C	-1.45406400	-0.91918800	0.00000000
C	-1.31455400	0.53069400	0.00000000
C	-2.48629000	1.32572500	0.00000000
C	-3.75647600	0.75886000	0.00000000
C	-0.31390300	-1.77779000	0.00000000
C	0.01877800	1.06518800	0.00000000
C	1.11036400	0.16269100	0.00000000
C	1.00194800	-1.24904600	0.00000000
C	2.23496500	-1.97080600	0.00000000
H	2.22833200	-3.05968400	0.00000000
C	3.45947000	-1.27848700	0.00000000
C	3.54274300	0.12873900	0.00000000
C	2.34511900	0.88075300	0.00000000
H	-0.47362200	-2.85531900	0.00000000
H	-4.89159400	-1.09286800	0.00000000
H	-2.88863900	-2.54154600	0.00000000
H	-2.38094200	2.40917700	0.00000000
H	-4.63778400	1.39662800	0.00000000
H	4.38324000	-1.85549200	0.00000000
H	4.51910400	0.61149900	0.00000000
C	1.99036700	2.27943600	0.00000000
C	0.59096100	2.38698900	0.00000000
H	2.68927300	3.11163700	-0.00000100
H	0.03557300	3.32093000	0.00000000

PAH(02) – acenaphthylene

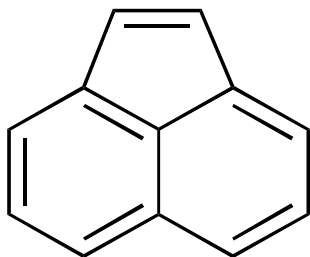
CAS: 208-96-8

Neutral Structure

C	0.00000000	2.43388200	1.10485700
C	0.00000000	1.28445500	1.88397000
C	0.00000000	0.00000000	1.25792600
C	0.00000000	0.00000000	-0.14152100
C	0.00000000	1.16336700	-0.95344000
C	0.00000000	2.39569400	-0.32266600
H	0.00000000	-1.36172300	2.96888500
H	0.00000000	3.40422200	1.59531300
H	0.00000000	1.36172300	2.96888500
C	0.00000000	-1.28445500	1.88397000
C	0.00000000	-1.16336700	-0.95344000
H	0.00000000	3.32890600	-0.88159900
C	0.00000000	-2.39569400	-0.32266600
C	0.00000000	-2.43388200	1.10485700
H	0.00000000	-3.32890600	-0.88159900
H	0.00000000	-3.40422200	1.59531300
C	0.00000000	-0.68420200	-2.34747200
C	0.00000000	0.68420200	-2.34747200
H	0.00000000	-1.32281000	-3.22470700
H	0.00000000	1.32281000	-3.22470700

Radical Anion

C	0.00000000	2.45284300	1.09539800
C	0.00000000	1.28552300	1.88541200
C	0.00000000	0.00000000	1.25845000
C	0.00000000	0.00000000	-0.15215100
C	0.00000000	1.17111300	-0.97036200
C	0.00000000	2.42814900	-0.31125000
H	0.00000000	-1.36522700	2.97133900
H	0.00000000	3.41924000	1.59867900
H	0.00000000	1.36522700	2.97133900
C	0.00000000	-1.28552300	1.88541200
C	0.00000000	-1.17111300	-0.97036200
H	0.00000000	3.36435700	-0.86811300
C	0.00000000	-2.42814900	-0.31125000
C	0.00000000	-2.45284300	1.09539800
H	0.00000000	-3.36435700	-0.86811300
H	0.00000000	-3.41924000	1.59867900
C	0.00000000	-0.70459600	-2.33317200
C	0.00000000	0.70459600	-2.33317200
H	0.00000000	-1.33545300	-3.21851600
H	0.00000000	1.33545300	-3.21851600

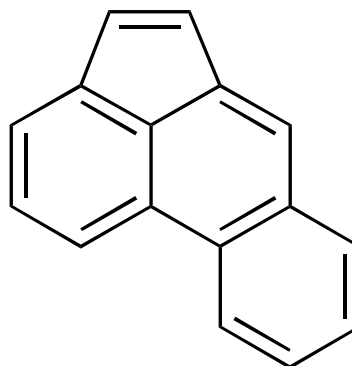


PAH(03) – acephenanthrylene

CAS: 201-06-9

Neutral Structure

C	-0.47568800	1.93452700	0.00000000
C	0.84254800	1.56643800	0.00000000
C	1.16104400	0.16846900	0.00000000
C	0.23374100	-0.87187400	0.00000000
C	0.77831100	-2.18557200	0.00000000
H	0.12895300	-3.05625500	0.00000000
C	2.15989100	-2.37260800	0.00000000
C	3.07690200	-1.28975700	0.00000000
C	2.56666000	0.00156500	0.00000000
H	-0.78646000	2.97755500	0.00000000
H	2.55064000	-3.38722700	0.00000000
H	4.14662100	-1.48639500	0.00000000
C	3.14183900	1.35771100	-0.00000100
C	2.12883800	2.27689400	0.00000100
H	4.20406900	1.57969400	-0.00000100
H	2.24257100	3.35577300	0.00000100
C	-3.87931800	0.35348400	0.00000000
C	-3.55613200	-1.01773600	0.00000000
C	-2.22872200	-1.42508200	0.00000000
C	-1.17407500	-0.48607900	0.00000000
C	-1.50210900	0.91578200	0.00000000
C	-2.86633400	1.29906500	0.00000000
H	-4.91989000	0.66780500	0.00000000
H	-4.34850100	-1.76221300	0.00000000
H	-1.99979000	-2.48696500	0.00000000
H	-3.10759800	2.35985600	0.00000000



Radical Anion

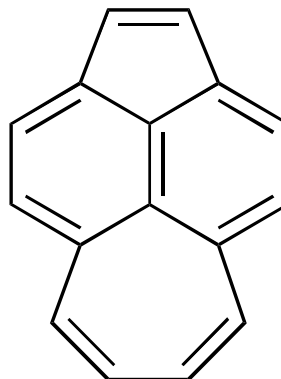
C	-0.50013500	1.95556800	0.00000000
C	0.85925800	1.58519900	0.00000000
C	1.17322200	0.18604300	0.00000000
C	0.24010300	-0.86106900	0.00000000
C	0.77143600	-2.17725100	0.00000000
H	0.11736800	-3.04523700	0.00000000
C	2.16994200	-2.37601100	0.00000000
C	3.08859200	-1.31610200	0.00000000
C	2.59541600	0.00971600	0.00000000
H	-0.81082200	2.99982800	0.00000000
H	2.54727900	-3.39763700	0.00000000
H	4.15770700	-1.52502400	0.00000000
C	3.16554700	1.33087200	0.00000000
C	2.11969700	2.27554700	0.00000000
H	4.22737200	1.56206100	0.00000100
H	2.24600700	3.35525600	-0.00000100
C	-3.89075400	0.34384200	0.00000000
C	-3.56062500	-1.03150800	0.00000000
C	-2.22215900	-1.41261500	0.00000000
C	-1.17258200	-0.46968900	0.00000000
C	-1.50466900	0.94602900	0.00000000
C	-2.89038500	1.29867200	0.00000000
H	-4.93452900	0.65199800	0.00000000
H	-4.34446000	-1.78524000	0.00000000
H	-1.97942900	-2.47274800	0.00000000
H	-3.15038700	2.35635700	0.00000000

PAH(04) – acepleiadylene

CAS: 194-32-1

Neutral Structure

C	-0.31481900	-1.55668100	-0.73082400
C	1.10836000	-1.64263700	-0.65880500
C	1.94224600	-1.27417600	0.36259400
C	-1.19743000	-1.08922800	0.20558700
H	-0.75448300	-1.91431600	-1.65997800
H	1.59300900	-2.05861300	-1.54008200
H	3.00328100	-1.43759500	0.18131700
H	-2.24670600	-1.12582300	-0.08243200
C	-2.12832200	-0.16169300	2.23899900
C	-0.97119300	-0.55188800	1.52227900
C	0.32563100	-0.37883300	2.16309100
C	0.29380900	0.17084600	3.44823100
C	-0.88257500	0.55915200	4.16071700
C	-2.11004600	0.38352000	3.53145600
H	-3.08955900	-0.29526000	1.74927800
C	1.65102600	-0.69992800	1.65075100
C	1.43237000	0.43509400	4.27052400
H	-3.04616300	0.65716200	4.01366000
C	2.68792700	0.12207200	3.76191200
C	2.77001200	-0.43358700	2.47640200
H	3.59782600	0.29500500	4.33271900
H	3.75288700	-0.67967300	2.08275500
C	-0.44598000	1.07004000	5.44275600
C	0.93347500	0.99613900	5.50816100
H	-1.10194100	1.44782200	6.22034600
H	1.54952400	1.30484200	6.34652900



Radical Anion

C	-0.32433100	-1.55657200	-0.74348700
C	1.11863900	-1.65038300	-0.66763900
C	1.93877200	-1.28081300	0.35970500
C	-1.19387000	-1.08758900	0.19923900
H	-0.76591400	-1.90902200	-1.67480000
H	1.60543400	-2.06964600	-1.54730500
H	3.00268300	-1.44722600	0.18605100
H	-2.24632500	-1.11676400	-0.08573000
C	-2.14149900	-0.16067100	2.24779700
C	-0.96947600	-0.55123600	1.52712400
C	0.32547600	-0.37656100	2.16996500
C	0.29342300	0.17694100	3.46122800
C	-0.89132800	0.56595800	4.17850000
C	-2.13962900	0.38034300	3.52835800
H	-3.09816300	-0.30022000	1.74597400
C	1.64896500	-0.69886900	1.65556400
C	1.44026900	0.44480500	4.28745300
H	-3.07890500	0.65217300	4.00772400
C	2.71758300	0.12280800	3.75871400
C	2.78279500	-0.42931600	2.48457300
H	3.63061900	0.29515800	4.32662800
H	3.76170700	-0.68064100	2.07838000
C	-0.46360300	1.06883800	5.43842200
C	0.95131100	0.99516100	5.50456400
H	-1.11369100	1.44794600	6.22260300
H	1.56122300	1.30716400	6.34833600

PAH(05) – anthracene

CAS: 120-12-7

Neutral Structure

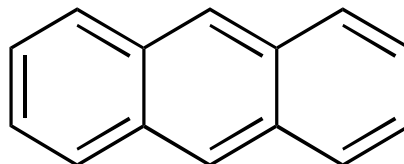
C	0.00000000	3.66609300	0.71452800
C	0.00000000	2.48247100	1.41088000
C	0.00000000	1.22502300	0.72356800
C	0.00000000	1.22502300	-0.72356800
C	0.00000000	2.48247100	-1.41088000
C	0.00000000	3.66609300	-0.71452800
C	0.00000000	0.00000000	1.40808600
C	0.00000000	0.00000000	-1.40808600
C	0.00000000	-1.22502300	-0.72356800
C	0.00000000	-1.22502300	0.72356800
C	0.00000000	-2.48247100	1.41088000
H	0.00000000	-2.47973900	2.49891000
C	0.00000000	-3.66609300	0.71452800
C	0.00000000	-3.66609300	-0.71452800
C	0.00000000	-2.48247100	-1.41088000
H	0.00000000	0.00000000	2.49670400
H	0.00000000	4.61345200	1.24798600
H	0.00000000	2.47973900	2.49891000
H	0.00000000	2.47973900	-2.49891000
H	0.00000000	4.61345200	-1.24798600
H	0.00000000	0.00000000	-2.49670400
H	0.00000000	-4.61345200	1.24798600
H	0.00000000	-4.61345200	-1.24798600
H	0.00000000	-2.47973900	-2.49891000

Radical Cation

C	0.00000000	3.66788300	0.70358400
C	0.00000000	2.46780500	1.40967800
C	0.00000000	1.23178700	0.72041700
C	0.00000000	1.23178700	-0.72041700
C	0.00000000	2.46780500	-1.40967800
C	0.00000000	3.66788300	-0.70358400
C	0.00000000	0.00000000	1.40951100
C	0.00000000	0.00000000	-1.40951100
C	0.00000000	-1.23178700	-0.72041700
C	0.00000000	-1.23178700	0.72041700
C	0.00000000	-2.46780500	1.40967800
H	0.00000000	-2.46836300	2.49637300
C	0.00000000	-3.66788300	0.70358400
C	0.00000000	-3.66788300	-0.70358400
C	0.00000000	-2.46780500	-1.40967800
H	0.00000000	0.00000000	2.49704900
H	0.00000000	4.61055000	1.24279100
H	0.00000000	2.46836300	2.49637300
H	0.00000000	2.46836300	-2.49637300
H	0.00000000	4.61055000	-1.24279100
H	0.00000000	0.00000000	-2.49704900
H	0.00000000	-4.61055000	1.24279100
H	0.00000000	-4.61055000	-1.24279100
H	0.00000000	-2.46836300	-2.49637300

Radical Anion

C	0.00000000	3.70741700	0.70381400
C	0.00000000	2.49632200	1.40202500
C	0.00000000	1.24388900	0.72678000
C	0.00000000	1.24388900	-0.72678000
C	0.00000000	2.49632200	-1.40202500
C	0.00000000	3.70741700	-0.70381400
C	0.00000000	0.00000000	1.40807000
C	0.00000000	0.00000000	-1.40807000
C	0.00000000	-1.24388900	-0.72678000
C	0.00000000	-1.24388900	0.72678000
C	0.00000000	-2.49632200	1.40202500
H	0.00000000	-2.49832300	2.49174800
C	0.00000000	-3.70741700	0.70381400
C	0.00000000	-3.70741700	-0.70381400
C	0.00000000	-2.49632200	-1.40202500
H	0.00000000	0.00000000	2.49831400
H	0.00000000	4.64878000	1.25028100
H	0.00000000	2.49832300	2.49174800
H	0.00000000	2.49832300	-2.49174800
H	0.00000000	4.64878000	-1.25028100
H	0.00000000	0.00000000	-2.49831400
H	0.00000000	-4.64878000	1.25028100
H	0.00000000	-4.64878000	-1.25028100
H	0.00000000	-2.49832300	-2.49174800



PAH(06) – azulene

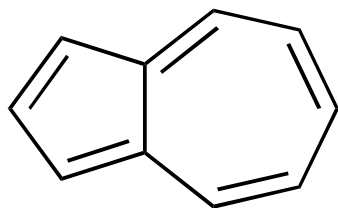
CAS: 275-51-4

Neutral Structure

C	-0.84949800	0.45427500	0.00027100
C	0.55166100	0.45072000	-0.00039000
C	1.42996500	1.54100800	-0.00035100
C	-1.74417300	1.53254700	0.00110400
C	1.13393300	2.90526700	0.00034100
C	-1.46212400	2.90395000	0.00148500
C	-0.22138600	3.54399900	0.00116700
H	-1.31351200	-0.53092300	0.00010800
H	1.02040300	-0.53105300	-0.00100100
H	2.49128200	1.29226700	-0.00094000
H	-2.79992900	1.26945400	0.00149600
H	-2.32920500	3.56457000	0.00211900
C	2.07447300	3.95651000	0.00031800
H	3.15183400	3.82968700	-0.00020900
C	1.37704300	5.17928500	0.00106200
H	1.83998400	6.16168200	0.00121200
C	-0.00987900	4.93850500	0.00159300
H	-0.79369900	5.68850100	0.00221600

Radical Anion

C	-0.86124400	0.42924100	0.00029100
C	0.56002700	0.44313800	-0.00040200
C	1.43573300	1.51850000	-0.00036500
C	-1.75506700	1.53443100	0.00110800
C	1.11946800	2.92500000	0.00037800
C	-1.48290900	2.89408400	0.00149300
C	-0.19693100	3.54544300	0.00116600
H	-1.32567200	-0.55615200	0.00011800
H	1.02827900	-0.54267700	-0.00103200
H	2.49978100	1.27688800	-0.00096000
H	-2.81367900	1.26852900	0.00148700
H	-2.34596000	3.56157500	0.00212700
C	2.07332000	3.97229300	0.00034000
H	3.15191800	3.83221400	-0.00018400
C	1.39308500	5.21359700	0.00105600
H	1.85647000	6.19657500	0.00121500
C	0.00274900	4.94762700	0.00158100
H	-0.79219400	5.68994600	0.00218500



PAH(07) – benz[*a*]anthracene

CAS: 56-55-3

Neutral Structure

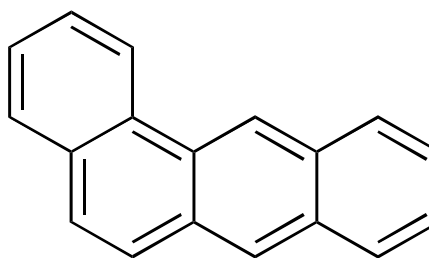
C	-0.85595900	-4.68776400	0.00000000
C	0.29323400	-3.93087900	0.00000000
C	0.22603000	-2.50346400	0.00000000
C	-1.06498700	-1.86634200	0.00000000
C	-2.23591300	-2.68556200	0.00000000
C	-2.13476700	-4.05801400	0.00000000
C	1.37515800	-1.69082600	0.00000000
C	-1.14044000	-0.45783600	0.00000000
C	-0.00123000	0.34874500	0.00000000
C	1.29169200	-0.29675800	0.00000000
C	2.48857300	0.50908000	0.00000000
H	3.44932500	-0.00084300	0.00000000
C	2.42481600	1.86650100	0.00000000
C	1.15773500	2.55913700	0.00000000
C	-0.06025500	1.81572400	0.00000000
H	2.35667000	-2.16119000	0.00000000
H	-0.79461900	-5.77328600	0.00000000
H	1.27127700	-4.40744900	0.00000000
H	-3.21069300	-2.20250800	0.00000000
H	-3.03272200	-4.67097500	0.00000000
H	-2.13073500	-0.01332800	0.00000000
H	3.33455900	2.46287200	0.00000000
C	1.11610600	3.97286700	0.00000000
H	2.05550800	4.52173100	0.00000000
C	-1.27773200	2.53557600	0.00000000
H	-2.22524500	2.00656600	0.00000000
C	-1.29658400	3.92457300	0.00000000
H	-2.24910700	4.44866700	0.00000000
C	-0.09228900	4.65276900	0.00000000
H	-0.11007700	5.73976700	0.00000000

Radical Cation

C	-1.18345000	-0.99487300	0.00760000
C	-0.08782700	-1.87962000	0.01340600
C	1.24633400	-1.41441700	0.01384800
C	1.51592100	-0.00150600	0.00758700
C	0.42291800	0.87454200	0.00185400
C	-0.92037600	0.41566200	0.00191200
C	2.31775000	-2.34640100	0.02096700
C	2.89654200	0.45628500	0.00816900
C	3.94825800	-0.52699700	0.01619600
C	3.62650100	-1.91148400	0.02223700
C	5.30714500	-0.11096100	0.01758800
H	6.08295300	-0.87229600	0.02358300
C	5.63049200	1.22904100	0.01137100
C	4.59911600	2.19762900	0.00336000
C	3.26609500	1.82146300	0.00179600
H	2.08994600	-3.40858400	0.02546900
H	-0.26833400	-2.95199300	0.01797200
H	0.57647300	1.94852200	-0.00255500
H	4.43911800	-2.63334500	0.02778600
H	6.66992900	1.54458500	0.01248100
H	4.85495500	3.25368900	-0.00158800
H	2.50822900	2.59704600	-0.00436200
C	-3.57701500	-0.54326000	0.00239900
C	-3.31872400	0.83846700	-0.00292100
C	-2.52363700	-1.45367500	0.00759400
C	-2.00712700	1.31545200	-0.00325200
H	-2.71727800	-2.52305900	0.01179500
H	-1.81175400	2.38446800	-0.00734800
H	-4.14597400	1.54237500	-0.00676000
H	-4.60216700	-0.90149000	0.00255100

Radical Anion

C	-0.75183300	-4.74409000	0.00000000
C	0.39013200	-3.93466100	0.00000000
C	0.29460100	-2.51585400	0.00000000
C	-1.02174800	-1.91193000	0.00000000
C	-2.15748000	-2.76319900	0.00000000
C	-2.02892700	-4.15845300	0.00000000
C	1.42451100	-1.65865400	0.00000000
C	-1.12614500	-0.49099700	0.00000000
C	0.00041800	0.36127800	0.00000000
C	1.31103300	-0.24659700	0.00000000
C	2.46889700	0.59293100	0.00000000
H	3.44737800	0.11382400	0.00000000
C	2.38004700	1.97028700	0.00000000
C	1.10968200	2.61443400	0.00000000
C	-0.09235500	1.81418200	0.00000000
H	2.42034700	-2.10151800	0.00000000
H	-0.64753000	-5.82759000	0.00000000
H	1.37991000	-4.39015700	0.00000000
H	-3.14821100	-2.30979800	0.00000000
H	-2.91866600	-4.78521800	0.00000000
H	-2.12822700	-0.07097200	0.00000000
H	3.28057000	2.58199300	0.00000000
C	1.00078600	4.03210000	0.00000000
H	1.91837000	4.61899300	0.00000000
C	-1.33769100	2.50350000	0.00000000
H	-2.26505700	1.93817600	0.00000000
C	-1.41288200	3.88639500	0.00000000
H	-2.38483600	4.37501100	0.00000000
C	-0.22812200	4.66566000	0.00000000
H	-0.28762800	5.75176200	0.00000000



PAH(08) – benzo[*b*]chrysene

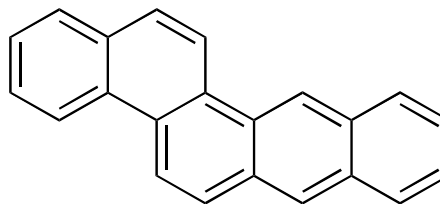
CAS: 214-17-5

Neutral Structure

C	1.87415800	-1.36744800	0.00000000
C	0.46646600	-1.67770100	0.00000000
C	-0.46940600	-0.61474500	0.00000000
C	2.32696900	-0.08268800	0.00000000
H	2.60180800	-2.17122700	0.00000000
H	3.39528200	0.12185700	0.00000000
C	-0.00005800	0.77196000	0.00000000
C	1.42050600	1.03020700	0.00000000
C	-0.86518300	1.87162600	0.00000000
C	1.89688900	2.34482300	0.00000000
C	-0.39400400	3.19892700	0.00000000
C	1.02539800	3.44710000	0.00000000
H	-1.94071700	1.73007400	0.00000000
H	2.97178300	2.51621700	0.00000000
C	-1.28681100	4.31633400	0.00000000
C	-0.80342100	5.60373700	0.00000000
H	-2.35815600	4.12672200	0.00000000
C	1.49142600	4.79914000	0.00000000
C	0.60216100	5.84810500	0.00000000
H	-1.49224400	6.44489000	0.00000000
H	2.56408000	4.98107800	0.00000000
H	0.96602000	6.87260200	0.00000000
H	-3.38441600	-2.42342500	0.00000000
C	-2.31663400	-2.21612600	0.00000000
C	-1.40657800	-3.31512900	0.00000000
C	-1.86683100	-0.92357800	0.00000000
C	0.00028700	-3.05329700	0.00000000
C	-1.87840700	-4.65424300	0.00000000
H	-2.59809400	-0.12281800	0.00000000
C	0.87844700	-4.17205400	0.00000000
C	-0.99688000	-5.71741100	0.00000000
H	-2.95274200	-4.82598000	0.00000000
C	0.39438400	-5.46831000	0.00000000
H	1.95224100	-4.02381100	0.00000000
H	-1.36704300	-6.73950200	0.00000000
H	1.09291900	-6.30145800	0.00000000

Radical Cation

C	1.84576200	-1.38451400	0.00000000
C	0.46175500	-1.68589900	0.00000000
C	-0.48511200	-0.60047600	0.00000000
C	2.31242500	-0.08418400	0.00000000
H	2.57649200	-2.18466000	0.00000000
H	3.38175600	0.10812500	0.00000000
C	-0.00003500	0.76833700	0.00000000
C	1.41837200	1.01431700	0.00000000
C	-0.85428000	1.87805400	0.00000000
C	1.91210900	2.33141600	0.00000000
C	-0.36793500	3.20956700	0.00000000
C	1.04836400	3.44558100	0.00000000
H	-1.93068900	1.74992800	0.00000000
H	2.98793100	2.48969600	0.00000000
C	-1.24898200	4.31623700	0.00000000
C	-0.74862800	5.61368500	0.00000000
H	-2.32124000	4.13893900	0.00000000
C	1.53129200	4.77812900	0.00000000
C	0.64205200	5.84508500	0.00000000
H	-1.43470100	6.45590400	0.00000000
H	2.60411900	4.95187500	0.00000000
H	1.01839100	6.86393100	0.00000000
H	-3.38970800	-2.40210500	0.00000000
C	-2.32163400	-2.19921200	0.00000000
C	-1.42051800	-3.30783200	0.00000000
C	-1.87522200	-0.90278200	0.00000000
C	-0.01405200	-3.06280200	0.00000000
C	-1.91033900	-4.63469100	0.00000000
H	-2.60865300	-0.10501600	0.00000000
C	0.85274300	-4.18185100	0.00000000
C	-1.03627200	-5.71012900	0.00000000
H	-2.98572000	-4.79457800	0.00000000
C	0.35173800	-5.47695200	0.00000000
H	1.92797000	-4.04762900	0.00000000
H	-1.41828200	-6.72725500	0.00000000
H	1.04237200	-6.31591300	0.00000000

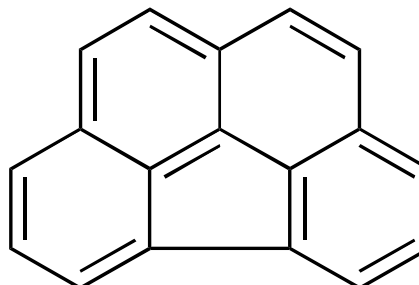


PAH(09) – benzo[ghi]fluoranthene

CAS: 203-12-3

Neutral Structure

C	-2.46612900	1.99808900	-0.08337000
C	-2.41762500	0.54815800	-0.08011600
C	-1.13400900	0.00680100	-0.03729200
C	-1.32358100	2.78931600	-0.04807300
H	-3.43690500	2.48842900	-0.11522600
H	-1.43641600	3.87129200	-0.05313000
C	-0.75389800	-1.36615200	-0.02321500
C	-1.79799200	-2.27751100	-0.05988200
C	-3.46221700	-0.42056200	-0.11692300
C	-3.13710300	-1.77783200	-0.10630900
H	-1.63449100	-3.35254900	-0.05449700
H	-4.50616000	-0.11706200	-0.15279700
H	-3.94620300	-2.50380000	-0.13478300
C	0.00034200	0.82472300	-0.00241300
C	0.00091000	2.20664200	-0.00513000
C	1.13398500	0.00600100	0.03626900
C	1.32587200	2.78838200	0.03582300
C	2.41802800	0.54646400	0.07763700
C	0.75270400	-1.36667300	0.02857800
C	2.46774600	1.99635200	0.07474100
H	1.43960400	3.87027500	0.03664100
C	3.46174900	-0.42298100	0.11981200
C	1.79597300	-2.27875800	0.07034600
H	3.43891800	2.48600300	0.10505500
C	3.13548300	-1.78000600	0.11529600
H	4.50591900	-0.12020400	0.15514600
H	1.63154500	-3.35366700	0.07004700
H	3.94395200	-2.50651200	0.14776400



Radical Anion

C	-2.46372900	2.00154700	-0.08225100
C	-2.42094100	0.54845200	-0.08040500
C	-1.12752300	0.01007100	-0.03777500
C	-1.31679600	2.80424500	-0.04726000
H	-3.43503800	2.49373900	-0.11359400
H	-1.44179000	3.88648100	-0.05222100
C	-0.73432300	-1.37402600	-0.02290000
C	-1.81264200	-2.29250700	-0.06041400
C	-3.46668900	-0.41584500	-0.11782500
C	-3.13189400	-1.79274500	-0.10671100
H	-1.65374200	-3.36975400	-0.05485600
H	-4.51239800	-0.11570200	-0.15344800
H	-3.94711500	-2.51458800	-0.13544900
C	0.00035000	0.83106200	-0.00257700
C	0.00091300	2.23441100	-0.00529500
C	1.12752100	0.00929200	0.03654700
C	1.31906200	2.80333700	0.03490400
C	2.42135100	0.54679500	0.07785300
C	0.73315100	-1.37452000	0.02827400
C	2.46532800	1.99985000	0.07354800
H	1.44492600	3.88548400	0.03581800
C	3.46622600	-0.41822900	0.12073700
C	1.81063800	-2.29375400	0.07096800
H	3.43701800	2.49137500	0.10351700
C	3.13027700	-1.79488300	0.11586100
H	4.51215500	-0.11880500	0.15593500
H	1.65081600	-3.37087700	0.07043300
H	3.94488500	-2.51724800	0.14858600

PAH(10) – benzo[ghi]perylene

CAS: 191-24-2

Neutral Structure

C	0.00000000	2.89227800	-2.74878800
C	0.00000000	3.57620400	-1.53980200
C	0.00000000	2.86441600	-0.32327000
C	0.00000000	1.43306100	-0.34534600
C	0.00000000	0.73593900	-1.59446300
C	0.00000000	1.49183700	-2.77613900
H	0.00000000	4.63422300	0.93975300
H	0.00000000	3.44310700	-3.68601900
H	0.00000000	4.66363000	-1.51856000
C	0.00000000	3.54652700	0.94120600
C	0.00000000	0.71457700	0.89644600
H	0.00000000	0.99963300	-3.74249700
C	0.00000000	1.42010800	2.13104000
C	0.00000000	2.85440800	2.11817200
H	0.00000000	3.38151000	3.06965200
C	0.00000000	-0.71457700	0.89644600
C	0.00000000	-1.43306100	-0.34534600
C	0.00000000	-1.42010800	2.13104000
C	0.00000000	-0.73593900	-1.59446300
C	0.00000000	-2.86441600	-0.32327000
C	0.00000000	-2.85440800	2.11817200
C	0.00000000	-1.49183700	-2.77613900
C	0.00000000	-3.57620400	-1.53980200
C	0.00000000	-3.54652700	0.94120600
H	0.00000000	-3.38151000	3.06965200
C	0.00000000	-2.89227800	-2.74878800
H	0.00000000	-0.99963300	-3.74249700
H	0.00000000	-4.66363000	-1.51856000
H	0.00000000	-4.63422300	0.93975300
H	0.00000000	-3.44310700	-3.68601900
C	0.00000000	-0.68894400	3.34845700
C	0.00000000	0.68894400	3.34845700
H	0.00000000	-1.23749000	4.28765100
H	0.00000000	1.23749000	4.28765100

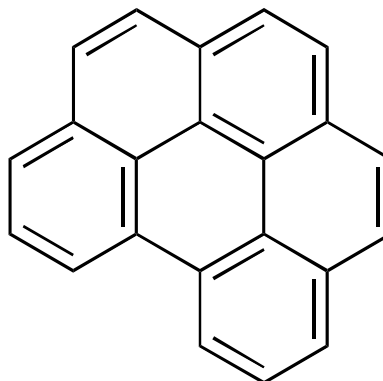
Radical Anion

C	0.00000000	2.88276200	-2.76298300
C	0.00000000	3.58025400	-1.55428000
C	0.00000000	2.87169200	-0.32270900
C	0.00000000	1.43078800	-0.34279100
C	0.00000000	0.72447000	-1.59080200
C	0.00000000	1.48868000	-2.79629500
H	0.00000000	4.63485500	0.93772600
H	0.00000000	3.43551000	-3.70134500
H	0.00000000	4.66833000	-1.54079600
C	0.00000000	3.54624900	0.93410900
C	0.00000000	0.71351600	0.90257300
H	0.00000000	0.99137700	-3.75993400
C	0.00000000	1.43195500	2.14731500
C	0.00000000	2.84663100	2.12869200
H	0.00000000	3.38308300	3.07638900
C	0.00000000	-0.71351600	0.90257300
C	0.00000000	-1.43078800	-0.34279100
C	0.00000000	-1.43195500	2.14731500
C	0.00000000	-0.72447000	-1.59080200
C	0.00000000	-2.87169200	-0.32270900
C	0.00000000	-2.84663100	2.12869200
C	0.00000000	-1.48868000	-2.79629500
C	0.00000000	-3.58025400	-1.55428000
C	0.00000000	-3.54624900	0.93410900
H	0.00000000	-3.38308300	3.07638900
C	0.00000000	-2.88276200	-2.76298300
H	0.00000000	-0.99137700	-3.75993400
H	0.00000000	-4.66833000	-1.54079600

H	0.00000000	-4.63485500	0.93772600
H	0.00000000	-3.43551000	-3.70134500
C	0.00000000	-0.68538500	3.36975800
C	0.00000000	0.68538500	3.36975800
H	0.00000000	-1.23323300	4.31080900
H	0.00000000	1.23323300	4.31080900

Radical Cation

C	0.02259200	2.87974900	-2.75847200
C	0.00603000	3.56235600	-1.54119500
C	-0.00415000	2.84955500	-0.32137600
C	-0.00200200	1.42208100	-0.34142600
C	0.00468600	0.72433400	-1.58645000
C	0.02279000	1.48908700	-2.78435200
H	-0.01889200	4.61739300	0.93143500
H	0.03591500	3.43391200	-3.69206300
H	0.00396500	4.64903700	-1.51899700
C	-0.01425300	3.53062000	0.92955500
C	-0.00365200	0.70862000	0.89455500
H	0.04118900	0.99411500	-3.74786400
C	-0.00886700	1.41952800	2.13686700
C	-0.01665600	2.83458000	2.12307200
H	-0.02293800	3.37058300	3.06822700
C	0.00365200	-0.70862000	0.89455500
C	0.00200200	-1.42208100	-0.34142600
C	0.00886700	-1.41952800	2.13686700
C	-0.00468600	-0.72433400	-1.58645000
C	0.00415000	-2.84955500	-0.32137600
C	0.01665600	-2.83458000	2.12307200
C	-0.02279000	-1.48908700	-2.78435200
C	-0.00603000	-3.56235600	-1.54119500
C	0.01425300	-3.53062000	0.92955500
H	0.02293800	-3.37058300	3.06822700
C	-0.02259200	-2.87974900	-2.75847200
H	-0.04118900	-0.99411500	-3.74786400
H	-0.00396500	-4.64903700	-1.51899700
H	0.01889200	-4.61739300	0.93143500
H	-0.03591500	-3.43391200	-3.69206300
C	0.00496000	-0.68411500	3.36561000
C	-0.00496000	0.68411500	3.36561000
H	0.00891400	-1.23808600	4.30036800
H	-0.00891400	1.23808600	4.30036800



PAH(11) – benzo[*a*]pyrene

CAS: 50-32-8

Neutral Structure

C	3.10709700	3.29119900	0.00000000
C	3.42923400	1.93825200	0.00000000
C	2.41209900	0.95783400	0.00000000
C	1.04368600	1.36591700	0.00000000
C	0.72624200	2.76266600	0.00000000
C	1.76657200	3.70198900	0.00000000
C	2.70122000	-0.44343700	0.00000000
C	0.00043900	0.38438600	0.00000000
C	0.31573200	-1.00151300	0.00000000
C	1.70030400	-1.37735300	0.00000000
C	-0.75371400	-1.97372300	0.00000000
C	-2.11430300	-1.51301200	0.00000000
C	-2.39049500	-0.12330200	0.00000000
C	-1.37588600	0.82094000	0.00000000
C	-1.65989000	2.23747400	0.00000000
C	-0.66193800	3.16116500	0.00000000
H	-0.89204300	4.22436200	0.00000000
H	-2.70201400	2.54901000	0.00000000
H	3.74163900	-0.76047200	0.00000000
H	3.89814200	4.03710700	0.00000000
H	4.46922000	1.61976500	0.00000000
H	1.52205100	4.76187800	0.00000000
H	1.97358600	-2.42689700	0.00000000
H	-3.42787100	0.20525700	0.00000000
C	-0.52846700	-3.37911000	0.00000000
C	-1.57898900	-4.27642100	0.00000000
H	0.48415300	-3.76734200	0.00000000
C	-3.17691900	-2.46356200	0.00000000
C	-2.91941100	-3.81710000	0.00000000
H	-1.37429500	-5.34415800	0.00000000
H	-4.20043900	-2.09512400	0.00000000
H	-3.73794600	-4.53259200	0.00000000

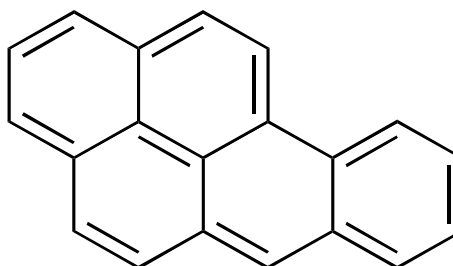
Radical Anion

C	3.15901600	3.27600400	0.00000000
C	3.46824000	1.90981900	0.00000000
C	2.43207100	0.93870600	0.00000000
C	1.06014400	1.36778100	0.00000000
C	0.76090900	2.77868000	0.00000000
C	1.83714000	3.71268800	0.00000000
C	2.69387600	-0.46207300	0.00000000
C	0.00017900	0.39825300	0.00000000
C	0.30114300	-1.00600200	0.00000000
C	1.66595800	-1.38795100	0.00000000
C	-0.79060500	-1.98354100	0.00000000
C	-2.15094000	-1.50030700	0.00000000
C	-2.41068800	-0.11012400	0.00000000
C	-1.37035800	0.84847600	0.00000000
C	-1.62589900	2.24975700	0.00000000
C	-0.60286000	3.18170000	0.00000000
H	-0.83409300	4.24593500	0.00000000
H	-2.66261400	2.58414700	0.00000000
H	3.72824700	-0.80130500	0.00000000
H	3.96552100	4.00781600	0.00000000
H	4.50463600	1.57809300	0.00000000
H	1.60835400	4.77691400	0.00000000
H	1.93098700	-2.44127300	0.00000000
H	-3.44477400	0.23195400	0.00000000
C	-0.57852200	-3.37890400	0.00000000
C	-1.63588600	-4.29330600	0.00000000
H	0.43455600	-3.77026500	0.00000000
C	-3.21186500	-2.45729300	0.00000000
C	-2.96248800	-3.82214400	0.00000000
H	-1.42941300	-5.36105500	0.00000000

H	-4.23708400	-2.09004600	0.00000000
H	-3.79234300	-4.52646000	0.00000000

Radical Cation

C	3.02950500	3.37346100	0.00000000
C	3.38000200	2.02095800	0.00000000
C	2.38575200	1.01263000	0.00000000
C	1.01214700	1.38606800	0.00000000
C	0.65864500	2.77061600	0.00000000
C	1.68829300	3.74724100	0.00000000
C	2.71132100	-0.36919700	0.00000000
C	0.00041400	0.38692000	0.00000000
C	0.35035900	-0.99682700	0.00000000
C	1.72538400	-1.33896500	0.00000000
C	-0.70922500	-1.99979000	0.00000000
C	-2.07889600	-1.56639600	0.00000000
C	-2.38214300	-0.18984700	0.00000000
C	-1.37343400	0.79260400	0.00000000
C	-1.70318800	2.17642900	0.00000000
C	-0.71493000	3.13910500	0.00000000
H	-0.97659100	4.19369200	0.00000000
H	-2.75080900	2.46401700	0.00000000
H	3.75740700	-0.66354000	0.00000000
H	3.80492100	4.13371600	0.00000000
H	4.42641900	1.72706200	0.00000000
H	1.41167800	4.79824200	0.00000000
H	2.02987000	-2.37912400	0.00000000
H	-3.42334400	0.12318500	0.00000000
C	-0.45811900	-3.38408400	0.00000000
C	-1.50472700	-4.30515900	0.00000000
H	0.55814700	-3.76036800	0.00000000
C	-3.12887300	-2.52598000	0.00000000
C	-2.84601700	-3.88006300	0.00000000
H	-1.27522600	-5.36718600	0.00000000
H	-4.15649100	-2.17247500	0.00000000
H	-3.64990400	-4.61044800	0.00000000



PAH(12) – benzo[*e*]pyrene

CAS: 192-97-2

Neutral Structure

C	-0.92144500	3.53396300	0.00000000
C	0.29981900	2.85197600	0.00000000
C	0.35727400	1.44887400	0.00000000
C	-0.86985700	0.71911100	0.00000100
C	-2.11637200	1.42403800	0.00000100
C	-2.12055600	2.83145200	0.00000100
C	1.62917000	0.71180700	0.00000000
C	-0.86985800	-0.71910900	0.00000100
C	0.35727000	-1.44887400	0.00000000
C	1.62916800	-0.71181000	0.00000000
C	0.29981300	-2.85197600	0.00000000
H	1.21128600	-3.43831400	0.00000000
C	-0.92145300	-3.53396000	0.00000000
C	-2.12056200	-2.83144700	0.00000100
C	-2.11637500	-1.42403300	0.00000100
C	-3.34753400	-0.68084900	0.00000100
C	-3.34753200	0.68085700	0.00000100
H	-4.28297800	1.23578100	0.00000100
H	-4.28298000	-1.23577100	0.00000100
H	-0.92591600	4.62113500	0.00000000
H	1.21129400	3.43831200	0.00000000
H	-3.07169200	3.35884300	0.00000100
H	-0.92592600	-4.62113200	0.00000000
H	-3.07170000	-3.35883600	0.00000100
C	2.87202900	1.38905900	0.00000000
C	4.07649800	0.70207000	0.00000000
C	4.07649600	-0.70208000	0.00000000
C	2.87202500	-1.38906600	0.00000000
H	2.89915500	2.47298500	0.00000000
H	5.01393000	1.25242400	0.00000000
H	5.01392700	-1.25243700	0.00000000
H	2.89914800	-2.47299200	0.00000000

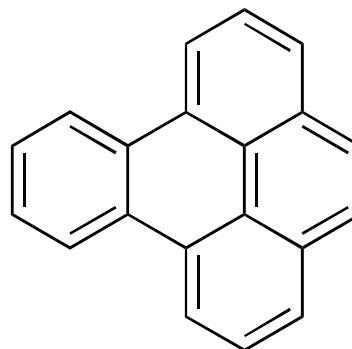
Radical Anion

C	-0.91763200	3.55469600	0.00000100
C	0.30857500	2.88187100	0.00000000
C	0.36209900	1.45489400	0.00000000
C	-0.86941400	0.72310800	0.00000000
C	-2.12800500	1.43233400	0.00000100
C	-2.12183100	2.86226400	0.00000100
C	1.61273400	0.72029000	0.00000000
C	-0.86941600	-0.72310600	0.00000100
C	0.36209600	-1.45489500	0.00000000
C	1.61273200	-0.72029400	0.00000000
C	0.30856800	-2.88187100	0.00000000
H	1.22100100	-3.46703700	0.00000000
C	-0.91764000	-3.55469400	0.00000100
C	-2.12183800	-2.86225900	0.00000100
C	-2.12800800	-1.43232900	0.00000100
C	-3.33755300	-0.69421900	0.00000100
C	-3.33755200	0.69422700	0.00000100
H	-4.27990200	1.24008900	0.00000100
H	-4.27990500	-1.24007800	0.00000100
H	-0.92282000	4.64409900	0.00000100
H	1.22100900	3.46703400	0.00000000
H	-3.07154600	3.39371400	0.00000100
H	-0.92283100	-4.64409600	0.00000100
H	-3.07155400	-3.39370600	0.00000100
C	2.86867600	1.38972100	0.00000000
C	4.07160100	0.70698100	0.00000000
C	4.07159900	-0.70699000	0.00000000
C	2.86867200	-1.38972700	0.00000000
H	2.89693700	2.47438200	0.00000000
H	5.00989300	1.25713100	0.00000000

H	5.00989000	-1.25714200	0.00000000
H	2.89693100	-2.47438900	0.00000000

Radical Cation

C	0.00000000	3.54513600	-0.92046300
C	0.00000000	2.85857000	0.29489300
C	0.00000000	1.43809700	0.35781500
C	0.00000000	0.71413300	-0.86382200
C	0.00000000	-1.41762600	-2.10909900
C	0.00000000	2.83993700	-2.11592700
C	0.00000000	0.72007400	1.61870700
C	0.00000000	-0.71413300	-0.86382200
C	0.00000000	-1.43809700	0.35781500
C	0.00000000	-0.72007400	1.61870700
C	0.00000000	-2.85857000	0.29489300
H	0.00000000	-3.44051900	1.20808200
C	0.00000000	-3.54513600	-0.92046300
C	0.00000000	-2.83993700	-2.11592700
C	0.00000000	-1.41762600	-2.10909900
C	0.00000000	-0.69303200	-3.32511100
C	0.00000000	0.69303200	-3.32511100
H	0.00000000	1.23983700	-4.26382600
H	0.00000000	-1.23983700	-4.26382600
H	0.00000000	4.63076300	-0.92329000
H	0.00000000	3.44051900	1.20808200
H	0.00000000	3.36054600	-3.06960400
H	0.00000000	-4.63076300	-0.92329000
H	0.00000000	-3.36054600	-3.06960400
C	0.00000000	1.39918500	2.86453000
C	0.00000000	0.70583300	4.05828300
C	0.00000000	-0.70583300	4.05828300
C	0.00000000	-1.39918500	2.86453000
H	0.00000000	2.48213300	2.89541300
H	0.00000000	1.24929500	4.99895800
H	0.00000000	-1.24929500	4.99895800
H	0.00000000	-2.48213300	2.89541300



PAH(13) – benzo[*b*]triphenylene

CAS: 215-58-7

Neutral Structure

C	0.00000000	0.73680200	-2.26074800
C	0.00000000	-0.73680200	-2.26074800
C	0.00000000	-1.45110700	-1.03137800
C	0.00000000	1.45110700	-1.03137800
H	0.00000000	-2.49743600	3.95373500
H	0.00000000	-1.24707700	6.09212100
C	0.00000000	-0.72071900	0.24880100
C	0.00000000	0.72071900	0.24880100
C	0.00000000	-1.39161200	1.47166700
C	0.00000000	1.39161200	1.47166700
C	0.00000000	-0.71669700	2.70962000
C	0.00000000	0.71669700	2.70962000
H	0.00000000	-2.47568500	1.50553900
H	0.00000000	2.47568500	1.50553900
C	0.00000000	-1.40940600	3.95799000
C	0.00000000	-0.71219300	5.14560700
C	0.00000000	1.40940600	3.95799000
C	0.00000000	0.71219300	5.14560700
H	0.00000000	2.49743600	3.95373500
H	0.00000000	1.24707700	6.09212100
H	0.00000000	-4.65130300	-2.26139100
C	0.00000000	-3.56423400	-2.26894000
C	0.00000000	-2.86017200	-3.48178600
C	0.00000000	-2.86478000	-1.07082900
C	0.00000000	-1.47268400	-3.46910500
C	0.00000000	1.47268400	-3.46910500
H	0.00000000	-3.43343400	-0.14852700
C	0.00000000	2.86478000	-1.07082900
C	0.00000000	2.86017200	-3.48178600
H	0.00000000	0.95650400	-4.42177300
C	0.00000000	3.56423400	-2.26894000
H	0.00000000	3.43343400	-0.14852700
H	0.00000000	3.39286600	-4.42934400
H	0.00000000	4.65130300	-2.26139100
H	0.00000000	-3.39286600	-4.42934400
H	0.00000000	-0.95650400	-4.42177300

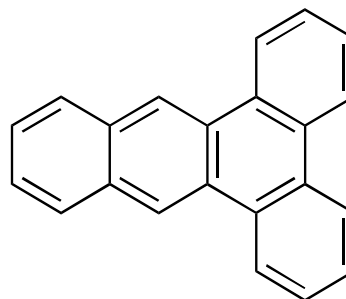
Radical Anion

C	0.00000000	0.72966200	-2.28601100
C	0.00000000	-0.72966200	-2.28601100
C	0.00000000	-1.43604900	-1.03805600
C	0.00000000	1.43604900	-1.03805600
H	0.00000000	-2.49167400	3.97538500
H	0.00000000	-1.24888800	6.13004700
C	0.00000000	-0.71730600	0.23314500
C	0.00000000	0.71730600	0.23314500
C	0.00000000	-1.39566000	1.47621100
C	0.00000000	1.39566000	1.47621100
C	0.00000000	-0.72179500	2.72832400
C	0.00000000	0.72179500	2.72832400
H	0.00000000	-2.48048800	1.50715800
H	0.00000000	2.48048800	1.50715800
C	0.00000000	-1.40211000	3.97457900
C	0.00000000	-0.70179000	5.18910200
C	0.00000000	1.40211000	3.97457900
C	0.00000000	0.70179000	5.18910200
H	0.00000000	2.49167400	3.97538500
H	0.00000000	1.24888800	6.13004700
H	0.00000000	-4.65044200	-2.26118900
C	0.00000000	-3.56266100	-2.27391500
C	0.00000000	-2.86462200	-3.49837200
C	0.00000000	-2.85925000	-1.08169500
C	0.00000000	-1.47794100	-3.48946700
C	0.00000000	1.47794100	-3.48946700

H	0.00000000	-3.42458900	-0.15670400
C	0.00000000	2.85925000	-1.08169500
C	0.00000000	2.86462200	-3.49837200
H	0.00000000	0.96368800	-4.44451700
C	0.00000000	3.56266100	-2.27391500
H	0.00000000	3.42458900	-0.15670400
H	0.00000000	3.40358800	-4.44276800
H	0.00000000	4.65044200	-2.26118900
H	0.00000000	-3.40358800	-4.44276800
H	0.00000000	-0.96368800	-4.44451700

Radical Cation

C	-0.00686600	0.72866300	-2.26373000
C	0.00686600	-0.72866300	-2.26373000
C	-0.00736000	-1.44931300	-1.02518100
C	0.00736000	1.44931300	-1.02518100
H	-0.04108400	-2.49474800	3.94096000
H	-0.02098000	-1.24261500	6.08783300
C	-0.00894200	-0.71562600	0.23244600
C	0.00894200	0.71562600	0.23244600
C	-0.02030200	-1.39018600	1.47038600
C	0.02030200	1.39018600	1.47038600
C	-0.01191700	-0.71430200	2.71080400
C	0.01191700	0.71430200	2.71080400
H	-0.03582400	-2.47325900	1.50403700
H	0.03582400	2.47325900	1.50403700
C	-0.02325500	-1.40809500	3.94134100
C	-0.01188600	-0.70142900	5.14641000
C	0.02325500	1.40809500	3.94134100
C	0.01188600	0.70142900	5.14641000
H	0.04108400	2.49474800	3.94096000
H	0.02098000	1.24261500	6.08783300
H	0.00250100	-4.64417700	-2.25482100
C	0.00592500	-3.55773500	-2.25677900
C	0.03433100	-2.85016800	-3.47501100
C	-0.01207500	-2.86706000	-1.06073200
C	0.03489200	-1.46784800	-3.47277400
C	-0.03489200	1.46784800	-3.47277400
H	-0.02746700	-3.43643000	-0.14010100
C	0.01207500	2.86706000	-1.06073200
C	-0.03433100	2.85016800	-3.47501100
H	-0.06367100	0.95434000	-4.42546800
C	-0.00592500	3.55773500	-2.25677900
H	0.02746700	3.43643000	-0.14010100
H	-0.05692500	3.38874300	-4.41836100
H	-0.00250100	4.64417700	-2.25482100
H	0.05692500	-3.38874300	-4.41836100
H	0.06367100	-0.95434000	-4.42546800



PAH(14) – chrysene

CAS: 218-01-9

Neutral Structure

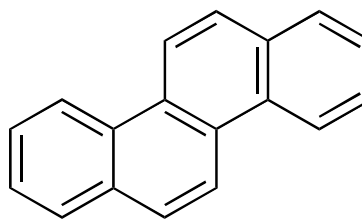
C	0.52736700	4.65078400	0.00000000
C	-0.64932600	3.92635900	0.00000000
C	-0.63161300	2.50743000	0.00000000
C	0.61593800	1.80893400	0.00000000
C	1.80643900	2.58488200	0.00000000
C	1.76432300	3.96882700	0.00000000
H	-2.79246700	2.29942000	0.00000000
H	0.50436300	5.73768500	0.00000000
H	-1.61150000	4.43417200	0.00000000
C	-1.84882900	1.75842500	0.00000000
C	0.61578500	0.35356700	0.00000000
H	2.77631800	2.10013700	0.00000000
H	2.69333300	4.53365500	0.00000000
C	-0.61578500	-0.35356700	0.00000000
C	-1.84064600	0.39151400	0.00000000
H	-2.79035300	-0.13112800	0.00000000
C	-0.61593800	-1.80893400	0.00000000
C	1.84064600	-0.39151400	0.00000000
C	0.63161300	-2.50743000	0.00000000
C	-1.80643900	-2.58488200	0.00000000
C	1.84882900	-1.75842500	0.00000000
H	2.79035300	0.13112800	0.00000000
C	0.64932600	-3.92635900	0.00000000
C	-1.76432300	-3.96882700	0.00000000
H	-2.77631800	-2.10013700	0.00000000
H	2.79246700	-2.29942000	0.00000000
C	-0.52736700	-4.65078400	0.00000000
H	1.61150000	-4.43417200	0.00000000
H	-2.69333300	-4.53365500	0.00000000
H	-0.50436300	-5.73768500	0.00000000

Radical Cation

C	-0.51344400	4.66504100	0.02269100
C	0.66344900	3.92837500	-0.01727300
C	0.62568900	2.51277400	-0.02328300
C	-0.62498300	1.82272200	0.00450800
C	-1.79961900	2.59568100	0.05116500
C	-1.74292700	3.99264000	0.05988200
H	2.77645200	2.29283100	-0.07649300
H	-0.48195100	5.75061400	0.02821000
H	1.62930100	4.42590200	-0.04220000
C	1.82865300	1.76172600	-0.05117900
C	-0.62786000	0.36059500	-0.01166400
H	-2.77545500	2.12569600	0.08824400
H	-2.66963500	4.55836600	0.09700500
C	0.62786000	-0.36059500	-0.01166400
C	1.82665000	0.37301200	-0.04138500
H	2.78276000	-0.13524700	-0.06579500
C	0.62498300	-1.82272200	0.00450800
C	-1.82665000	-0.37301200	-0.04138500
C	-0.62568900	-2.51277400	-0.02328300
C	1.79961900	-2.59568100	0.05116500
C	-1.82865300	-1.76172600	-0.05117900
H	-2.78276000	0.13524700	-0.06579500
C	-0.66344900	-3.92837500	-0.01727300
C	1.74292700	-3.99264000	0.05988200
H	2.77545500	-2.12569600	0.08824400
H	-2.77645200	-2.29283100	-0.07649300
C	0.51344400	-4.66504100	0.02269100
H	-1.62930100	-4.42590200	-0.04220000
H	2.66963500	-4.55836600	0.09700500
H	0.48195100	-5.75061400	0.02821000

Radical Anion

C	0.54789700	4.68363500	0.00000000
C	-0.63697100	3.94873600	0.00000000
C	-0.63346300	2.52814600	0.00000000
C	0.62660100	1.82990500	0.00000000
C	1.80607000	2.60906500	0.00000000
C	1.77708300	4.00996900	0.00000000
H	-2.79743700	2.31049900	0.00000000
H	0.51574300	5.77145000	0.00000000
H	-1.59707500	4.46306200	0.00000000
C	-1.84917400	1.77643100	0.00000000
C	0.63400000	0.35926500	0.00000000
H	2.77614800	2.12106700	0.00000000
H	2.71128300	4.56747300	0.00000000
C	-0.63400000	-0.35926500	0.00000000
C	-1.82978400	0.38312500	0.00000000
H	-2.78547400	-0.13401000	0.00000000
C	-0.62660100	-1.82990500	0.00000000
C	1.82978400	-0.38312500	0.00000000
C	0.63346300	-2.52814600	0.00000000
C	-1.80607000	-2.60906500	0.00000000
C	1.84917400	-1.77643100	0.00000000
H	2.78547400	0.13401000	0.00000000
C	0.63697100	-3.94873600	0.00000000
C	-1.77708300	-4.00996900	0.00000000
H	-2.77614800	-2.12106700	0.00000000
H	2.79743700	-2.31049900	0.00000000
C	-0.54789700	-4.68363500	0.00000000
H	1.59707500	-4.46306200	0.00000000
H	-2.71128300	-4.56747300	0.00000000
H	-0.51574300	-5.77145000	0.00000000



PAH(15) – coronene

CAS: 191-07-1

Neutral Structure

C	0.96405300	-2.80735300	-0.00068100
C	2.39056600	-2.81120700	-0.00044700
C	3.08024000	-1.56630600	0.00001000
C	2.34358300	-0.34132000	0.00026100
C	0.92086400	-0.36662900	0.00001900
C	0.25546300	-1.62862400	-0.00044900
C	4.50912300	-1.54100000	0.00026300
C	3.03631300	0.90895300	0.00070400
C	4.46519500	0.93425900	0.00095700
C	5.20185200	-0.29072700	0.00070700
C	5.15486900	2.17916000	0.00141400
C	4.39478100	3.38643200	0.00164900
C	3.01971900	3.36215400	0.00142100
C	2.30281800	2.12864500	0.00095100
C	0.87724500	2.07391000	0.00071600
C	0.21074200	0.87086500	0.00027100
H	-0.87683000	0.84784100	0.00010600
H	0.31984300	3.00798100	0.00090800
H	0.44012400	-3.76062500	-0.00104600
H	-0.83219700	-1.64442700	-0.00062800
H	4.92528800	4.33598400	0.00201800
H	2.45604700	4.29245800	0.00161700
C	3.15065500	-4.01847900	-0.00068200
C	4.52571600	-3.99420100	-0.00045400
C	5.24261700	-2.76069200	0.00001600
H	2.62014800	-4.96803100	-0.00105100
H	5.08938900	-4.92450500	-0.00065000
C	6.66819000	-2.70595600	0.00025100
C	7.33469300	-1.50291200	0.00069600
C	6.62457100	-0.26541800	0.00094800
H	7.22559200	-3.64002800	0.00005900
H	8.42226600	-1.47988800	0.00086100
C	6.58138300	2.17530600	0.00164800
H	7.10531200	3.12857800	0.00201300
C	7.28997200	0.99657700	0.00141700
H	8.37763300	1.01238000	0.00159500

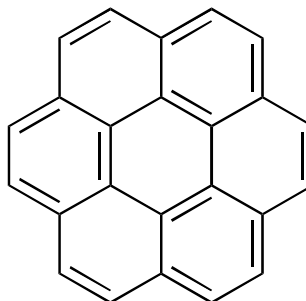
Radical Anion

C	0.97257700	-2.81942200	-0.00067600
C	2.37976200	-2.82583900	-0.00044400
C	3.08306100	-1.56894300	0.00001300
C	2.34385900	-0.34065000	0.00026200
C	0.90902400	-0.36730200	0.00001800
C	0.24886900	-1.62782600	-0.00044500
C	4.50723500	-1.54365100	0.00026800
C	3.03820000	0.91160400	0.00070000
C	4.46237500	0.93689700	0.00095400
C	5.20157600	-0.29139600	0.00070600
C	5.16567300	2.19379300	0.00141100
C	4.38957000	3.40842700	0.00165500
C	3.02173200	3.38281800	0.00142300
C	2.29108400	2.14436200	0.00094500
C	0.88255400	2.08670200	0.00071100
C	0.20258500	0.87485100	0.00027000
H	-0.88559800	0.85787000	0.00011100
H	0.32120500	3.02034200	0.00090600
H	0.44406400	-3.77191500	-0.00104900
H	-0.83924800	-1.65016600	-0.00063000
H	4.91965100	4.35960700	0.00204300
H	2.45797600	4.31473500	0.00163400
C	3.15586500	-4.04047400	-0.00068700
C	4.52370400	-4.01486400	-0.00045500
C	5.25435100	-2.77640800	0.00002300
H	2.62578400	-4.99165400	-0.00107600

H	5.08746000	-4.94678100	-0.00066700
C	6.66288200	-2.71874900	0.00025600
C	7.34285000	-1.50689800	0.00069700
C	6.63641200	-0.26474500	0.00094900
H	7.22423000	-3.65238900	0.00006100
H	8.43103300	-1.48991700	0.00085600
C	6.57285800	2.18737500	0.00164300
H	7.10137100	3.13986900	0.00201600
C	7.29656600	0.99577900	0.00141300
H	8.38468300	1.01811900	0.00159700

Radical Cation

C	-0.00005000	1.23010700	3.53696000
C	-0.00001300	2.43358400	2.83920400
C	-0.00009800	2.46063400	1.42018100
C	0.00180700	1.23016200	0.70965700
C	-0.00164300	-0.00301900	1.42233400
C	0.00019300	-0.00291300	2.85482500
C	0.00002500	3.67960300	0.68462800
C	-0.00185400	1.23061300	-0.71327200
C	0.00003600	2.47325500	-1.43072300
C	-0.00004500	3.68259600	-0.70282200
C	-0.00003800	2.44622800	-2.86805600
H	0.00022200	3.39249500	-3.40223800
C	0.00009600	1.26311600	-3.55082300
C	-0.00019300	0.00291300	-2.85482500
C	0.00164300	0.00301900	-1.42233400
H	-0.00015000	4.61984300	1.22973400
H	0.00009900	1.23478100	4.62356900
H	-0.00030700	3.37448600	3.38318700
H	0.00026200	4.62472800	-1.24391500
H	0.00014100	1.25227400	-4.63755400
H	-0.00026200	-4.62472800	1.24391500
C	0.00004500	-3.68259600	0.70282200
C	-0.00003600	-2.47325500	1.43072300
C	-0.00002500	-3.67960300	-0.68462800
C	0.00003800	-2.44622800	2.86805600
C	0.00185400	-1.23061300	0.71327200
C	0.00009800	-2.46063400	-1.42018100
H	0.00015000	-4.61984300	-1.22973400
C	-0.00009600	-1.26311600	3.55082300
H	-0.00022200	-3.39249500	3.40223800
C	-0.00180700	-1.23016200	-0.70965700
C	0.00001300	-2.43358400	-2.83920400
H	-0.00014100	-1.25227400	4.63755400
H	0.00030700	-3.37448600	-3.38318700
C	0.00005000	-1.23010700	-3.53696000
H	-0.00009900	-1.23478100	-4.62356900

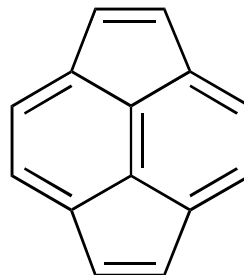


PAH(16) – cyclopent[fg]acenaphthylene

CAS: 187-78-0

Neutral Structure

C	-4.10875800	-1.28468000	-0.03235500
C	-2.73090900	-1.08490500	-0.02566200
C	-2.29850100	0.25505600	-0.00621300
C	-3.15653200	1.30610100	0.00620400
C	-4.55620700	1.15033900	-0.00021300
C	-5.02746300	-0.15964600	-0.01943200
H	-4.53899200	-2.28351700	-0.04729500
C	-0.89882600	0.41081800	0.00020200
C	-2.72412400	2.64606200	0.02565100
H	-6.09230900	-0.38154400	-0.02558600
C	-1.34627500	2.84583700	0.03234200
C	-0.42757000	1.72080300	0.01941900
H	-0.91604100	3.84467500	0.04728000
H	0.63727500	1.94270100	0.02557100
C	-5.06150400	2.55550400	0.01771100
C	-3.99998800	3.42200900	0.03268800
H	-6.10665700	2.84664500	0.01879600
H	-4.07623300	4.50419200	0.04745700
C	-0.39352900	-0.99434700	-0.01772400
C	-1.45504500	-1.86085200	-0.03270100
H	0.65162400	-1.28548800	-0.01881100
H	-1.37880000	-2.94303500	-0.04747200



Radical Anion

C	-4.13347000	-1.28740300	-0.03255000
C	-2.72581300	-1.09573900	-0.02590800
C	-2.29552400	0.25137100	-0.00627400
C	-3.15950900	1.30978600	0.00626300
C	-4.56578600	1.15754500	-0.00001000
C	-5.03505600	-0.18314400	-0.01988000
H	-4.56113200	-2.28942600	-0.04748900
C	-0.88924700	0.40361100	-0.00000200
C	-2.72922100	2.65689500	0.02589700
H	-6.10249500	-0.40189400	-0.02586500
C	-1.32156300	2.84856000	0.03253800
C	-0.41997800	1.74430100	0.01986700
H	-0.89390100	3.85058300	0.04747500
H	0.64746100	1.96305100	0.02585100
C	-5.06350800	2.53445900	0.01746300
C	-3.97892100	3.41966200	0.03265800
H	-6.10769900	2.83574200	0.01873700
H	-4.06557000	4.50290200	0.04726400
C	-0.39152500	-0.97330200	-0.01747600
C	-1.47611300	-1.85850500	-0.03267200
H	0.65266600	-1.27458500	-0.01875000
H	-1.38946400	-2.94174500	-0.04727900

PAH(17) – cyclopent[hi]acephenanthrylene

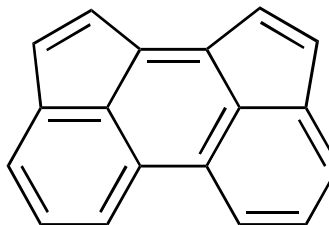
CAS: 114959-37-4

Neutral Structure

C	-4.77703800	-4.04634400	-0.00089300
C	-3.39504800	-3.91105500	-0.00447800
C	-2.83641300	-2.61128300	-0.00248200
C	-3.59616800	-1.43315500	0.00265500
C	-5.00638500	-1.59429000	0.00627000
C	-5.56890000	-2.86994200	0.00451900
C	-1.39222700	-2.71953000	-0.00736600
C	-2.83895900	-0.18364900	0.00358100
C	-1.44312900	-0.31177900	-0.00102700
C	-0.67859700	-1.54187200	-0.00645000
C	-0.54963300	0.78514000	-0.00105300
C	-1.06952200	2.07275000	0.00362900
C	-2.47878500	2.23020000	0.00840700
C	-3.34901100	1.14103400	0.00840900
H	-5.25656300	-5.02245300	-0.00225700
H	-5.65687000	-0.72367400	0.01033600
H	-6.65163900	-2.96772000	0.00732100
H	-0.42623900	2.94963500	0.00379200
H	-2.89332100	3.23516600	0.01219100
H	-4.42178700	1.31456200	0.01219700
C	0.80992300	0.21731400	-0.00665900
C	0.73278300	-1.14823500	-0.00991300
H	1.72338700	0.80312600	-0.00801600
H	1.57016900	-1.83704000	-0.01425400
C	-2.26212900	-4.85323900	-0.01077000
C	-1.08746300	-4.15268100	-0.01241800
H	-2.35856800	-5.93411600	-0.01365400
H	-0.08930100	-4.57606400	-0.01682200

Radical Anion

C	-4.80017100	-4.04897100	-0.00060900
C	-3.40005400	-3.94009900	-0.00447600
C	-2.82190200	-2.63215700	-0.00250400
C	-3.58650100	-1.44644600	0.00254700
C	-4.98880600	-1.59296500	0.00621100
C	-5.57311700	-2.87469000	0.00464900
C	-1.38659000	-2.74832600	-0.00746600
C	-2.82257600	-0.18613900	0.00337800
C	-1.41777200	-0.31501500	-0.00127000
C	-0.65024900	-1.53356300	-0.00655100
C	-0.52608700	0.80307400	-0.00111500
C	-1.07789900	2.09448700	0.00370200
C	-2.47650400	2.23600400	0.00833400
C	-3.34200700	1.12467800	0.00821200
H	-5.29185500	-5.02073400	-0.00186600
H	-5.63335500	-0.71694100	0.01020500
H	-6.65833300	-2.95615500	0.00754500
H	-0.44421500	2.98017900	0.00403200
H	-2.90669600	3.23556000	0.01217800
H	-4.41692000	1.29048600	0.01196400
C	0.81630500	0.25862500	-0.00641000
C	0.73074700	-1.13708400	-0.00976000
H	1.73341200	0.84023800	-0.00769600
H	1.57833300	-1.81678800	-0.01402100
C	-2.29583400	-4.87783100	-0.01087900
C	-1.09834100	-4.15589200	-0.01255500
H	-2.38687200	-5.96000900	-0.01383500
H	-0.10357500	-4.59271900	-0.01714800



PAH(18) – cyclopenta[hi]chrysene

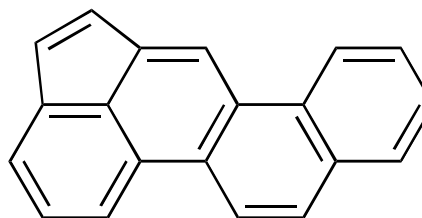
CAS: 216-48-8

Neutral Structure

C	0.20936700	4.66582300	0.00001400
C	-0.92016200	3.87137100	-0.00020600
C	-0.81758600	2.45513600	-0.00018800
C	0.47100300	1.83126700	0.00006600
C	1.61105100	2.68061400	0.00028400
C	1.48509800	4.05892900	0.00025900
H	0.12078300	5.74923100	-0.00000100
C	-1.99174300	1.64229700	-0.00042000
C	0.56140100	0.37719900	0.00009100
H	2.60895900	2.25767000	0.00047000
H	2.37866000	4.67823500	0.00043000
C	-0.64486500	-0.39192400	-0.00016900
C	-1.90646800	0.27662500	-0.00041700
H	-2.81838900	-0.31230000	-0.00060100
C	-0.56473800	-1.84480500	-0.00017600
C	1.84659200	-0.27752100	0.00038800
C	0.71290800	-2.39899100	0.00012100
C	-1.63911700	-2.78172400	-0.00047500
C	1.92356900	-1.64798800	0.00041200
H	2.75457100	0.31578800	0.00060300
C	1.00596800	-3.78455000	0.00017400
C	-1.37541500	-4.14907600	-0.00044700
H	-2.67218700	-2.44750100	-0.00073200
C	-0.05554600	-4.67674300	-0.00012100
H	-2.21253900	-4.84289100	-0.00068400
H	0.09572300	-5.75376800	-0.00011000
C	3.01546100	-2.63285200	0.00068300
C	2.47562800	-3.89029300	0.00055000
H	4.07272500	-2.38949600	0.00094500
H	3.03022900	-4.82292600	0.00068800
H	-1.91157500	4.31919200	-0.00039900
H	-2.96323800	2.13123300	-0.00060600

Radical Anion

C	0.20340300	4.68551300	0.00003900
C	-0.92226200	3.87984700	-0.00016600
C	-0.81910000	2.46363500	-0.00017300
C	0.47511300	1.84714700	0.00004300
C	1.60512000	2.70471300	0.00024100
C	1.48018900	4.08743600	0.00024200
H	0.10486000	5.76857900	0.00004300
C	-1.99366900	1.64536600	-0.00039200
C	0.59088800	0.38200000	0.00006100
H	2.60449500	2.28296000	0.00039600
H	2.37312200	4.70826500	0.00040000
C	-0.63424300	-0.39550400	-0.00020000
C	-1.88679000	0.27422600	-0.00041200
H	-2.79761400	-0.31935400	-0.00058800
C	-0.55804900	-1.85406700	-0.00021900
C	1.85527600	-0.25672300	0.00034900
C	0.72749900	-2.41240000	0.00009300
C	-1.63645700	-2.78264700	-0.00052200
C	1.94359000	-1.66310000	0.00039100
H	2.76541200	0.33559000	0.00057300
C	1.01838600	-3.81198400	0.00018600
C	-1.37652400	-4.16939900	-0.00046500
H	-2.66920900	-2.44487200	-0.00079700
C	-0.07836500	-4.70453000	-0.00011000
H	-2.22415400	-4.85319700	-0.00070600
H	0.06411700	-5.78426500	-0.00007100
C	3.00972400	-2.62891000	0.00071200
C	2.45611300	-3.92201800	0.00059500
H	4.07152300	-2.39665700	0.00099200
H	3.01889200	-4.85156400	0.00077400
H	-1.91563400	4.32514500	-0.00032900
H	-2.96952400	2.12603200	-0.00055000



PAH(19) – cyclopenta[*cd*]fluoranthene

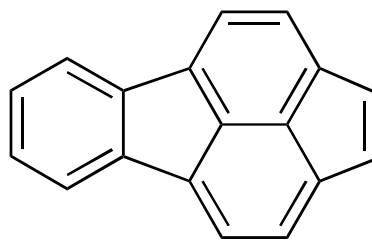
CAS: 193-54-4

Neutral Structure

C	0.00004500	2.18576400	1.03604200
C	0.00104700	1.05147400	0.22710000
C	-0.00101600	-0.19395600	0.88909200
C	-0.00391000	-0.29606900	2.24604000
C	-0.00508500	0.82381500	3.09998100
C	-0.00307900	2.07176500	2.47783800
H	0.00152000	3.18572100	0.60908000
C	-0.00001100	-1.32634200	0.04829000
C	-0.00609800	-1.53125000	2.92260100
H	-0.00376700	2.99369700	3.05529300
C	-0.00520100	-2.67197500	2.12030000
C	-0.00210200	-2.56904300	0.67772300
H	-0.00679300	-3.66990600	2.55321100
H	-0.00154600	-3.49396700	0.10595900
C	0.00307600	-0.75032500	-1.32617600
C	0.00499600	-1.35475200	-2.57769600
C	0.00380400	0.68774400	-1.21807500
C	0.00765000	-0.54703200	-3.73084200
H	0.00442200	-2.43812100	-2.67038200
C	0.00643700	1.47222000	-2.36550400
C	0.00837100	0.84557500	-3.62628900
H	0.00912800	-1.01530400	-4.71190700
H	0.00698100	2.55738800	-2.29560800
H	0.01041800	1.45492100	-4.52657100
C	-0.00896900	-1.14406400	4.35768500
C	-0.00834300	0.22557600	4.46096600
H	-0.01118100	-1.83437600	5.19481900
H	-0.00999800	0.78225800	5.39227800

Radical Anion

C	0.00022100	2.20463400	1.05061500
C	0.00133500	1.05328300	0.22137400
C	-0.00067200	-0.19384200	0.88803900
C	-0.00370400	-0.29667100	2.25373900
C	-0.00506400	0.82648300	3.11383900
C	-0.00297700	2.09587400	2.46751100
H	0.00168500	3.20361000	0.61697900
C	0.00029900	-1.32724700	0.04233300
C	-0.00603500	-1.53595700	2.93586900
H	-0.00377200	3.01799600	3.04772900
C	-0.00509900	-2.69435900	2.10641500
C	-0.00193500	-2.58972600	0.68927000
H	-0.00682700	-3.69284400	2.54211800
H	-0.00142300	-3.51264200	0.11096600
C	0.00321600	-0.76044100	-1.31188200
C	0.00498400	-1.35518100	-2.57920600
C	0.00394000	0.69558900	-1.20242300
C	0.00742400	-0.55208100	-3.72881800
H	0.00440700	-2.43958500	-2.67634600
C	0.00642300	1.47287500	-2.36699700
C	0.00816600	0.85021700	-3.62351300
H	0.00876800	-1.01952200	-4.71118900
H	0.00699000	2.55973700	-2.30151000
H	0.01010500	1.45884700	-4.52525700
C	-0.00914000	-1.15898300	4.34280600
C	-0.00851800	0.24262400	4.44858500
H	-0.01158400	-1.84271600	5.18758300
H	-0.01042000	0.79146600	5.38661800



PAH(20) – cyclopenta[*cd*]perylene

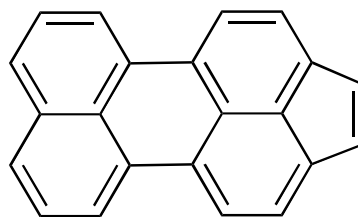
CAS: 189-01-5

Neutral Structure

C	0.01527500	2.44290100	-2.76241800
C	0.00832800	1.27067500	-3.48936800
C	0.00062000	0.01338500	-2.82742900
C	-0.00045700	-0.03912400	-1.39250900
C	0.00142700	1.19674000	-0.65265200
C	0.01171500	2.40190200	-1.35475500
H	-0.00565900	-1.13068000	-4.66589700
H	0.02306400	3.40474000	-3.26836300
H	0.00952300	1.28951700	-4.57660900
C	-0.00595900	-1.19198100	-3.58015200
C	-0.00321700	-1.32575700	-0.74510900
H	0.01839300	3.34447200	-0.81721900
C	-0.01204000	-2.47590200	-1.53378300
C	-0.01357700	-2.41413400	-2.94072600
H	-0.01876800	-3.45473100	-1.06615400
H	-0.02030100	-3.33668700	-3.51523500
C	0.00336200	-1.38577300	0.72475700
C	-0.00233500	-0.14331400	1.43660400
C	0.01368400	-2.57010800	1.47983900
C	-0.00747200	1.14784600	0.81763700
C	-0.00347900	-0.19415000	2.82839300
C	0.01413500	-2.58751900	2.89781300
H	0.02276500	-3.53121800	0.97590100
C	-0.01980200	2.27343400	1.65738400
C	-0.01296100	0.93820400	3.67984200
C	0.00419500	-1.38581700	3.59457900
H	0.02217200	-3.54744400	3.40977900
C	-0.02239000	2.18755800	3.07284000
H	-0.02895800	3.26809600	1.22406600
H	-0.03182200	3.10769000	3.65330600
C	-0.00039400	-0.96145500	4.99940300
C	-0.01103500	0.41175900	5.04987500
H	0.00379600	-1.63004400	5.85407700
H	-0.01688500	1.01543800	5.95152600

Radical Anion

C	-0.00122500	2.45035700	-2.75270100
C	0.00020100	1.27327200	-3.48775800
C	0.00071600	0.01343900	-2.82883500
C	-0.00040900	-0.03936000	-1.38679000
C	-0.00200500	1.19745700	-0.64034300
C	-0.00230400	2.41728600	-1.35323500
H	0.00307100	-1.13817700	-4.66494200
H	-0.00156500	3.41101700	-3.26392300
H	0.00098000	1.29652900	-4.57542600
C	0.00228200	-1.19481100	-3.57844500
C	0.00021400	-1.32734000	-0.73297100
H	-0.00336700	3.35894400	-0.81370500
C	0.00185300	-2.49162600	-1.53325400
C	0.00286500	-2.42245200	-2.93139800
H	0.00242600	-3.46967900	-1.066341000
H	0.00413500	-3.34334100	-3.51121900
C	-0.00091300	-1.38333800	0.71786900
C	-0.00261700	-0.14305500	1.43479700
C	-0.00041300	-2.58803200	1.48585000
C	-0.00336700	1.14626800	0.81074300
C	-0.00381300	-0.19432600	2.83383900
C	-0.00155700	-2.60714000	2.88447400
H	0.00089100	-3.54551100	0.97297500
C	-0.00541400	2.29135600	1.66492500
C	-0.00580700	0.94228000	3.68890900
C	-0.00328100	-1.39052500	3.60321800
H	-0.00105200	-3.56773100	3.39847800
C	-0.00664200	2.20818300	3.06128200
H	-0.00623200	3.28321000	1.22271200
H	-0.00828100	3.12869100	3.64406600
C	-0.00493200	-0.97436500	4.98533200
C	-0.00651600	0.42547000	5.03695000
H	-0.00499800	-1.63704700	5.84644800
H	-0.00798300	1.02261700	5.94472700



PAH(21) – cyclopenta[*cd*]pyrene

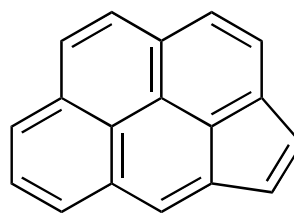
CAS: 27208-37-3

Neutral Structure

C	-4.33548600	-4.96202400	-0.00031100
C	-2.93691900	-5.01704400	0.00016100
C	-2.16878700	-3.83628800	0.00009100
C	-2.87626500	-2.58750000	-0.00045100
C	-4.29626700	-2.52678400	-0.00095300
C	-5.01373400	-3.73824000	-0.00086200
C	-0.71664400	-3.85941500	0.00056200
C	-2.14162300	-1.37223600	-0.00053600
C	-0.75790200	-1.44979400	-0.00006800
C	-0.01592000	-2.67642500	0.00046900
C	0.09620100	-0.33889000	-0.00010000
C	-0.49821100	0.93422900	-0.00061400
C	-1.90263900	1.04677500	-0.00110000
C	-2.75495900	-0.08474700	-0.00107600
C	-4.19572100	-0.05899600	-0.00158300
C	-4.92282700	-1.22246900	-0.00151500
H	-6.00982700	-1.18002400	-0.00189700
H	-4.70729200	0.90119500	-0.00201900
H	-0.21901500	-4.82746300	0.00097000
H	-4.90477100	-5.88800100	-0.00024300
H	-2.43319000	-5.98098100	0.00058300
H	-6.10138800	-3.71934700	-0.00122400
H	0.10482300	1.83970800	-0.00066500
H	-2.34982300	2.03840900	-0.00150900
C	1.39754100	-2.26550800	0.00079400
C	1.46202200	-0.89444900	0.00045200
H	2.24527000	-2.94242600	0.00122000
H	2.37415100	-0.30620700	0.00056800

Radical Anion

C	-4.34823000	-4.97233400	-0.00033600
C	-2.95308100	-5.03937500	0.00014400
C	-2.15874200	-3.85273500	0.00009500
C	-2.87405000	-2.59318400	-0.00044200
C	-4.29821900	-2.53028500	-0.00094400
C	-5.03089400	-3.74867800	-0.00086700
C	-0.73013000	-3.87718500	0.00057600
C	-2.13266400	-1.37489000	-0.00052000
C	-0.74184500	-1.45089700	-0.00004500
C	0.00089300	-2.66988500	0.00049200
C	0.12223800	-0.32332800	-0.00009600
C	-0.49912200	0.95732600	-0.00063600
C	-1.88981100	1.06314700	-0.00110600
C	-2.75218800	-0.08491700	-0.00106200
C	-4.17700900	-0.06056200	-0.00156200
C	-4.91574200	-1.23209400	-0.00149500
H	-6.00331800	-1.18098800	-0.00187800
H	-4.69289300	0.89905900	-0.00200300
H	-0.23045000	-4.84576100	0.00098800
H	-4.92085100	-5.89851100	-0.00027700
H	-2.45651000	-6.00807000	0.00056400
H	-6.11873200	-3.72449400	-0.00122600
H	0.09935400	1.86803500	-0.00071300
H	-2.34620700	2.05202800	-0.00153200
C	1.38798000	-2.26672600	0.00080600
C	1.45975000	-0.86098700	0.00043500
H	2.24266400	-2.93804500	0.00123800
H	2.37860800	-0.28060600	0.00054600



PAH(22) – dibenz[*a,h*]anthracene

CAS: 53-70-5

Neutral Structure

C	-0.77388100	3.70545600	0.00000000
C	0.38749300	2.87503500	0.00000000
C	0.21898500	1.42027000	0.00000000
C	-1.10789400	0.87095900	0.00000000
C	-2.24502400	1.75541200	0.00000000
C	-2.08521000	3.10674600	0.00000000
C	1.29222300	0.52074500	0.00000000
C	-1.29222300	-0.52074500	0.00000000
C	-0.21898500	-1.42027000	0.00000000
C	1.10789400	-0.87095900	0.00000000
C	2.24502400	-1.75541200	0.00000000
H	3.23965300	-1.31508000	0.00000000
C	2.08521000	-3.10674600	0.00000000
C	0.77388100	-3.70545600	0.00000000
C	-0.38749300	-2.87503500	0.00000000
H	2.31495800	0.88471800	0.00000000
H	-3.23965300	1.31508000	0.00000000
H	-2.95056600	3.76584100	0.00000000
H	-2.31495800	-0.88471800	0.00000000
H	2.95056600	-3.76584100	0.00000000
C	-1.65550200	-3.50371200	0.00000000
C	0.62808800	-5.11338200	0.00000000
C	-1.77542900	-4.88660700	0.00000000
H	-2.56048400	-2.90493100	0.00000000
C	-0.62654200	-5.70152400	0.00000000
H	1.52437400	-5.72999200	0.00000000
H	-2.76344300	-5.34023900	0.00000000
H	-0.72481300	-6.78415400	0.00000000
C	1.65550200	3.50371200	0.00000000
C	1.77542900	4.88660700	0.00000000
H	2.56048400	2.90493100	0.00000000
C	-0.62808800	5.11338200	0.00000000
C	0.62654200	5.70152400	0.00000000
H	2.76344300	5.34023900	0.00000000
H	-1.52437400	5.72999200	0.00000000
H	0.72481300	6.78415400	0.00000000

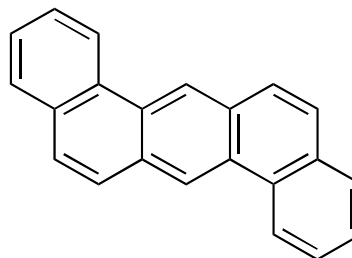
Radical Anion

C	-0.80112300	3.73115800	0.00000000
C	0.36829500	2.88437300	0.00000000
C	0.21177400	1.43255900	0.00000000
C	-1.12071600	0.88540900	0.00000000
C	-2.24054900	1.76517800	0.00000000
C	-2.09538900	3.14324400	0.00000000
C	1.29188900	0.53025500	0.00000000
C	-1.29188900	-0.53025500	0.00000000
C	-0.21177400	-1.43255900	0.00000000
C	1.12071600	-0.88540900	0.00000000
C	2.24054900	-1.76517800	0.00000000
H	3.23781200	-1.32665200	0.00000000
C	2.09538900	-3.14324400	0.00000000
C	0.80112300	-3.73115800	0.00000000
C	-0.36829500	-2.88437300	0.00000000
H	2.31352400	0.89997000	0.00000000
H	-3.23781200	1.32665200	0.00000000
H	-2.96981000	3.79136300	0.00000000
H	-2.31352400	-0.89997000	0.00000000
H	2.96981000	-3.79136300	0.00000000
C	-1.64067500	-3.51528300	0.00000000
C	0.62815100	-5.14516900	0.00000000
C	-1.77852700	-4.89435500	0.00000000
H	-2.54099800	-2.90776300	0.00000000
C	-0.62706600	-5.72181300	0.00000000
H	1.51798200	-5.77308200	0.00000000

H	-2.77038100	-5.34057400	0.00000000
H	-0.73346300	-6.80443300	0.00000000
C	1.64067500	3.51528300	0.00000000
C	1.77852700	4.89435500	0.00000000
H	2.54099800	2.90776300	0.00000000
C	-0.62815100	5.14516900	0.00000000
C	0.62706600	5.72181300	0.00000000
H	2.77038100	5.34057400	0.00000000
H	-1.51798200	5.77308200	0.00000000
H	0.73346300	6.80443300	0.00000000

Radical Cation

C	-0.76191900	3.71116900	0.00000000
C	0.40815600	2.87842300	0.00000000
C	0.23106100	1.42922000	0.00000000
C	-1.09620300	0.88268100	0.00000000
C	-2.21891100	1.74420000	0.00000000
C	-2.05294100	3.11745700	0.00000000
C	1.29188900	0.52589700	0.00000000
C	-1.29188900	-0.52589700	0.00000000
C	-0.23106100	-1.42922000	0.00000000
C	1.09620300	-0.88268100	0.00000000
C	2.21891100	-1.74420000	0.00000000
H	3.21622100	-1.31336800	0.00000000
C	2.05294100	-3.11745700	0.00000000
C	0.76191900	-3.71116900	0.00000000
C	-0.40815600	-2.87842300	0.00000000
H	2.31908100	0.87465100	0.00000000
H	-3.21622100	1.31336800	0.00000000
H	-2.92406800	3.76750800	0.00000000
H	-2.31908100	-0.87465100	0.00000000
H	2.92406800	-3.76750800	0.00000000
C	-1.66977600	-3.50890100	0.00000000
C	0.62589900	-5.12630200	0.00000000
C	-1.77500100	-4.89375900	0.00000000
H	-2.57996100	-2.91931200	0.00000000
C	-0.62387900	-5.71159900	0.00000000
H	1.52665000	-5.73465300	0.00000000
H	-2.76026400	-5.35212700	0.00000000
H	-0.72611900	-6.79301200	0.00000000
C	1.66977600	3.50890100	0.00000000
C	1.77500100	4.89375900	0.00000000
H	2.57996100	2.91931200	0.00000000
C	-0.62589900	5.12630200	0.00000000
C	0.62387900	5.71159900	0.00000000
H	2.76026400	5.35212700	0.00000000
H	-1.52665000	5.73465300	0.00000000
H	0.72611900	6.79301200	0.00000000



PAH(23) – dibenz[*a,j*]anthracene

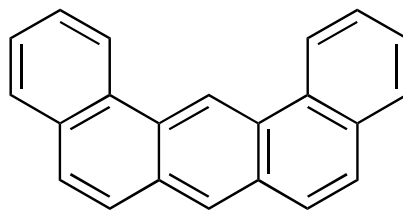
CAS: 224-41-9

Neutral Structure

C	0.00000000	3.66336800	1.73022200
C	0.00000000	3.72455600	0.28974000
C	0.00000000	2.51816200	-0.47465000
C	0.00000000	2.47147600	2.38627200
H	0.00000000	4.59969800	2.28393100
H	0.00000000	2.43565000	3.47349800
C	0.00000000	1.23219900	0.22723600
C	0.00000000	1.22557600	1.66310300
C	0.00000000	0.00000000	-0.44438200
C	0.00000000	0.00000000	2.34122900
C	0.00000000	-1.23219900	0.22723600
C	0.00000000	-1.22557600	1.66310300
H	0.00000000	0.00000000	-1.52683800
H	0.00000000	0.00000000	3.42963300
C	0.00000000	-2.51816200	-0.47465000
C	0.00000000	-3.72455600	0.28974000
C	0.00000000	-2.47147600	2.38627200
C	0.00000000	-3.66336800	1.73022200
H	0.00000000	-2.43565000	3.47349800
H	0.00000000	-4.59969800	2.28393100
H	0.00000000	3.91194200	-3.60231200
C	0.00000000	3.86269600	-2.51619300
C	0.00000000	5.04941100	-1.75759500
C	0.00000000	2.62608200	-1.88579100
C	0.00000000	4.97477300	-0.37402400
C	0.00000000	-2.62608200	-1.88579100
H	0.00000000	1.73198900	-2.50025700
C	0.00000000	-4.97477300	-0.37402400
C	0.00000000	-3.86269600	-2.51619300
H	0.00000000	-1.73198900	-2.50025700
C	0.00000000	-5.04941100	-1.75759500
H	0.00000000	-5.88248900	0.22571600
H	0.00000000	-3.91194200	-3.60231200
H	0.00000000	-6.01605400	-2.25494900
H	0.00000000	6.01605400	-2.25494900
H	0.00000000	5.88248900	0.22571600

Radical Cation

C	0.00000000	3.66423400	1.71663800
C	0.00000000	3.72525200	0.29651700
C	0.00000000	2.50859100	-0.47790500
C	0.00000000	2.45694400	2.38134500
H	0.00000000	4.59530600	2.27721300
H	0.00000000	2.42310000	3.46736300
C	0.00000000	1.23984100	0.22391800
C	0.00000000	1.23412200	1.65391000
C	0.00000000	0.00000000	-0.44763500
C	0.00000000	0.00000000	2.33600900
C	0.00000000	-1.23984100	0.22391800
C	0.00000000	-1.23412200	1.65391000
H	0.00000000	0.00000000	-1.52948600
H	0.00000000	0.00000000	3.42333300
C	0.00000000	-2.50859100	-0.47790500
C	0.00000000	-3.72525200	0.29651700
C	0.00000000	-2.45694400	2.38134500
C	0.00000000	-3.66423400	1.71663800
H	0.00000000	-2.42310000	3.46736300
H	0.00000000	-4.59530600	2.27721300
H	0.00000000	3.91546700	-3.59087700
C	0.00000000	3.85785000	-2.50577200
C	0.00000000	5.05158500	-1.74252400
C	0.00000000	2.61950300	-1.89007000
C	0.00000000	4.98327500	-0.36654000
C	0.00000000	-2.61950300	-1.89007000
H	0.00000000	1.73001100	-2.50957500
C	0.00000000	-4.98327500	-0.36654000
C	0.00000000	-3.85785000	-2.50577200
H	0.00000000	-1.73001100	-2.50957500
C	0.00000000	-5.05158500	-1.74252400
H	0.00000000	-5.88753900	0.23642000
H	0.00000000	-3.91546700	-3.59087700
H	0.00000000	-6.01441200	-2.24563500
H	0.00000000	6.01441200	-2.24563500
H	0.00000000	5.88753900	0.23642000



PAH(24) – dibenzo[*ghi,mno*]fluoranthene

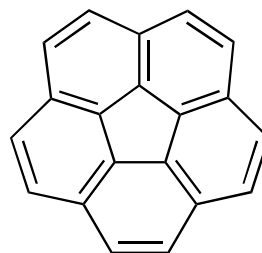
CAS: 5821-51-2

Neutral Structure

C	-0.27081300	2.36731700	0.72334500
C	-0.80267800	1.14833100	0.32740900
C	-0.80222700	0.00035200	1.16129500
C	-0.26878000	0.00020200	2.44237800
C	0.08763300	1.31247600	2.94433400
C	0.08640000	2.43917300	2.12630400
C	-0.80356200	-1.14770600	0.32749500
C	0.08664700	-1.31230800	2.94443900
H	0.45521500	1.41238200	3.96351500
H	0.45347700	3.37781400	2.53624900
C	0.08458800	-2.43905700	2.12648900
C	-0.27258200	-2.36704000	0.72351900
H	0.45412200	-1.41241100	3.96363800
H	0.45093400	-3.37795400	2.53650100
C	-0.80314500	-0.70914100	-1.02181900
C	-0.27132300	-1.46252000	-2.05870500
C	-0.80258300	0.70966700	-1.02187200
C	0.08376100	-0.69631900	-3.23671200
C	-0.27019100	1.46255700	-2.05881600
C	0.08431200	0.69599200	-3.23676000
H	0.44942100	-1.21469200	-4.12068600
H	0.45037300	1.21401400	-4.12077500
C	0.08578500	3.24976500	-0.36995300
C	0.08559600	2.81943000	-1.69411400
H	0.45203300	4.25049400	-0.15040400
H	0.45226200	3.49957800	-2.46016100
C	0.08335300	-3.24984900	-0.36970000
C	0.08346700	-2.81962400	-1.69389700
H	0.44885400	-4.25083200	-0.15006900
H	0.44965000	-3.50009200	-2.45989000

Radical Anion

C	-0.26539900	2.40063600	0.73785600
C	-0.77294300	1.15331900	0.32338100
C	-0.75456800	0.00049700	1.15181500
C	-0.24551200	0.00009700	2.45008700
C	0.08099400	1.31985100	2.95574100
C	0.08861600	2.46221400	2.12200100
C	-0.77390900	-1.15253700	0.32320900
C	0.08031300	-1.31930800	2.95566200
H	0.44924400	1.42715100	3.97488700
H	0.46104300	3.39593700	2.54288600
C	0.08684600	-2.46210000	2.12167000
C	-0.26743600	-2.40006500	0.73795800
H	0.44920300	-1.42678800	3.97455600
H	0.45908400	-3.39598600	2.54233800
C	-0.76341400	-0.71380400	-1.01307900
C	-0.25483500	-1.46905000	-2.07658600
C	-0.76246700	0.71433700	-1.01300300
C	0.09655000	-0.71458000	-3.23704000
C	-0.25315400	1.46903500	-2.07629800
C	0.09716200	0.71410000	-3.23710200
H	0.48537300	-1.22386300	-4.11783400
H	0.48645100	1.22302100	-4.11788600
C	0.06174800	3.27974400	-0.37267100
C	0.05640100	2.85112800	-1.69727300
H	0.39731500	4.29609500	-0.16732900
H	0.38883600	3.55030000	-2.46364600
C	0.05819900	-3.27997500	-0.37301100
C	0.05337600	-2.85143600	-1.69734500
H	0.39224000	-4.29681300	-0.16762800
H	0.38464600	-3.55115600	-2.46373900



PAH(25) – dibenzo[fg,ij]pentaphene

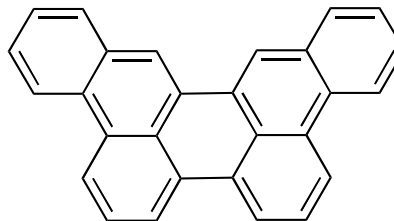
CAS: 197-69-3

Neutral Structure

C	-3.25523000	1.47314800	-0.05846300
C	-2.06170500	0.74707800	-0.01820700
C	-0.82243700	1.46010400	-0.00976800
C	-0.82436600	2.89337600	-0.02009400
C	-2.06302500	3.57359600	-0.05118600
C	-3.25565600	2.87290800	-0.07493300
C	0.43489000	0.73907100	0.00986900
C	0.43594100	3.62505600	0.00178100
C	1.65026800	2.88189800	0.03944700
C	1.60917700	1.45721600	0.04498600
C	2.89534600	3.56511500	0.06674100
H	3.81072600	2.97802800	0.09577200
C	2.94639800	4.94624500	0.05464100
C	1.74540500	5.68716100	0.01535400
C	0.51988500	5.03964600	-0.01049500
H	-4.21199200	0.96539200	-0.08073700
H	-2.09168000	4.65724300	-0.05929200
H	-4.20098400	3.40865000	-0.10513100
H	2.56775900	0.95060900	0.07769300
H	3.90378300	5.46078800	0.07496600
H	1.77899700	6.77378900	0.00523100
H	-0.38162100	5.64161600	-0.04042700
C	2.91496200	-4.96494400	-0.05385600
C	2.87249700	-3.58354200	-0.06695900
C	1.63173700	-2.89256300	-0.03961100
C	0.41277700	-3.62803700	-0.00095300
C	0.48792900	-5.04313800	0.01240000
C	1.70938200	-5.69830000	-0.01347800
C	1.59974500	-1.46767600	-0.04588900
C	-0.84285600	-2.88830300	0.02090400
C	-0.83177000	-1.45504900	0.01003700
C	0.43011100	-0.74202900	-0.01035200
C	-2.06646600	-0.73411000	0.01865500
C	-3.26462900	-1.45249100	0.05934600
C	-3.27399300	-2.85220800	0.07626700
C	-2.08586400	-3.56050400	0.05254500
H	2.56152200	-0.96725600	-0.07922500
H	3.86910600	-5.48546500	-0.07420000
H	3.79148000	-3.00214400	-0.09677300
H	-0.41720500	-5.63961100	0.04329300
H	1.73618000	-6.78511200	-0.00250300
H	-4.21816900	-0.93866800	0.08169900
H	-4.22270400	-3.38191400	0.10684700
H	-2.12152700	-4.64391000	0.06104600

Radical Anion

C	-3.27383700	1.47834400	0.00074600
C	-2.07035500	0.73739700	0.00061800
C	-0.82159400	1.44929500	0.00052700
C	-0.82600600	2.89190100	0.00054100
C	-2.06096600	3.57020000	0.00066600
C	-3.26720000	2.86826300	0.00077400
C	0.42919800	0.72674200	0.00042700
C	0.44211400	3.62305300	0.00042700
C	1.66368000	2.87190600	0.00033900
C	1.63014600	1.45949400	0.00034800
C	2.90470900	3.58062900	0.00022800
H	3.82821300	3.00391800	0.00015900
C	2.94641500	4.96106300	0.00019400
C	1.74190000	5.70218900	0.00027400
C	0.52238100	5.03542800	0.00039000
H	-4.23177600	0.97107500	0.00083600
H	-2.09002800	4.65439000	0.00068900
H	-4.20919900	3.41262600	0.00088100
H	2.58693100	0.94906400	0.00025900
H	3.90376400	5.47816400	0.00010100
H	1.76690500	6.78920700	0.00024000
H	-0.38549400	5.63038000	0.00044600
C	2.91487700	-4.97977800	0.00000500
C	2.88183500	-3.59911900	0.00009700
C	1.64527700	-2.88262800	0.00022600
C	0.41899300	-3.62604200	0.00027000
C	0.49040800	-5.03890900	0.00018000
C	1.70572600	-5.71330500	0.00005100
C	1.62075700	-1.47004700	0.00030200
C	-0.84447100	-2.88681100	0.00039700
C	-0.83083900	-1.44423800	0.00045500
C	0.42451700	-0.72964900	0.00039700
C	-2.07504800	-0.72437800	0.00057100
C	-3.28325500	-1.45759500	0.00063900
C	-3.28549500	-2.84752200	0.00058900
C	-2.08376300	-3.55715400	0.00046800
H	2.58078300	-0.96576100	0.00027100
H	3.86895400	-5.50288300	-0.00010500
H	3.80891600	-3.02818300	0.00005800
H	-0.42110700	-5.62828200	0.00021300
H	1.72389300	-6.80045900	-0.00001600
H	-4.23796400	-0.94423600	0.00073000
H	-4.23093900	-3.38588100	0.00064900
H	-2.11983700	-4.64111200	0.00043000



PAH(26) – dibenzo[*a,e*]pyrene

CAS: 192-65-4

Neutral Structure

C	3.35267000	2.82855200	-0.00000700
C	2.11297100	3.44581400	-0.00000100
C	0.93525100	2.66757600	0.00000200
C	1.01892900	1.23886000	0.00000100
C	2.30625900	0.61417100	-0.00000200
C	3.44528400	1.42916300	-0.00000800
C	-0.35266100	3.28563100	0.00000600
C	-0.18963800	0.45646900	0.00000100
C	-1.45665800	1.10588000	0.00000400
C	-1.49542500	2.53817400	0.00000700
C	-2.67213300	0.32293100	0.00000200
C	-2.56430600	-1.10263900	-0.00000300
C	-1.28522700	-1.71428500	-0.00000500
C	-0.10946000	-0.98512400	-0.00000200
C	1.21188700	-1.63904100	-0.00000100
C	2.39698000	-0.85546700	0.00000100
H	-0.40729600	4.37182900	0.00000800
H	4.26246100	3.42352800	-0.00001100
H	2.02951100	4.53010500	0.00000000
H	4.43489800	0.98793800	-0.00001300
H	-2.45097800	3.05003900	0.00001000
H	-1.26641700	-2.79846800	-0.00000800
C	-3.97635800	0.89155800	0.00000500
C	-5.10611100	0.09494300	0.00000200
H	-4.10403000	1.96823200	0.00000900
C	-3.74437900	-1.90019500	-0.00000600
C	-4.99329700	-1.31656400	-0.00000300
H	-6.08986700	0.55762600	0.00000400
H	-3.63855800	-2.98288200	-0.00001000
H	-5.88869500	-1.93302300	-0.00000500
C	1.33303200	-3.04798000	0.00000000
C	2.57075000	-3.67482800	0.00000300
H	0.44550300	-3.66996500	-0.00000200
C	3.64735300	-1.51663200	0.00000600
C	3.74082000	-2.90087600	0.00000700
H	2.62762800	-4.76039600	0.00000400
H	4.56674100	-0.94212000	0.00001100
H	4.71758100	-3.37788800	0.00001100

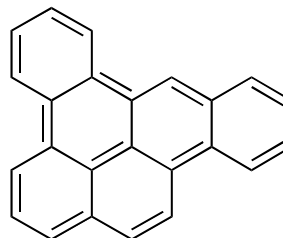
Radical Anion

C	3.37612100	2.83255300	0.00000100
C	2.12875600	3.45402800	0.00000100
C	0.94440000	2.67493900	0.00000100
C	1.03193900	1.23659000	0.00000100
C	2.32504900	0.61415400	0.00000100
C	3.47975400	1.44261900	0.00000100
C	-0.34247300	3.28288600	0.00000100
C	-0.17846600	0.44664900	0.00000100
C	-1.46096500	1.10417700	0.00000100
C	-1.49284100	2.51847400	0.00000100
C	-2.69344500	0.31215900	0.00000100
C	-2.57911500	-1.12071100	0.00000000
C	-1.30151900	-1.73116900	0.00000000
C	-0.09981400	-0.98679900	0.00000000
C	1.20637600	-1.62449800	0.00000000
C	2.40798200	-0.83704400	0.00000000
H	-0.40758600	4.36924800	0.00000100
H	4.28271000	3.43519700	0.00000100
H	2.04683300	4.53904900	0.00000100
H	4.46956000	1.00049500	0.00000100
H	-2.44809100	3.03447700	0.00000100
H	-1.27774900	-2.81563300	0.00000000
C	-3.98614200	0.87859700	0.00000100
C	-5.14208400	0.09101700	0.00000100

H	-4.10550000	1.95776700	0.00000100
C	-3.77311600	-1.90243900	0.00000000
C	-5.02930900	-1.31101600	0.00000000
H	-6.12058300	0.56562800	0.00000100
H	-3.68000600	-2.98745100	0.00000000
H	-5.92310300	-1.93202600	0.00000000
C	1.33956300	-3.04222200	0.00000000
C	2.57228400	-3.66976400	0.00000000
H	0.45109800	-3.66408700	0.00000000
C	3.65758100	-1.51270200	0.00000000
C	3.75194500	-2.89387300	0.00000000
H	2.62857500	-4.75608500	-0.00000100
H	4.57846700	-0.93890800	0.00000000
H	4.72793200	-3.37362800	0.00000000

Radical Cation

C	3.36657500	2.82520300	0.00000100
C	2.12011000	3.44283200	0.00000100
C	0.94135700	2.66290100	0.00000100
C	1.02318800	1.23719700	0.00000100
C	2.30271700	0.60972200	0.00000000
C	3.45503500	1.43497200	0.00000100
C	-0.33463900	3.28009100	0.00000100
C	-0.17992800	0.46041300	0.00000100
C	-1.45557200	1.11648700	0.00000100
C	-1.49338300	2.52925000	0.00000100
C	-2.68044300	0.32578300	0.00000100
C	-2.56785600	-1.09937300	0.00000000
C	-1.29476600	-1.70446800	0.00000000
C	-0.09724600	-0.96600100	0.00000000
C	1.19788000	-1.62737300	0.00000000
C	2.39752000	-0.84076500	0.00000000
H	-0.39240700	4.36521700	0.00000200
H	4.27409200	3.42137800	0.00000100
H	2.03602200	4.52626300	0.00000100
H	4.44158900	0.98919200	0.00000000
H	-2.44369800	3.04940000	0.00000100
H	-1.27062000	-2.78753400	0.00000000
C	-3.97185900	0.88444200	0.00000100
C	-5.10530000	0.07116400	0.00000100
H	-4.11248200	1.95884900	0.00000100
C	-3.73550700	-1.90978300	0.00000000
C	-4.99265600	-1.33057700	0.00000000
H	-6.08830700	0.53379500	0.00000100
H	-3.61981700	-2.99040900	-0.00000100
H	-5.88452400	-1.95028900	0.00000000
C	1.31243000	-3.04144400	0.00000000
C	2.54628900	-3.66182600	0.00000000
H	0.42577300	-3.66285000	0.00000000
C	3.64785700	-1.50892000	0.00000000
C	3.72487300	-2.88844800	0.00000000
H	2.60575000	-4.74661300	0.00000000
H	4.57086800	-0.94189100	0.00000000
H	4.69610200	-3.37533900	0.00000000



PAH(27) – dicyclopenta[hi,qr]chrysene

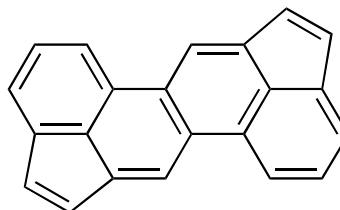
CAS: 225226-02-8

Neutral Structure

C	0.09533700	4.66678700	0.00006300
C	-0.97976400	3.79239600	-0.00001100
C	-0.71229500	2.40085100	-0.00001200
C	0.55707100	1.82460000	0.00005300
C	1.64633600	2.74606500	0.00012900
C	1.40637900	4.11677600	0.00013300
H	-0.03828900	5.74607600	0.00007000
C	-1.93912100	1.67577200	-0.00008600
C	0.61858800	0.36991800	0.00003900
H	2.67410600	2.39674200	0.00018700
H	2.25539900	4.79586400	0.00019400
C	-0.61858800	-0.36991800	-0.00003400
C	-1.88788900	0.30262100	-0.00009500
H	-2.80034400	-0.28640300	-0.00014900
C	-0.55707100	-1.82460000	-0.00004800
C	1.88788900	-0.30262100	0.00010000
C	0.71229500	-2.40085100	0.00001700
C	-1.64633600	-2.74606500	-0.00012500
C	1.93912100	-1.67577200	0.00009100
H	2.80034400	0.28640300	0.00015400
C	0.97976400	-3.79239600	0.00001600
C	-1.40637900	-4.11677600	-0.00012900
H	-2.67410600	-2.39674200	-0.00018200
C	-0.09533700	-4.66678700	-0.00005800
H	-2.25539900	-4.79586400	-0.00018900
H	0.03828900	-5.74607600	-0.00006500
C	-3.01128300	2.68072600	-0.00014300
C	-2.44680500	3.92713200	-0.00009200
H	-4.07284300	2.45729500	-0.00020800
H	-2.98246900	4.87072900	-0.00011300
C	3.01128300	-2.68072600	0.00014700
C	2.44680500	-3.92713200	0.00009800
H	4.07284300	-2.45729500	0.00021200
H	2.98246900	-4.87072900	0.00011800

Radical Anion

C	0.10429100	4.69359800	0.00006300
C	-0.98765900	3.81395200	-0.00000900
C	-0.71633400	2.41500500	-0.00001000
C	0.56135300	1.84153100	0.00005400
C	1.64329900	2.76164000	0.00012900
C	1.40272200	4.14532600	0.00013300
H	-0.02956600	5.77389100	0.00007100
C	-1.94343900	1.68763800	-0.00008400
C	0.63210600	0.37517100	0.00003800
H	2.67267100	2.41415000	0.00018600
H	2.25652900	4.82018000	0.00019300
C	-0.63210600	-0.37517100	-0.00003300
C	-1.87597400	0.28992800	-0.00009200
H	-2.79112900	-0.29797300	-0.00014800
C	-0.56135300	-1.84153100	-0.00004900
C	1.87597400	-0.28992800	0.00009600
C	0.71633400	-2.41500500	0.00001400
C	-1.64329900	-2.76164000	-0.00012500
C	1.94343900	-1.68763800	0.00008800
H	2.79112900	0.29797300	0.00015100
C	0.98765900	-3.81395200	0.00001500
C	-1.40272200	-4.14532600	-0.00012800
H	-2.67267100	-2.41415000	-0.00018100
C	-0.10429100	-4.69359800	-0.00005800
H	-2.25652900	-4.82018000	-0.00018800
H	0.02956600	-5.77389100	-0.00006400
C	-3.00082000	2.67387100	-0.00014800
C	-2.43610800	3.94548600	-0.00008700
H	-4.06460100	2.45372000	-0.00021800
H	-2.98195100	4.88420000	-0.00010500
C	3.00082000	-2.67387100	0.00015000
C	2.43610800	-3.94548600	0.00009500
H	4.06460100	-2.45372000	0.00021800
H	2.98195100	-4.88420000	0.00011500



PAH(28) – dicyclopenta[*cd,lm*]perylene

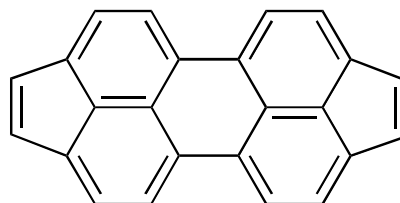
CAS: 80879-80-7

Neutral Structure

C	0.01514900	2.19502100	-2.95994700
C	0.00799000	0.96485600	-3.60027900
C	0.00085500	-0.19578000	-2.78737100
C	-0.00039100	-0.19313500	-1.39444700
C	0.00182200	1.08581000	-0.73890400
C	0.01215900	2.23571600	-1.54038700
H	0.02285100	3.13142500	-3.51321200
C	-0.00483300	-1.35951500	-3.59583900
C	-0.00358100	-1.46956400	-0.73401600
H	0.01970200	3.21401200	-1.06949100
C	-0.01228500	-2.62256100	-1.53110900
C	-0.01287000	-2.58723200	-2.95082100
H	-0.02027300	-3.59913400	-1.05660300
H	-0.01945100	-3.52572200	-3.50055100
C	0.00301900	-1.46667900	0.73525100
C	-0.00270300	-0.18774100	1.39078700
C	0.01407900	-2.61656000	1.53675800
C	-0.00745000	1.08867700	0.73034900
C	-0.00387700	-0.18508600	2.78371200
C	0.01466500	-2.57585200	2.95632200
H	0.02403400	-3.59485500	1.06591200
C	-0.02002900	2.24165400	1.52741700
C	-0.01326300	0.97863700	3.59216200
C	0.00422100	-1.34570200	3.59663600
H	0.02320500	-3.51224000	3.50960300
C	-0.02287400	2.20633400	2.94712400
H	-0.02952900	3.21818700	1.05285400
H	-0.03242800	3.14480900	3.49683600
C	-0.00016300	-0.86581600	4.98884900
C	-0.01100300	0.50410600	4.98620900
H	0.00431300	-1.50260800	5.86722600
H	-0.01678300	1.14428600	5.86211500
C	-0.00124500	-0.88497400	-4.98987800
C	0.00678700	0.48496700	-4.99249700
H	-0.00434000	-1.52515800	-5.86579500
H	0.01135500	1.12177300	-5.87086500

Radical Anion

C	-0.00123900	2.20921300	-2.94710300
C	0.00045300	0.96768600	-3.60498900
C	0.00095800	-0.19577200	-2.78946200
C	-0.00027900	-0.19309800	-1.39018000
C	-0.00204900	1.08458900	-0.72849900
C	-0.00245000	2.25071600	-1.54445100
H	-0.00168600	3.14573700	-3.50293800
C	0.00283000	-1.36234500	-3.60051700
C	0.00043400	-1.46824900	-0.72360100
H	-0.00371800	3.22699100	-1.06776900
C	0.00234600	-2.63750000	-1.53507900
C	0.00355400	-2.60134800	-2.93787700
H	0.00304300	-3.61198300	-1.05470800
H	0.00505900	-3.53998200	-3.49013800
C	-0.00090400	-1.46544800	0.72483800
C	-0.00267400	-0.18776000	1.38651900
C	-0.00050300	-2.63157400	1.54079000
C	-0.00338700	1.08739100	0.71994000
C	-0.00391100	-0.18508700	2.78580100
C	-0.00171400	-2.59007100	2.94344200
H	0.00076500	-3.60784900	1.06410900
C	-0.00529900	2.25664200	1.53141900
C	-0.00578300	0.98148700	3.59685600
C	-0.00340600	-1.34854500	3.60132900
H	-0.00126700	-3.52659500	3.49927800
C	-0.00650700	2.22049000	2.93421700
H	-0.00599600	3.23112500	1.05104800
H	-0.00801200	3.15912300	3.48647800
C	-0.00498400	-0.87558100	4.97557600
C	-0.00647000	0.51382000	4.97289900
H	-0.00504200	-1.50695900	5.85924700
H	-0.00785400	1.14861700	5.85411900
C	0.00351700	-0.89467800	-4.97656000
C	0.00203100	0.49472200	-4.97923600
H	0.00490100	-1.52947500	-5.85778000
H	0.00208900	1.12610100	-5.86290800



PAH(29) – dicyclopenta[*cd,fg*]pyrene

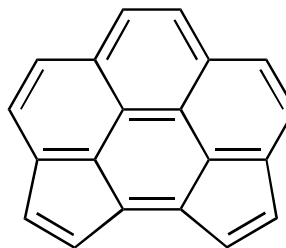
CAS: 173678-72-3

Neutral Structure

C	-3.92601300	-4.79203400	-0.00765400
C	-2.53789600	-4.58138200	-0.00821900
C	-2.08151600	-3.25837700	-0.00431500
C	-2.94245100	-2.16654700	0.00002600
C	-4.34729100	-2.35287000	0.00058700
C	-4.81180500	-3.68855600	-0.00328900
C	-0.63477700	-3.20520300	-0.00586600
C	-2.35558700	-0.88152500	0.00334400
C	-0.96668500	-0.81737800	0.00202000
C	-0.05941200	-1.94551500	-0.00268600
C	-0.26560400	0.39407100	0.00468600
C	-1.01561000	1.58119500	0.00892400
C	-2.42963200	1.52812300	0.01025300
C	-3.13486200	0.30228200	0.00743800
C	-4.57557500	0.11191800	0.00812000
C	-5.14701900	-1.13942400	0.00485900
H	-6.23107700	-1.23055300	0.00547600
H	-5.21668300	0.99077200	0.01125000
H	-4.34134100	-5.79721600	-0.01064100
H	-5.88264700	-3.88042300	-0.00307200
H	-0.52801800	2.55345200	0.01118800
H	-2.98596200	2.46299800	0.01349600
C	1.16846700	0.02141800	0.00165800
C	1.28740900	-1.34296500	-0.00267100
H	1.99368900	0.72618000	0.00271400
H	2.21856400	-1.89844500	-0.00559900
C	-0.20807300	-4.61757700	-0.01106500
C	-1.31701900	-5.42121200	-0.01238800
H	0.82162000	-4.95717100	-0.01345500
H	-1.30892100	-6.50639600	-0.01603300

Radical Anion

C	-3.94406200	-4.80060900	-0.00775000
C	-2.53859900	-4.60855000	-0.00828400
C	-2.07039600	-3.27285200	-0.00418000
C	-2.93489800	-2.17375000	0.00023800
C	-4.34164800	-2.35372900	0.00071900
C	-4.81690400	-3.70340300	-0.00337800
C	-0.63198900	-3.22776400	-0.00579800
C	-2.34511300	-0.88262000	0.00359100
C	-0.94842100	-0.81637400	0.00225300
C	-0.04042800	-1.93292100	-0.00247200
C	-0.24546700	0.41232300	0.00479800
C	-1.02095900	1.60035500	0.00885100
C	-2.42166900	1.54157600	0.01020100
C	-3.13045200	0.29851800	0.00752600
C	-4.55843600	0.11023900	0.00814700
C	-5.13459200	-1.15119400	0.00489200
H	-6.22017100	-1.23789700	0.00545500
H	-5.20385400	0.98731800	0.01120800
H	-4.36628800	-5.80473500	-0.01088800
H	-5.89053300	-3.88506000	-0.00324400
H	-0.53873700	2.57717800	0.01097700
H	-2.98747800	2.47194700	0.01333300
C	1.16364100	0.05674700	0.00175200
C	1.28010400	-1.33591600	-0.00259500
H	1.99403400	0.75703000	0.00265400
H	2.21889000	-1.88228800	-0.00558700
C	-0.21825700	-4.61659500	-0.01105400
C	-1.34691200	-5.44073700	-0.01246000
H	0.80964300	-4.96769700	-0.01354400
H	-1.33177500	-6.52689900	-0.01627300



PAH(30) – dicyclopenta[*cd,jk*]pyrene

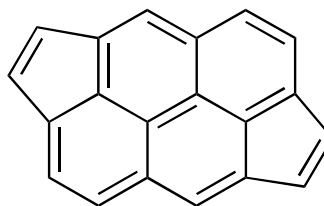
CAS: 98791-43-6

Neutral Structure

C	-2.84955300	-2.04440400	0.00000000
C	-1.56337600	-2.63484000	0.00000000
C	-0.36969500	-1.86943200	0.00000000
C	-0.54168900	-0.45245000	0.00000000
C	-1.80257500	0.10395300	0.00000000
C	-2.98427300	-0.64454000	0.00000000
C	0.99066700	-2.39523500	0.00000000
C	0.54168900	0.45245000	0.00000000
C	1.80257500	-0.10395300	0.00000000
C	2.05541400	-1.51714800	0.00000000
C	2.98427300	0.64454000	0.00000000
C	2.84955300	2.04440400	0.00000000
C	1.56337600	2.63484000	0.00000000
C	0.36969500	1.86943200	0.00000000
C	-0.99066700	2.39523500	0.00000000
C	-2.05541400	1.51714800	0.00000000
H	-1.13752600	3.47370100	0.00000000
H	1.13752600	-3.47370100	0.00000000
H	-3.72124100	-2.69487900	0.00000000
H	-1.49336800	-3.72050500	0.00000000
H	3.72124100	2.69487900	0.00000000
H	1.49336800	3.72050500	0.00000000
C	4.07421000	-0.35822500	0.00000000
C	3.53214800	-1.61747100	0.00000000
H	5.13469600	-0.12860900	0.00000000
H	4.09275500	-2.54632500	0.00000000
C	-4.07421000	0.35822500	0.00000000
C	-3.53214800	1.61747100	0.00000000
H	-5.13469600	0.12860900	0.00000000
H	-4.09275500	2.54632500	0.00000000

Radical Anion

C	-2.85604400	-2.06059100	0.00000000
C	-1.58253800	-2.64654700	0.00000000
C	-0.36656100	-1.87784600	0.00000000
C	-0.54452800	-0.45205500	0.00000000
C	-1.80997200	0.10513700	0.00000000
C	-3.00681300	-0.64751600	0.00000000
C	0.96946900	-2.39747400	0.00000000
C	0.54452800	0.45205500	0.00000000
C	1.80997200	-0.10513700	0.00000000
C	2.06325300	-1.51392600	0.00000000
C	3.00681300	0.64751600	0.00000000
C	2.85604400	2.06059100	0.00000000
C	1.58253800	2.64654700	0.00000000
C	0.36656100	1.87784600	0.00000000
C	-0.96946900	2.39747400	0.00000000
C	-2.06325300	1.51392600	0.00000000
H	-1.11708600	3.47732000	0.00000000
H	1.11708600	-3.47732000	0.00000000
H	-3.72789600	-2.71375900	0.00000000
H	-1.51020300	-3.73323200	0.00000000
H	3.72789600	2.71375900	0.00000000
H	1.51020300	3.73323200	0.00000000
C	4.07514900	-0.33718500	0.00000000
C	3.51869500	-1.61727500	0.00000000
H	5.13942200	-0.11905700	0.00000000
H	4.08436300	-2.54473800	0.00000000
C	-4.07514900	0.33718500	0.00000000
C	-3.51869500	1.61727500	0.00000000
H	-5.13942200	0.11905700	-0.00000100
H	-4.08436300	2.54473800	0.00000100



PAH(31) – dicyclopenta[*cd,mn*]pyrene

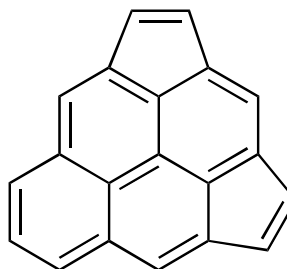
CAS: 96915-04-7

Neutral Structure

C	0.00000000	0.00000000	-3.97395600
C	0.00000000	-1.22875800	-3.29664400
C	0.00000000	-1.26605800	-1.88735100
C	0.00000000	0.00000000	-1.22733100
C	0.00000000	1.26605800	-1.88735100
C	0.00000000	1.22875800	-3.29664400
C	0.00000000	-2.50184700	-1.10116200
C	0.00000000	0.00000000	0.17620500
C	0.00000000	-1.17324700	0.89662300
C	0.00000000	-2.46086700	0.28262900
C	0.00000000	-1.21947200	2.30046800
C	0.00000000	0.00000000	3.02887200
C	0.00000000	1.21947200	2.30046800
C	0.00000000	1.17324700	0.89662300
C	0.00000000	2.46086700	0.28262900
C	0.00000000	2.50184700	-1.10116200
H	0.00000000	3.44369000	-1.64683000
H	0.00000000	-3.44369000	-1.64683000
H	0.00000000	0.00000000	-5.06087500
H	0.00000000	-2.15584000	-3.86556100
H	0.00000000	2.15584000	-3.86556100
H	0.00000000	0.00000000	4.11735600
C	0.00000000	-3.39446000	1.42724900
C	0.00000000	-2.67063100	2.59838500
H	0.00000000	-4.47710300	1.35818500
H	0.00000000	-3.10201100	3.59462900
C	0.00000000	3.39446000	1.42724900
C	0.00000000	2.67063100	2.59838500
H	0.00000000	4.47710300	1.35818500
H	0.00000000	3.10201100	3.59462900

Radical Anion

C	0.00000000	0.00000000	-3.99058300
C	0.00000000	-1.23248700	-3.32164900
C	0.00000000	-1.27601000	-1.89431600
C	0.00000000	0.00000000	-1.23179300
C	0.00000000	1.27601000	-1.89431600
C	0.00000000	1.23248700	-3.32164900
C	0.00000000	-2.49402400	-1.11646900
C	0.00000000	0.00000000	0.17676300
C	0.00000000	-1.17860200	0.89948200
C	0.00000000	-2.45513100	0.29537500
C	0.00000000	-1.22350400	2.32271800
C	0.00000000	0.00000000	3.04448200
C	0.00000000	1.22350400	2.32271800
C	0.00000000	1.17860200	0.89948200
C	0.00000000	2.45513100	0.29537500
C	0.00000000	2.49402400	-1.11646900
H	0.00000000	3.44026100	-1.65663500
H	0.00000000	-3.44026100	-1.65663500
H	0.00000000	0.00000000	-5.07951500
H	0.00000000	-2.15904500	-3.89249800
H	0.00000000	2.15904500	-3.89249800
H	0.00000000	0.00000000	4.13482000
C	0.00000000	-3.38137000	1.42974500
C	-0.00000100	-2.65454100	2.61972700
H	0.00000000	-4.46587500	1.36473800
H	-0.00000100	-3.09422200	3.61345000
C	-0.00000100	3.38137000	1.42974500
C	0.00000100	2.65454100	2.61972700
H	-0.00000100	4.46587500	1.36473800
H	0.00000200	3.09422200	3.61345000



PAH(32) – 9,10-dimethylantracene

CAS: 781-43-1

Neutral Structure

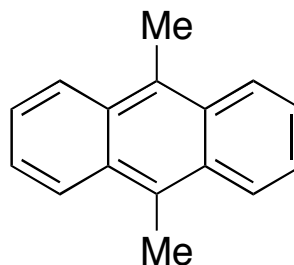
C	-3.67197000	0.74839900	0.00035000
C	-2.47998800	1.42910200	0.00034900
C	-1.21256600	0.74987200	0.00034900
C	-1.22738300	-0.70220200	0.00034900
C	-2.50029300	-1.36837300	0.00035100
C	-3.68400000	-0.67388400	0.00035100
C	0.02162900	1.44500400	0.00035100
C	-0.02162900	-1.44500400	0.00035100
C	1.21256600	-0.74987200	0.00034900
C	1.22738300	0.70220100	0.00034900
C	2.50029300	1.36837300	0.00035200
H	2.52932600	2.45204900	0.00035300
C	3.68400000	0.67388400	0.00035200
C	3.67197000	-0.74839900	0.00035000
C	2.47998800	-1.42910200	0.00034900
H	-4.61022200	1.29787200	0.00034900
H	-2.50801100	2.51214400	0.00034800
H	-2.52932600	-2.45204900	0.00035300
H	-4.63077500	-1.20852600	0.00035300
H	4.63077500	1.20852600	0.00035300
H	4.61022200	-1.29787200	0.00034900
H	2.50801100	-2.51214400	0.00034800
C	0.09521500	2.95763500	0.00035500
H	-0.88423900	3.43362200	0.00035500
H	0.63291600	3.32902700	0.88231500
H	0.63291700	3.32903400	-0.88160300
C	-0.09521400	-2.95763500	0.00035400
H	-0.63291600	-3.32903400	-0.88160300
H	0.88423900	-3.43362200	0.00035500
H	-0.63291600	-3.32902700	0.88231500

Radical Cation

C	0.70929400	3.68350800	0.00040900
C	1.40615500	2.48280300	0.00041000
C	0.73436800	1.23143500	0.00041000
C	-0.70922800	1.23346700	0.00040900
C	-1.38576000	2.47897800	0.00040600
C	-0.69341800	3.68276500	0.00040700
C	1.44856600	-0.00659500	0.00041200
C	-1.44856600	0.00659500	0.00041200
C	-0.73436800	-1.23143500	0.00041000
C	0.70922800	-1.23346700	0.00040900
C	1.38576000	-2.47897800	0.00040600
H	2.46845200	-2.50519500	0.00040300
C	0.69341800	-3.68276500	0.00040700
C	-0.70929400	-3.68350800	0.00040900
C	-1.40615500	-2.48280300	0.00041000
H	1.25610200	4.62186400	0.00041100
H	2.48756800	2.52277000	0.00041100
H	-2.46845200	2.50519500	0.00040300
H	-1.24192700	4.62017500	0.00040600
H	1.24192700	-4.62017500	0.00040600
H	-1.25610200	-4.62186400	0.00041100
H	-2.48756800	-2.52277000	0.00041100
C	2.94979500	-0.06261200	0.00041700
H	3.42021100	0.91727900	0.00041800
H	3.31241500	-0.60493200	0.88254200
H	3.31242500	-0.60493300	-0.88170300
C	-2.94979500	0.06261200	0.00041700
H	-3.31242500	0.60493300	-0.88170300
H	-3.42021100	-0.91727900	0.00041800
H	-3.31241500	0.60493200	0.88254200

Radical Anion

C	-3.69664000	0.76460900	-0.11972500
C	-2.47327000	1.43767000	-0.06379600
C	-1.22326600	0.75156300	0.01141800
C	-1.24829500	-0.70644200	0.01162000
C	-2.51987100	-1.35114100	-0.06357900
C	-3.72045400	-0.63804800	-0.11960800
C	0.02542300	1.43931000	0.08054500
C	-0.02542700	-1.43930400	0.08065800
C	1.22326500	-0.75156200	0.01152900
C	1.24829300	0.70644300	0.01160900
C	2.51987100	1.35113700	-0.06359100
H	2.56319100	2.43554100	-0.08925900
C	3.72045800	0.63804000	-0.11950800
C	3.69664400	-0.76461700	-0.11950200
C	2.47327200	-1.43767500	-0.06357200
H	-4.62377500	1.33244900	-0.17556600
H	-2.48225700	2.52286700	-0.08998400
H	-2.56319200	-2.43554700	-0.08915800
H	-4.66610100	-1.17449100	-0.17541100
H	4.66610600	1.17447900	-0.17531500
H	4.62378200	-1.33246200	-0.17525100
H	2.48226100	-2.52287400	-0.08966700
C	0.05816800	2.94907800	0.17529400
H	-0.82625400	3.34556600	0.68482300
H	0.92503500	3.30118400	0.74582900
H	0.10642700	3.44718400	-0.80859200
C	-0.05817300	-2.94906600	0.17551300
H	-0.10640100	-3.44723900	-0.80834100
H	0.82623400	-3.34551800	0.68509500
H	-0.92505600	-3.30113400	0.74604500



PAH(33) – 7,12-dimethylbenz[*a*]anthracene

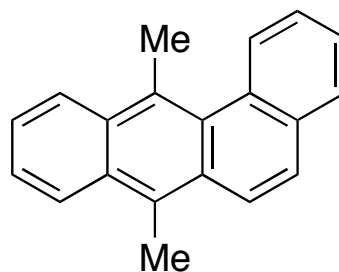
CAS: 57-97-6

Neutral Structure

C	-4.62432400	-0.31293900	-0.30372700
C	-3.72172800	0.72539400	-0.30283200
C	-2.32006700	0.51044700	-0.09784100
C	-1.86408500	-0.84512800	0.10619000
C	-2.84049400	-1.89276700	0.11140500
C	-4.17816600	-1.64187400	-0.09201400
C	-1.37832800	1.57552200	-0.04355800
C	-0.47601800	-1.13805300	0.26925200
C	0.46415700	-0.10293400	0.09366800
C	-0.00876900	1.26813400	0.05975100
C	0.95941500	2.33463300	0.20603400
H	0.60544300	3.35729300	0.26217000
C	2.29185900	2.09492400	0.30956800
C	2.81827700	0.76628400	0.14106800
C	1.91734400	-0.32719600	-0.03640600
H	-5.68014300	-0.11392600	-0.47054800
H	-4.09240500	1.72907100	-0.47338500
H	-2.51927000	-2.91903300	0.24675000
H	-4.89090000	-2.46295800	-0.10057100
H	2.99121200	2.91541600	0.45470900
C	4.21459100	0.56208500	0.06229200
H	4.87359100	1.41234400	0.22466600
C	2.48425500	-1.56401000	-0.43146900
H	1.84475700	-2.39187800	-0.70596100
C	3.86000800	-1.74222000	-0.53301600
H	4.25098100	-2.70771800	-0.84458500
C	4.73901800	-0.68227100	-0.25347900
H	5.81450100	-0.82663800	-0.31917600
C	-0.09461800	-2.53497000	0.72263400
H	-0.06541800	-3.27022700	-0.09294900
H	0.88013900	-2.54411500	1.21336500
H	-0.82084600	-2.90064600	1.45571200
C	-1.81416000	3.02648400	-0.07696500
H	-1.56372500	3.53730400	0.86217200
H	-1.31793400	3.57837700	-0.88440500
H	-2.88737000	3.14366800	-0.22222200

Radical Cation

C	-4.61602100	-0.33016700	-0.36703800
C	-3.71409400	0.72530100	-0.31733500
C	-2.33149800	0.50610000	-0.08319500
C	-1.87353800	-0.84199200	0.11211600
C	-2.82026100	-1.89019900	0.07919300
C	-4.16826100	-1.64250900	-0.16675500
C	-1.39024900	1.57656500	-0.00227000
C	-0.47372700	-1.12753500	0.30432800
C	0.47750200	-0.09451700	0.09156700
C	0.00681400	1.26683300	0.08762600
C	0.95164000	2.32673100	0.20696400
H	0.60484000	3.35010100	0.27043200
C	2.30233900	2.08331800	0.26568600
C	2.81914900	0.77104100	0.10054700
C	1.91111200	-0.33147100	-0.04860500
H	-5.66663300	-0.13257400	-0.55861600
H	-4.08882900	1.72857700	-0.47401500
H	-2.49923000	-2.91560700	0.21720600
H	-4.86853500	-2.47206000	-0.20513600
H	2.99822000	2.90924000	0.38806800
C	4.22091500	0.56555400	0.01320500
H	4.87943900	1.41898000	0.15240300
C	2.47146000	-1.58051600	-0.41602400
H	1.83187000	-2.41616000	-0.66399600
C	3.84298300	-1.75144000	-0.52512900
H	4.23511400	-2.72173900	-0.81783100
C	4.73162200	-0.68209600	-0.28014700
H	5.80434200	-0.83611600	-0.35648600
C	-0.09728900	-2.49094400	0.82197500
H	-0.08578200	-3.24987300	0.02739900
H	0.88276900	-2.48590000	1.29903100
H	-0.82694000	-2.81925200	1.56794400
C	-1.82165400	3.01492800	-0.02262900
H	-1.51014000	3.51646800	0.90259200
H	-1.35127600	3.55496000	-0.85312400
H	-2.89872300	3.13881600	-0.11005100

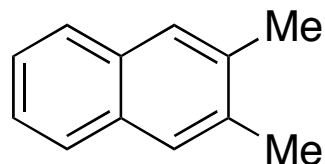


PAH(34) – 2,3-dimethylnaphthalene

CAS: 581-40-8

Neutral Structure

C	3.19162600	-0.70976600	-0.00000100
C	1.99902200	-1.40601800	-0.00000200
C	0.75388000	-0.71598900	-0.00000100
C	0.75388000	0.71598900	0.00000000
C	1.99902200	1.40601800	0.00000100
C	3.19162600	0.70976500	0.00000000
H	-0.49291500	-2.48362900	-0.00000200
H	4.13679000	-1.24741300	-0.00000200
H	1.99598200	-2.49434600	-0.00000300
C	-0.49664900	-1.39465600	-0.00000100
C	-0.49664900	1.39465600	0.00000100
H	1.99598200	2.49434600	0.00000200
H	4.13679000	1.24741300	0.00000100
C	-1.70292000	0.71903300	0.00000000
C	-1.70292000	-0.71903200	-0.00000100
H	-0.49291400	2.48362900	0.00000200
C	-3.00701200	1.47959800	0.00000000
H	-3.61653500	1.23649800	-0.88074000
H	-3.61654200	1.23648800	0.88073300
H	-2.82982300	2.56017700	0.00000700
C	-3.00701300	-1.47959800	0.00000000
H	-3.61653400	-1.23649800	0.88074200
H	-3.61654300	-1.23648700	-0.88073200
H	-2.82982300	-2.56017600	-0.00000700



Radical Cation

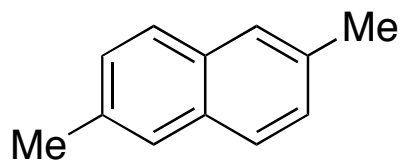
C	-0.00448900	-0.00171000	-0.03056900
C	-0.00135900	-0.01235000	1.37646800
C	1.21562900	-0.00531200	2.09020200
C	2.44837900	0.01263500	1.36838700
C	2.42307500	0.02387600	-0.04190800
C	1.19808500	0.01623300	-0.73431000
H	0.32218300	-0.03028200	4.05576600
H	-0.95000900	-0.00746100	-0.56405200
H	-0.94031400	-0.02595100	1.92325500
C	1.25958600	-0.01685600	3.50504500
C	3.66062200	0.01849700	2.09913300
H	3.35990100	0.03765900	-0.59239200
H	1.19635800	0.02440900	-1.82004900
C	3.69299600	0.00623400	3.50839000
C	2.47323700	-0.01124500	4.22261600
H	4.59952600	0.03189100	1.55083100
C	5.01187400	0.01228800	4.22599100
H	5.09960600	0.89106700	4.87870000
H	5.11070600	-0.86955800	4.87278200
H	5.84642500	0.02012500	3.51995300
C	2.45513100	-0.02558300	5.72334100
H	2.98264400	-0.90681300	6.11214700
H	2.97189600	0.85402000	6.12958600
H	1.43162700	-0.03586300	6.10710600

PAH(35) – 2,6-dimethylnaphthalene

CAS: 581-42-0

Neutral Structure

C	2.56066600	-0.07734300	0.00000000
C	1.56699900	-1.03959600	0.00000000
C	0.18661300	-0.69124900	0.00000000
C	-0.18661300	0.69124900	0.00000000
C	0.84823300	1.66940400	0.00000000
C	2.17517200	1.29596700	0.00000000
H	-0.57512800	-2.72291900	0.00000000
H	1.83481400	-2.09508800	0.00000000
C	-0.84823300	-1.66940400	0.00000000
C	-1.56699900	1.03959600	0.00000000
H	0.57512800	2.72291900	0.00000000
H	2.95027200	2.06032800	0.00000000
C	-2.56066600	0.07734300	0.00000000
C	-2.17517200	-1.29596700	0.00000000
H	-1.83481400	2.09508800	0.00000000
H	-2.95027200	-2.06032800	0.00000000
C	-4.02479500	0.44571300	0.00000000
H	-4.53706800	0.03813900	-0.88178300
H	-4.53706800	0.03814000	0.88178500
H	-4.16356900	1.53213000	-0.00000100
C	4.02479500	-0.44571300	0.00000000
H	4.53706800	-0.03814000	-0.88178400
H	4.53706800	-0.03813900	0.88178400
H	4.16356900	-1.53213000	0.00000100



Radical Cation

C	-0.00136500	0.00436500	-0.05205700
C	0.01423200	-0.03183000	1.36887300
C	1.21482800	-0.02251400	2.09119200
C	2.45903800	0.02263100	1.38112900
C	2.43197200	0.05868400	-0.04220600
C	1.22414500	0.04843400	-0.73588400
H	0.30119400	-0.09299800	4.05773500
H	-0.92949900	-0.06646400	1.90820200
C	1.24189400	-0.05856700	3.51452600
C	3.65963500	0.03194700	2.10344800
H	3.37267200	0.09311500	-0.58541400
H	1.22863000	0.07529300	-1.82169200
C	3.67523200	-0.00424800	3.52437700
C	2.44972200	-0.04831700	4.20820400
H	4.60336600	0.06658100	1.56411900
H	2.44523600	-0.07517600	5.29401300
C	4.98495100	0.00383600	4.25236200
H	4.84334600	0.00315700	5.33645600
H	5.58283800	-0.87521800	3.97518500
H	5.57597200	0.88617000	3.97285600
C	-1.31108400	-0.00371900	-0.78004100
H	-1.16947900	-0.00304000	-1.86413600
H	-1.90210500	-0.88605300	-0.50053600
H	-1.90897100	0.87533500	-0.50286400

PAH(36) – 2,3,3',2'-dipyrenylene

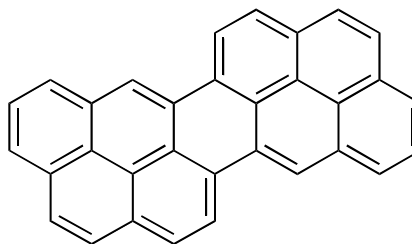
CAS: 188-91-0

Neutral Structure

C	-6.11873500	-5.10278400	-0.02769100
C	-4.70673300	-5.13810000	-0.03398000
C	-3.99795700	-3.91029700	-0.02782800
C	-4.72390100	-2.67371800	-0.01538100
C	-6.15161500	-2.67451600	-0.00813600
C	-6.82338500	-3.91114300	-0.01503400
C	-2.54682500	-3.87663800	-0.03506200
C	-4.03248300	-1.42425400	-0.00893800
C	-2.60603300	-1.41094300	-0.01638800
C	-1.90520900	-2.65558500	-0.02960200
C	-1.92971800	-0.17402900	-0.00961200
H	-0.84211400	-0.16493300	-0.01469400
C	-2.64306300	1.02570200	0.00385500
C	-4.03985300	1.02213200	0.01076200
C	-4.75584600	-0.19086100	0.00435400
C	-6.19247500	-0.23280100	0.01153300
C	-6.85884100	-1.42461700	0.00532100
H	-7.94637200	-1.44924800	0.01082100
H	-6.73973800	0.70709500	0.02209100
H	-6.68491700	-6.02691100	-0.03289400
H	-7.91088800	-3.92597000	-0.01033800
H	-0.82190300	-2.59862100	-0.03524800
H	-2.10667800	1.97133900	0.00929600
H	-4.58954700	1.96049500	0.02142600
C	-3.87017300	-11.31602000	-0.08495600
C	-2.47338300	-11.31245000	-0.09186300
C	-1.75739100	-10.09945700	-0.08545500
C	-2.48075400	-8.86606400	-0.07216300
C	-3.90720300	-8.87937500	-0.06471300
C	-4.58351800	-10.11628900	-0.07148800
C	-0.32076100	-10.05751700	-0.09263400
C	-1.78933500	-7.61660000	-0.06571900
C	-0.36162100	-7.61580200	-0.07296500
C	0.34560400	-8.86570100	-0.08642200
C	0.31014900	-6.37917500	-0.06606700
H	1.39765200	-6.36434800	-0.07076300
C	-0.39450100	-5.18753300	-0.05341000
C	-1.80650300	-5.15221800	-0.04712100
C	-2.51527900	-6.38002100	-0.05327300
C	-3.96641100	-6.41368000	-0.04603800
C	-4.60802700	-7.63473300	-0.05149900
H	-5.69133300	-7.69169700	-0.04585300
H	0.22650200	-10.99741300	-0.10319200
H	-4.40655800	-12.26165700	-0.09039700
H	-1.92369000	-12.25081300	-0.10252600
H	-5.67112200	-10.12538500	-0.06640600
H	1.43313600	-8.84107000	-0.09192200
H	0.17168100	-4.26340700	-0.04820700

Radical Anion

C	-6.12080500	-5.10790700	-0.02614900
C	-4.69648800	-5.14955700	-0.03360700
C	-3.98508400	-3.91151600	-0.02763800
C	-4.71550100	-2.67065600	-0.01509600
C	-6.14576200	-2.67506600	-0.00782800
C	-6.82055600	-3.92216200	-0.01392800
C	-2.54177300	-3.87854000	-0.03484200
C	-4.02455900	-1.41753400	-0.00876800
C	-2.58821700	-1.40393500	-0.01557000
C	-1.89166100	-2.63492600	-0.02835600
C	-1.92072900	-0.14779000	-0.00846200
H	-0.83263500	-0.13013000	-0.01272900
C	-2.64270800	1.04405700	0.00406900
C	-4.04158900	1.04174200	0.01025300
C	-4.75247500	-0.18296700	0.00389800
C	-6.18437000	-0.23377000	0.01058000
C	-6.84974300	-1.43385200	0.00482600
H	-7.93816200	-1.45712500	0.01019300
H	-6.73862700	0.70276200	0.02061300
H	-6.68542100	-6.03364000	-0.03052600
H	-7.90893700	-3.93280800	-0.00878000
H	-0.80773700	-2.58271100	-0.03322000
H	-2.10888000	1.99269200	0.00965400
H	-4.59589500	1.97761700	0.02048700
C	-3.87052800	-11.33437500	-0.08516900
C	-2.47164700	-11.33206000	-0.09135300
C	-1.76076100	-10.10735000	-0.08499900
C	-2.48867700	-8.87278400	-0.07233300
C	-3.92501900	-8.88638300	-0.06553100
C	-4.59250700	-10.14252800	-0.07263900
C	-0.32886600	-10.05654800	-0.09168000
C	-1.79773500	-7.61966200	-0.06600500
C	-0.36747400	-7.61525200	-0.07327400
C	0.33650700	-8.85646500	-0.08592700
C	0.30731900	-6.36815600	-0.06717400
H	1.39570100	-6.35751000	-0.07232200
C	-0.39243100	-5.18241000	-0.05495300
C	-1.81674800	-5.14076100	-0.04749500
C	-2.52815200	-6.37880200	-0.05346300
C	-3.97146300	-6.41177800	-0.04625900
C	-4.62157500	-7.65539200	-0.05274500
H	-5.70549900	-7.70760700	-0.04788100
H	0.22539000	-10.99308000	-0.10171400
H	-4.40435600	-12.28301000	-0.09075300
H	-1.91734100	-12.26793500	-0.10158600
H	-5.68060200	-10.16018800	-0.06837100
H	1.42492600	-8.83319300	-0.09129400
H	0.17218400	-4.25667800	-0.05057600



PAH(37) – fluoranthene

CAS: 206-44-0

Neutral Structure

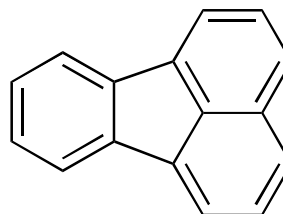
C	0.00000000	2.40219700	0.74082000
C	0.00000000	1.17376300	0.10561000
C	0.00000000	0.00000000	0.90426500
C	0.00000000	0.00000000	2.30977700
C	0.00000000	1.28079500	2.93895400
C	0.00000000	2.43408900	2.16648500
H	0.00000000	3.33687100	0.18520400
C	0.00000000	-1.17376300	0.10561000
C	0.00000000	-1.28079500	2.93895400
H	0.00000000	1.35167000	4.02428700
H	0.00000000	3.40194100	2.66190500
C	0.00000000	-2.43408900	2.16648500
C	0.00000000	-2.40219700	0.74082000
H	0.00000000	-1.35167000	4.02428700
H	0.00000000	-3.40194100	2.66190500
H	0.00000000	-3.33687100	0.18520400
C	0.00000000	-0.71492300	-1.29879300
C	0.00000000	-1.41848100	-2.50280700
C	0.00000000	0.71492300	-1.29879300
C	0.00000000	-0.70083000	-3.70851800
H	0.00000000	-2.50600700	-2.51268200
C	0.00000000	1.41848100	-2.50280700
C	0.00000000	0.70083000	-3.70851800
H	0.00000000	-1.23909000	-4.65315700
H	0.00000000	2.50600700	-2.51268200
H	0.00000000	1.23909000	-4.65315700

Radical Cation

C	0.69735900	2.42155100	0.00000000
C	0.07625400	1.15567900	0.00000000
C	0.90120400	-0.01012100	0.00000000
C	2.30382700	0.01774600	0.00000000
C	2.89809700	1.30631800	0.00000000
C	2.09372700	2.47207900	0.00000000
H	0.11499000	3.33782800	0.00000000
C	0.13056900	-1.18273100	0.00000000
C	2.96498900	-1.24073800	0.00000000
H	3.98002100	1.40777900	0.00000000
H	2.58725600	3.43912100	0.00000000
C	2.20874600	-2.41671000	0.00000000
C	0.79467900	-2.41030000	0.00000000
H	4.05031500	-1.28802300	0.00000000
H	2.72409700	-3.37270500	0.00000000
H	0.25176400	-3.35110300	0.00000000
C	-1.28593100	-0.74128300	0.00000000
C	-2.47272800	-1.44318600	0.00000000
C	-1.29724200	0.69246700	0.00000000
C	-3.69750400	-0.71563000	0.00000000
H	-2.48895300	-2.52944800	0.00000000
C	-2.50607600	1.39995500	0.00000000
C	-3.71321200	0.67626400	0.00000000
H	-4.63414500	-1.26576400	0.00000000
H	-2.51301300	2.48638600	0.00000000
H	-4.65930900	1.20882600	0.00000000

Radical Anion

C	0.00000000	2.43390200	0.75095000
C	0.00000000	1.17936900	0.09434000
C	0.00000000	0.00000000	0.89626300
C	0.00000000	0.00000000	2.31376200
C	0.00000000	1.28295700	2.93983300
C	0.00000000	2.45518600	2.15581400
H	0.00000000	3.36945900	0.19445100
C	0.00000000	-1.17936900	0.09434000
C	0.00000000	-1.28295700	2.93983300
H	0.00000000	1.35854500	4.02598100
H	0.00000000	3.41903100	2.66338600
C	0.00000000	-2.45518600	2.15581400
C	0.00000000	-2.43390200	0.75095000
H	0.00000000	-1.35854500	4.02598100
H	0.00000000	-3.41903100	2.66338600
H	0.00000000	-3.36945900	0.19445100
C	0.00000000	-0.72844700	-1.28194700
C	0.00000000	-1.42064800	-2.50728600
C	0.00000000	0.72844700	-1.28194700
C	0.00000000	-0.70852200	-3.70811100
H	0.00000000	-2.50997100	-2.52372900
C	0.00000000	1.42064800	-2.50728600
C	0.00000000	0.70852200	-3.70811100
H	0.00000000	-1.24555700	-4.65458900
H	0.00000000	2.50997100	-2.52372900
H	0.00000000	1.24555700	-4.65458900

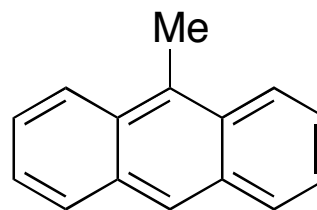


PAH(38) – 9-methylantracene

CAS: 779-02-2

Neutral Structure

C	3.67384800	0.42008000	0.00000200
C	2.50194100	1.13909400	0.00000200
C	1.22265400	0.48790800	0.00000000
C	1.21128600	-0.95805800	0.00000000
C	2.45348600	-1.67192400	0.00000000
C	3.65331400	-1.00569900	0.00000100
C	0.00294000	1.21506100	-0.00000100
C	-0.01347400	-1.63634600	-0.00000100
C	-1.22720700	-0.94082500	-0.00000100
C	-1.22915300	0.51090200	-0.00000100
C	-2.51244600	1.15991700	0.00000000
H	-2.56971500	2.24233300	0.00000000
C	-3.68473300	0.44363400	0.00000000
C	-3.67077800	-0.98259400	0.00000000
C	-2.47328500	-1.65004300	0.00000000
H	4.62803800	0.94150900	0.00000400
H	2.54851000	2.22277000	0.00000300
H	2.42207700	-2.75957100	0.00000000
H	4.58970300	-1.55811400	0.00000200
H	-0.02221900	-2.72470500	-0.00000100
H	-4.63655200	0.96935500	0.00000100
H	-4.60893800	-1.53193400	0.00000100
H	-2.44336200	-2.73772400	0.00000000
C	0.06191800	2.72712900	-0.00000100
H	0.59764200	3.10189500	0.88177100
H	0.59766000	3.10189300	-0.88176200
H	-0.92330900	3.19211300	-0.00001200



Radical Cation

C	3.67766500	0.40701100	0.00000000
C	2.49284300	1.13851500	0.00000000
C	1.23389200	0.49072900	0.00000000
C	1.22024700	-0.94828400	0.00000000
C	2.43987800	-1.66925900	0.00000000
C	3.65577300	-0.99886800	0.00000000
C	0.00051800	1.22566700	0.00000000
C	-0.01102300	-1.62956800	0.00000000
C	-1.23407900	-0.93340200	0.00000000
C	-1.24092500	0.51022000	0.00000000
C	-2.50347400	1.15613600	0.00000000
H	-2.56936800	2.23694500	0.00000000
C	-3.68929700	0.42600900	0.00000000
C	-3.67118700	-0.97874500	0.00000000
C	-2.45534200	-1.65013700	0.00000000
H	4.62826700	0.93248000	0.00000000
H	2.54762100	2.22086300	0.00000000
H	2.40601700	-2.75549100	0.00000000
H	4.58695700	-1.55764100	0.00000000
H	-0.01864100	-2.71682000	0.00000000
H	-4.63810000	0.95456000	0.00000000
H	-4.60291900	-1.53652000	0.00000000
H	-2.42352300	-2.73640000	0.00000000
C	0.05300000	2.72521300	0.00000000
H	0.59685900	3.08755300	0.88155600
H	0.59685900	3.08755300	-0.88155600
H	-0.92968200	3.19129900	0.00000000

PAH(39) – 3-methylcholanthrene

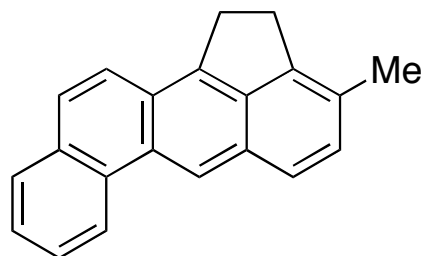
CAS: 56-49-5

Neutral Structure

C	-4.05431000	-0.65616200	-0.00229200
C	-3.12122200	0.36272600	0.00281100
C	-1.73932800	0.04862900	0.00198300
C	-1.22768400	-1.27394500	-0.00327300
C	-2.20495900	-2.31591600	-0.00839100
C	-3.55209300	-2.00197200	-0.00786800
C	-0.92505900	1.18681900	0.00620000
C	0.17643900	-1.41702100	-0.00375000
C	1.02727400	-0.30122700	0.00033200
C	0.46585000	1.04125800	0.00514100
C	1.34434300	2.18353800	0.00815900
H	0.90126900	3.17612800	0.01164100
C	2.69624300	2.03808600	0.00638400
C	3.30788800	0.73189000	0.00198300
C	2.49159200	-0.43957200	-0.00065200
H	-1.88726500	-3.35653400	-0.01280200
H	-4.27827000	-2.81313000	-0.01195400
H	0.58708200	-2.42152800	-0.00784900
H	3.34707000	2.90975000	0.00842900
C	4.71749400	0.60726200	0.00044400
H	5.31916900	1.51376000	0.00234500
C	3.14368800	-1.69595000	-0.00421600
H	2.56244400	-2.61195700	-0.00595300
C	4.52884900	-1.79666400	-0.00554200
H	4.99530300	-2.77877200	-0.00829700
C	5.32711800	-0.63743400	-0.00331300
H	6.41122600	-0.71840100	-0.00444600
C	-5.53976200	-0.38585200	-0.00133500
H	-5.84375200	0.18604800	0.88605100
H	-5.84174000	0.20418500	-0.87738100
H	-6.11456300	-1.31805900	-0.01153200
C	-1.80448600	2.42562300	0.01053400
H	-1.61310400	3.05133300	0.89131700
H	-1.61363000	3.05688200	-0.86640100
C	-3.27188400	1.87321200	0.00916600
H	-3.82986600	2.21645900	0.88980400
H	-3.83115400	2.22398400	-0.86766800

Radical Cation

C	-4.05895200	-0.66867200	0.00019800
C	-3.10811100	0.37045100	0.00034400
C	-1.74141500	0.04919800	0.00029300
C	-1.23247200	-1.27012200	0.00011800
C	-2.19554100	-2.30641500	-0.00001400
C	-3.56103300	-1.99220300	0.00002600
C	-0.93008300	1.19119700	0.00040900
C	0.17243100	-1.41287900	0.00006200
C	1.03472900	-0.29007600	0.00015800
C	0.48126400	1.04442300	0.00033900
C	1.33829400	2.17860000	0.00042900
H	0.90030100	3.17207500	0.00056800
C	2.70334300	2.02586500	0.00033000
C	3.30578100	0.73405900	0.00013600
C	2.48224400	-0.44316500	0.00005300
H	-1.88074200	-3.34654100	-0.00015300
H	-4.27860500	-2.80906400	-0.00008400
H	0.58218900	-2.41654800	-0.00006900
H	3.35048100	2.89923600	0.00039200
C	4.71991800	0.60825900	0.00001600
H	5.32124000	1.51388800	0.00007800
C	3.13149200	-1.70387500	-0.00014300
H	2.55248300	-2.62032700	-0.00021200
C	4.51211500	-1.79738400	-0.00025700
H	4.98125600	-2.77760100	-0.00040700
C	5.31731700	-0.63539000	-0.00017800
H	6.40009600	-0.72549000	-0.00027200
C	-5.53319300	-0.38196500	0.00023400
H	-5.81680600	0.20820400	0.88184700
H	-5.81677900	0.20858800	-0.88113000
H	-6.11951800	-1.30522600	0.00002600
C	-1.80259400	2.41713900	0.00057200
H	-1.59989600	3.04375400	0.87859400
H	-1.59993300	3.04396000	-0.87731100
C	-3.26298600	1.86836200	0.00053700
H	-3.82627200	2.20830400	0.87913000
H	-3.82631200	2.20852900	-0.87794400



PAH(40) – 1-methylnaphthalene

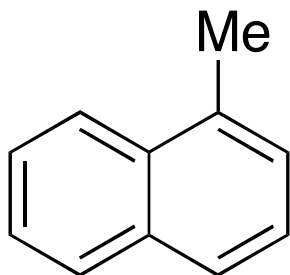
CAS: 90-12-0

Neutral Structure

C	0.97267400	1.45982100	0.00000000
C	-0.00093000	0.41902700	0.00000000
C	-1.41331100	0.68536600	0.00000000
H	2.19736600	-2.23657800	0.00000000
H	-0.12967500	-3.03100300	0.00000000
C	-2.29250500	-0.38395200	0.00000000
C	-1.83764700	-1.72734200	0.00000000
C	-0.48850900	-2.00399400	0.00000000
C	1.86033200	-1.20203600	0.00000000
C	2.77487700	-0.16910800	0.00000000
C	0.46044000	-0.94244400	0.00000000
C	2.32433600	1.17471900	0.00000000
H	3.84111100	-0.38216400	0.00000000
H	3.04921600	1.98530900	0.00000000
H	0.64699600	2.49567400	0.00000000
H	-3.36295600	-0.18940500	0.00000000
H	-2.56421100	-2.53651200	0.00000000
C	-1.93553500	2.10222000	0.00000000
H	-1.59631900	2.66106300	0.88212100
H	-1.59631900	2.66106300	-0.88212100
H	-3.03032700	2.10761200	0.00000000

Radical Cation

C	0.95272100	1.46637300	0.00000000
C	0.00023400	0.42625000	0.00000000
C	-1.41246200	0.67930900	0.00000000
H	2.21005000	-2.21391500	0.00000000
H	-0.09224800	-3.01821100	0.00000000
C	-2.29967700	-0.42604900	0.00000000
C	-1.83765300	-1.73498400	0.00000000
C	-0.45599800	-1.99451400	0.00000000
C	1.86341700	-1.18427400	0.00000000
C	2.78575500	-0.12983900	0.00000000
C	0.47245800	-0.92867000	0.00000000
C	2.33038400	1.18788800	0.00000000
H	3.85028300	-0.34311300	0.00000000
H	3.03896800	2.01074900	0.00000000
H	0.62730100	2.50119800	0.00000000
H	-3.36806000	-0.23129500	0.00000000
H	-2.54149200	-2.56165800	0.00000000
C	-1.96964300	2.06747800	0.00000000
H	-1.62972400	2.62720400	0.88122500
H	-1.62972400	2.62720400	-0.88122500
H	-3.06194200	2.04904400	0.00000000



PAH(41) – 2-methylnaphthalene

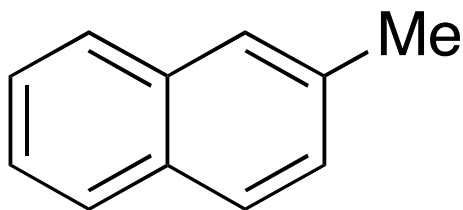
CAS: 91-57-6

Neutral Structure

C	1.40958000	-1.51999400	0.00000000
C	0.30947600	-0.61621300	0.00000000
C	-1.04196500	-1.06698500	0.00000000
H	2.11822100	2.31489900	0.00000000
H	-0.33958900	2.76099800	0.00000000
C	-2.10495100	-0.18294500	0.00000000
C	-1.82647400	1.21678900	0.00000000
C	-0.53282000	1.69007100	0.00000000
C	1.92356600	1.24418000	0.00000000
C	2.96925500	0.34242100	0.00000000
C	0.57396900	0.79329100	0.00000000
C	2.70877800	-1.05273700	0.00000000
H	3.99683300	0.69774600	0.00000000
H	3.53935200	-1.75458600	0.00000000
H	1.20835800	-2.58941100	0.00000000
H	-2.65871200	1.91831200	0.00000000
C	-3.53670500	-0.66068900	0.00000000
H	-3.59282300	-1.75438800	0.00000000
H	-4.07730500	-0.29210900	0.88192500
H	-4.07730500	-0.29210900	-0.88192500
H	-1.22937700	-2.13964700	0.00000000

Radical Cation

C	-1.40181300	-1.51699900	0.00000000
C	-0.30980000	-0.61137900	0.00000000
C	1.02420800	-1.06084700	0.00000000
H	-2.10605500	2.31563700	0.00000000
H	0.33989500	2.76253400	0.00000000
C	2.11934400	-0.15415100	0.00000000
C	1.84656200	1.21976800	0.00000000
C	0.53192700	1.69279000	0.00000000
C	-1.90295500	1.24801800	0.00000000
C	-2.97074100	0.32880800	0.00000000
C	-0.57091300	0.79705100	0.00000000
C	-2.72100500	-1.04366200	0.00000000
H	-3.99195900	0.69739500	0.00000000
H	-3.54599900	-1.74942100	0.00000000
H	-1.20261800	-2.58523100	0.00000100
H	2.66927500	1.92884000	-0.00000100
C	3.52075000	-0.68365400	0.00000000
H	3.69098400	-1.31737300	-0.88064200
H	4.25744000	0.12407700	-0.00000500
H	3.69098600	-1.31736400	0.88064900
H	1.22150500	-2.13042200	0.00000000



PAH(42) – naphthacene

CAS: 92-24-0

Neutral Structure

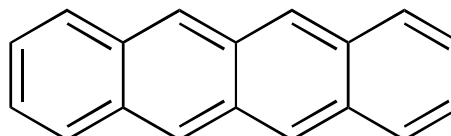
C	0.00000000	4.89534700	0.71676700
C	0.00000000	3.71509300	1.41311300
C	0.00000000	2.45264100	0.72687400
C	0.00000000	2.45264100	-0.72687400
C	0.00000000	3.71509300	-1.41311300
C	0.00000000	4.89534700	-0.71676700
H	0.00000000	1.23618000	2.49948600
H	0.00000000	5.84365100	1.24849300
H	0.00000000	3.71261700	2.50112800
C	0.00000000	1.23639000	1.41098000
C	0.00000000	1.23639000	-1.41098000
H	0.00000000	3.71261700	-2.50112800
H	0.00000000	5.84365100	-1.24849300
C	0.00000000	0.00000000	-0.72700100
C	0.00000000	0.00000000	0.72700100
H	0.00000000	1.23618000	-2.49948600
C	0.00000000	-1.23639000	-1.41098000
C	0.00000000	-1.23639000	1.41098000
C	0.00000000	-2.45264100	-0.72687400
H	0.00000000	-1.23618000	-2.49948600
C	0.00000000	-2.45264100	0.72687400
H	0.00000000	-1.23618000	2.49948600
C	0.00000000	-3.71509300	-1.41311300
C	0.00000000	-3.71509300	1.41311300
C	0.00000000	-4.89534700	-0.71676700
H	0.00000000	-3.71261700	-2.50112800
C	0.00000000	-4.89534700	0.71676700
H	0.00000000	-3.71261700	2.50112800
H	0.00000000	-5.84365100	-1.24849300
H	0.00000000	-5.84365100	1.24849300

Radical Cation

C	0.00000000	4.89010700	0.70801600
C	0.00000000	3.69838500	1.41164300
C	0.00000000	2.45662900	0.72237900
C	0.00000000	2.45662900	-0.72237900
C	0.00000000	3.69838500	-1.41164300
C	0.00000000	4.89010700	-0.70801600
H	0.00000000	1.22876200	2.50014200
H	0.00000000	5.83518200	1.24358800
H	0.00000000	3.69712400	2.49849600
C	0.00000000	1.22778300	1.41264200
C	0.00000000	1.22778300	-1.41264200
H	0.00000000	3.69712400	-2.49849600
H	0.00000000	5.83518200	-1.24358800
C	0.00000000	0.00000000	-0.72591900
C	0.00000000	0.00000000	0.72591900
H	0.00000000	1.22876200	-2.50014200
C	0.00000000	-1.22778300	-1.41264200
C	0.00000000	-1.22778300	1.41264200
C	0.00000000	-2.45662900	-0.72237900
H	0.00000000	-1.22876200	-2.50014200
C	0.00000000	-2.45662900	0.72237900
H	0.00000000	-1.22876200	2.50014200
C	0.00000000	-3.69838500	-1.41164300
C	0.00000000	-3.69838500	1.41164300
C	0.00000000	-4.89010700	-0.70801600
H	0.00000000	-3.69712400	-2.49849600
C	0.00000000	-4.89010700	0.70801600
H	0.00000000	-3.69712400	2.49849600
H	0.00000000	-5.83518200	-1.24358800
H	0.00000000	-5.83518200	1.24358800

Radical Anion

C	0.00000000	4.93612600	0.70821600
C	0.00000000	3.73437300	1.40330600
C	0.00000000	2.48037700	0.72557300
C	0.00000000	2.48037700	-0.72557300
C	0.00000000	3.73437300	-1.40330600
C	0.00000000	4.93612600	-0.70821600
H	0.00000000	1.24412100	2.49753800
H	0.00000000	5.87916400	1.25101800
H	0.00000000	3.73497100	2.49275700
C	0.00000000	1.24178600	1.40749000
C	0.00000000	1.24178600	-1.40749000
H	0.00000000	3.73497100	-2.49275700
H	0.00000000	5.87916400	-1.25101800
C	0.00000000	0.00000000	-0.73232600
C	0.00000000	0.00000000	0.73232600
H	0.00000000	1.24412100	-2.49753800
C	0.00000000	-1.24178600	-1.40749000
C	0.00000000	-1.24178600	1.40749000
C	0.00000000	-2.48037700	-0.72557300
H	0.00000000	-1.24412100	-2.49753800
C	0.00000000	-2.48037700	0.72557300
H	0.00000000	-1.24412100	2.49753800
C	0.00000000	-3.73437300	-1.40330600
C	0.00000000	-3.73437300	1.40330600
C	0.00000000	-4.93612600	-0.70821600
H	0.00000000	-3.73497100	-2.49275700
C	0.00000000	-4.93612600	0.70821600
H	0.00000000	-3.73497100	2.49275700
H	0.00000000	-5.87916400	-1.25101800
H	0.00000000	-5.87916400	1.25101800



PAH(43) – naphthalene

CAS: 91-20-3

Neutral Structure

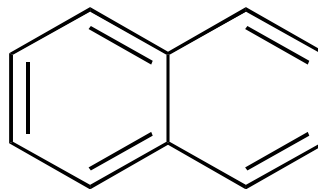
C	0.00000000	2.43798400	0.70993600
C	0.00000000	1.24674400	1.40640300
C	0.00000000	0.00000000	0.71794100
C	0.00000000	0.00000000	-0.71794100
C	0.00000000	1.24674400	-1.40640300
C	0.00000000	2.43798400	-0.70993600
H	0.00000000	-1.24390000	2.49452900
H	0.00000000	3.38334200	1.24701000
H	0.00000000	1.24390000	2.49452900
C	0.00000000	-1.24674400	1.40640300
C	0.00000000	-1.24674400	-1.40640300
H	0.00000000	1.24390000	-2.49452900
H	0.00000000	3.38334200	-1.24701000
C	0.00000000	-2.43798400	-0.70993600
C	0.00000000	-2.43798400	0.70993600
H	0.00000000	-1.24390000	-2.49452900
H	0.00000000	-3.38334200	-1.24701000
H	0.00000000	-3.38334200	1.24701000

Radical Cation

C	0.00000000	2.45125900	0.69654900
C	0.00000000	1.23532800	1.40445800
C	0.00000000	0.00000000	0.71640400
C	0.00000000	0.00000000	-0.71640400
C	0.00000000	1.23532800	-1.40445800
C	0.00000000	2.45125900	-0.69654900
H	0.00000000	-1.23878900	2.49115500
H	0.00000000	3.38881000	1.24367600
H	0.00000000	1.23878900	2.49115500
C	0.00000000	-1.23532800	1.40445800
C	0.00000000	-1.23532800	-1.40445800
H	0.00000000	1.23878900	-2.49115500
H	0.00000000	3.38881000	-1.24367600
C	0.00000000	-2.45125900	-0.69654900
C	0.00000000	-2.45125900	0.69654900
H	0.00000000	-1.23878900	-2.49115500
H	0.00000000	-3.38881000	-1.24367600
H	0.00000000	-3.38881000	1.24367600

Radical Anion

C	0.00000000	2.47693400	0.69763500
C	0.00000000	1.25345300	1.40642900
C	0.00000000	0.00000000	0.72770600
C	0.00000000	0.00000000	-0.72770600
C	0.00000000	1.25345300	-1.40642900
C	0.00000000	2.47693400	-0.69763500
H	0.00000000	-1.25700900	2.49621100
H	0.00000000	3.41785600	1.24629300
H	0.00000000	1.25700900	2.49621100
C	0.00000000	-1.25345300	1.40642900
C	0.00000000	-1.25345300	-1.40642900
H	0.00000000	1.25700900	-2.49621100
H	0.00000000	3.41785600	-1.24629300
C	0.00000000	-2.47693400	-0.69763500
C	0.00000000	-2.47693400	0.69763500
H	0.00000000	-1.25700900	-2.49621100
H	0.00000000	-3.41785600	-1.24629300
H	0.00000000	-3.41785600	1.24629300



PAH(44) – pentacene

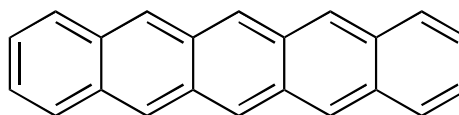
CAS: 135-48-8

Neutral Structure

C	0.00000000	1.22742900	0.72938100
C	0.00000000	1.22742900	-0.72938100
C	0.00000000	0.00000000	-1.41317000
C	0.00000000	0.00000000	1.41317000
H	0.00000000	-4.94434800	-2.50227500
H	0.00000000	-7.07399500	-1.24880000
C	0.00000000	-1.22742900	-0.72938100
C	0.00000000	-1.22742900	0.72938100
C	0.00000000	-2.46957300	-1.41254100
C	0.00000000	-2.46957300	1.41254100
C	0.00000000	-3.68167100	-0.72862900
C	0.00000000	-3.68167100	0.72862900
H	0.00000000	-2.46948700	-2.50102300
H	0.00000000	-2.46948700	2.50102300
C	0.00000000	-4.94661600	-1.41426300
C	0.00000000	-6.12523200	-0.71792200
C	0.00000000	-4.94661600	1.41426300
C	0.00000000	-6.12523200	0.71792200
H	0.00000000	-4.94434800	2.50227500
H	0.00000000	-7.07399500	1.24880000
H	0.00000000	0.00000000	-2.50154200
C	0.00000000	3.68167100	-0.72862900
C	0.00000000	3.68167100	0.72862900
C	0.00000000	2.46957300	-1.41254100
C	0.00000000	2.46957300	1.41254100
C	0.00000000	4.94661600	-1.41426300
H	0.00000000	2.46948700	-2.50102300
C	0.00000000	4.94661600	1.41426300
C	0.00000000	6.12523200	-0.71792200
H	0.00000000	4.94434800	-2.50227500
C	0.00000000	6.12523200	0.71792200
H	0.00000000	4.94434800	2.50227500
H	0.00000000	7.07399500	-1.24880000
H	0.00000000	7.07399500	1.24880000
H	0.00000000	0.00000000	2.50154200
H	0.00000000	2.46948700	2.50102300

Radical Anion

C	0.00000000	1.24032100	0.73259600
C	0.00000000	1.24032100	-0.73259600
C	0.00000000	0.00000000	-1.40972900
C	0.00000000	0.00000000	1.40972900
H	0.00000000	-4.96950400	-2.49467300
H	0.00000000	-7.10946300	-1.25096500
C	0.00000000	-1.24032100	-0.73259600
C	0.00000000	-1.24032100	0.73259600
C	0.00000000	-2.48001800	-1.40725900
C	0.00000000	-2.48001800	1.40725900
C	0.00000000	-3.71333900	-0.72547900
C	0.00000000	-3.71333900	0.72547900
H	0.00000000	-2.48273200	-2.49712200
H	0.00000000	-2.48273200	2.49712200
C	0.00000000	-4.96972200	-1.40549900
C	0.00000000	-6.16495100	-0.71120500
C	0.00000000	-4.96972200	1.40549900
C	0.00000000	-6.16495100	0.71120500
H	0.00000000	-4.96950400	2.49467300
H	0.00000000	-7.10946300	1.25096500
H	0.00000000	0.00000000	-2.49954800
C	0.00000000	3.71333900	-0.72547900
C	0.00000000	3.71333900	0.72547900
C	0.00000000	2.48001800	-1.40725900
C	0.00000000	2.48001800	1.40725900
C	0.00000000	4.96972200	-1.40549900
H	0.00000000	2.48273200	-2.49712200
C	0.00000000	4.96972200	1.40549900
C	0.00000000	6.16495100	-0.71120500
H	0.00000000	4.96950400	-2.49467300
C	0.00000000	6.16495100	0.71120500
H	0.00000000	4.96950400	2.49467300
H	0.00000000	7.10946300	-1.25096500
H	0.00000000	7.10946300	1.25096500
H	0.00000000	0.00000000	2.49954800
H	0.00000000	2.48273200	2.49712200



PAH(45) – periflanthene

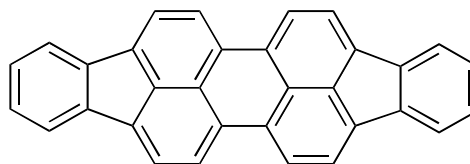
CAS: 188-94-3

Neutral Structure

C	-4.91861800	-0.86469600	0.01379400
C	-3.52126900	-0.97935300	0.02529300
C	-2.74361600	0.22750100	0.01298600
C	-3.43974900	1.44147900	-0.00818800
C	-4.85356900	1.55087900	-0.01914700
C	-5.59511700	0.38005300	-0.00794100
H	-5.52780300	-1.76336700	0.02002600
C	-1.30941500	0.28936500	0.01764200
C	-2.82004300	2.71705300	-0.02677400
H	-6.68237300	0.38941500	-0.01654000
C	-1.43513900	2.76588300	-0.02339700
C	-0.70281100	1.55321300	-0.00139100
H	-0.89394400	3.70873400	-0.03877600
H	0.38039700	1.62452300	-0.00158900
C	-2.66429400	-4.72959800	0.08793500
C	-1.27939000	-4.68076900	0.09131300
C	-0.65968400	-3.40519400	0.07272600
C	-1.35581700	-2.19121700	0.05155200
C	-2.79001800	-2.25308000	0.04689600
C	-3.39662200	-3.51692800	0.06592900
H	-3.20548900	-5.67244900	0.10331400
C	0.75413600	-3.51459400	0.08368500
C	-0.57816400	-0.98436200	0.03924500
H	-4.47983000	-3.58823800	0.06612700
C	0.81918500	-1.09902000	0.05074400
C	1.49568400	-2.34376900	0.07248000
H	1.42837000	-0.20034800	0.04451200
H	2.58294000	-2.35313100	0.08107800
C	1.02562200	-7.75237800	0.16125000
C	2.24159500	-7.05512400	0.15450600
C	2.26497700	-5.65220700	0.12876100
C	1.05600900	-4.95735700	0.11039700
C	-0.18594800	-5.66963000	0.11607800
C	-0.19700200	-7.06381300	0.14214700
H	1.02860600	-8.83943300	0.18131700
H	3.17826600	-7.60684900	0.16910600
H	3.21340200	-5.12020600	0.12365600
H	-1.13535000	-7.61346500	0.14710700
C	-5.15544200	2.99364100	-0.04585800
C	-3.91348500	3.70591400	-0.05153900
C	-3.90243100	5.10009800	-0.07760900
C	-5.12505500	5.78866300	-0.09671200
C	-6.34102800	5.09140900	-0.08996800
C	-6.36441000	3.68849100	-0.06422300
H	-2.96408300	5.64974900	-0.08256800
H	-5.12803900	6.87571800	-0.11677800
H	-7.27769900	5.64313300	-0.10456800
H	-7.31283500	3.15649100	-0.05911800

Radical Anion

C	-4.93422000	-0.86973400	0.01558100
C	-3.51571800	-0.98770700	0.02573500
C	-2.74079200	0.22268000	0.01382400
C	-3.44018700	1.44217600	-0.00640600
C	-4.85597400	1.55120600	-0.01696400
C	-5.60067500	0.36333500	-0.00514000
H	-5.53897500	-1.77194700	0.02317300
C	-1.30494700	0.28051000	0.01880300
C	-2.81927200	2.71926200	-0.02457600
H	-6.68910600	0.37670500	-0.01290600
C	-1.41809000	2.76226300	-0.02015000
C	-0.69048300	1.56428900	0.00135600
H	-0.87997200	3.70832100	-0.03471500
H	0.39359000	1.63020500	0.00287500
C	-2.68134300	-4.72597800	0.08468800
C	-1.28016200	-4.68297700	0.08911400
C	-0.65924600	-3.40589100	0.07094500
C	-1.35864200	-2.18639600	0.05071500
C	-2.79448600	-2.24422500	0.04573500
C	-3.40895000	-3.52800400	0.06318200
H	-3.21946200	-5.67203700	0.09925300
C	0.75654100	-3.51492100	0.08150200
C	-0.58371500	-0.97600800	0.03880300
H	-4.49302300	-3.59392000	0.06166300
C	0.83478600	-1.09398200	0.04895700
C	1.50124200	-2.32705000	0.06967800
H	1.43954200	-0.19176800	0.04136500
H	2.58967200	-2.34042100	0.07744400
C	1.02031900	-7.75030700	0.16350700
C	2.24236500	-7.04965600	0.15598800
C	2.26471900	-5.65105200	0.12821400
C	1.05484100	-4.94333800	0.10878600
C	-0.19729500	-5.66141700	0.11481100
C	-0.19799700	-7.06282300	0.14312000
H	1.02440900	-8.83784300	0.18544300
H	3.17892400	-7.60260800	0.17168000
H	3.21541200	-5.12122100	0.12267000
H	-1.13580300	-7.61518800	0.14881300
C	-5.15427400	2.97962300	-0.04424800
C	-3.90213900	3.69770200	-0.05027300
C	-3.90143600	5.09910800	-0.07858100
C	-5.11975200	5.78659200	-0.09896900
C	-6.34179900	5.08594100	-0.09145000
C	-6.36415200	3.68733700	-0.06367500
H	-2.96363000	5.65147300	-0.08427500
H	-5.12384300	6.87412800	-0.12090500
H	-7.27835700	5.63889300	-0.10714100
H	-7.31484600	3.15750500	-0.05813200



PAH(46) – perylene

CAS: 198-55-0

Neutral Structure

C	-0.05194200	2.42627300	-2.88959700
C	-0.02601200	1.23420000	-3.58144700
C	0.00000000	0.00000000	-2.87822400
C	0.00000000	0.00000000	-1.44096100
C	-0.01237100	1.25192100	-0.73926500
C	-0.04489200	2.43228800	-1.48015800
H	0.02726600	-1.21890500	-4.66888700
H	-0.07681200	3.37238300	-3.42441300
H	-0.02726600	1.21890500	-4.66888700
C	0.02601200	-1.23420000	-3.58144700
C	0.01237100	-1.25192100	-0.73926500
H	-0.06722500	3.39411700	-0.98011300
C	0.04489200	-2.43228800	-1.48015800
C	0.05194200	-2.42627300	-2.88959700
H	0.06722500	-3.39411700	-0.98011300
H	0.07681200	-3.37238300	-3.42441300
C	-0.01237100	-1.25192100	0.73926500
C	0.00000000	0.00000000	1.44096100
C	-0.04489200	-2.43228800	1.48015800
C	0.01237100	1.25192100	0.73926500
C	0.00000000	0.00000000	2.87822400
C	-0.05194200	-2.42627300	2.88959700
H	-0.06722500	-3.39411700	0.98011300
C	0.04489200	2.43228800	1.48015800
C	0.02601200	1.23420000	3.58144700
C	-0.02601200	-1.23420000	3.58144700
H	-0.07681200	-3.37238300	3.42441300
C	0.05194200	2.42627300	2.88959700
H	0.06722500	3.39411700	0.98011300
H	0.02726600	1.21890500	4.66888700
H	-0.02726600	-1.21890500	4.66888700
H	0.07681200	3.37238300	3.42441300

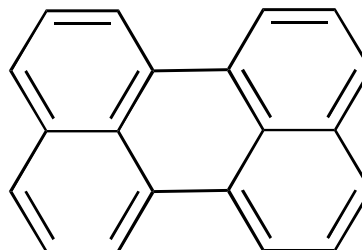
Radical Anion

C	-0.00000200	2.44007700	-2.87831200
C	-0.00000100	1.23841000	-3.57968100
C	0.00000000	0.00000000	-2.88195200
C	0.00000000	0.00000000	-1.43432000
C	0.00000000	1.25265600	-0.72836100
C	-0.00000200	2.45472900	-1.48117200
H	0.00000100	-1.22926400	-4.66792500
H	-0.00000300	3.38413700	-3.42071800
H	-0.00000100	1.22926400	-4.66792500
C	0.00000100	-1.23841000	-3.57968100
C	0.00000000	-1.25265600	-0.72836100
H	-0.00000300	3.41504400	-0.97735300
C	0.00000200	-2.45472900	-1.48117200
C	0.00000200	-2.44007700	-2.87831200
H	0.00000300	-3.41504400	-0.97735300
H	0.00000300	-3.38413700	-3.42071800
C	0.00000000	-1.25265600	0.72836100
C	0.00000000	0.00000000	1.43432000
C	-0.00000200	-2.45472900	1.48117200
C	0.00000000	1.25265600	0.72836100
C	0.00000000	0.00000000	2.88195200
C	-0.00000200	-2.44007700	2.87831200

H	-0.00000300	-3.41504400	0.97735300
C	0.00000200	2.45472900	1.48117200
C	0.00000100	1.23841000	3.57968100
C	-0.00000100	-1.23841000	3.57968100
H	-0.00000300	-3.38413700	3.42071800
C	0.00000200	2.44007700	2.87831200
H	0.00000300	3.41504400	0.97735300
H	0.00000100	1.22926400	4.66792500
H	-0.00000100	-1.22926400	4.66792500
H	0.00000300	3.38413700	3.42071800

Radical Cation

C	-0.06142900	2.43399900	-2.87206500
C	-0.03113000	1.22851000	-3.56293100
C	0.00000000	0.00000000	-2.86006100
C	0.00000000	0.00000000	-1.42686800
C	-0.01340400	1.24629600	-0.72628900
C	-0.05145400	2.44309200	-1.47714600
H	0.03404600	-1.21319600	-4.64960400
H	-0.09156900	3.37444000	-3.41391900
H	-0.03404600	1.21319600	-4.64960400
C	0.03113000	-1.22851000	-3.56293100
C	0.01340400	-1.24629600	-0.72628900
H	-0.07854500	3.40233400	-0.97482400
C	0.05145400	-2.44309200	-1.47714600
C	0.06142900	-2.43399900	-2.87206500
H	0.07854500	-3.40233400	-0.97482400
H	0.09156900	-3.37444000	-3.41391900
C	-0.01340400	-1.24629600	0.72628900
C	0.00000000	0.00000000	1.42686800
C	-0.05145400	-2.44309200	1.47714600
C	0.01340400	1.24629600	0.72628900
C	0.00000000	0.00000000	2.86006100
C	-0.06142900	-2.43399900	2.87206500
H	-0.07854500	-3.40233400	0.97482400
C	0.05145400	2.44309200	1.47714600
C	0.03113000	1.22851000	3.56293100
C	-0.03113000	-1.22851000	3.56293100
H	-0.09156900	-3.37444000	3.41391900
C	0.06142900	2.43399900	2.87206500
H	0.07854500	3.40233400	0.97482400
H	0.03404600	1.21319600	4.64960400
H	-0.03404600	-1.21319600	4.64960400
H	0.09156900	3.37444000	3.41391900



PAH(47) – phenanthrene

CAS: 85-01-8

Neutral Structure

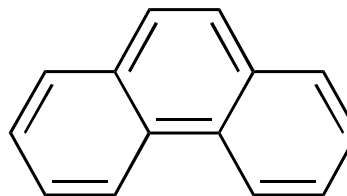
C	0.00000000	3.56785800	-0.29579900
C	0.00000000	2.84167200	0.88226500
C	0.00000000	1.42442800	0.86666300
C	0.00000000	0.73019600	-0.38278300
C	0.00000000	1.50242300	-1.57167100
C	0.00000000	2.88831300	-1.53160700
C	0.00000000	0.68134900	2.09751200
C	0.00000000	-0.73019600	-0.38278300
C	0.00000000	-1.42442800	0.86666300
C	0.00000000	-0.68134900	2.09751200
C	0.00000000	-2.84167200	0.88226500
H	0.00000000	-3.35125600	1.84354800
C	0.00000000	-3.56785800	-0.29579900
C	0.00000000	-2.88831300	-1.53160700
C	0.00000000	-1.50242300	-1.57167100
H	0.00000000	1.23506000	3.03381800
H	0.00000000	4.65474300	-0.27077500
H	0.00000000	3.35125600	1.84354800
H	0.00000000	1.01299500	-2.53995200
H	0.00000000	3.45272300	-2.46087400
H	0.00000000	-1.23506000	3.03381800
H	0.00000000	-4.65474300	-0.27077500
H	0.00000000	-3.45272300	-2.46087400
H	0.00000000	-1.01299500	-2.53995200

Radical Cation

C	-4.94472600	-4.56638000	-0.00416700
C	-3.56198200	-4.55128500	-0.00473400
C	-2.84795500	-3.31441400	-0.00327400
C	-3.56373500	-2.06731400	-0.00091200
C	-4.96080200	-2.11784800	-0.00038700
C	-5.64065500	-3.34608000	-0.00206800
C	-1.44110500	-3.31646500	-0.00459400
C	-2.80346100	-0.81349400	0.00060500
C	-1.36679900	-0.87046300	-0.00128200
C	-0.71420900	-2.11699100	-0.00375200
C	-0.60040300	0.33493700	-0.00013300
H	0.48357900	0.25843200	-0.00166800
C	-1.22745500	1.56753900	0.00303300
C	-2.63126800	1.61934200	0.00515900
C	-3.40522800	0.44825900	0.00391300
H	-0.91060900	-4.26454700	-0.00634700
H	-5.48766800	-5.50636300	-0.00538100
H	-2.99237200	-5.47658300	-0.00637200
H	-5.54782700	-1.20621200	0.00104400
H	-6.72711900	-3.34431300	-0.00176300
H	0.37173300	-2.14903500	-0.00489300
H	-0.64604500	2.48425200	0.00395200
H	-3.13582000	2.58142600	0.00773000
H	-4.48477100	0.54683500	0.00571600

Radical Anion

C	0.31529400	3.58723300	0.00000000
C	-0.87377700	2.87421600	0.00000000
C	-0.89615400	1.43704300	0.00000000
C	0.37838600	0.74115200	0.00000000
C	1.55757200	1.50359200	0.00000000
C	1.55100500	2.91086800	0.00000000
C	-2.10370400	0.70665700	0.00000000
C	0.37838900	-0.74115100	0.00000000
C	-0.89614700	-1.43704800	0.00000000
C	-2.10370100	-0.70666900	0.00000000
C	-0.87376200	-2.87422100	0.00000000
H	-1.82615000	-3.40342200	0.00000000
C	0.31531200	-3.58723200	0.00000000
C	1.55102000	-2.91086100	0.00000000
C	1.55758000	-1.50358500	0.00000000
H	-3.04694600	1.25157000	0.00000000
H	0.29063700	4.67628900	0.00000000
H	-1.82616700	3.40341200	0.00000000
H	2.52165200	1.00158100	0.00000000
H	2.48820000	3.46221500	0.00000000
H	-3.04694000	-1.25158600	0.00000000
H	0.29066000	-4.67628800	0.00000000
H	2.48821700	-3.46220300	0.00000000
H	2.52165600	-1.00156900	0.00000000



PAH(48) – picene

CAS: 213-46-7

Neutral Structure

C	-2.84293000	1.99924400	-0.00308500
C	-3.59236800	0.78064400	-0.00031800
C	-2.89283000	-0.46462300	-0.00310900
C	-1.47703500	1.99564500	-0.00597600
H	-3.38543100	2.94203100	-0.00123700
H	-0.96276100	2.94910500	-0.00583700
C	-3.66455400	-1.65663600	0.00562900
C	-5.04918300	-1.61736800	0.01370100
H	-3.17703100	-2.62529300	0.00876000
C	-5.01057700	0.79649100	0.00742300
C	-5.73303800	-0.38212000	0.01367600
H	-5.61216300	-2.54745300	0.02077700
H	-5.52033800	1.75763400	0.00899000
H	-6.81995200	-0.36089700	0.01974900
C	-1.43620500	-0.46034600	-0.01226400
C	-0.72511100	0.77147500	-0.00937400
C	-0.68590100	-1.67072600	-0.02523000
C	0.72511300	0.77147400	-0.00920700
C	0.68590400	-1.67072700	-0.02511500
C	1.43620700	-0.46034700	-0.01200100
H	-1.19660500	-2.62688800	-0.03795100
H	1.19660800	-2.62689000	-0.03776400
H	0.96276200	2.94910400	-0.00540500
C	1.47703500	1.99564400	-0.00556700
C	2.84293000	1.99924200	-0.00242000
C	3.59236700	0.78064200	0.00038800
H	3.38543100	2.94203000	-0.00038900
C	2.89283100	-0.46462500	-0.00257700
C	5.01057600	0.79649000	0.00836700
C	3.66455400	-1.65663800	0.00624200
C	5.73303700	-0.38212000	0.01467800
H	5.52033500	1.75763400	0.01006400
C	5.04918200	-1.61736900	0.01454000
H	3.17703300	-2.62529600	0.00925700
H	6.81994900	-0.36089700	0.02092400
H	5.61216100	-2.54745400	0.02166700

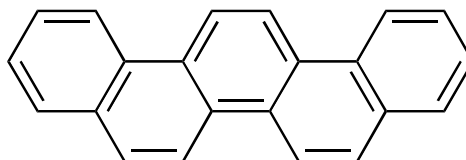
Radical Anion

C	-2.87986300	2.00583600	-0.00061400
C	-3.62019700	0.79333100	-0.00076800
C	-2.91766500	-0.46188300	-0.00062900
C	-1.48772200	1.98547500	-0.00030400
H	-3.41420800	2.95366100	-0.00071200
H	-0.97255100	2.94117800	-0.00018900
C	-3.68715200	-1.64865800	-0.00079800
C	-5.07937300	-1.62929800	-0.00108900
H	-3.19060100	-2.61409200	-0.00071300
C	-5.04554700	0.78746100	-0.00107000
C	-5.76382000	-0.39548000	-0.00121800
H	-5.63441800	-2.56441300	-0.00121100
H	-5.56580900	1.74408200	-0.00117400
H	-6.85172900	-0.37422400	-0.00143600
C	-1.44599900	-0.47126000	-0.00030600
C	-0.73861600	0.78741600	-0.00016000
C	-0.70322900	-1.66340000	-0.00015400
C	0.73861600	0.78741600	0.00016000
C	0.70322900	-1.66340000	0.00015500
C	1.44599900	-0.47126000	0.00030700
H	-1.20766800	-2.62442100	-0.00025900
H	1.20766800	-2.62442100	0.00026100
H	0.97255100	2.94117800	0.00018900
C	1.48772100	1.98547500	0.00030400
C	2.87986200	2.00583600	0.00061400
C	3.62019600	0.79333100	0.00076900

H	3.41420700	2.95366100	0.00071200
C	2.91766500	-0.46188200	0.00062900
C	5.04554700	0.78746200	0.00107000
C	3.68715200	-1.64865800	0.00079800
C	5.76382000	-0.39548000	0.00121700
H	5.56580900	1.74408200	0.00117400
C	5.07937300	-1.62929800	0.00108900
H	3.19060100	-2.61409100	0.00071200
H	6.85172900	-0.37422300	0.00143600
H	5.63441800	-2.56441300	0.00121000

Radical Cation

C	-2.85621100	1.97592000	0.07097000
C	-3.60343900	0.77316500	0.03400900
C	-2.90738000	-0.47629300	-0.01120900
C	-1.46946600	1.97865300	0.05619100
H	-3.38956100	2.92212100	0.11021100
H	-0.96642300	2.93675700	0.09281100
C	-3.67714900	-1.65637100	-0.06260200
C	-5.06806600	-1.60382700	-0.05887800
H	-3.20099000	-2.62902500	-0.11227800
C	-5.02383300	0.80328500	0.03940700
C	-5.74988700	-0.37199300	-0.00499700
H	-5.63314300	-2.53113000	-0.09944300
H	-5.52433100	1.76740700	0.07729500
H	-6.83593300	-0.34983300	-0.00137900
C	-1.44649600	-0.46688300	-0.00665300
C	-0.73226500	0.77673200	0.00927600
C	-0.69832400	-1.65270400	-0.00400300
C	0.73226500	0.77673200	-0.00927500
C	0.69832300	-1.65270400	0.00400300
C	1.44649600	-0.46688300	0.00665300
H	-1.19425400	-2.61606600	0.00008200
H	1.19425300	-2.61606600	-0.00008200
H	0.96642400	2.93675700	-0.09281100
C	1.46946700	1.97865300	-0.05619100
C	2.85621200	1.97592000	-0.07096900
C	3.60343900	0.77316400	-0.03400900
H	3.38956200	2.92212000	-0.11021000
C	2.90737900	-0.47629400	0.01120900
C	5.02383300	0.80328400	-0.03940600
C	3.67714900	-1.65637200	0.06260200
C	5.74988700	-0.37199500	0.00499700
H	5.52433200	1.76740600	-0.07729400
C	5.06806600	-1.60382800	0.05887800
H	3.20099000	-2.62902600	0.11227800
H	6.83593300	-0.34983500	0.00138000
H	5.63314200	-2.53113100	0.09944300



PAH(49) – pyrene

CAS: 129-00-0

Neutral Structure

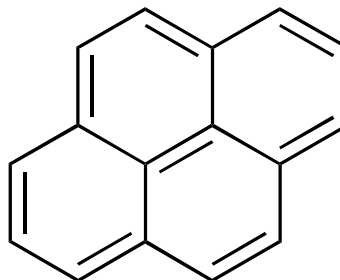
C	3.52922800	0.00000000	0.00036300
C	2.83750500	-1.21368800	0.00030500
C	1.43086100	-1.23820400	0.00015700
C	0.71436700	0.00000000	0.00007500
C	1.43086100	1.23820400	0.00013500
C	2.83750500	1.21368800	0.00028200
C	0.68233600	-2.46871400	0.00009400
C	-0.71436700	0.00000000	-0.00007500
C	-1.43086100	-1.23820400	-0.00013500
C	-0.68233600	-2.46871400	-0.00004800
C	-2.83750500	-1.21368800	-0.00028200
H	-3.38410500	-2.15412100	-0.00033000
C	-3.52922800	0.00000000	-0.00036300
C	-2.83750500	1.21368700	-0.00030500
C	-1.43086100	1.23820400	-0.00015700
C	-0.68233600	2.46871400	-0.00009400
C	0.68233600	2.46871400	0.00004800
H	1.23285300	3.40693500	0.00009500
H	-1.23285300	3.40693500	-0.00015900
H	1.23285300	-3.40693500	0.00015900
H	4.61651300	0.00000000	0.00047400
H	3.38410500	-2.15412100	0.00037000
H	3.38410500	2.15412100	0.00033000
H	-1.23285300	-3.40693500	-0.00009500
H	-4.61651300	0.00000000	-0.00047400
H	-3.38410500	2.15412000	-0.00037000

Radical Cation

C	3.54032700	0.00000100	0.00036500
C	2.84467100	-1.20871800	0.00030600
C	1.42130200	-1.23479100	0.00015600
C	0.70864700	0.00000000	0.00007500
C	1.42130100	1.23479200	0.00013200
C	2.84467000	1.20872000	0.00028200
C	0.69323200	-2.45306000	0.00009500
C	-0.70864700	0.00000000	-0.00007500
C	-1.42130100	-1.23479200	-0.00013200
C	-0.69323000	-2.45306000	-0.00004800
C	-2.84467000	-1.20872000	-0.00028200
H	-3.38531800	-2.15148800	-0.00032900
C	-3.54032700	-0.00000100	-0.00036500
C	-2.84467100	1.20871800	-0.00030600
C	-1.42130200	1.23479100	-0.00015600
C	-0.69323200	2.45306000	-0.00009500
C	0.69323000	2.45306000	0.00004800
H	1.23807200	3.39302400	0.00009400
H	-1.23807400	3.39302400	-0.00015800
H	1.23807400	-3.39302400	0.00015800
H	4.62596400	0.00000100	0.00047700
H	3.38531900	-2.15148600	0.00037100
H	3.38531800	2.15148800	0.00032900
H	-1.23807200	-3.39302400	-0.00009400
H	-4.62596400	-0.00000100	-0.00047700
H	-3.38531900	2.15148600	-0.00037100

Radical Anion

C	-3.55161800	0.00000000	-0.00036400
C	-2.86980900	-1.21859800	-0.00030900
C	-1.43914100	-1.24735900	-0.00015900
C	-0.71800400	0.00000000	-0.00007600
C	-1.43914100	1.24735900	-0.00013600
C	-2.86980900	1.21859800	-0.00028700
C	-0.69468300	-2.45645300	-0.00009800
C	0.71800400	0.00000000	0.00007600
C	1.43914100	-1.24735900	0.00013600
C	0.69468300	-2.45645300	0.00005200
C	2.86980900	-1.21859800	0.00028700
H	3.41749700	-2.15912900	0.00033300
C	3.55161800	0.00000000	0.00036400
C	2.86980900	1.21859800	0.00030900
C	1.43914100	1.24735900	0.00015900
C	0.69468300	2.45645300	0.00009800
C	-0.69468300	2.45645300	-0.00005200
H	-1.23588800	3.40180000	-0.00009800
H	1.23588800	3.40180000	0.00016300
H	-1.23588800	-3.40180000	-0.00016300
H	-4.64130500	0.00000000	-0.00047300
H	-3.41749700	-2.15912900	-0.00037400
H	-3.41749700	2.15912900	-0.00033300
H	1.23588800	-3.40180000	0.00009800
H	4.64130500	0.00000000	0.00047300
H	3.41749700	2.15912900	0.00037400



PAH(50) – rubicene

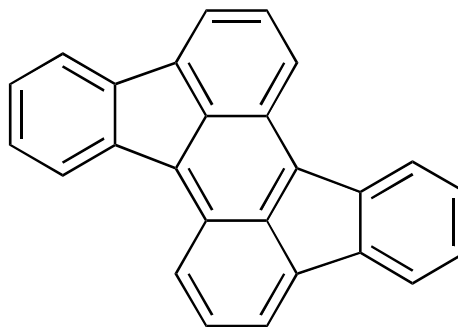
CAS: 197-61-5

Neutral Structure

C	-2.78476500	0.15571300	-0.00247200
C	-3.50628200	1.38660700	-0.02632400
C	-4.91332800	1.54090200	-0.05486400
C	-1.35626600	0.26341700	0.02441200
C	-2.85864500	2.66082700	-0.02688400
C	-1.48372100	2.72289400	-0.00018200
C	-0.74307300	1.50165300	0.02550900
H	-0.95254000	3.67148000	0.00063100
H	0.34265400	1.55307100	0.04600300
C	-7.01346900	-2.19501400	-0.06180200
C	-5.63854600	-2.13294700	-0.03510100
C	-4.99090800	-0.85872600	-0.03566000
C	-5.71242600	0.37216800	-0.05951200
C	-7.14092500	0.26446400	-0.08639700
C	-7.75411800	-0.97377300	-0.08749400
H	-7.54465000	-3.14360000	-0.06261500
C	-3.58386300	-1.01302100	-0.00712000
H	-8.83984400	-1.02519100	-0.10798700
C	-3.43442600	-5.26891300	0.03872300
C	-2.19954700	-4.60821300	0.05142800
C	-2.12972700	-3.20714600	0.03856900
C	-3.31461900	-2.46477100	0.01244300
C	-4.57169200	-3.14629200	-0.00236300
C	-4.63140100	-4.53787900	0.01168900
H	-3.46664600	-6.35555200	0.04911000
H	-1.27914800	-5.18660400	0.07127100
H	-1.15873300	-2.72256100	0.04882000
H	-5.58886000	-5.05341700	0.00046700
C	-5.18257200	2.99265200	-0.07442700
C	-3.92549800	3.67417200	-0.05962100
C	-3.86578900	5.06575900	-0.07367400
C	-5.06276500	5.79679400	-0.10070800
C	-6.29764300	5.13609300	-0.11341300
C	-6.36746300	3.73502700	-0.10055400
H	-2.90833100	5.58129800	-0.06245200
H	-5.03054400	6.88343200	-0.11109500
H	-7.21804300	5.71448400	-0.13325500
H	-7.33845700	3.25044200	-0.11080500
H	-7.75396700	1.15878000	-0.10568800
H	-0.74322300	-0.63089900	0.04370300

Radical Anion

C	-2.77002600	0.16381600	-0.00241200
C	-3.49617600	1.39463800	-0.02603600
C	-4.91563100	1.54589100	-0.05491800
C	-1.35450800	0.27381000	0.02384600
C	-2.85161200	2.66668800	-0.02660300
C	-1.45558500	2.73272500	0.00008100
C	-0.72614300	1.52730700	0.02491200
H	-0.93077800	3.68594400	0.00086100
H	0.36114300	1.56774700	0.04540100
C	-7.04160500	-2.20484500	-0.06206500
C	-5.64557800	-2.13880700	-0.03538200
C	-5.00101500	-0.86675800	-0.03594900
C	-5.72716400	0.36406400	-0.05957300
C	-7.14268200	0.25407100	-0.08583100
C	-7.77104800	-0.99942700	-0.08689700
H	-7.56641300	-3.15806400	-0.06284600
C	-3.58155900	-1.01801000	-0.00706700
H	-8.85833300	-1.03986600	-0.10738500
C	-3.44083100	-5.26999600	0.03837100
C	-2.20078500	-4.60277100	0.05177600
C	-2.13162200	-3.20634300	0.03895100
C	-3.31834000	-2.44847800	0.01235300
C	-4.58550400	-3.14067300	-0.00294500
C	-4.63381400	-4.53894800	0.01095800
H	-3.47078300	-6.35721300	0.04878400
H	-1.27990200	-5.18195100	0.07226300
H	-1.15886900	-2.72281500	0.04979200
H	-5.59091700	-5.05762000	-0.00069000
C	-5.17885000	2.97635900	-0.07433800
C	-3.91168600	3.66855400	-0.05904000
C	-3.86337600	5.06682800	-0.07294200
C	-5.05636000	5.79787700	-0.10035500
C	-6.29640500	5.13065200	-0.11376000
C	-6.36556800	3.73422400	-0.10093600
H	-2.90627400	5.58550000	-0.06129400
H	-5.02640700	6.88509300	-0.11076900
H	-7.21728800	5.70983100	-0.13424800
H	-7.33832100	3.25069600	-0.11177600
H	-7.75895000	1.14770600	-0.10518200
H	-0.73824100	-0.61982600	0.04319700



PAH(51) – triphenylene

CAS: 217-59-4

Neutral Structure

C	0.00000000	3.56224300	-1.24552400
C	0.00000000	2.86132500	-0.04946000
C	0.00000000	1.44600500	-0.01371200
C	0.00000000	0.73458100	-1.24641500
C	0.00000000	1.47441100	-2.45391000
C	0.00000000	2.86073600	-2.46148700
C	0.00000000	0.71147700	1.25895600
C	0.00000000	-0.73458100	-1.24641500
C	0.00000000	-1.44600500	-0.01371200
C	0.00000000	-0.71147700	1.25895600
C	0.00000000	-2.86132500	-0.04946000
H	0.00000000	-3.42764500	0.87424500
C	0.00000000	-3.56224300	-1.24552400
C	0.00000000	-2.86073600	-2.46148700
C	0.00000000	-1.47441100	-2.45391000
H	0.00000000	4.64932100	-1.23635700
H	0.00000000	3.42764500	0.87424500
H	0.00000000	0.96024900	-3.40779600
H	0.00000000	3.39702300	-3.40704500
H	0.00000000	-4.64932100	-1.23635700
H	0.00000000	-3.39702300	-3.40704500
H	0.00000000	-0.96024900	-3.40779600
C	0.00000000	1.38830000	2.50298000
C	0.00000000	0.70195600	3.70751200
H	0.00000000	2.47179600	2.53324000
C	0.00000000	-1.38830000	2.50298000
C	0.00000000	-0.70195600	3.70751200
H	0.00000000	1.25286800	4.64463200
H	0.00000000	-2.47179600	2.53324000
H	0.00000000	-1.25286800	4.64463200

Radical Cation

C	0.00217700	3.53160400	-1.25072900
C	0.02146600	2.84404100	-0.04200900
C	0.00920300	1.44126500	0.00553000
C	-0.00840400	0.71441900	-1.24865000
C	-0.04092300	1.45930300	-2.47525100
C	-0.03585500	2.83193700	-2.47890800
C	0.01043600	0.71040600	1.27264700
C	0.00840400	-0.71442400	-1.24864900
C	-0.00920300	-1.44126700	0.00552400
C	-0.01043600	-0.71040500	1.27264700
C	-0.02146600	-2.84403900	-0.04201400
H	-0.04293500	-3.42344100	0.87177600
C	-0.00217700	-3.53160600	-1.25073800
C	0.03585500	-2.83194300	-2.47891300
C	0.04092300	-1.45930600	-2.47525200
H	0.01122500	4.61792900	-1.24637000
H	0.04293500	3.42344200	0.87178200
H	-0.07851500	0.94017200	-3.42335400
H	-0.06186300	3.37779100	-3.41689500
H	-0.01122500	-4.61793100	-1.24637500
H	0.06186300	-3.37779500	-3.41690200
H	0.07851500	-0.94017300	-3.42335400
C	0.02244600	1.38833900	2.50968400
C	0.01207500	0.69674200	3.72277000
H	0.03877500	2.47103900	2.54288800
C	-0.02244600	-1.38833500	2.50968100
C	-0.01207500	-0.69673400	3.72276900
H	0.02175900	1.25091000	4.65674900
H	-0.03877500	-2.47103500	2.54288900
H	-0.02176000	-1.25090300	4.65674700

Radical Anion

C	0.00000000	3.58778300	-1.24963500
C	0.00000000	2.86053500	-0.04872700
C	0.00000000	1.45808400	-0.00783900
C	0.00000000	0.71093800	-1.25652100
C	0.00000000	1.48857700	-2.47600000
C	0.00000000	2.86976300	-2.46913000
C	0.00000000	0.71554500	1.26586900
C	0.00000000	-0.71093800	-1.25652100
C	0.00000000	-1.45808400	-0.00783900
C	0.00000000	-0.71554500	1.26586900
C	0.00000000	-2.86053500	-0.04872700
H	0.00000000	-3.42450000	0.87926800
C	0.00000000	-3.58778300	-1.24963500
C	0.00000000	-2.86976300	-2.46913000
C	0.00000000	-1.48857700	-2.47600000
H	0.00000000	4.67476200	-1.23725400
H	0.00000000	3.42450000	0.87926800
H	0.00000000	0.98089800	-3.43532800
H	0.00000000	3.40761800	-3.41661600
H	0.00000000	-4.67476200	-1.23725400
H	0.00000000	-3.40761800	-3.41661600
H	0.00000000	-0.98089800	-3.43532800
C	0.00000000	1.38340500	2.51462100
C	0.00000000	0.69967200	3.72824000
H	0.00000000	2.46783800	2.54453000
C	0.00000000	-1.38340500	2.51462100
C	0.00000000	-0.69967200	3.72824000
H	0.00000000	1.25519400	4.66340400
H	0.00000000	-2.46783800	2.54453000
H	0.00000000	-1.25519400	4.66340400

