

1 **A G4MP2 theoretical study on the gas phase enthalpies of formation for various polycyclic**
2 **aromatic hydrocarbons (PAHs) and other C₁₀ through C₂₀ unsaturated hydrocarbons**

3
4 Sierra Rayne^{*,†} and Kaya Forest[‡]

5
6 [†] Chemologica Research, Mortlach, Saskatchewan, S0H 3E0, Canada; [‡]Department of
7 Environmental Engineering, Saskatchewan Institute of Applied Science and Technology, Palliser
8 Campus, Moose Jaw, Saskatchewan, S6H 4R6, Canada

9
10 Corresponding Author: *E-mail: rayne.sierra@gmail.com.

11

12 The thermodynamic properties of polycyclic aromatic hydrocarbons (PAHs) and other large
13 unsaturated hydrocarbons play a fundamental role¹ in our understanding of petroleum processing
14^{2,3} and combustion chemistry.⁴ Due to advances in theoretical methods and associated computing
15 power, many of these compounds are now coming within the reach of modern high-level and
16 accurate computational approaches. In the current work, we present a survey of estimated gas
17 phase enthalpies of formation at 298.15 and 1 atm ($\Delta_f H_{(g),298K}$) obtained at the G4MP2⁵ level of
18 theory for 86 PAHs and other C₁₀ through C₂₀ unsaturated hydrocarbons (Table 1). Calculations
19 were conducted using Gaussian 09 (G09; rev. B.01)⁶ and employed standard atomization
20 enthalpy approaches for $\Delta_f H_{(g)}^\circ$ estimates.⁷⁻¹¹ We have previously shown G4MP2 calculations are
21 expected to yield near chemically accurate (± 4.2 -8.4 kJ/mol) $\Delta_f H_{(g)}$ estimates,^{12,13} consistent with
22 the thermochemical accuracy obtained at the more expensive Gaussian-4 (G4) level.^{9-11,14-16} All
23 final structures were confirmed as true minima on their respective potential energy surfaces and
24 are absent any imaginary frequencies. Structures were visualized using Gabedit 2.2.12.¹⁷
25 Enthalpies of formation at 0 K and 1 atm ($\Delta_f H_{(g),0K}$) are also provided in Table 1 since the 298 K
26 data may be less accurate due to anharmonicity.

27
28 Experimental $\Delta_f H_{(g)}$ were obtained from the NIST Chemistry WebBook¹⁸ and other literature
29 sources for 21 of the compounds under investigation. For a number of these compounds, multiple
30 experimental datapoints are available, often ranging widely. As an example, phenanthrene has six
31 experimental $\Delta_f H_{(g)}$ reports¹⁹⁻²⁵ in the NIST database that range over 46 kJ/mol. Similarly, the
32 error bar on the single experimental $\Delta_f H_{(g)}$ report²⁶ for 9,10-dehydrophenanthrene is 40 kJ/mol.
33 If the best agreement between a $\Delta_f H_{(g)}$ report and the corresponding G4MP2 estimate is taken for
34 each compound, the error metrics include mean signed (MSD), mean unsigned (MUD), and root
35 mean squared (RMSD) deviations of -14.0, 14.6, and 18.0 kJ/mol, respectively.

36
37 A survey of other theoretical $\Delta_f H_{(g)}$ estimates for these compounds was also undertaken, and
38 these prior literature values are compiled in Table 1. The quality of the previous estimates varies
39 widely from the application of semiempirical computational methods (e.g., AM1) through ab
40 initio (e.g., Hartree-Fock) and density functional theory (DFT) approaches up to other high-level
41 calculations (e.g., Gaussian-n and coupled cluster) using atomization, isodesmic, and
42 homodesmotic reaction schemes with and without group corrections, as well as additivity systems
43 and hybrid computational/additivity methods. Our G4MP2 estimates are in excellent agreement
44 (i.e., typically <1-2 kJ/mol deviation) with other high-level Gaussian-n $\Delta_f H_{(g)}$ reports (e.g., G3
45 level and lower) where available (see, e.g., comparisons with data from ref.^{27, 28}).

46
47 As the error metrics suggest, the G4MP2 $\Delta_f H_{(g),298K}$ estimates are generally lower than the
48 experimental values. In light of previous work showing that $\Delta_f H_{(g),298K}$ estimates at the
49 G4MP2/G4 levels of theory are at or near thermochemical accuracy,⁹⁻¹⁶ and the excellent
50 agreement between our values and prior Gn (n \leq 3) level estimates, it is not clear whether the
51 theoretical $\Delta_f H_{(g),298K}$ presented herein are more accurate than the experimental values or vice
52 versa. None of the compounds under consideration have a boiling point of <298.15 K at 1 atm.
53 Thus, experimental $\Delta_f H_{(g)}$ reports for these molecules are often comprised of a solid-phase
54 enthalpy of formation at 298.15 and 1 atm ($\Delta_f H_{(s)}$) coupled with a measured or estimated
55 enthalpy of sublimation, obtained through the use of various reactions such as the enthalpy of
56 hydrogenation, or other indirect approaches.

57

58 Consequently, the present study offers some of the highest level thermochemical calculations
59 currently available in the literature for a suite of 86 PAHs and other C₁₀ through C₂₀ unsaturated
60 hydrocarbons, and includes high-level $\Delta_f H_{(g),298K}$ estimates for 65 compounds not having
61 available experimental data. The findings provide a thermodynamic benchmark dataset for a
62 large set of molecules relevant to petroleum processing and combustion chemistry against which
63 future experimental reports and theoretical studies can be assessed. As part of the method
64 validation process, we also conducted triplet state calculations on all compounds to confirm all
65 ground states were singlets. For the 30 compounds whose triplet state calculations converged
66 without imaginary frequencies, G4MP2 estimated adiabatic singlet-triplet excitation energies
67 (AE_{S-T}) were all positive, ranging from 141.6 kJ/mol (1,8-dihydro-as-indacene) to 425.7 kJ/mol
68 (2a,3,8,8a-tetrahydro-(2a α ,3 α ,8 α ,8a α)-3,8-methanocyclobuta[b]naphthalene) (Table 2). For the
69 remaining 56 compounds, triplet state calculations at the G4MP2 level of theory either failed to
70 converge, or yielded structures with one or more imaginary frequencies. Where available, good
71 agreement was obtained between the experimental and G4MP2 AE_{S-T} , suggesting this level of
72 theory is at or near chemical accuracy for AE_{S-T} calculations.

73
74 Because of the computational expense of G4MP2 calculations, groups wishing to conduct
75 thermochemical studies on larger hydrocarbons and/or without access to high-performance
76 computing facilities will need to employ lower level theoretical approaches. The MOPAC suite
77 of semiempirical methods (e.g., MNDO, MNDO-d, AM1,⁸⁰ PM3,⁸¹ RM1,⁸² and PM6⁸³) is
78 commonly used for this purpose. Thus, we conducted $\Delta_f H_{(g),298K}$ calculations at these
79 semiempirical levels of theory using MOPAC 11.052W (<http://openmopac.net>) on the 86
80 unsaturated hydrocarbons of interest using both the restricted (RHF) and unrestricted (UHF)
81 Hartree-Fock Hamiltonians (Supplementary Information Table S1). There is emerging interest in
82 the open-shell singlet states of large unsaturated systems (particularly the polyacenes),⁸⁴⁻⁹⁸ but the
83 field remains controversial with strong theoretical evidence against the claims of some open-shell
84 ground singlet state hydrocarbons.^{99,100} Thus, while we present the UHF semiempirical data,
85 noting that UHF $\Delta_f H_{(g),298K}$ are always lower than RHF $\Delta_f H_{(g),298K}$ (by up to tens of kJ/mol; and
86 often in better agreement with the G4MP2 and experimental results than the RHF data), the UHF
87 dataset was not considered further owing to the speculative nature of the findings. Indeed, the
88 UHF semiempiricals yield lower $\Delta_f H_{(g),298K}$ than the RHF counterparts for polyacenes as small as
89 anthracene that are present in our dataset, which is far smaller than the onset of open-shell
90 ground singlet states predicted as occurring at octacene and longer acene lengths using density
91 functional theory (DFT) approaches, and contrary to the known closed-shell singlet ground state
92 for this compound (see ref.⁹⁹⁻¹⁰¹ and references therein). The G4MP2 results are stable to
93 breaking the closed-shell restriction.

94
95 No difference was observed between $\Delta_f H_{(g),298K}$ predicted by the PM6 Hamiltonian
96 (keyword=PM6) and the PM6 Hamiltonian with corrections for dispersion and hydrogen-bonding
97 (keywords=PM6-DH+¹⁰⁴ and PM6-DH2¹⁰⁵), and as such, only the PM6 data are reported. MSD,
98 MUD, and RMSD between the various semiempirical methods and the G4MP2 $\Delta_f H_{(g),298K}$ are
99 given in Table 3. All semiempirical methods systematically overestimate $\Delta_f H_{(g),298K}$ when
100 compared to the G4MP2 data, with MSD ranging from 15.5 (RM1) to 66.4 (AM1) kJ/mol and
101 MUD ranging from 21.5 (RM1) to 66.4 (AM1) kJ/mol. Consequently, if semiempirical methods
102 are to be used to estimate $\Delta_f H_{(g),298K}$ of large unsaturated hydrocarbons, their $\Delta_f H_{(g),298K}$ must be
103 adjusted via calibration regressions against high-level (e.g., G4MP2) $\Delta_f H_{(g),298K}$ estimates -

104 believed to be at or near chemical accuracy - based on a training set of compounds such as
105 investigated herein. Thus, we linearly regressed the semiempirical $\Delta_f H_{(g),298K}$ estimates against
106 the corresponding G4MP2 estimates, and obtained the regression parameters provided in Table 3.

107
108 Using these calibration regressions of semiempirical $\Delta_f H_{(g),298K}$ versus G4MP2 $\Delta_f H_{(g),298K}$, the
109 semiempirical $\Delta_f H_{(g),298K}$ for an additional suite of 156 large unsaturated hydrocarbons and PAHs
110 were calculated and the resulting corrected $\Delta_f H_{(g),298K}$ are provided in Table 4 (both RHF and
111 UHF $\Delta_f H_{(g),298K}$ are given in Supplementary Information Table S2; only RHF data were used to
112 obtain corrected $\Delta_f H_{(g),298K}$). The corrected semiempirical $\Delta_f H_{(g),298K}$ still range broadly across the
113 various methods, with $\Delta_f H_{(g),298K}$ ranges for each compound varying from a minimum of 7.6
114 kJ/mol to a maximum of 236.6 kJ/mol, with an average range of 44.8 kJ/mol. Based on the
115 quality of the regression statistics and error reductions for the calibration set following $\Delta_f H_{(g),298K}$
116 correction, the corrected PM6 $\Delta_f H_{(g),298K}$ data may be of the highest quality. However, validation
117 of which suite of corrected semiempirical $\Delta_f H_{(g),298K}$ data for these 156 molecules is most
118 accurate awaits experimental data for several members of the dataset. Overall, high-level
119 calculations remain the best approach for reliable $\Delta_f H_{(g),298K}$ estimates, and where molecular size
120 renders such approaches too computationally expensive, corrected lower level theoretical
121 $\Delta_f H_{(g),298K}$ estimates will carry substantial residual uncertainty.

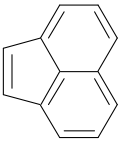
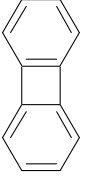
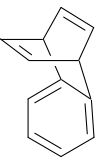
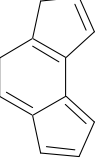

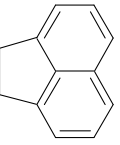
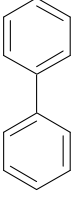
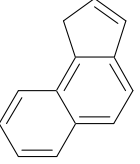
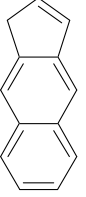
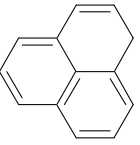
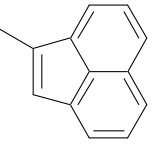
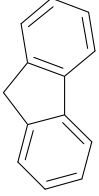
122
123 **Acknowledgments.** This work was made possible by the facilities of the Western Canada
124 Research Grid (WestGrid: project 100185), the Shared Hierarchical Academic Research
125 Computing Network (SHARCNET: project sn4612), and Compute/Calcul Canada.

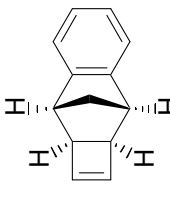
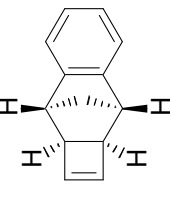
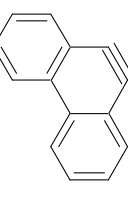
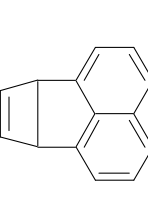
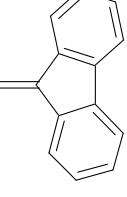
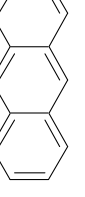
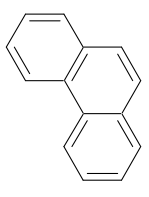
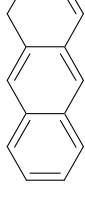
126
127 **Supporting Information Available.** Full G09 archive entries including optimized geometries
128 and energies at each stage of the composite method process, as well as semiempirical method
129 enthalpies of formation using the unrestricted and restricted wave functions.

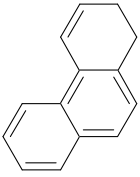
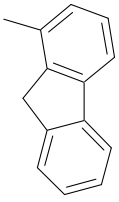
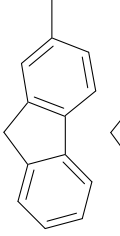
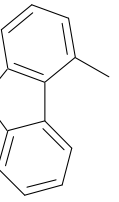
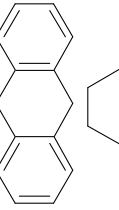
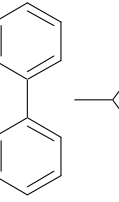
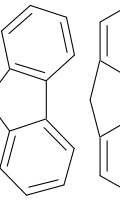
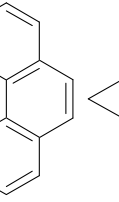
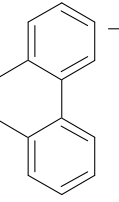
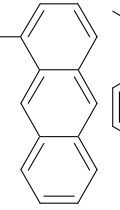
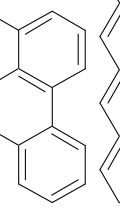
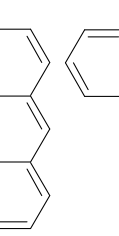
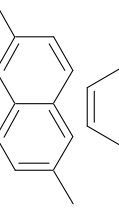
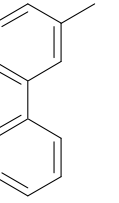
130

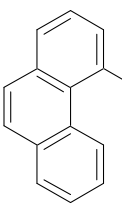
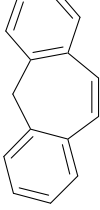
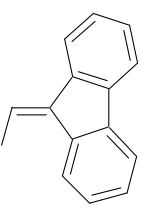
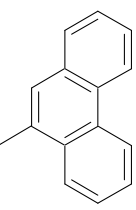
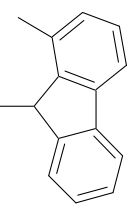
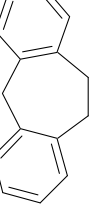
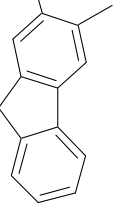
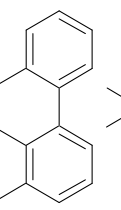
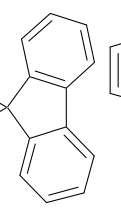
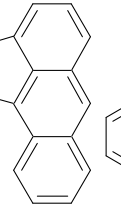
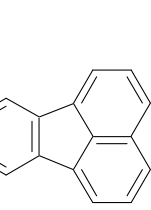
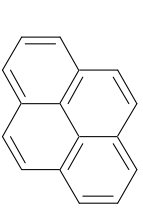
Table 1. G4MP2 estimated enthalpies of formation at 298.15 K and 1 atm ($\Delta_f H_{(g),298K}$) and 0 K and 1 atm ($\Delta_f H_{(g),0K}$) for various polycyclic aromatic and other C_{10} through C_{20} unsaturated hydrocarbons. Where available, experimental values and other theoretical estimates are also provided.

name	structure	CAS-RN	formula	MW (g/mol)	expt. $\Delta_f H_{(g)}$ (kJ/mol)	G4MP2 $\Delta_f H_{(g),298K}$ (kJ/mol)	other theoretical $\Delta_f H_{(g)}$ (kJ/mol)	G4MP2 $\Delta_f H_{(g),0K}$ (kJ/mol)
1,4-diethynylbenzene		935-14-8	$C_{10}H_6$	126.15	n/a	546.9	n/a	557.2
[4.2.2]propella-2,4,7,9-tetraene		88090-34-0	$C_{10}H_8$	128.17	n/a	555.0	n/a	577.4
1-methylene-1H-indene		2471-84-3	$C_{10}H_8$	128.17	n/a	227.3	n/a	249.7
azulene		275-51-4	$C_{10}H_8$	128.17	280, ^{58,59} 308 ⁶⁰	284.2	240.2, ^{61,62} 244.3, ⁶² 247.0, ⁶³ 247.7, ⁶⁴ 248.4, ⁶³ 249.4, ⁶⁴ 254.3, ⁶³ 254.4, ⁶⁴ 255.1, ⁶³ 255.6, ⁶⁴ 280.7, ⁵⁶ 282.0, ⁶¹ 282.4, ^{61,62} 284.1, ⁵⁷ 285.3, ⁶⁵ 288.2, ⁵⁷ 295.0, ⁶¹ 300.8, ⁶⁵ 308.5, ⁴⁸ 319.6, ^{43,44} 319.9, ⁴⁴ 320.2, ^{43,44} 320.3, ^{43,44} 320.8, ⁴⁴ 320.9, ⁴⁴ 321.8, ^{41,42} 322.0, ⁴¹ 322.3, ⁴² 338.1, ⁴⁰ 338.5, ⁵⁰ 352.7, ⁵⁷ 353.5, ⁵⁰ 396.2 ^{40,50}	307.0
naphthalene		91-20-3	$C_{10}H_8$	128.17	recommended: 150.6±1.5 ²² other: 141.6, ⁵² 145.6, ⁷⁷ 150.6, ²⁵ 150.6±1.1, ²⁴ 150.9, ⁷⁸ 151.7±1.9, ³⁰ 160.1 ⁵³	137.1	101.3, ^{61,62} 112.2, ³⁹ 134.9, ²⁷ 135.1, ²⁸ 137.0, ³⁹ 138.5, ⁴⁷ 138.9, ³⁹ 140.9, ⁴³ 141.3, ⁴³ 141.8, ⁴³ 142.0, ⁴⁴ 142.3, ⁴⁴ 142.4, ⁴² 143.1, ⁴² 143.4, ⁴⁸ 143.9, ⁴⁴ 144.0, ⁴⁴ 144.2, ⁴⁴ 144.3, ⁴⁴ 145.6, ⁵⁷ 146.0, ³¹ 146.8, ⁵⁷ 147.3, ³¹ 147.4, ⁴⁷ 148.1, ^{31,40,50} 148.3, ³⁹ 148.5, ^{40,50} 148.8, ²⁷ 149.0, ^{31,50} 149.4, ⁴⁷ 149.5, ³⁹ 149.8, ³¹ 150.6, ^{31,49} 151.0, ⁶² 152.1, ⁵⁴ 152.3, ^{61,62} 152.6, ⁶³ 152.8, ⁵⁶ 153.1, ⁴⁹ 153.6, ⁶¹ 153.9, ⁵⁴ 155.2, ⁴⁹ 155.5, ⁵⁴ 155.8, ⁵⁴ 156.0, ⁶³ 156.4, ⁶³ 156.6, ⁶⁴ 157.9, ⁵⁴ 158.4, ⁴⁵ 159.4, ⁶⁴ 159.9, ³⁹ 160.2, ⁶⁴ 162.5, ⁶³ 163.6, ⁶¹ 166.5, ⁶⁴ 169.9, ³¹ 214.1 ⁵⁷	160.7
1,4-dihydro-1,4-methanonaphthalene		4453-90-1	$C_{11}H_{10}$	142.20	n/a	236.4	n/a	268.1
1-methylnaphthalene		90-12-0	$C_{11}H_{10}$	142.20	116.9±2.7 ³⁰	103.8	102.3, ²⁸ 118.8, ³¹ 120.5, ³¹ 142.0 ³¹	132.7
2-methylnaphthalene		91-57-6	$C_{11}H_{10}$	142.20	106.2, ¹⁹ 116.1±2.6 ³⁰	102.9	101.2, ²⁸ 114.6, ³¹ 116.3, ³¹ 137.6 ³¹	131.3
bicyclo[4.4.1]undeca-1,3,5,7,9-pentaene		2443-46-1	$C_{11}H_{10}$	142.20	315±3, ⁶⁶ 323 ⁶⁷	301.4	n/a	331.8

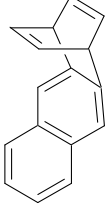
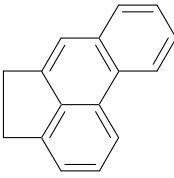
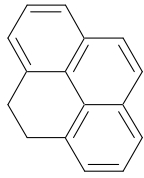
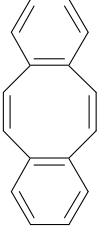
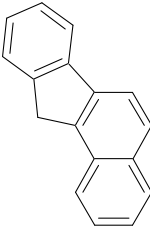
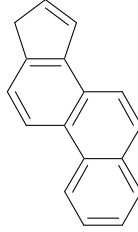
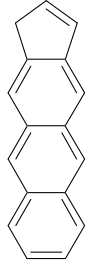
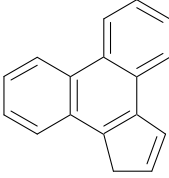
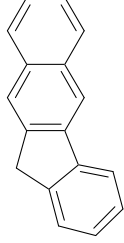
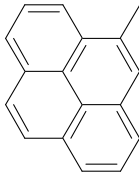
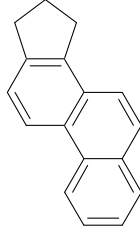
acenaphthylene		208-96-8	C ₁₂ H ₈	152.19	recommended: 263.2±3.7 ²² other: 258.0±5.9, ³⁸ 264.0 ⁴⁶	245.9	176.9, ⁴⁵ 233.0, ⁴⁷ 257.2, ⁴⁸ 258.2, ⁴⁹ 259.4, ⁴⁷ 259.8, ³¹ 263.6, ⁴⁹ 264.0, ⁴⁰ 264.4, ⁵⁰ 264.9, ⁴³ 265.9, ⁴³ 266.0, ^{43,44} 266.1, ⁴² 266.5, ^{41,42} 266.7, ⁴¹ 266.9, ^{44,47} 267.0, ⁴⁴ 267.6, ⁴¹ 267.8, ⁴⁴ 269.4, ⁴⁹ 274.9, ⁵⁰ 278.7, ^{40,50} 337.6 ³¹	269.4
biphenylene		259-79-0	C ₁₂ H ₈	152.19	recommended: 417.2±1.9 ²² other: 420.4±1.9, ⁷² 440.0 ⁷³	403.1	410.6, ⁴¹ 410.7, ⁴⁴ 410.9, ⁴⁴ 411.2, ⁴⁴ 411.3, ⁴⁴ 411.4, ⁴⁴ 411.5, ⁴³ 411.6, ⁴³ 411.8, ⁴¹ 412.1, ⁴³ 412.6, ^{41,42} 413.2, ⁴² 415.1, ⁷⁴ 416.3, ⁴⁸ 417.6, ⁷⁴ 419.2, ⁵⁰ 419.7, ⁴⁰ 446.0, ⁵⁰ 450.0 ^{40,50}	425.4
1,4-dihydro-1,4-ethenonaphthalene		7322-47-6	C ₁₂ H ₁₀	154.2078	n/a	288.3	n/a	319.4
1,8-dihydro-as-indacene		18837-46-2	C ₁₂ H ₁₀	154.21	n/a	327.0	n/a	355.9
2,5-etheno[4.2.2]propella-3,7,9-triene		88090-38-4	C ₁₂ H ₁₀	154.21	n/a	607.9	n/a	638.8
acenaphthene		83-32-9	C ₁₂ H ₁₀	154.21	recommended: 156.8±3.1 ²² other: 156±4 ³⁸	143.3	124.2, ³⁹ 146.0, ⁴⁰ 152.4, ^{41,42} 152.7, ⁴² 153.7, ⁴³ 153.8, ⁴⁴ 154.0, ⁴⁵ 154.2, ⁴³ 154.8, ⁴³ 155.0, ^{41,44} 155.1, ⁴¹ 155.6, ³⁹ 155.7, ³⁹ 156.1, ³⁹ 156.4, ⁴⁴ 156.5, ⁴⁴ 157.0, ⁴⁴ 157.1, ⁴⁴ 157.3, ³⁹ 183.1 ³⁹	173.4
biphenyl		92-52-4	C ₁₂ H ₁₀	154.21	recommended: 180.3±3.3 ²² other: 178.4, ⁵² 178.8, ⁶⁸ 181.1±1.8, ⁶⁹ 182.0±0.7, ^{70,71} 182.1±2.6 ²⁴	165.7	140.5, ³⁹ 163.0, ²⁸ 170.0, ⁵⁶ 170.2, ^{43,44} 170.4, ⁴⁴ 170.6, ⁴³ 171.8, ³⁹ 172.0, ⁴⁸ 172.3, ⁴⁴ 172.5, ⁴² 172.7, ⁴⁴ 172.8, ^{41,42} 173.7, ⁴¹ 174.8, ⁴¹ 175.4, ²⁸ 178.7, ³⁹ 180.2, ⁴⁵ 181.3, ³⁹ 184.5, ³⁹ 191.9, ⁴⁵ 199.2, ³¹ 202.1 ³⁹	194.4
1H-benz[e]indene		232-54-2	C ₁₃ H ₁₀	166.22	n/a	209.8	n/a	239.2
1H-benz[f]indene		268-40-6	C ₁₃ H ₁₀	166.22	n/a	209.6	n/a	239.0
1H-phenalene		203-80-5	C ₁₃ H ₁₀	166.22	n/a	192.2	n/a	221.8
1-methylacenaphthylene		n/a	C ₁₃ H ₁₀	166.22	n/a	207.2	n/a	235.4
fluorene		86-73-7	C ₁₃ H ₁₀	166.22	recommended: 176.7±3.1 ²² other: 166.9±4.1, ⁷⁶ 175.0±1.5 ³⁴	172.2	167.0 ⁴⁵	201.8

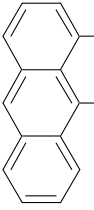
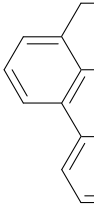
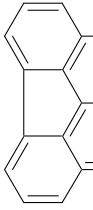
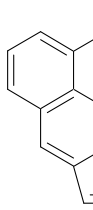
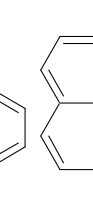
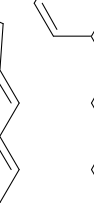
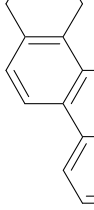
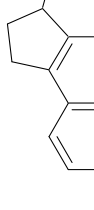
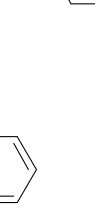
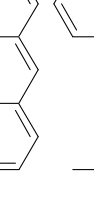
2a,3,8,8a-tetrahydro-(2 α ,3 α ,8 α ,8 α)-3,8-methanocyclobuta[b]naphthalene		54443-68-4	C ₁₃ H ₁₂	168.23	n/a	313.6	n/a	352.1
2a,3,8,8a-tetrahydro-(2 α ,3 β ,8 β ,8 α)-3,8-methanocyclobuta[b]naphthalene		54483-73-7	C ₁₃ H ₁₂	168.23	n/a	302.1	n/a	340.7
9,10-dehydrophenanthrene		7048-96-6	C ₁₄ H ₈	176.21	600±40 ²⁶	550.9	n/a	571.2
6b,8a-dihydrocyclobut[a]acenaphthylene		30736-79-9	C ₁₄ H ₁₀	178.23	n/a	361.1	n/a	390.9
9-methylene-9H-fluorene		4425-82-5	C ₁₄ H ₁₀	178.23	n/a	248.1	n/a	276.2
anthracene		120-12-7	C ₁₄ H ₁₀	178.23	recommended: 229.4±2.9 ²² other: 209.1, ⁵¹ 217.6, ⁵² 218.3, ²⁵ 221.6, ²³ 227.1, ⁵³ 230.8±4.6 ²⁴	210.8	168.7, ³⁹ 188.7, ⁴⁷ 208.3, ²⁷ 208.5, ²⁸ 218.4, ^{31,39} 218.4, ⁴⁷ 218.7, ³⁹ 220.9, ³⁹ 223.0, ³¹ 224.3, ³⁹ 225.1, ³¹ 226.4, ⁴⁵ 226.8, ⁴⁸ 227.1, ⁵⁴ 227.6, ⁵⁴ 228.0, ³¹ 228.6, ⁵⁴ 229.2, ⁵⁴ 229.7, ^{43,47} 230.1, ^{27,31,40,55} 230.2, ⁴⁴ 230.7, ⁴³ 231.0, ^{31,50} 231.1, ⁴² 231.2, ⁴² 231.3, ⁴³ 231.4, ^{31,44} 231.8, ⁴⁴ 232.3, ⁴⁴ 232.4, ⁴⁴ 232.6, ³¹ 233.4, ⁵⁴ 233.5, ⁵⁰ 233.9, ⁴⁹ 236.4, ⁴⁹ 234.3, ⁴⁹ 234.7, ³¹ 237.7, ⁵⁶ 238.1, ⁵⁷ 238.5, ^{40,50} 238.6, ⁵⁷ 261.7, ³⁹ 263.2, ³¹ 330.7, ⁵⁷	239.9
phenanthrene		85-01-8	C ₁₄ H ₁₀	178.23	recommended: 202.2±2.3 ²² other: 163.6, ¹⁹ 201.2±4.7, ²⁰ 201.7±2.9, ²¹ 203.8, ²³ 206.9±4.6, ²⁴ 209.1 ²⁵	187.8	168.2, ⁴⁷ 168.6, ³⁹ 185.2, ²⁷ 185.4, ²⁸ 199.6, ^{40,50} 200.0, ⁴⁷ 200.8, ⁵⁰ 201.3, ^{40,49} 201.7, ⁵⁰ 201.8, ²⁷ 202.4, ⁴³ 203.1, ⁴⁴ 201.3, ⁵⁶ 203.3, ⁴⁹ 203.4, ⁴³ 203.5, ⁴³ 203.8, ^{42,44} 204.1, ⁴² 204.6, ⁴⁹ 204.8, ⁴⁴ 204.9, ⁴⁴ 205.4, ³¹ 205.9, ³¹ 206.5, ⁵⁴ 206.6, ⁵⁴ 207.0, ⁴⁵ 207.1, ^{31,55} 207.5, ³¹ 209.2, ³¹ 210.0, ³¹ 210.5, ⁵⁴ 210.9, ^{39,47,54} 211.7, ³¹ 212.1, ³¹ 212.9, ⁵⁴ 213.8, ⁴⁷ 217.5, ⁵⁷ 218.2, ^{39,57} 218.4, ³¹ 225.3, ³⁹ 231.3, ³⁹ 240.2, ³¹ 249.6, ³⁹ 310.9 ⁵⁷	217.0
1,2-dihydroanthracene		58746-82-0	C ₁₄ H ₁₂	180.24	n/a	172.9	n/a	208.9

1,2-dihydrophenanthrene		56179-83-0	C ₁₄ H ₁₂	180.24	n/a	180.5	n/a	216.4
1-methyl-9H-fluorene		1730-37-6	C ₁₄ H ₁₂	180.24	n/a	136.1	n/a	170.5
2-methyl-9H-fluorene		1430-97-3	C ₁₄ H ₁₂	180.24	n/a	140.3	n/a	174.2
4-methyl-9H-fluorene		1556-99-6	C ₁₄ H ₁₂	180.24	n/a	139.6	n/a	174.5
9,10-dihydroanthracene		613-31-0	C ₁₄ H ₁₂	180.24	n/a	146.6	n/a	182.8
9,10-dihydrophenanthrene		776-35-2	C ₁₄ H ₁₂	180.24	154.6±1.6, ³⁶ 155.1±1.6 ³⁷	136.6	n/a	173.0
9-methyl-9H-fluorene		2523-37-7	C ₁₄ H ₁₂	180.24	148.0±1.1 ³⁴	142.0	n/a	177.0
4H-cyclopenta[def]phenanthrene		203-64-5	C ₁₅ H ₁₀	190.24	n/a	228.1	n/a	258.1
1a,9b-dihydro-1H-cyclopropa[l]phenanthrene		949-41-7	C ₁₅ H ₁₂	192.26	n/a	252.3	n/a	288.2
1-methylanthracene		610-48-0	C ₁₅ H ₁₂	192.26	n/a	176.2	198.2 ²⁹	210.6
1-methylphenanthrene		832-69-9	C ₁₅ H ₁₂	192.26	n/a	156.4	n/a	190.7
2-methylanthracene		613-12-7	C ₁₅ H ₁₂	192.26	n/a	175.3	191.2 ²⁹	209.3
2-methylphenanthrene		2531-84-2	C ₁₅ H ₁₂	192.26	n/a	153.7	n/a	187.4
3-methylphenanthrene		832-71-3	C ₁₅ H ₁₂	192.26	n/a	153.9	n/a	187.6

4-methylphenanthrene		832-64-4	C ₁₅ H ₁₂	192.26	195.8±1.1 ³³	179.4	n/a	214.3
5H-dibenzo[a,d]cycloheptene		256-81-5	C ₁₅ H ₁₂	192.26	n/a	220.6	n/a	256.2
9-ethylidenefluorene		7151-64-6	C ₁₅ H ₁₂	192.26	n/a	221.6	n/a	254.7
9-methylphenanthrene		883-20-5	C ₁₅ H ₁₂	192.26	n/a	154.5	n/a	189.0
1,9-dimethyl-9H-fluorene		17057-98-6	C ₁₅ H ₁₄	194.27	n/a	108.4	n/a	148.5
10,11-dihydro-5H-dibenzo(a,d)cycloheptene		833-48-7	C ₁₅ H ₁₄	194.27	161.4±3.7 ³²	141.5	152.4, ³² 154.7, ³² 154.8, ³² 154.9, ³² 156.1, ³² 157.6, ³² 158.2, ³² 158.5, ³² 158.8, ³² 158.9, ³² 161.5, ³² 163.8, ³² 165.1, ³² 168.0, ³² 183.3, ³² 186.9, ³² 189.8 ³²	184.2
2,3-dimethyl-9H-fluorene		4612-63-9	C ₁₅ H ₁₄	194.27	n/a	107.1	n/a	146.8
9,10-dihydro-1-methylphenanthrene		95676-48-5	C ₁₅ H ₁₄	194.27	n/a	106.3	n/a	147.9
9,9-dimethyl-9H-fluorene		4569-45-3	C ₁₅ H ₁₄	194.27	n/a	105.3	n/a	145.8
aceanthrylene		202-03-9	C ₁₆ H ₁₀	202.25	n/a	316.3	n/a	345.1
fluoranthene		206-44-0	C ₁₆ H ₁₀	202.25	recommended: 291.4±4.0 ²² other: 289.8, ⁷⁵ 292.0±2.2 ³⁸	262.6	215.2, ³⁹ 241.0, ⁴⁷ 277.0, ⁴⁷ 279.9, ⁴⁷ 280.4, ⁵⁶ 283.8, ³⁹ 284.0, ³⁹ 284.3, ⁴³ 284.7, ⁴⁵ 284.9, ⁴¹ 285.0, ³⁹ 285.1, ⁴⁴ 285.2, ⁴² 285.3, ⁴⁴ 285.4, ^{41,44} 285.5, ^{41,42} 285.8, ⁴³ 285.9, ⁴³ 286.2, ⁴⁴ 289.5, ⁴⁷ 293.5, ⁴⁸ 293.6, ³⁹ 295.0, ⁴⁹ 304.2, ⁴⁹ 308.8, ⁴⁹ 339.5 ³⁹	291.6
pyrene		129-00-0	C ₁₆ H ₁₀	202.25	recommended: 225.5±2.5 ²² other: 214.9, ^{19,75} 225.7±1.3 ⁷⁹	203.4	175.6, ³⁹ 181.2, ⁴⁷ 200.7, ²⁷ 214.2, ⁵⁰ 214.6, ⁴⁰ 215.9, ⁵⁰ 217.6, ⁴⁷ 219.7, ^{40,50} 223.8, ⁴⁷ 224.3, ³¹ 224.5, ⁵⁴ 225.2, ⁵⁴ 225.5, ³¹ 225.8, ⁴⁵ 226.1, ²⁷ 227.2, ^{31,39} 227.4, ⁵⁴ 227.9, ⁵⁴ 228.1, ³⁹ 228.2, ⁵⁴	233.1

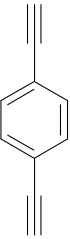

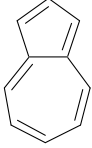
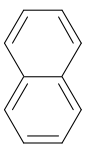
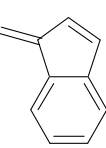

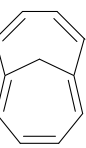
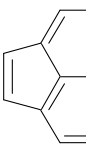
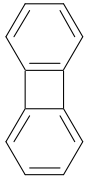
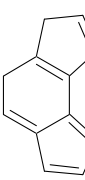
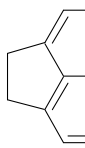
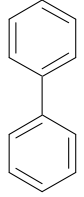
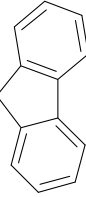
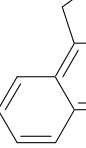
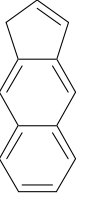
228.7,³⁹ 228.9,⁴³ 229.5,⁴² 230.2,^{41,42}
 230.4,⁴⁴ 230.5,^{31,43} 230.6,⁴¹ 230.7,^{41,44}
 230.8,⁴⁴ 231.0,^{43,44} 231.1,⁴⁴ 231.4,³¹
 231.7,⁴⁴ 234.3,⁴⁹ 234.9,³⁹ 237.5,⁵⁶
 237.7,⁴⁹ 239.7,³¹ 243.5,³¹ 245.2,³¹
 250.2,⁴⁹ 269.4,³⁹ 281.6,³¹

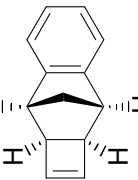
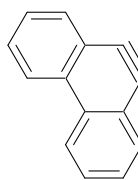
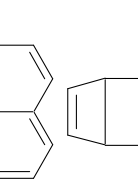
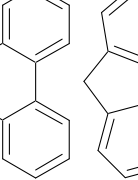

1,4-dihydro-1,4-ethenoanthracene		27765-96-4	C ₁₆ H ₁₂	204.27	n/a	340.9	n/a	377.5
4,5-dihydroacephenanthrylene		6232-48-0	C ₁₆ H ₁₂	204.27	n/a	189.6	n/a	225.2
4,5-dihydropyrene		6628-98-4	C ₁₆ H ₁₂	204.27	n/a	157.4	n/a	194.1
dibenzo[a,e]cyclooctene		262-89-5	C ₁₆ H ₁₂	204.27	n/a	342.5	n/a	376.3
1,2-benzofluorene		238-84-6	C ₁₇ H ₁₂	216.28	n/a	228.3	n/a	263.4
17H-cyclopenta[a]phenanthrene		219-08-9	C ₁₇ H ₁₂	216.28	n/a	261.5	n/a	296.2
1H-cyclopent[b]anthracene		259-06-3	C ₁₇ H ₁₂	216.28	n/a	282.0	n/a	316.8
1H-cyclopenta[1]phenanthrene		235-92-7	C ₁₇ H ₁₂	216.28	n/a	261.3	n/a	296.0
2,3-benzofluorene		243-17-4	C ₁₇ H ₁₂	216.28	n/a	230.0	n/a	265.1
4-methylpyrene		3353-12-6	C ₁₇ H ₁₂	216.28	n/a	168.8	n/a	203.7
1,2-cyclopentenophenanthrene		482-66-6	C ₁₇ H ₁₄	218.29	n/a	161.9	n/a	203.8

4,5,6-trihydrobenz[de]anthracene		n/a	C ₁₇ H ₁₄	218.29	n/a	168.1	n/a	210.8
5,6-dihydro-4H-benz[de]anthracene		4389-09-7	C ₁₇ H ₁₄	218.29	n/a	141.9	n/a	184.5
benzo[ghi]fluoranthene		203-12-3	C ₁₈ H ₁₀	226.27	n/a	335.5	n/a	364.8
cyclopenta[cd]pyrene		27208-37-3	C ₁₈ H ₁₀	226.27	n/a	316.2	n/a	345.5
3,4-dihydrocyclopenta(cd)pyrene		25732-74-5	C ₁₈ H ₁₂	228.29	n/a	213.3	n/a	249.3
benz[a]anthracene		56-55-3	C ₁₈ H ₁₂	228.29	recommended: 290.3±6.0 ²² other: 276.9 ²⁵	254.7	225.1, ³⁹ 231.8, ⁴⁷ 271.5, ⁴⁷ 277.0, ³¹ 278.7, ⁴⁷ 281.9, ⁴¹ 282.4, ³¹ 282.5, ⁴⁴ 282.6, ⁴⁴ 282.7, ⁴¹ 282.8, ³¹ 283.0, ⁴³ 283.1, ⁴⁴ 283.3, ⁴⁴ 283.7, ³¹ 283.8, ⁴⁴ 284.1, ⁴¹⁻⁴³ 284.3, ⁴² 284.6, ⁴³ 284.9, ³¹ 286.9, ⁵⁴ 287.0, ³¹ 287.6, ⁵⁴ 289.2, ⁵⁴ 289.3, ⁵⁴ 289.5, ⁴⁷ 291.2, ⁴⁷ 291.4, ⁵⁴ 291.6, ³¹ 293.3, ⁴⁹ 294.8, ³⁹ 295.7, ³⁹ 297.7, ³⁹ 303.8, ^{45,49} 306.0, ³⁹ 307.1, ⁴⁹ 327.2, ³¹ 351.4 ³⁹	289.3
1,2,3,4-tetrahydrochrysene		2091-90-9	C ₁₈ H ₁₆	232.32	n/a	128.3	n/a	177.0
17-methyl-16,17-dihydro-15h-cyclopenta(a)phenanthrene		n/a	C ₁₈ H ₁₆	232.32	n/a	129.9	n/a	177.3
10-methylbenz[a]anthracene		2381-15-9	C ₁₉ H ₁₄	242.31	n/a	219.8	n/a	259.2
11-methylbenz[a]anthracene		6111-78-0	C ₁₉ H ₁₄	242.31	n/a	220.4	n/a	260.3

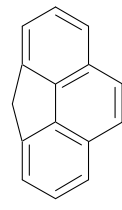
2-methylbenz[a]anthracene		2498-76-2	C ₁₉ H ₁₄	242.31	n/a	220.8	n/a	260.0
2-methylchrysene		3351-32-4	C ₁₉ H ₁₄	242.31	n/a	209.6	n/a	248.5
3-methyl-1,2-benzanthracene		2319-96-2	C ₁₉ H ₁₄	242.31	n/a	220.9	n/a	260.7
5-methylbenzo[c]phenanthrene		652-04-0	C ₁₉ H ₁₄	242.31	n/a	232.8	n/a	273.1
6-methylbenz[a]anthracene		316-14-3	C ₁₉ H ₁₄	242.31	n/a	220.1	n/a	260.1
6-methylbenzo[c]phenanthrene		2381-34-2	C ₁₉ H ₁₄	242.31	n/a	234.2	n/a	274.5
8-methylbenz[a]anthracene		2381-31-9	C ₁₉ H ₁₄	242.31	n/a	220.4	n/a	260.2
9-methylbenz[a]anthracene		2381-16-0	C ₁₉ H ₁₄	242.31	n/a	219.7	n/a	259.0
1,2-dihydrobenz[j]aceanthrylene		479-23-2	C ₂₀ H ₁₄	254.32	n/a	260.0	n/a	301.0
9,10-dihydro-9,10[1',2']-benzoanthracene		477-75-8	C ₂₀ H ₁₄	254.32	322±13 ³⁵	294.6	n/a	336.9

Table 2. G4MP2 estimated adiabatic singlet-triplet excitation energies (AE_{S-T}) at 298.15 K and 1 atm for various polycyclic aromatic and other C_{10} through C_{16} unsaturated hydrocarbons. Experimental values (where available) are provided in parentheses.

name	structure	CAS-RN	formula	MW (g/mol)	G4MP2 AE_{S-T} (kJ/mol)	Experimental AE_{S-T} (kJ/mol)
1,4-diethynylbenzene		935-14-8	$C_{10}H_6$	126.15	269.4	
[4.2.2]propella-2,4,7,9-tetraene		88090-34-0	$C_{10}H_8$	128.17	212.0	
azulene		275-51-4	$C_{10}H_8$	128.17	168.6	
naphthalene		91-20-3	$C_{10}H_8$	128.17	255.5 (253.5 ¹⁰²)	
1-methylene-1H-indene		2471-84-3	$C_{10}H_8$	128.17	210.2	
1,4-dihydro-1,4-methanonaphthalene		4453-90-1	$C_{11}H_{10}$	142.20	281.5	
bicyclo[4.4.1]undeca-1,3,5,7,9-pentaene		2443-46-1	$C_{11}H_{10}$	142.20	201.5	
acenaphthylene		208-96-8	$C_{12}H_8$	152.19	199.1	
biphenylene		259-79-0	$C_{12}H_8$	152.19	186.1	
1,8-dihydro-as-indacene		18837-46-2	$C_{12}H_{10}$	154.21	141.6	
acenaphthene		83-32-9	$C_{12}H_{10}$	154.21	246.0 (247.7 ¹⁰²)	
biphenyl		92-52-4	$C_{12}H_{10}$	154.21	289.5 (273.8 ¹⁰²)	
fluorene		86-73-7	$C_{13}H_{10}$	166.22	290.1 (278.2 ¹⁰³)	
1H-benz[e]indene		232-54-2	$C_{13}H_{10}$	166.22	240.3	
1H-benz[f]indene		268-40-6	$C_{13}H_{10}$	166.22	250.3	

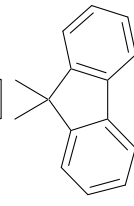
1H-phenalene	203-80-5	C ₁₃ H ₁₀	166.22	211.3	
2a,3,8,8a-tetrahydro-(2α,3α,8α,8α)-3,8-methanocyclobuta[b]naphthalene	54443-68-4	C ₁₃ H ₁₂	168.23	425.7	
2a,3,8,8a-tetrahydro-(2α,3β,8β,8α)-3,8-methanocyclobuta[b]naphthalene	54483-73-7	C ₁₃ H ₁₂	168.23	380.6	
9,10-dehydrophenanthrene	7048-96-6	C ₁₄ H ₈	176.21	230.7	
anthracene	120-12-7	C ₁₄ H ₁₀	178.23	174.8	
phenanthrene	85-01-8	C ₁₄ H ₁₀	178.23	273.3 (258.4 ¹⁰²)	
6b,8a-dihydrocyclobut[a]acenaphthylene	30736-79-9	C ₁₄ H ₁₀	178.23	239.9	
1,2-dihydroanthracene	58746-82-0	C ₁₄ H ₁₂	180.24	243.6	
1,2-dihydrophenanthrene	56179-83-0	C ₁₄ H ₁₂	180.24	212.2	
9,10-dihydrophenanthrene	776-35-2	C ₁₄ H ₁₂	180.24	279.2	
2-methyl-9H-fluorene	1430-97-3	C ₁₄ H ₁₂	180.24	283.1	
9-methyl-9H-fluorene	2523-37-7	C ₁₄ H ₁₂	180.24	285.5	

4H-cyclopenta[def]phenanthrene



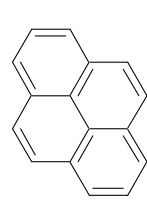
203-64-5 C₁₅H₁₀ 190.24 263.1

9,9-dimethyl-9H-fluorene



4569-45-3 C₁₅H₁₄ 194.27 281.8

pyrene



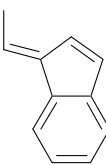
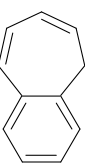
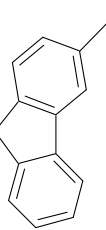
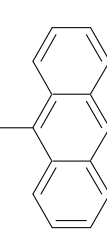
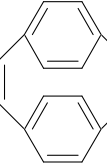
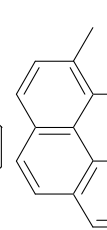
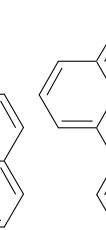
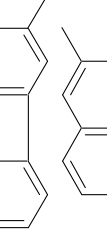
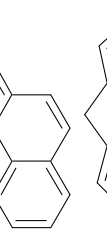
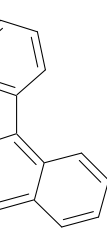
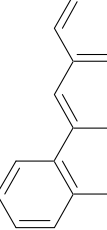
129-00-0 C₁₆H₁₀ 202.25 199.2 (199.4¹⁰³)

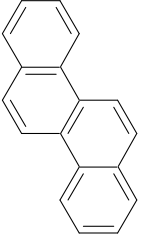
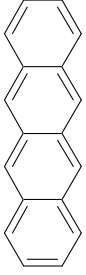
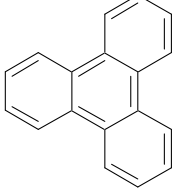
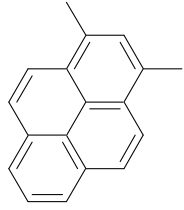
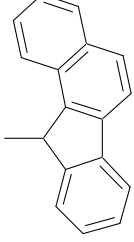
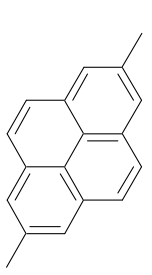
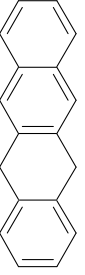
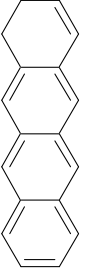
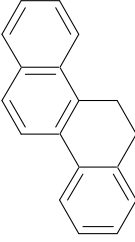
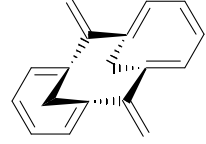
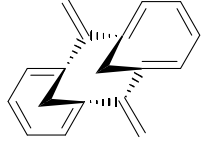
Table 3. Linear regression statistics and uncorrected/corrected error metrics between estimated enthalpies of formation at 298.15 K and 1 atm ($\Delta_f H_{(g),298K}$) for various polycyclic aromatic and other C_{10} through C_{20} unsaturated hydrocarbons obtained by semiempirical methods and the corresponding G4MP2 $\Delta_f H_{(g),298K}$ estimates. Values are in kJ/mol.

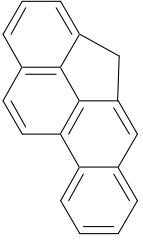
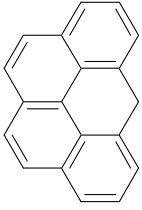
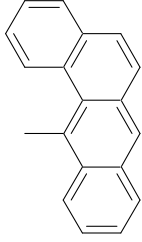
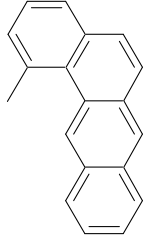
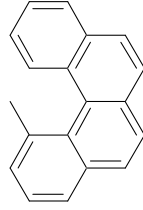
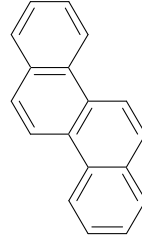
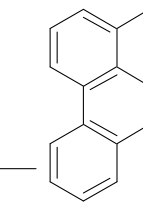
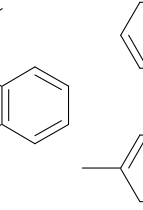
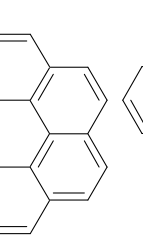
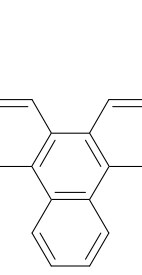
	r^a	SE ^b	CV ^c	m ^d	b ^e	uncorrected			corrected		
						MSD	MUD	RMSD	MSD	MUD	RMSD
MNDO	0.967	25.6	0.113	0.944±0.027	-22.1±7.6	37.0	39.0	45.2	0.0	18.8	25.3
MNDO-d	0.967	25.7	0.113	0.943±0.027	-22.9±7.7	37.8	39.7	45.9	0.0	18.9	25.4
AM1	0.974	23.1	0.101	0.814±0.021	-11.7±6.6	66.4	66.4	73.7	0.0	15.7	22.8
PM3	0.984	18.2	0.080	0.927±0.019	-22.2±5.4	41.7	42.2	46.1	0.0	12.5	18.0
RM1	0.975	22.3	0.098	0.993±0.024	-13.9±6.4	15.5	21.5	26.9	0.0	15.3	23.0
PM6	0.978	21.0	0.092	0.999±0.023	-28.0±6.3	28.2	30.7	35.0	0.0	7.9	12.0

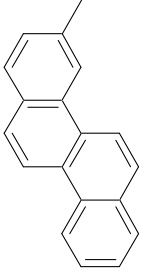
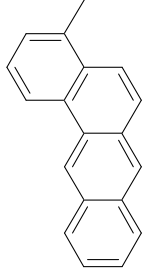
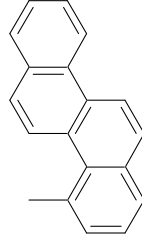
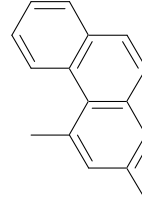
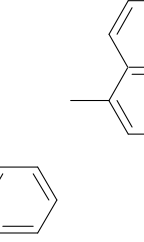
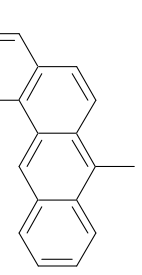
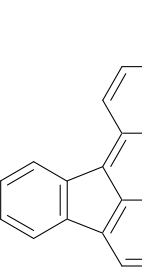
^a correlation coefficient. ^b standard error. ^c coefficient of variation. ^d regression slope (\pm standard error). ^e regression y-intercept (\pm standard error).

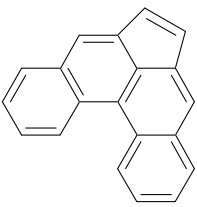
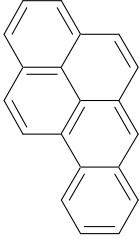
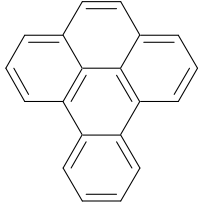
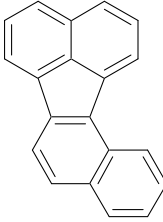
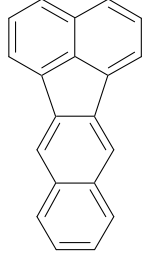
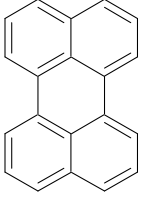
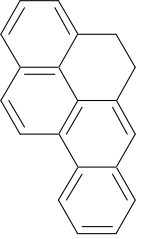
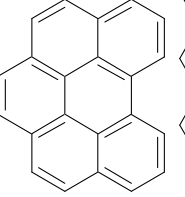
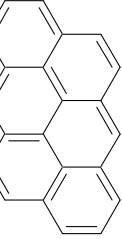
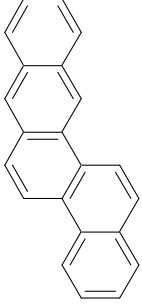
Table 4. Corrected enthalpies of formation at 298.15 K and 1 atm ($\Delta_f H_{(g),298K}$) for various polycyclic aromatic and other C_{42} unsaturated hydrocarbons obtained by semiempirical methods. Values are in kJ/mol.

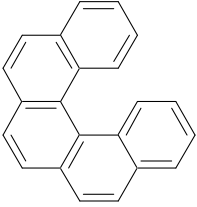
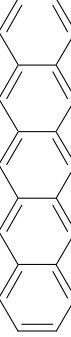
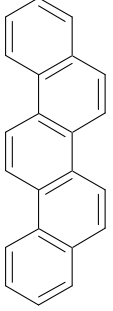
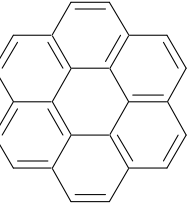
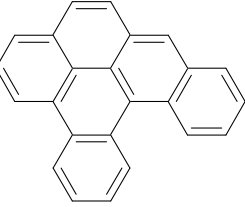
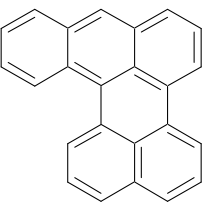
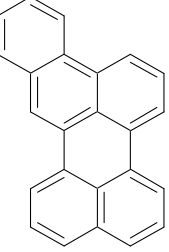
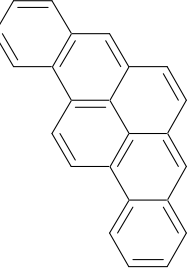
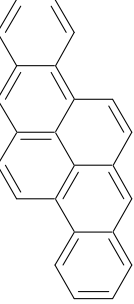
name	structure	CAS-RN	formula	MW (g/mol)	MNDO	MNDO-d	AM1	PM3	RM1	PM6
1-ethylidene-1H-indene		2471-83-2	$C_{11}H_{10}$	142.20	180.6	180.4	195.9	188.0	200.9	189.3
3,4-benzotropolilidene		264-09-5	$C_{11}H_{10}$	142.20	164.2	164.0	160.3	182.1	183.1	170.3
3-methyl-9H-fluorene		2523-39-9	$C_{14}H_{12}$	180.24	124.8	124.8	147.2	131.4	136.4	131.1
9-methylanthracene		779-02-2	$C_{15}H_{12}$	192.26	209.0	209.0	188.2	187.8	194.4	191.3
[2.2]paracyclophanediene		6572-60-7	$C_{16}H_{12}$	204.27	459.9	459.9	416.1	446.0	429.8	418.2
1-methylpyrene		2381-21-7	$C_{17}H_{12}$	216.28	200.9	201.1	197.9	191.9	186.1	192.9
2-methylfluoranthene		33543-31-6	$C_{17}H_{12}$	216.28	235.8	235.9	262.0	252.1	251.2	251.4
2-methylpyrene		3442-78-2	$C_{17}H_{12}$	216.28	187.1	187.2	191.3	190.0	180.9	187.1
7H-benzo[c]fluorene		205-12-9	$C_{17}H_{12}$	216.28	241.3	241.4	246.1	236.2	244.9	244.6
benz[a]anthracene		56-55-3	$C_{18}H_{12}$	228.29	272.5	272.7	254.0	265.9	268.3	274.3
benzo[c]phenanthrene		195-19-7	$C_{18}H_{12}$	228.29	291.7	291.8	264.1	277.9	278.8	283.8

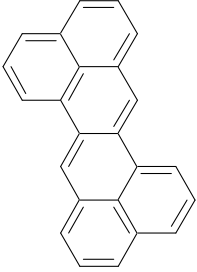
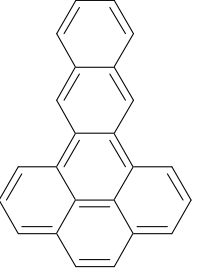
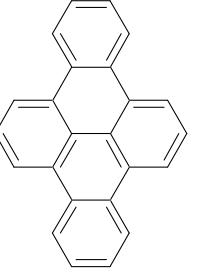
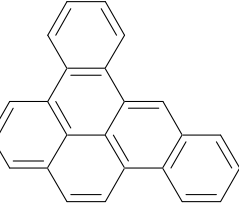
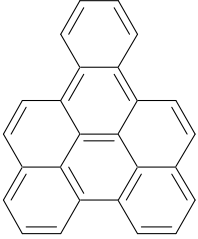
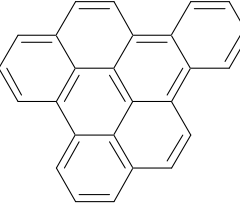
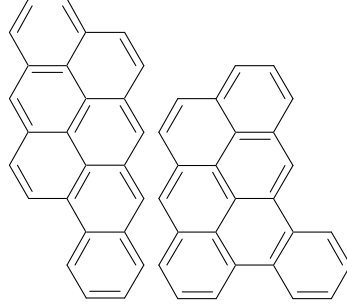
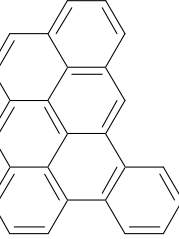
chrysene		218-01-9	C ₁₈ H ₁₂	228.29	272.6	272.8	247.1	251.9	256.8	264.1
naphthacene		92-24-0	C ₁₈ H ₁₂	228.29	296.3	296.4	283.6	304.3	304.8	308.4
triphenylene		217-59-4	C ₁₈ H ₁₂	228.29	280.2	280.4	244.6	241.9	250.4	259.1
1,3-dimethylpyrene		64401-21-4	C ₁₈ H ₁₄	230.30	182.3	182.5	175.4	160.6	151.2	154.8
11-methylbenzo[a]fluorene		71265-25-3	C ₁₈ H ₁₄	230.30	224.9	225.0	229.2	218.4	219.2	223.0
2,7-dimethylpyrene		15679-24-0	C ₁₈ H ₁₄	230.30	157.4	157.6	165.8	154.0	142.2	145.7
5,12-dihydronaphthacene		959-02-4	C ₁₈ H ₁₄	230.30	191.0	191.2	181.8	191.0	188.6	189.0
9,10-dihydronaphthacene		n/a	C ₁₈ H ₁₄	230.30	224.5	224.7	219.4	237.1	232.0	232.5
dihydrochrysene		41593-31-1	C ₁₈ H ₁₄	230.30	210.3	210.5	188.8	194.8	194.6	198.5
anti-7,14-dihydro-7,14-dimethylene-1,6,8,13-bismethano[14]annulene		109281-33-6	C ₁₈ H ₁₆	232.32	477.6	477.7	407.8	457.3	420.8	394.0
syn-7,14-dihydro-7,14-dimethylene-1,6,8,13-bismethano[14]annulene		109216-46-8	C ₁₈ H ₁₆	232.32	466.2	466.3	423.8	464.3	438.0	401.2

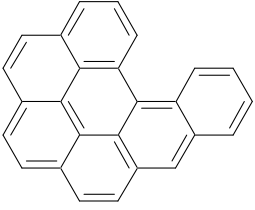
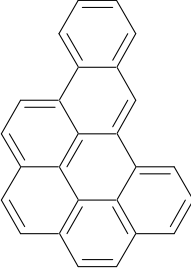
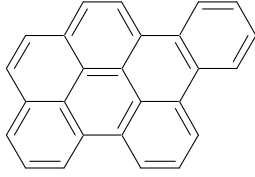
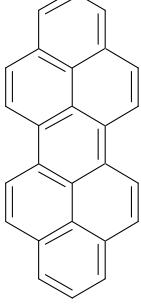
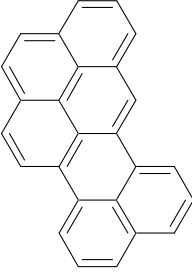
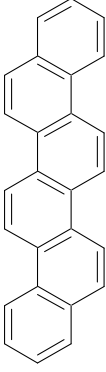
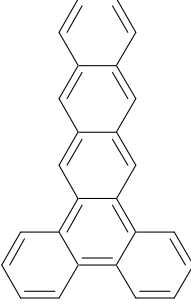
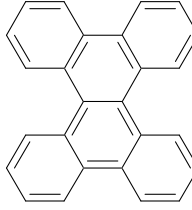
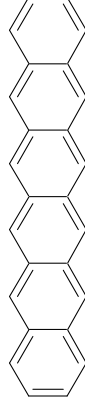
4H-cyclopenta[def]chrysene		202-98-2	C ₁₉ H ₁₂	240.30	284.6	284.8	302.6	298.9	292.9	300.3
6H-benzo[cd]pyrene		191-33-3	C ₁₉ H ₁₂	240.30	224.3	224.6	227.7	233.1	218.5	229.4
12-methylbenz[a]anthracene		2422-79-9	C ₁₉ H ₁₄	242.31	291.3	291.6	255.9	261.5	261.6	263.8
1-methylbenz[a]anthracene		2498-77-3	C ₁₉ H ₁₄	242.31	276.6	277.0	249.6	258.5	254.2	255.1
1-methylbenzo[c]phenanthrene		4076-39-5	C ₁₉ H ₁₄	242.31	292.4	292.5	260.6	271.7	258.3	310.3
1-methylchrysene		3351-28-8	C ₁₉ H ₁₄	242.31	254.4	254.6	225.0	221.1	222.3	227.4
1-methyltriphenylene		2871-91-2	C ₁₉ H ₁₄	242.31	280.1	280.3	240.4	237.9	237.3	242.2
2-methylbenzo[c]phenanthrene		2606-85-1	C ₁₉ H ₁₄	242.31	261.7	261.9	238.0	241.4	239.7	241.6
2-methyltriphenylene		1705-84-6	C ₁₉ H ₁₄	242.31	250.1	250.3	218.6	205.4	211.3	217.1
3-methylbenz[a]anthracene		2498-75-1	C ₁₉ H ₁₄	242.31	241.9	242.1	227.8	229.5	229.3	232.2

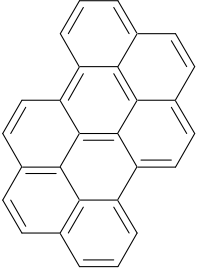
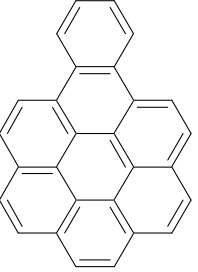
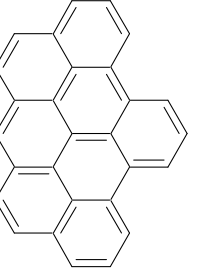
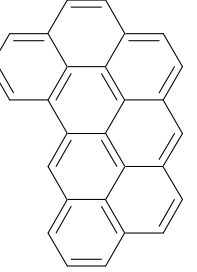
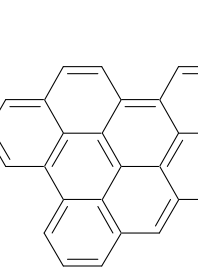
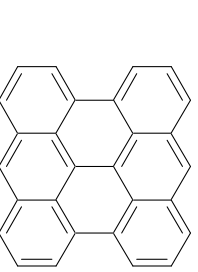
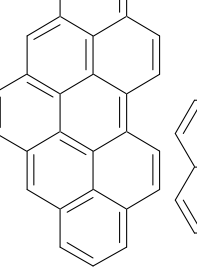
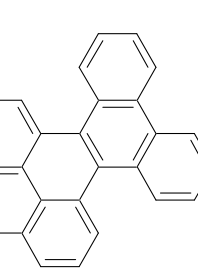
3-methylbenzo[c]phenanthrene		2381-19-3	C ₁₉ H ₁₄	242.31	260.8	260.9	237.8	241.2	239.5	241.4
3-methylchrysene		3351-31-3	C ₁₉ H ₁₄	242.31	242.9	243.1	221.0	215.3	217.5	222.2
4-methylbenz[a]anthracene		242.3145	C ₁₉ H ₁₄	242.31	255.0	255.2	232.2	235.4	234.2	238.0
4-methylbenzo[c]phenanthrene		4076-40-8	C ₁₉ H ₁₄	242.31	272.8	273.1	242.1	245.8	246.3	248.8
4-methylchrysene		3351-30-2	C ₁₉ H ₁₄	242.31	276.1	276.4	243.6	243.3	244.4	246.8
5-methylchrysene		3697-24-3	C ₁₉ H ₁₄	242.31	276.8	277.0	244.4	244.2	244.7	247.8
6-methylchrysene		1705-85-7	C ₁₉ H ₁₄	242.31	255.7	255.9	225.2	221.0	222.2	227.5
7-methylbenz[a]anthracene		2541-69-7	C ₁₉ H ₁₄	242.31	274.3	274.3	241.4	237.7	242.5	245.5
1,2-benzfluoranthene		203-33-8	C ₂₀ H ₁₂	252.31	356.3	356.6	366.7	366.3	369.7	375.9
benz[e]acephenanthrylene		205-99-2	C ₂₀ H ₁₂	252.31	325.8	326.0	339.0	340.2	338.6	347.5

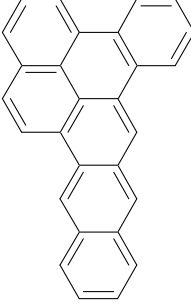
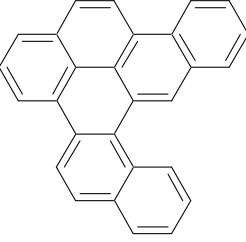
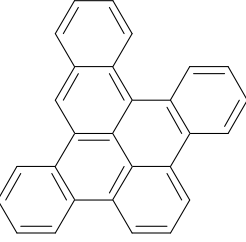
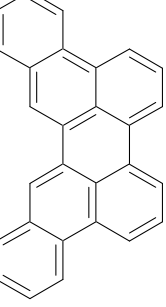
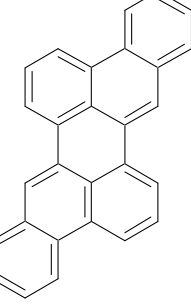
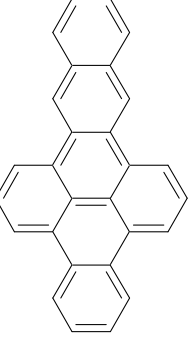
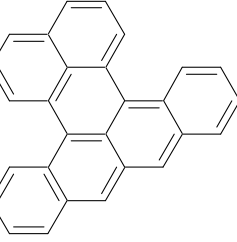
benzo[a]acephenanthrylene		n/a	C ₂₀ H ₁₂	252.31	392.7	392.9	388.6	385.3	386.8	391.8
benzo[a]pyrene		50-32-8	C ₂₀ H ₁₂	252.31	296.5	296.8	285.5	293.8	285.7	300.1
benzo[e]pyrene		192-97-2	C ₂₀ H ₁₂	252.31	293.3	293.6	273.4	273.9	269.2	285.4
benzo[j]fluoranthene		205-82-3	C ₂₀ H ₁₂	252.31	348.2	348.5	358.9	357.2	359.8	367.6
benzo[k]fluoranthene		207-08-9	C ₂₀ H ₁₂	252.31	327.5	327.7	345.2	349.0	345.5	353.8
perylene		198-55-0	C ₂₀ H ₁₂	252.31	310.5	310.7	291.6	295.2	290.2	304.6
4,5-dihydrobenzo[a]pyrene		57652-66-1	C ₂₀ H ₁₄	254.32	220.7	220.9	213.6	218.0	205.8	216.6
benzo[ghi]perylene		191-24-2	C ₂₂ H ₁₂	276.33	302.6	302.9	298.3	300.5	282.0	306.8
dibenzo[def,mno]chrysene		191-26-4	C ₂₂ H ₁₂	276.33	323.1	323.5	325.9	337.1	316.1	337.7
benzo[b]chrysene		214-17-5	C ₂₂ H ₁₄	278.35	351.0	351.3	320.1	329.7	330.4	342.1

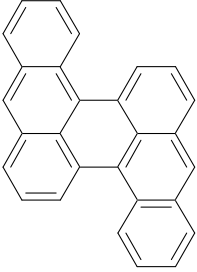
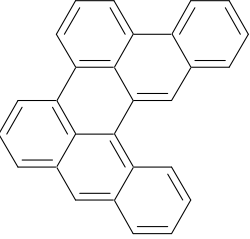
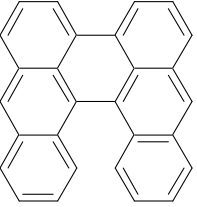
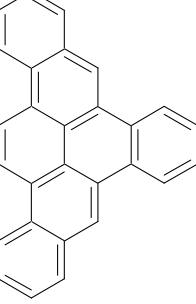
dibenzo[c,g]phenanthrene		188-52-3	C ₂₂ H ₁₄	278.35	377.2	377.5	339.7	362.2	345.8	360.6
pentacene		135-48-8	C ₂₂ H ₁₄	278.35	386.4	386.8	368.2	395.4	392.7	399.7
picene		213-46-7	C ₂₂ H ₁₄	278.35	345.8	346.1	308.7	311.1	314.2	327.2
coronene		191-07-1	C ₂₄ H ₁₂	300.35	304.5	305.0	315.0	316.2	283.9	318.7
1,2,9,10-dibenzopyrene		191-30-0	C ₂₄ H ₁₄	302.37	394.6	395.1	363.1	374.3	361.2	381.5
benzo[a]perylene		191-85-5	C ₂₄ H ₁₄	302.37	415.6	416.0	387.4	403.9	389.4	408.0
benzo[b]perylene		197-70-6	C ₂₄ H ₁₄	302.37	383.3	383.8	351.5	351.9	345.6	366.1
dibenzo(a,i)pyrene		189-55-9	C ₂₄ H ₁₄	302.37	371.8	372.3	349.8	357.0	346.9	366.6
dibenzo[b,def]chrysene		189-64-0	C ₂₄ H ₁₄	302.37	382.5	382.9	359.0	367.0	357.8	377.4

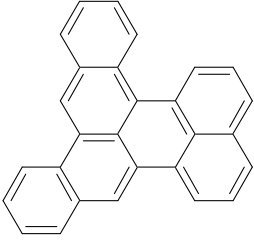
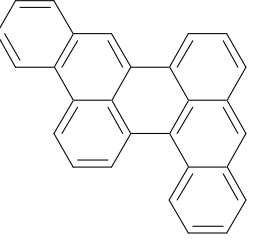
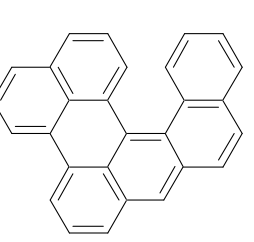
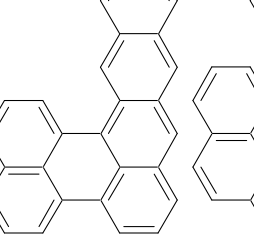
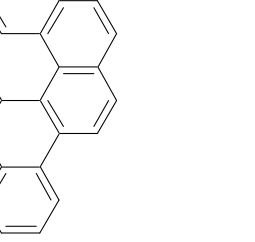
dibenzo[de,mn]naphthacene		214-63-1	C ₂₄ H ₁₄	302.37	409.6	410.1	387.2	399.0	389.4	405.7
dibenzo[de,qr]naphthacene		193-09-9	C ₂₄ H ₁₄	302.37	365.6	366.0	340.6	344.9	335.5	356.7
dibenzo[fg,op]naphthacene		192-51-8	C ₂₄ H ₁₄	302.37	375.8	376.2	333.8	324.1	321.1	344.6
naphtho[1,2,3,4-def]chrysene		192-65-4	C ₂₄ H ₁₄	302.37	373.1	373.6	340.8	339.4	333.0	354.8
1,12-phenyleneperylene		190-84-1	C ₂₆ H ₁₄	326.39	392.4	392.9	367.1	361.0	344.2	375.2
1,12-phenyleneperylene		190-84-1	C ₂₆ H ₁₄	326.39	392.4	392.9	367.1	361.0	344.2	375.2
anthra[2,1,9,8-opqra]naphthacene		92586-98-6	C ₂₆ H ₁₄	326.39	410.6	411.1	401.3	412.6	390.5	417.0
benzo[f]naphtho[7,8,1,2,3-nopqr]tetraphene		n/a	C ₂₆ H ₁₄	326.39	397.8	398.3	380.0	381.9	362.5	391.4

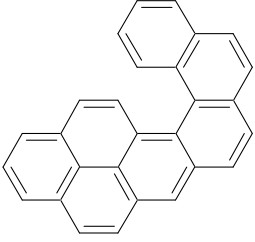
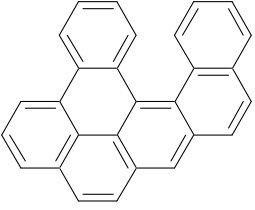
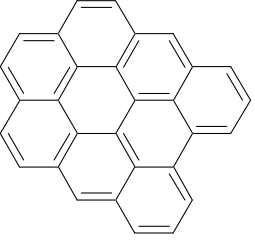
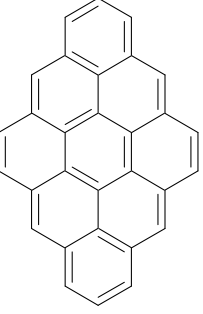
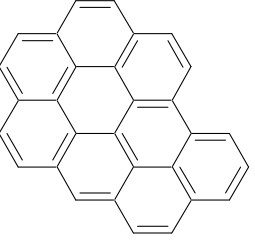
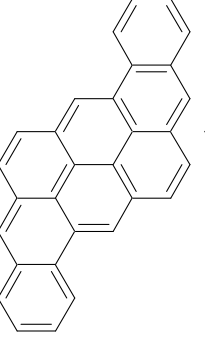
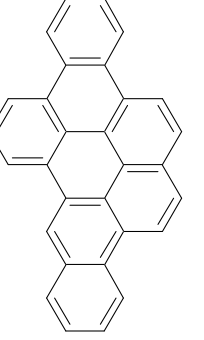
dibenzo[a,ghi]perylene		6596-37-8	C ₂₆ H ₁₄	326.39	409.4	409.9	391.3	402.7	377.3	405.6
dibenzo[b,ghi]perylene		5869-30-7	C ₂₆ H ₁₄	326.39	379.5	380.1	363.1	363.3	343.1	375.2
dibenzo[b,pqr]perylene		190-95-4	C ₂₆ H ₁₄	326.39	385.4	385.9	359.7	352.5	335.9	367.5
dibenzo[cd,lm]perylene		188-96-5	C ₂₆ H ₁₄	326.39	400.5	401.0	383.3	386.1	366.5	395.2
naphtho[8,1,2-bcd]perylene		188-89-6	C ₂₆ H ₁₄	326.39	398.1	400.4	382.9	385.6	366.2	394.6
benzo(c)picene		217-37-8	C ₂₆ H ₁₆	328.40	419.6	420.2	370.9	371.1	372.3	391.0
dibenzo(a,c)naphthacene		216-00-2	C ₂₆ H ₁₆	328.40	436.7	437.3	390.6	397.4	397.8	415.0
dibenzo[g,p]chrysene		191-68-4	C ₂₆ H ₁₆	328.40	458.8	459.3	399.7	415.6	405.3	424.8
hexacene		258-31-1	C ₂₆ H ₁₆	328.40	478.4	479.0	454.7	488.7	482.9	493.0

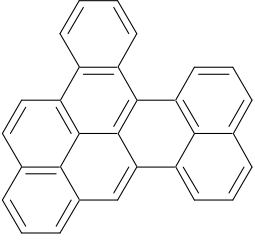
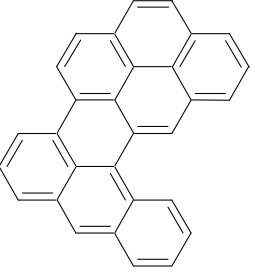
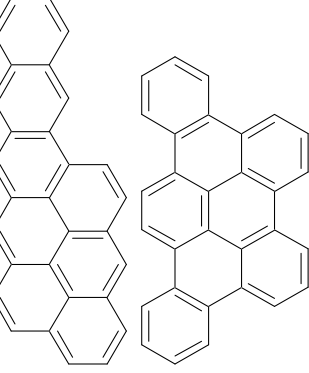
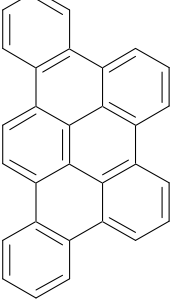
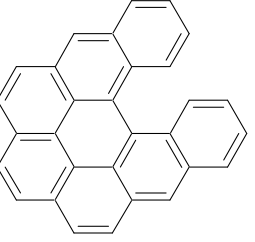
benzo(pqr)naphtho(8,1,2-bcd)perylene		190-71-6	C ₂₈ H ₁₄	350.41	396.7	397.4	386.8	382.3	352.3	392.0
benzo[a]coronene		190-70-5	C ₂₈ H ₁₄	350.41	388.9	389.6	379.0	372.3	341.6	382.7
n/a		n/a	C ₂₈ H ₁₄	350.41	401.2	401.8	390.9	386.8	357.0	396.3
n/a		n/a	C ₂₈ H ₁₄	350.41	402.9	403.6	400.9	403.9	370.7	408.5
n/a		n/a	C ₂₈ H ₁₄	350.41	413.6	414.2	403.9	401.8	372.0	410.0
phenanthro(1,10,9,8-opqra)perylene		190-39-6	C ₂₈ H ₁₄	350.41	457.0	457.6	446.9	451.2	422.8	457.9
phenanthro[2,1,10,9,8,7-pqrstuv]pentaphene		4552-79-8	C ₂₈ H ₁₄	350.41	428.9	429.5	426.5	433.6	401.0	436.3
benzo(p)naphtho(1,8,7-ghi)chrysene		385-14-8	C ₂₈ H ₁₆	352.43	478.5	479.2	432.4	449.5	426.5	453.7

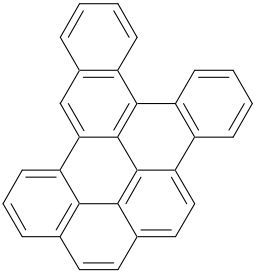
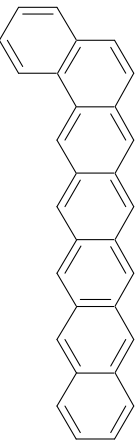
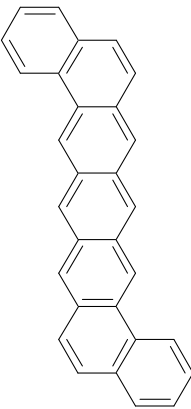
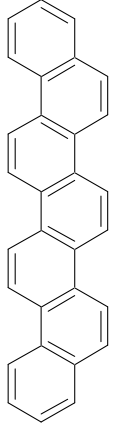
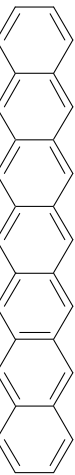
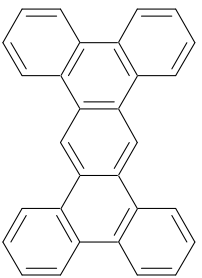
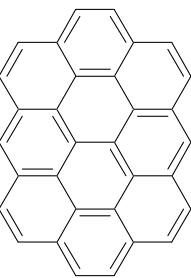
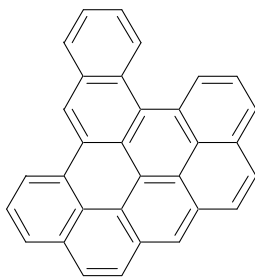
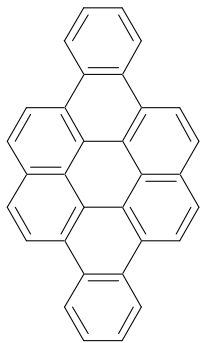
benzo[a]naphtho[8,1,2-cde]naphthacene		192-70-1	C ₂₈ H ₁₆	352.43	453.0	453.6	415.2	418.7	408.3	434.3
benzo[a]naphtho[8,1,2-fgh]tetraphene		n/a	C ₂₈ H ₁₆	352.43	466.6	467.3	424.5	434.0	418.0	444.5
benzo[fg]naphtho[1,2,3-op]tetracene		n/a	C ₂₈ H ₁₆	352.43	466.1	466.7	418.4	422.2	409.3	437.4
dibenzo(fg,ij)pentaphene		197-69-3	C ₂₈ H ₁₆	352.43	455.9	450.8	411.3	408.7	400.8	427.3
dibenzo(fg,qr)pentacene		197-74-0	C ₂₈ H ₁₆	352.43	456.2	456.8	411.5	409.0	401.0	427.5
dibenzo(fg,st)pentacene		192-59-6	C ₂₈ H ₁₆	352.43	449.0	449.6	401.7	395.7	388.3	416.5
dibenzo[a,f]perylene		191-81-1	C ₂₈ H ₁₆	352.43	549.0	549.6	498.7	526.9	507.3	528.0

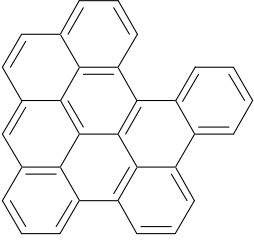
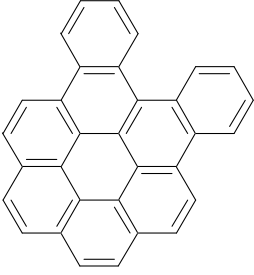
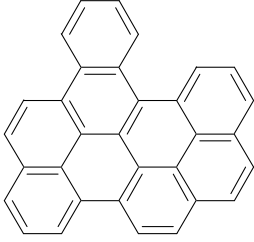
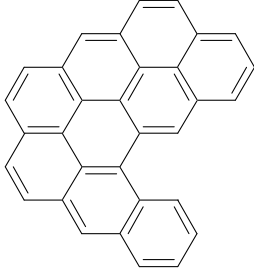
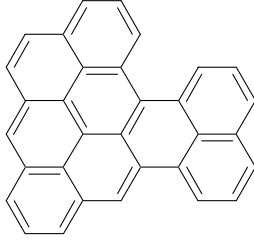
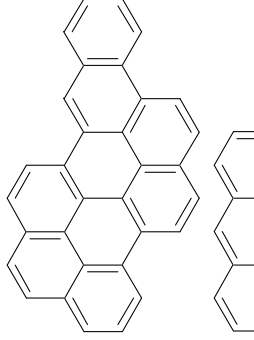
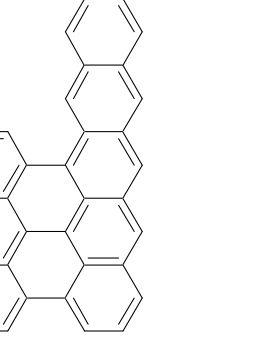
dibenzo[a,j]perylene		191-87-7	C ₂₈ H ₁₆	352.43	547.8	548.5	496.5	523.4	504.3	524.7
dibenzo[a,n]perylene		n/a	C ₂₈ H ₁₆	352.43	484.3	484.9	445.5	460.6	443.4	468.1
dibenzo[a,o]perylene		190-36-3	C ₂₈ H ₁₆	352.43	516.5	517.2	479.6	506.7	476.7	502.8
dibenzo[b,e]perylene		n/a	C ₂₈ H ₁₆	352.43	479.0	479.6	432.8	442.8	428.3	453.4
dibenzo[de,qr]pentacene		n/a	C ₂₈ H ₁₆	352.43	480.9	481.6	446.5	456.1	444.9	466.9
dibenzo[h,rst]pentaphene		192-47-2	C ₂₈ H ₁₆	352.43	449.6	450.3	405.0	401.6	393.3	420.7
n/a		n/a	C ₂₈ H ₁₆	352.43	467.0	467.6	430.8	446.5	428.2	453.4

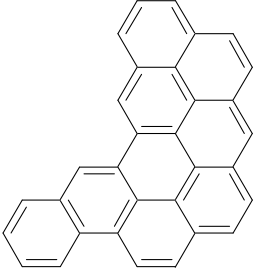
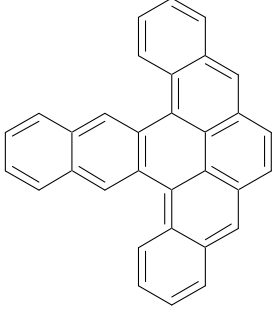
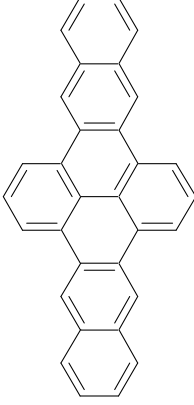
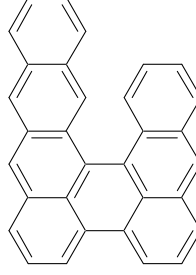
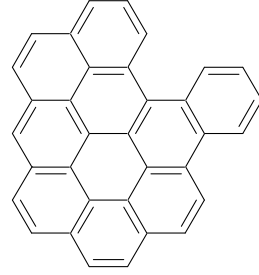
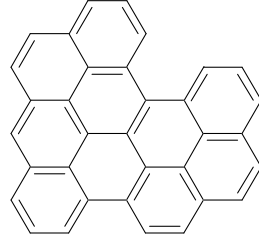
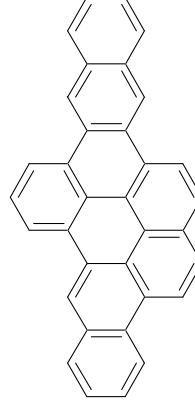
n/a		n/a	C ₂₈ H ₁₆	352.43	480.5	481.1	441.5	455.5	438.3	463.6
n/a		n/a	C ₂₈ H ₁₆	352.43	483.1	483.7	442.9	461.7	432.4	461.5
n/a		n/a	C ₂₈ H ₁₆	352.43	484.3	484.9	445.7	461.0	443.9	468.6
n/a		n/a	C ₂₈ H ₁₆	352.43	492.0	492.6	456.1	477.9	447.8	475.3
n/a		n/a	C ₂₈ H ₁₆	352.43	495.9	496.5	449.7	469.4	449.1	472.8
n/a		n/a	C ₂₈ H ₁₆	352.43	502.1	502.7	468.4	491.3	472.9	495.4
naphtho[2,1,8-def]pentahelicene		n/a	C ₂₈ H ₁₆	352.43	471.0	471.6	431.5	449.3	419.9	449.7

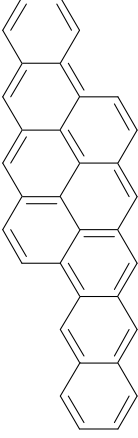
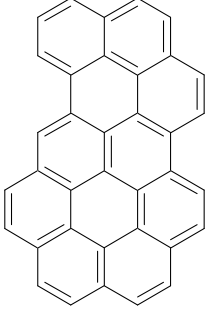
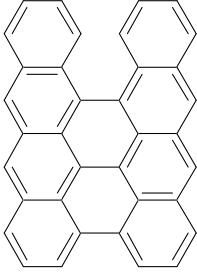
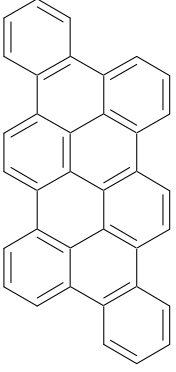
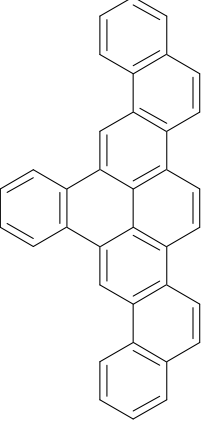
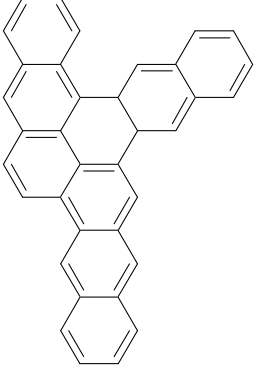
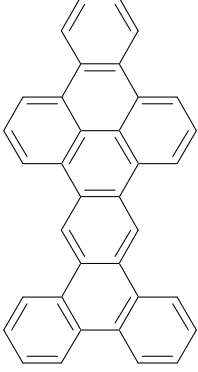
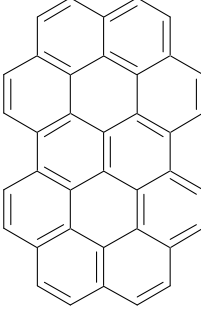
naphtho[8,1,2-cde]pentahelicene		n/a	$C_{28}H_{16}$	352.43	473.6	474.3	438.7	462.5	431.0	458.7
naphtho[8,1,2-fgh]pentahelicene		n/a	$C_{28}H_{16}$	352.43	474.3	474.9	434.3	452.5	423.3	452.8
dibenzo(bc,ef)coronene		190-31-8	$C_{30}H_{14}$	374.43	434.1	434.9	439.1	439.7	396.8	443.0
dibenzo[bc,kl]coronene		190-55-6	$C_{30}H_{14}$	374.43	459.3	460.0	471.1	481.6	435.9	478.3
naphtho(8,1,2-abc)coronene		6596-38-9	$C_{30}H_{14}$	374.43	407.6	408.4	412.7	409.3	365.7	414.2
1,2:7,8-dibenzanthanthrene		191-13-9	$C_{30}H_{16}$	376.45	472.2	472.9	451.9	460.1	435.3	468.0
benzo(qr)naphtho(2,1,8,7-fghi)pentacene		190-87-4	$C_{30}H_{16}$	376.45	464.1	464.8	425.9	416.6	398.2	435.4

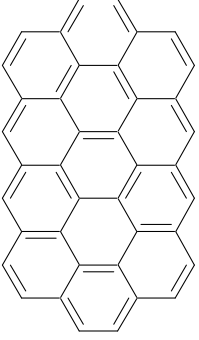
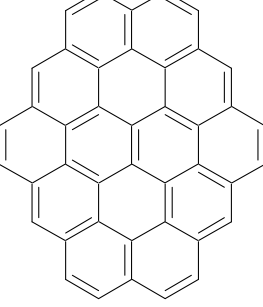
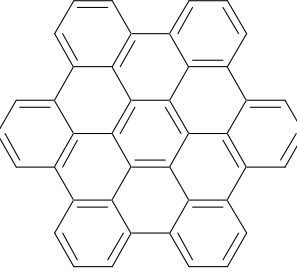
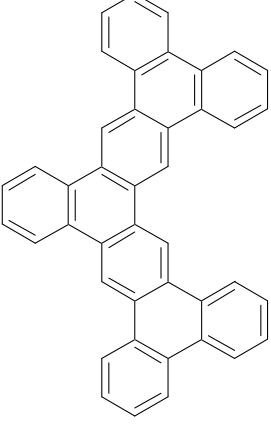
benzo[a]naphtho[2,1,8-cde]perylene		n/a	C ₃₀ H ₁₆	376.45	504.4	505.1	472.7	483.5	455.3	489.5
benzo[a]naphtho[2,1,8-lmn]perylene		n/a	C ₃₀ H ₁₆	376.45	503.8	504.5	478.0	494.3	464.8	497.5
benzo[b]naphtho[1,2,3,4-pqr]perylene		n/a	C ₃₀ H ₁₆	376.45	486.4	487.2	445.9	446.2	422.0	459.3
n/a		n/a	C ₃₀ H ₁₆	376.45	494.3	495.0	479.4	496.3	470.5	500.9
tribenzo(b,n,pqr)perylene		190-81-8	C ₃₀ H ₁₆	376.45	463.8	464.6	420.8	404.0	389.1	427.8
tribenzo[a,e,ghi]perylene		n/a	C ₃₀ H ₁₆	376.45	484.3	485.0	448.4	452.2	427.0	463.0
tribenzo[a,ghi,o]perylene		n/a	C ₃₀ H ₁₆	376.45	506.2	506.9	478.3	499.2	457.7	494.5

tribenzo[b,e,ghi]perylene		n/a	C ₃₀ H ₁₆	376.45	479.3	480.0	444.6	448.8	422.8	459.0
benzo[a]hexacene		n/a	C ₃₀ H ₁₈	378.46	536.4	537.1	501.8	532.6	524.6	541.0
dibenzo(a,l)pentacene		227-09-8	C ₃₀ H ₁₈	378.46	504.7	505.5	464.9	486.0	479.0	498.3
dibenzo[c,m]picene		n/a	C ₃₀ H ₁₈	378.46	493.1	493.9	432.9	430.7	430.1	454.5
heptacene		258-38-8	C ₃₀ H ₁₈	378.46	571.7	572.4	542.1	583.1	574.3	587.5
tetrabenz[a,c,h,j]anthracene		215-11-2	C ₃₀ H ₁₈	378.46	504.1	504.8	429.6	417.3	421.6	448.1
ovalene		190-26-1	C ₃₂ H ₁₄	398.45	423.5	424.3	442.8	440.5	383.9	441.3
benzo[e]phenanthro[2,3,4,5-pqab]perylene		n/a	C ₃₂ H ₁₆	400.47	501.2	502.1	478.9	484.5	446.5	490.1
dibenzo(a,j)coronene		190-72-7	C ₃₂ H ₁₆	400.47	476.4	477.2	445.4	430.3	401.4	448.6

dibenzo[a,cd]naphtho[8,1,2,3-fghi]perylene		n/a	C ₃₂ H ₁₆	400.47	511.8	512.6	484.6	487.3	450.9	495.1
dibenzo[a,d]coronene		n/a	C ₃₂ H ₁₆	400.47	490.9	491.8	463.3	462.2	425.1	471.6
dibenzo[a,ghi]naphtho[2,1,8-cde]perylene		n/a	C ₃₂ H ₁₆	400.47	504.4	505.3	476.2	477.1	440.7	485.9
dibenzo[a,ghi]naphtho[2,1,8-lmn]perylene		n/a	C ₃₂ H ₁₆	400.47	511.0	511.8	495.3	508.3	467.6	509.2
dinaphtho[1,8-ab:8',1',2',3'-fghi]perylene		n/a	C ₃₂ H ₁₆	400.47	530.1	531.0	512.2	525.5	485.2	526.2
dinaphtho[2,1,8,7-defg:2',1',8',7'-qrst]pentacene		n/a	C ₃₂ H ₁₆	400.47	476.2	477.1	453.8	447.3	415.8	461.0
n/a		n/a	C ₃₂ H ₁₆	400.47	571.6	572.4	548.6	565.2	528.6	567.7

tetrapheno[10,11,12,1,2-defghij]pentaphene	n/a	C ₃₂ H ₁₆	400.47	478.1	479.0	463.9	464.7	429.9	473.4
									
anthra(1,2,3,4-rst)pentaphene	31541-07-8	C ₃₂ H ₁₈	402.48	580.2	581.0	526.6	553.2	527.3	554.7
									
dibenzo(hi,uv)hexacene	192-54-1	C ₃₂ H ₁₈	402.48	522.5	523.3	469.8	467.6	455.8	488.8
									
n/a	n/a	C ₃₂ H ₁₈	402.48	602.7	603.6	560.7	593.6	560.0	589.8
									
benzo[p]naphtho[8,1,2-abc]coronene	n/a	C ₃₄ H ₁₆	424.49	514.2	515.2	499.6	500.2	451.0	504.8
									
n/a	n/a	C ₃₄ H ₁₆	424.49	529.4	530.4	515.0	518.3	469.9	521.8
									
benzo[uv]naphtho[2,1,8,7-fghi]hexacene	n/a	C ₃₄ H ₁₈	426.51	535.4	536.4	494.9	489.7	467.0	509.0
									

n/a		n/a	C ₃₄ H ₁₈	426.51	587.6	588.5	559.6	577.2	551.1	586.5
pyreno[1,10,9-abc]coronene		n/a	C ₃₆ H ₁₆	448.51	495.2	496.2	494.9	483.6	427.9	492.1
benzo[fg]benzo[8,9]phenaleno[1,2,3,4,5-rstuv]pentaphene		n/a	C ₃₆ H ₁₈	450.53	679.4	680.4	646.1	673.4	622.2	668.9
dibenzo[ij,rst]phenanthro[9,10,1,2-defg]pentaphene		n/a	C ₃₆ H ₁₈	450.53	557.1	558.2	508.1	484.2	457.8	511.5
n/a		n/a	C ₃₆ H ₂₀	452.54	598.4	599.3	528.8	518.5	507.0	546.2
n/a		n/a	C ₃₆ H ₂₀	452.54	626.2	627.3	574.1	594.6	569.4	604.9
tetrabenzo[a,c,hi,qr]pentacene		n/a	C ₃₆ H ₂₀	452.54	599.5	600.6	518.8	499.3	492.1	533.4
naphtho[7,8,1',2':5,10,4]anthra[1,9,8-abcd]coronene		41163-25-1	C ₃₈ H ₁₆	472.53	508.2	509.4	515.5	498.6	432.2	506.4

phenanthro[3,4,5,6-bcdef]ovalene		n/a	$C_{40}H_{16}$	496.55	557.8	559.0	585.7	582.1	501.7	580.3
dinaphtho[2,1,8,7-hijk:2',1',8',7'-stuv]ovalene		n/a	$C_{42}H_{16}$	520.58	557.2	558.5	593.5	582.8	490.4	579.9
hexabenzozo[bc,ef,hi,kl,no,qr]coronene		190-24-9	$C_{42}H_{18}$	522.59	620.2	621.9	592.5	554.7	498.3	579.4
n/a		n/a	$C_{42}H_{24}$	528.64	727.9	729.3	614.7	592.5	592.7	637.1

References

- (1) Slayden, S. W.; Liebman, J. F. *Chem. Rev.* **2001**, *101*, 1541-1566.
- (2) Robinson, P. R. In *Practical Advances in Petroleum Processing - Volume 1*; Hsu, C. S.; Robinson, P. R., Eds.; Springer: New York, 2006, pp. 1-39.
- (3) Rahimi, P. M.; Gentzis, T. In *Practical Advances in Petroleum Processing - Volume 2*; Hsu, C. S.; Robinson, P. R., Eds.; Springer: New York, 2006, pp. 149-186.
- (4) Richter, H.; Howard, J. B. *Prog. Energy Comb. Sci.* **2000**, *26*, 565-608.
- (5) Curtiss, L. A.; Redfern, P. C.; Raghavachari, K. *J. Chem. Phys.* **2007**, *127*, 124105-124108.
- (6) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J.C.; Iyengar, S.S.; Tomasi, J. *Gaussian 09, Revision B.02*; Gaussian, Inc.: Wallingford, CT, USA, 2009.
- (7) Notario, R.; Castano, O.; Abboud, J. L. M.; Gomperts, R.; Frutos, L. M.; Palmeiro, R. *J. Org. Chem.* **1999**, *64*, 9011-9014.
- (8) Notario, R.; Castano, O.; Gomperts, R.; Frutos, L. M.; Palmeiro, R. *J. Org. Chem.* **2000**, *65*, 4298-4302.
- (9) Curtiss, L. A.; Redfern, P. C.; Raghavachari, K. *J. Chem. Phys.* **2007**, *126*, 84108-84112.
- (10) Rayne, S.; Forest, K. *J. Chem. Eng. Data* **2010**, *55*, 5359-5364.
- (11) Rayne, S.; Forest, K. *J. Chem. Eng. Data* **2011**, *56*, 684-685.
- (12) Rayne, S.; Forest, K. *J. Mol. Struct. (Theochem)* **2010**, *948*, 111-112.
- (13) Rayne, S.; Forest, K. *J. Mol. Struct. (Theochem)* **2010**, *948*, 102-107.
- (14) Rayne, S.; Forest, K. *J. Mol. Struct. (Theochem)* **2010**, *953*, 47-48.
- (15) Rayne, S.; Forest, K. *Theor. Chem. Acc.* **2010**, *127*, 697-709.
- (16) Rayne, S.; Forest, K. *Comp. Theor. Chem.* **2011**, doi:10.1016/j.comptc.2011.05.018.
- (17) Allouche, A. R. *J. Comp. Chem.* **2010**, *32*, 174-182.
- (18) Linstrom, P. J.; Mallard, W. G. *J. Chem. Eng. Data* **2001**, *46*, 1059-1063.
- (19) Richardson, J. W.; Parks, G. S. *J. Am. Chem. Soc.* **1939**, *61*, 3543-3546.
- (20) Steele, W. V.; Chirico, R. D.; Nguyen, A.; Hossenlopp, I. A.; Smith, N. K. *Am. Inst. Chem. Eng. Symp. Ser.* **1990**, 138-154.
- (21) Nagano, Y. *J. Chem. Thermodyn.* **2002**, *34*, 377-383.
- (22) Roux, M. V.; Temprado, M.; Chickos, J. S.; Nagano, Y. *J. Phys. Chem. Ref. Data* **2008**, *37*, 1855-1996.
- (23) Bender, P.; Farber, J. *J. Am. Chem. Soc.* **1952**, *74*, 1450-1452.
- (24) Coleman, D. J.; Pilcher, G. *Trans. Faraday Soc.* **1966**, *62*, 821-827.
- (25) Alberty, R. A.; Reif, A. K. *J. Phys. Chem. Ref. Data* **1988**, *17*, 241-253.
- (26) Grutzmacher, H. F.; Lohmann, J. *Liebigs Ann. Chem.* **1969**, *726*, 47-56.
- (27) Blanquart, G.; Pitsch, H. *J. Phys. Chem. A* **2007**, *111*, 6510-6520.
- (28) Taskinen, E. *J. Phys. Org. Chem.* **2009**, *22*, 632-642.
- (29) Ribeiro da Silva, M. A. V.; Amaral, L. M. P. F.; Santos, A. F. L. O. M.; Gomes, J. R. B. *J. Chem. Thermodyn.* **2006**, *38*, 367-375.
- (30) Speros, D. M.; Rossini, F. D. *J. Phys. Chem.* **1960**, *64*, 1723-1727.

- (31) Wang, H.; Frenklach, M. *J. Phys. Chem.* **1993**, *97*, 3861-3874.
- (32) Miranda, M. S.; Matos, M. A. R.; Morais, V. M. F.; Liebman, J. F. *J. Chem. Thermodyn.* **2011**, *43*, 364-370.
- (33) Chirico, R. D.; Hossenlopp, I. A.; Nguyen, A.; Steele, W. V.; Gammon, B. E. *J. Chem. Thermodyn.* **1989**, *21*, 179-201.
- (34) Rakus, K.; Verevkin, S. P.; Schatzer, J.; Beckhaus, H. D.; Ruchardt, C. *Chem. Ber.* **1994**, *127*, 1095-1103.
- (35) Rodgers, D. L.; Westrum, E. F.; Andrews, J. T. S. *J. Chem. Thermodyn.* **1973**, *5*, 733-739.
- (36) Shaw, R. G.; David, M.; Benson, S. W. *J. Phys. Chem.* **1977**, *81*, 1716-1729.
- (37) Lee-Bechtold, S. H.; Hossenlopp, I. A.; Scott, D. W.; Osborn, A. G.; Good, W. D. *J. Chem. Thermodyn.* **1979**, *11*, 469-482.
- (38) Boyd, R. H.; Christensen, R. L.; Pua, R. *J. Am. Chem. Soc.* **1965**, *87*, 3554-3559.
- (39) Mercader, A.; Castro, E. A.; Toropov, A. A. *Chem. Phys. Lett.* **2000**, *330*, 612-623.
- (40) Peck, R. C.; Schulman, J. M.; Disch, R. L. *J. Phys. Chem.* **1990**, *94*, 6637-6641.
- (41) Duchowicz, P.; Castro, E. A. *J. Korean Chem. Soc.* **2000**, *44*, 501-506.
- (42) Duchowicz, P.; Castro, E. A. *J. Korean Chem. Soc.* **1999**, *43*, 621-627.
- (43) Herndon, W. C. *Chem. Phys. Lett.* **1995**, *234*, 82-86.
- (44) Castro, E. A. *Computers Chem.* **1997**, *21*, 305-308.
- (45) Welsh, W. J.; Tong, W.; Collantes, E. R.; Chickos, J. S.; Gagarin, S. G. *Thermochim. Acta* **1996**, *290*, 55-64.
- (46) Sadowska, K. W. *Przem. Chem.* **1966**, *45*, 66-67.
- (47) Yu, J.; Sumathi, R.; Green, W. H. *J. Am. Chem. Soc.* **2004**, *126*, 12685-12700.
- (48) Liu, M. H.; Chen, C. *J. Comp. Chem.* **2006**, *27*, 537-544.
- (49) Sivaramakrishnan, R.; Tranter, R. S.; Brezinsky, L. *J. Phys. Chem. A* **2005**, *109*, 1621-1628.
- (50) Schulman, J. M.; Peck, R. C.; Disch, R. L. *J. Am. Chem. Soc.* **1989**, *111*, 5675-5680.
- (51) Parks, G. S.; West, T. J.; Naylor, B. F.; Fujii, P. S.; McClaine, L. A. *J. Am. Chem. Soc.* **1946**, *68*, 2524-2527.
- (52) Mackle, H.; O'Hare, P. A. G. *Trans. Faraday Soc.* **1963**, *59*, 2693-2701.
- (53) Metzger, R. M.; Kuo, C. S.; Arafat, E. S. *J. Chem. Thermodyn.* **1983**, *15*, 841-851.
- (54) Herndon, W. C.; Biedermann, P. U.; Agranat, I. *J. Org. Chem.* **1998**, *63*, 7445-7448.
- (55) Kudchadker, S. A.; Kudchadker, A. P.; Zwolinski, B. J. *J. Chem. Thermodyn.* **1979**, *11*, 1051-1059.
- (56) Mestechkin, M. M.; Vysotskii, Y. B. *Zhurnal Strukturnoi Khimii* **1983**, *24*, 164-167.
- (57) Winget, P.; Clark, T. *J. Comp. Chem.* **2004**, *25*, 725-733.
- (58) Kovats, E.; Gunthard, H. H.; Plattner, P. A. *Helv. Chim. Acta* **1955**, *38*, 1912-1919.
- (59) Kovats, E.; Gunthard, H.; Plattner, A. *Helv. Chim. Acta* **1957**, *40*, 1-2.
- (60) Roth, W. R.; Bohm, M.; Lenhartz, H. W.; Vogel, E. *Angew. Chem.* **1983**, *95*, 1011-1012.
- (61) Curtiss, L. A.; Raghavachari, K.; Redfern, P. C.; Pople, J. A. *J. Chem. Phys.* **2000**, *112*, 7374-7383.
- (62) Kristyan, S.; Ruzsinszky, A.; Csonka, G. I. *Theor. Chem. Acc.* **2001**, *106*, 404-411.
- (63) Ruzsinszky, A.; Van Alsenoy, C.; Csonka, G. I. *J. Phys. Chem. A* **2002**, *106*, 12139-12150.
- (64) Ruzsinszky, A.; Van Alsenoy, C.; Csonka, G. I. *J. Phys. Chem. A* **2003**, *107*, 736-744.
- (65) De Yonker, N. J.; Grimes, T.; Yockel, S.; Dinescu, A.; Mintz, B.; Cundari, T. R.; Wilson, A. K. *J. Chem. Phys.* **2006**, *125*, 10411.
- (66) Bremser, W.; Hagen, R.; Heilbronner, E.; Vogel, E. *Helv. Chim. Acta* **1969**, *52*, 418-431.
- (67) Roth, W. R.; Klarner, F. G.; Siepert, G.; Lennartz, H. W. *Chem. Ber.* **1992**, *125*, 217-224.

- (68) Parks, G. S.; Vaughan, L. M. *J. Am. Chem. Soc.* **1951**, *73*, 2380-2381.
- (69) Montgomery, R. L.; Rossini, F. D.; Mansson, M. *J. Chem. Eng. Data* **1978**, *23*, 125-129.
- (70) Chirico, R. D.; Knipmeyer, S. E.; Nguyen, A.; Steele, W. V. *J. Chem. Thermodyn.* **1989**, *21*, 1307-1331.
- (71) Cox, J. D.; Pilcher, G. *Thermochemistry of Organic and Organometallic Compounds*; Academic Press: New York, NY, USA, 1970.
- (72) Douslin, D. R.; Scott, D. W.; Good, W. D.; Osborn, A. G. *Gov. Rep. Announce. Index U.S.* **1976**, *76*, 97-110.
- (73) Bedford, A. F.; Carey, J. G.; Millar, I. T.; Mortimer, C. T.; Springall, H. D. *J. Chem. Soc.* **1962**, 3895-3898.
- (74) Schulman, J. M.; Disch, R. L. *J. Mol. Struct. (Theochem)* **1992**, *259*, 173-179.
- (75) Westrum, E. F.; Wong, S. *AEC Rept. COO-1149-92, Contract AT(11-1)-1149* **1967**, 1-7.
- (76) Sabbah, R. *Bull. Soc. Chim. Fr.* **1991**, *128*, 350-356.
- (77) Keffler, L. J. P.; Guthrie, F. C. *J. Phys. Chem.* **1927**, *31*, 58-67.
- (78) Ammar, M. M.; El Sayed, N.; Morsi, S. E.; El Azmirly, A. *Egypt. J. Phys.* **1977**, *8*, 111-118.
- (79) Smith, N. K.; Stewart, R. C.; Osborn, A. G.; Scott, D. W. *J. Chem. Thermodyn.* **1980**, *12*, 919-926.
- (80) Dewar, M. J. S.; Zoebisch, E. G.; Healy, E. F. *J. Am. Chem. Soc.* **1985**, *107*, 3902-3909.
- (81) Stewart, J. J. P. *J. Comp. Chem.* **1989**, *10*, 209-220.
- (82) Rocha, G. B.; Freire, R. O.; Simas, A. M.; Stewart, J. J. P. *J. Comp. Chem.* **2006**, *27*, 1101-1111.
- (83) Stewart, J. J. P. *J. Mol. Model.* **2007**, *13*, 1173-1213.
- (84) Mondal, R.; Shah, B. K.; Neckers, D. C. *J. Am. Chem. Soc.* **2006**, *128*, 9612-9613.
- (85) Bettinger, H. F. *Pure Appl. Chem.* **2010**, *82*, 905-915.
- (86) Houk, K. N.; Lee, P. S.; Nendel, M. *J. Org. Chem.* **2001**, *66*, 5517-5521.
- (87) dos Santos, M. C. *Phys. Rev. B* **2006**, *74*, 045426-045429.
- (88) Schug, J. C.; Lengsfeld, B. H.; Brewer, D. A. *J. Phys. Chem.* **1978**, *82*, 1436-1438.
- (89) Bendikov, M.; Duong, H.; Starkey, K.; Houk, K. N.; Carter, E. A.; Wudl, F. *J. Am. Chem. Soc.* **2004**, *126*, 7416-7417.
- (90) Gao, H.; Hodgson, J. L.; Jiang, D.; Zhang, S. B.; Nagase, S.; Miller, G. P.; Chen, Z. *Org. Lett.* **2011**, *13*, 3316-3319.
- (91) Qu, Z.; Zhang, D.; Liu, C.; Jiang, Y. *J. Phys. Chem. A* **2009**, *113*, 7909-7914.
- (92) Norton, J.E.; Houk, K. N. *J. Am. Chem. Soc.* **2005**, *127*, 4162-4163.
- (93) Hachmann, J.; Dorando, J. J.; Aviles, M.; Chan, G. K. L. *J. Chem. Phys.* **2007**, *127*, 134309.
- (94) Jiang, D. E.; Dai, S. *J. Phys. Chem. A* **2008**, *112*, 332-335.
- (95) Zade, S. S.; Zamoshchik, N.; Reddy, A. R.; Fridman-Marueli, G.; Sheberla, D.; Bendikov, M. *J. Am. Chem. Soc.* **2011**, doi: 10.1021/ja106594v.
- (96) Motomura, S.; Nakano, M.; Fukui, H.; Yoneda, K.; Kubo, T.; Carion, R.; Champagne, B. *Phys. Chem. Chem. Phys.* **2011**, doi: 10.1039/c1cp20773c.
- (97) Pelzer, K.; Greenman, L.; Gidofalvi, G.; Mazziotti, D. A. *J. Phys. Chem. A* **2011**, *115*, 5632-5640.
- (98) Lambert, C. *Angew. Chem. Int. Ed.* **2011**, *50*, 1756-1758.
- (99) Hajgato, B.; Szieberth, D.; Geerlings, P.; De Proft, F.; Deleuze, M. S. *J. Chem. Phys.* **2009**, *131*, 224321.
- (100) Hajgato, B.; Huzak, M.; Deleuze, M.S. *J. Phys. Chem. A* **2011**, doi: 10.1021/jp2043043.
- (101) Rayne, S.; Forest, K., *Comp. Theor. Chem.* (2011) submitted.

- (102) Marchetti, A. P.; Kearns, D. R. *J. Am. Chem. Soc.* **1967**, *89*, 768-777.
- (103) Vo-Dinh, T.; Gammage, R. B. *Anal. Chem.* **1978**, *50*, 2054-2058.
- (104) Korth, M. *J. Chem. Theory Comput.* **2010**, *6*, 3808-3816.
- (105) Korth, M.; Pitonak, M.; Rezac, J.; Hobza, P. *J. Chem. Theory Comp.* **2010**, *6*, 344-352.
- (106) Rezac, J.; Fanfrlik, J.; Salahub, D.; Hobza, P. *J. Chem. Theory Comp.* **2009**, *5*, 1749-1760.

Supplementary Material:
A G4MP2 Theoretical Study on the Gas Phase Enthalpies of Formation
for Various Polycyclic Aromatic Hydrocarbons (PAHs) and Other C₁₀
Through C₂₀ Unsaturated Hydrocarbons

Sierra Rayne^{a,*}, Kaya Forest^b

^aChemologica Research, Mortlach, Saskatchewan, S0H 3E0, Canada

^bDepartment of Environmental Engineering, Saskatchewan Institute of Applied Science and Technology,
Palliser Campus, Moose Jaw, Saskatchewan, S6H 4R6, Canada

*Corresponding author. Tel.: +1 250 487 0166. E-mail address: rayne.sierra@gmail.com (S. Rayne).

Gaussian-4 (G4) archive entries

[4.2.2]propella-2,4,7,9-tetraene

1\1\GINC-BUL75\Mixed\G4MP2\G4MP2\C10H8\KFOREST\15-Dec-2010\0\#\# G4MP2\
\name\0,1\C,0,4.5955764131,3.7952497607,2.3036265982\C,0,4.4356258264
,3.2750886404,3.5275021322\C,0,3.553691285,2.8808192583,1.649323241\C,
0,3.3654236274,2.2688120942,3.0894452086\C,0,3.8453921881,0.9541679819
,2.4640164612\C,0,1.9947628888,2.3464537441,3.6806969367\C,0,4.0054567
503,1.4742988651,1.240142999\C,0,2.3440079067,3.4817498453,1.009114292
8\C,0,1.1676492239,3.4853783063,1.6540270584\C,0,0.992424296,2.9157729
775,2.9944478357\H,0,5.2410395936,4.5646354399,1.8943848098\H,0,4.9019
936763,3.4621045855,4.4885340539\H,0,4.0140669147,-0.0293176802,2.8887
048835\H,0,1.8283447568,1.9340689319,4.6730548916\H,0,4.3533263133,1.0
731566488,0.2945593787\H,0,2.4372301523,3.9133838033,0.0153674977\H,0,
0.2939504918,3.9243775637,1.1807936427\H,0,-0.0003722174,2.9676195758,
3.4322682353\Version=AM64L-G09RevB.01\State=1-A\MP2/GTbas1=-384.44238
08\CCSD(T)/GTbas1=-384.5623737\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2Lar
geXP=-383.288717\MP2/GTMP2LargeXP=-384.8636685\HF/GFHFB3=-383.2915118\
HF/GFHFB4=-383.3181022\G4MP2=-385.1058768\FreqCoord=8.6843808435,7.171
9826536,4.353223383,8.3821180399,6.1890205913,6.666012963,6.7155032895
,5.4439594365,3.11676923,6.3597289769,4.287433505,5.8382053468,7.26673
81091,1.8031161706,4.6563162985,3.7695555598,4.4341549598,6.9555091885
,7.5692162951,2.7860210931,2.3435306338,4.429532997,6.5795536708,1.906
9496502,2.2065372524,6.5864104684,3.1256581568,1.8754101271,5.51001239
32,5.6586863287,9.9041294835,8.6259108779,3.5798684808,9.2634255533,6.
54242951,8.4821000999,7.5854871478,-0.0554023865,5.4588611086,3.455070
8669,3.6548606035,8.8307939491,8.2265944992,2.0279721639,0.5566365556,
4.6056975107,7.3952236411,0.0290403619,0.5554859261,7.4159988375,2.231
3766042,-0.0007033889,5.6079882649,6.4860469793\PG=C01 [X(C10H8)]\NIma
g=0\

1, 2, 3, 4-tetrahydrochrysene

1\1\GINC-SAW190\Mixed\G4MP2\G4MP2\C18H16\KFOREST\29-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,-1.8719874047,-1.7509342899,-0.0420146457\C,0,-1.8828
62505,-0.3285797687,0.0064055559\C,0,-3.0907125332,-2.4635748037,-0.05
98044386\C,0,-0.6190021618,-2.4360074581,-0.0736069515\C,0,-3.14052357
2,0.3154774034,0.0372781677\C,0,-0.6197387234,0.3921279064,0.021509696
4\C,0,-4.319237502,-0.40097954,0.0200521045\C,0,-4.2993140055,-1.80507
99197,-0.0297444614\C,0,0.5589036934,-1.7615206585,-0.0473314303\C,0,0
.6096365787,-0.3279351016,0.0069212069\C,0,1.8583069073,0.3665831239,0
.0333645688\C,0,-0.5575644849,1.8020197405,0.0430939755\C,0,1.87307506
75,1.7552735752,0.0350805331\C,0,3.1574654137,-0.4237933774,0.03437386
11\C,0,0.6497447085,2.4554341286,0.0415354493\C,0,3.1607815088,2.55675
86244,0.0355147671\C,0,4.3767407866,1.740470862,-0.4067075641\C,0,4.40
14523522,0.4150548459,0.3545254769\H,0,-3.0551572133,-3.5484383601,-0.
0972886649\H,0,-0.6274738857,-3.521198566,-0.118695138\H,0,-3.19325380
52,1.3962795894,0.0783770311\H,0,-5.2679293563,0.1251002672,0.04540146
66\H,0,-5.229680404,-2.3628409262,-0.0434573336\H,0,1.4845363225,-2.32
14945895,-0.0796988601\H,0,-1.4679161127,2.3882393259,0.047153264\H,0,
3.2868996539,-0.9000018886,-0.948615288\H,0,3.0904717932,-1.2474047732
,0.7534969927\H,0,0.6708401821,3.5418597205,0.0431901976\H,0,3.3387524
34,2.9466970262,1.0487631341\H,0,3.0338381888,3.4392605894,-0.60250880
34\H,0,5.2965078963,2.3096552369,-0.2353455903\H,0,4.3200021794,1.5435
064679,-1.4853907666\H,0,5.3017216218,-0.1613688664,0.1165352069\H,0,4
.4379963808,0.6227844538,1.4321872804\Version=EM64L-G09RevB.01\State=
1-A\MP2/GTBas1=-693.2832364\CCSD(T)/GTBas1=-693.4832241\MP2/GTBas2=0.\
MP2/GTBas3=0.\HF/GTMP2LargeXP=-691.1856421\MP2/GTMP2LargeXP=-694.05259
99\HF/GFHFB3=-691.1920712\HF/GFHFB4=-691.2408005\G4MP2=-694.4540268\Fr
eqCoord=-3.5375435191,-3.3087862847,-0.0793961739,-3.5580944804,-0.620
9257756,0.0121047464,-5.8406002432,-4.6554816868,-0.1130140104,-1.1697
445615,-4.6033869535,-0.1390969798,-5.9347294649,0.5961658935,0.070445
5277,-1.1711364612,0.7410143521,0.0406474355,-8.1621759817,-0.75774151
56,0.0378929859,-8.1245260296,-3.4111066963,-0.0562088861,1.0561749152
, -3.328791622,-0.0894434408,1.1520461744,-0.6197075313,0.0130791855,3.
5116911257,0.6927417092,0.0630498975,-1.0536441778,3.4053237956,0.0814
358117,3.539598904,3.3169863454,0.0662926002,5.9667449059,-0.800853420
2,0.0649571837,1.2278395554,4.6400980405,0.078490624,5.9730114176,4.83
1573588,0.0671131834,8.2708414414,3.2890132714,-0.7685659123,8.3175395
327,0.7843399889,0.6699560585,-5.773410426,-6.7055767,-0.1838489326,-1
.1857537995,-6.6541009492,-0.2243013042,-6.0343751646,2.638586029,0.14
8111124,-9.9549437708,0.2364052442,0.085796338,-9.8826637261,-4.465122
246,-0.082122459,2.8053670838,-4.3869889932,-0.1506090188,-2.773959439
1,4.5131182658,0.0891067552,6.2113401722,-1.7007570885,-1.7926230998,5
.8401453105,-2.3572533982,1.4239029581,1.2677042231,6.6931448728,0.081
6176451,6.3093277258,5.5684503761,1.9818751017,5.7331233082,6.49926061
37,-1.1385766312,10.0089493847,4.3646158591,-0.4447387122,8.1636210125
,2.9168045087,-2.8069817491,10.0188018981,-0.3049429639,0.2202196258,8
.3865977384,1.1768920575,2.7064417309\PG=C01 [X(C18H16)]\NImag=0\

1,2-benzofluorene

1\1\GINC-SAW55\Mixed\G4MP2\G4MP2\C17H12\KFOREST\29-Jan-2011\0\#\# G4MP2
\name\0,1\C,0,2.9208676911,1.5545147318,5.0239603192\C,0,3.796001196
2,1.8514800377,6.0609376655\C,0,3.2917051694,1.74649098,3.673470359\C,
0,1.6130128563,1.0329301257,5.5786829277\C,0,3.1423708915,1.5538304353
,7.3389708242\C,0,5.0886550076,2.3565526758,5.794897782\C,0,4.60537182
57,2.2596134011,3.4074513068\C,0,2.437207402,1.4595948193,2.5779134751
\C,0,1.8473656297,1.0674957718,7.0735066806\C,0,3.5931756769,1.6780555
634,8.6512491798\C,0,5.4752711864,2.5527829101,4.4929323398\C,0,4.9982
866943,2.4598982738,2.060993047\C,0,2.8529578205,1.6666421068,1.285125
1696\C,0,1.0043200215,0.7061377501,8.1122737294\C,0,2.7411405053,1.313
1560747,9.6925428968\C,0,4.1462864522,2.1718511959,1.0224151422\C,0,1.
4584202203,0.8315076036,9.4278673309\H,0,0.7596706246,1.6574101143,5.2
826310452\H,0,1.3874476462,0.0191148393,5.2221366318\H,0,5.7668836189,
2.5862678953,6.610217709\H,0,1.443002618,1.0714521931,2.7739227915\H,0
,4.5893982227,2.0518228158,8.8650483821\H,0,6.4647559442,2.9401557125,
4.2688330026\H,0,5.9931377242,2.8483590985,1.8632094492\H,0,2.18722353
64,1.44213573,0.4581672854\H,0,0.0051093877,0.3307003132,7.9126878062\
H,0,3.0785889972,1.4044823691,10.7198431723\H,0,4.462852299,2.33102219
75,-0.0029864207\H,0,0.808313134,0.5520622643,10.2503189695\Version=E
M64L-G09RevB.01\State=1-A\MP2/GTBas1=-652.9344717\CCSD(T)/GTBas1=-653.
1103984\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-650.9689431\MP2/G
TMP2LargeXP=-653.6315101\HF/GFHFB3=-650.9769145\HF/GFHFB4=-651.0209259
\G4MP2=-654.0185699\FreqCoord=5.5196400066,2.9376071126,9.4939091057,7
.173402661,3.4987902118,11.4535122963,6.2204212803,3.3003896458,6.9418
529357,3.0481525472,1.9519550519,10.5421829156,5.9382203929,2.93631397
97,13.8686449549,9.6161643491,4.453239175,10.9507697761,8.7028914907,4
.2700504944,6.4391497811,4.6056545188,2.7582344735,4.8715504622,3.4910
151075,2.0172746566,13.3669904254,6.7901179767,3.1710654506,16.3484916
572,10.3467630456,4.8240605767,8.4904116558,9.4453929859,4.6485340522,
3.8947124205,5.3913089493,3.1494971435,2.428534617,1.8978897904,1.3344
069598,15.3299756636,5.1800048467,2.481505351,18.3162516063,7.83534586
31,4.1042039617,1.9320846129,2.7560148031,1.5713216482,17.8160872726,1
.4355694317,3.1320512059,9.9827259366,2.621896075,0.0361218113,9.86840
80626,10.89783068,4.8873380284,12.4915011488,2.726879757,2.0247512094,
5.2419543898,8.6727057556,3.8773831951,16.752513597,12.2166182506,5.55
60890846,8.066925282,11.3253889753,5.3826186242,3.5209555871,4.1332534
751,2.7252415761,0.8658106925,0.0096553435,0.6249330241,14.9528129288,
5.8176900805,2.654087036,20.2575677831,8.4335686166,4.4049935629,-0.00
56435172,1.5274904528,1.0432464879,19.3702956271\PG=C01 [X(C17H12)]\NI
mag=0\

1,2-cyclopentenophenanthrene

```
1\1\GINC-SAW185\Mixed\G4MP2\G4MP2\C17H14\KFOREST\28-Jan-2011\0\#\# G4MP
2\name\0,1\C,0,-3.9708941719,-0.5477509583,-0.0998696471\C,0,-3.8524
243023,-1.9471733507,-0.0778413172\C,0,-2.6008622189,-2.5193168851,-0.
0272552989\C,0,-2.8454183767,0.2497472794,-0.070154379\C,0,-1.54679600
45,-0.3039159936,-0.0171658913\C,0,-1.4347378405,-1.7241870268,0.00331
80123\C,0,-0.1391986152,-2.3302647139,0.0547622606\C,0,0.9902935117,-1
.5790382444,0.0805481279\C,0,-0.3374654789,0.5046271522,0.0184931249\C
,0,0.9322482424,-0.1475207943,0.0617080893\C,0,0.792265257,2.669567595
8,0.0531882681\C,0,-0.3652918171,1.9178717874,0.0143972437\C,0,2.03515
84714,2.0243608842,0.0866101589\C,0,2.1018903429,0.6421544718,0.085441
7015\C,0,3.5422506247,0.1769247836,0.1455588147\C,0,4.3413362406,1.454
0113304,-0.2182487061\C,0,3.4153442633,2.6363855594,0.1591046171\H,0,-
4.9533938768,-0.0890020948,-0.1406665454\H,0,-4.7405354733,-2.56970569
41,-0.1010512931\H,0,-2.4902340742,-3.5996053318,-0.0102356156\H,0,-2.
9727697614,1.3250290911,-0.0895431077\H,0,-0.0806473051,-3.4145984967,
0.0715927579\H,0,1.962244013,-2.0584721681,0.1215682341\H,0,0.73449578
74,3.753835846,0.0513629542\H,0,-1.3157029318,2.436052,-0.0183525381\H
,0,3.7912827917,-0.1742089153,1.1570100262\H,0,3.7605351797,-0.6536396
375,-0.5333323504\H,0,4.5228391813,1.4687585228,-1.2980174066\H,0,5.31
50694693,1.5001618726,0.2756572517\H,0,3.5400721305,3.5003020299,-0.50
18498591\H,0,3.6210867416,2.9913300987,1.1787223124\Version=EM64L-G09
RevB.01\State=1-A\MP2/GTBas1=-654.1130328\CCSD(T)/GTBas1=-654.2968579\
MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-652.1372081\MP2/GTMP2Larg
eXP=-654.8282046\HF/GFHFB3=-652.1439717\HF/GFHFB4=-652.1892482\G4MP2=-
655.2100054\FreqCoord=-7.5039024875,-1.0350993002,-0.1887262819,-7.280
026879,-3.679624366,-0.1470987713,-4.914917303,-4.7608189549,-0.051505
0505,-5.3770614654,0.4719539605,-0.1325725634,-2.9230208319,-0.5743179
952,-0.0324388334,-2.711261591,-3.2582412824,0.0062701346,-0.263047260
9,-4.4035621264,0.103485675,1.8713835283,-2.9839498352,0.1522139023,-0
.6377173344,0.9536071169,0.0349469413,1.761693866,-0.2787739002,0.1166
11389,1.4971643603,5.0447516492,0.1005112602,-0.6903014929,3.624252436
2,0.0272068476,3.8458921479,3.8254876652,0.1636694807,3.9719971095,1.2
134960868,0.1614614162,6.6938835747,0.334339387,0.2750662961,8.2039365
454,2.7476832086,-0.4124302833,6.4540653072,4.982046688,0.3006641527,-
9.3605578555,-0.1681895844,-0.2658212468,-8.9583137679,-4.856040004,-0
.1909592693,-4.705860407,-6.8022682635,-0.0193425102,-5.6177207053,2.5
039421003,-0.1692119507,-0.1524013199,-6.4526560126,0.1352907055,3.708
1037905,-3.8899486499,0.2297306688,1.387995884,7.0937216968,0.09706191
68,-2.4863182134,4.6034711255,-0.0346812709,7.1644861687,-0.3292071397
,2.1864320825,7.1063816027,-1.2351999045,-1.00785208,8.5469273958,2.77
55513634,-2.4528974142,10.0440256742,2.8348950942,0.5209167122,6.68976
68173,6.614612219,-0.9483587935,6.8428622451,5.6527946596,2.2274623571
\PG=C01 [X(C17H14)]\NImag=0\
```

1,2-dihydroanthracene

1\1\GINC-BUL27\Mixed\G4MP2\G4MP2\C14H12\KFOREST\17-Dec-2010\0\#\# G4MP2
\name\0,1\C,0,-2.4302470357,-1.3912634424,0.0372601152\C,0,-1.191599
8216,-0.7049313638,-0.0270474003\C,0,-3.6150528754,-0.7010870539,0.128
900846\C,0,0.0499979199,-1.3799375559,-0.1145919595\C,0,1.2463604842,-
0.6967245151,-0.1694970142\C,0,2.5316598705,-1.3940383679,-0.200249663
4\C,0,3.6883054584,-0.7642959372,0.0402349742\C,0,-3.6150760276,0.7113
396488,0.1612836146\C,0,-1.1923013263,0.7245150919,0.0056053638\C,0,1.
24199936,0.7362862952,-0.1619606551\C,0,3.7312254478,0.7123665761,0.33
88445764\C,0,-2.4297414505,1.4056220312,0.1013582656\C,0,0.0510500882,
1.4073949865,-0.0682773882\C,0,2.5648299818,1.4483685972,-0.3389980371
\H,0,-2.4259041617,-2.4770885455,0.0135187205\H,0,-4.5561814609,-1.238
8860105,0.1775014406\H,0,0.0530127764,-2.4670799158,-0.1228489445\H,0,
2.512257539,-2.4666583106,-0.3744231635\H,0,4.6198387272,-1.3222094396
,0.0666572935\H,0,-4.5562277023,1.2463767534,0.2339663648\H,0,4.682915
1568,1.1442995679,0.0112237499\H,0,3.6922610583,0.8612899859,1.4291223
056\H,0,-2.4265819989,2.4914927676,0.1251616636\H,0,0.0441177853,2.494
8144027,-0.0602961349\H,0,2.4942489561,2.4800950805,0.0194635719\H,0,2
.780503251,1.5055886732,-1.4162925051\\Version=AM64L-G09RevB.01\State=
1-A\MP2\GTBas1=-538.9303548\CCSD(T)/GTBas1=-539.0887451\MP2\GTBas2=0.\
MP2\GTBas3=0.\HF/GTMP2LargeXP=-537.312033\MP2\GTMP2LargeXP=-539.524367
9\HF/GFHFB3=-537.3173976\HF/GFHFB4=-537.355092\G4MP2=-539.8440544\Freq
Coord=-4.5925013327,-2.6291068848,0.0704114133,-2.2517973229,-1.332127
22,-0.0511121791,-6.8314598904,-1.3248625271,0.2435872971,0.0944823759
, -2.6077040611,-0.2165474206,2.3552799781,-1.3166185237,-0.3203029372,
4.7841438169,-2.634350734,-0.378417022,6.9698872109,-1.4443100058,0.07
60330822,-6.8315036417,1.3442371236,0.3047818613,-2.2531229747,1.36913
51029,0.0105926024,2.3470386476,1.3913794533,-0.3060612825,7.050994236
4,1.346177735,0.6403234509,-4.5915459151,2.6562406853,0.1915393633,0.0
964706857,2.6595910853,-0.1290255648,4.8468262431,2.7370199883,-0.6406
134498,-4.5842944903,-4.681018958,0.0255466794,-8.6099351728,-2.341155
2697,0.3354291109,0.1001796288,-4.6621053888,-0.2321508608,4.747478723
9,-4.6613086705,-0.7075572369,8.7302299725,-2.4986137312,0.1259640294,
-8.6100225565,2.3553107224,0.4421323537,8.8494271499,2.1624127974,0.02
12098134,6.9773622114,1.6276021943,2.700649768,-4.5855754169,4.7082389
928,0.2365212666,0.0833705318,4.7145159735,-0.1139431818,4.7134474343,
4.6867004857,0.0367808204,5.254389656,2.8451502611,-2.6764049587\PG=C0
1 [X(C14H12)]\NImag=0\

1,2-dihydrobenz[j]aceanthrylene

1\1\GINC-SAW186\Mixed\G4MP2\G4MP2\C20H14\KFOREST\31-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,1.0683140819,3.0715576003,-0.0249672836\C,0,2.6350632
681,3.1332848737,-0.0249536517\C,0,3.0812730284,1.683211024,-0.0151441
396\C,0,3.2729751757,-1.1364282379,0.0032658411\C,0,4.3914208571,-0.33
53538656,-0.00108061\C,0,4.315161543,1.0892351593,-0.0103625353\C,0,1.
9296931816,0.8619983599,-0.0106533465\C,0,0.7410593049,1.5895146947,-0
.0159832365\C,0,0.7381561322,-1.2213427001,0.0019794564\C,0,1.97368600
99,-0.5523703293,-0.0014744524\C,0,-0.4766382473,-0.5292135345,-0.0033
414786\C,0,-0.480584467,0.9211635266,-0.0124588659\C,0,-1.7307888012,1
.6276372471,-0.0173767915\C,0,-2.9135409687,0.9713541395,-0.0136825751
\C,0,-1.7672770745,-1.2231029936,0.0000817425\C,0,-2.9714155711,-0.464
5625101,-0.00496154\C,0,-4.2153914896,-1.1261643936,-0.0015266872\C,0,
-4.2935582987,-2.5033903112,0.0065781763\C,0,-3.1124354511,-3.25766658
48,0.0113947532\C,0,-1.8818877463,-2.6281485807,0.0081809753\H,0,0.648
9195136,3.5732313786,-0.9044633981\H,0,0.6485733669,3.5837612397,0.848
284524\H,0,3.0133570128,3.6644041642,-0.9049973701\H,0,3.0130042906,3.
6763309665,0.847919695\H,0,3.3749433548,-2.217394906,0.0103349096\H,0,
5.3731721775,-0.7989023036,0.002656374\H,0,5.2306254346,1.6724476437,-
0.0134560702\H,0,0.7465362544,-2.3048736681,0.0091235298\H,0,-1.706422
386,2.7125001933,-0.0241019729\H,0,-3.8507359416,1.5199157948,-0.01736
54933\H,0,-5.1201066431,-0.5252635934,-0.0054658272\H,0,-5.2587176191,
-2.9985895477,0.0091362204\H,0,-3.1606364813,-4.3415825181,0.017643858
7\H,0,-0.9902368012,-3.2425174276,0.0119072698\Version=EM64L-G09RevB.
01\State=1-A\MP2/GTBas1=-768.096526\CCSD(T)/GTBas1=-768.30187\MP2/GTBas
2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-765.7749149\MP2/GTMP2LargeXP=-768
.9151821\HF/GFHFB3=-765.7841915\HF/GFHFB4=-765.8358062\G4MP2=-769.3682
383\FreqCoord=2.0188210387,5.8044026659,-0.0471813283,4.9795479195,5.9
210503077,-0.0471555677,5.8227621643,3.1808078593,-0.0286182764,6.1850
267217,-2.1475381392,0.0061715453,8.2985827541,-0.6337269636,-0.002042
057,8.1544735354,2.0583561453,-0.0195823539,3.6465916336,1.6289408272,
-0.0201319073,1.4003991345,3.0037474572,-0.0302039398,1.3949129331,-2.
3080032176,0.0037406304,3.729726031,-1.0438286462,-0.0027863113,-0.900
7157519,-1.0000686459,-0.0063144794,-0.9081730263,1.7407467889,-0.0235
438445,-3.2707168281,3.0757886406,-0.032837377,-5.5057945078,1.8355933
016,-0.0258563197,-3.3396696718,-2.3113296902,0.0001544709,-5.61516165
63,-0.8778959156,-0.0093759519,-7.9659354583,-2.1281422844,-0.00288502
07,-8.1136493201,-4.7307220919,0.0124309516,-5.8816506089,-6.156097677
5,0.0215329628,-3.5562524533,-4.966481054,0.0154598029,1.226280163,6.7
524287151,-1.7091881197,1.2256260405,6.7723272687,1.6030254331,5.69441
94949,6.9247203105,-1.7101971804,5.6937529465,6.9472587005,1.602336006
2,6.3777186547,-4.1902691009,0.0195301487,10.1538238803,-1.5097065607,
0.0050198193,9.8844495752,3.1604680182,-0.0254282875,1.4107490691,-4.3
555800037,0.0172409727,-3.2246709766,5.1258825008,-0.045546128,-7.2768
363397,2.8722245971,-0.0328160265,-9.6755993266,-0.9926043391,-0.01032
89165,-9.9375361103,-5.6665130301,0.0172649544,-5.9727373553,-8.204401
9425,0.0333420608,-1.871276361,-6.1274699193,0.022501479\PG=C01 [X(C20
H14)]\NImag=0\

1,2-dihydrophenanthrene

1\1\GINC-SAW59\Mixed\G4MP2\G4MP2\C14H12\KFOREST\26-Jan-2011\0\#\# G4MP2
\name\0,1\C,0,0.7871810762,-1.458875953,0.1324279471\C,0,2.082483279
5,-2.2265153656,0.2970188763\C,0,0.8134663716,-0.0668733027,0.16042982
1\C,0,-0.4392091759,-2.1444538739,0.019789585\C,0,3.2769484059,-1.4977
247586,-0.3301969679\C,0,3.2677888074,-0.0457977115,0.0707298808\C,0,2
.1153599919,0.597811152,0.2950106115\C,0,-0.4133671278,0.6688617772,0.
058124105\C,0,-1.6275560728,-1.4634802036,-0.0651009917\C,0,-1.6495805
848,-0.0486456212,-0.0493316099\C,0,-2.8683031179,0.6707004933,-0.1441
902803\C,0,-0.4723685585,2.0881104913,0.0458999582\C,0,-1.6696474694,2
.7555299495,-0.0485034435\C,0,-2.8846605032,2.0422429857,-0.1410217261
\H,0,1.9801636757,-3.2332067063,-0.1207439682\H,0,2.2764658445,-2.3545
271769,1.3732975096\H,0,-0.4324918323,-3.2306646612,0.004642181\H,0,3.
2338904652,-1.573058936,-1.4283658277\H,0,4.2126010345,-1.9798092309,-
0.0289691858\H,0,4.2132560764,0.4835794493,0.1414788672\H,0,2.13700837
23,1.6459841801,0.5700118276\H,0,-2.567206602,-2.00087765,-0.150618764
1\H,0,-3.7938656976,0.1078588038,-0.2229267975\H,0,0.4441189327,2.6624
565975,0.0988105284\H,0,-1.6824783553,3.8405928577,-0.0551334514\H,0,-
3.8237772365,2.580532414,-0.2138286843\Version=EM64L-G09RevB.01\State
=1-A\MP2/GTbas1=-538.927362\CCSD(T)/GTbas1=-539.0852072\MP2/GTbas2=0.\
MP2/GTbas3=0.\HF/GTimp2LargeXP=-537.3066764\MP2/GTimp2LargeXP=-539.52212
58\HF/GFHFB3=-537.3119369\HF/GFHFB4=-537.3496749\G4MP2=-539.8412174\Fr
eqCoord=1.487556651,-2.756876013,0.2502525524,3.9353230746,-4.20750427
17,0.5612843324,1.5372286607,-0.1263722276,0.3031684252,-0.8299850574,
-4.0524305264,0.0373968959,6.1925350388,-2.8302896162,-0.6239818393,6.
1752259062,-0.0865451323,0.1336601041,3.9974510571,1.1296993565,0.5574
89262,-0.7811506638,1.2639655798,0.1098386401,-3.0756352434,-2.7655767
858,-0.1230230453,-3.1172555394,-0.0919269016,-0.0932232325,-5.4203073
589,1.2674402496,-0.2724801407,-0.8926472093,3.9459569638,0.0867383506
, -3.1551764556,5.2071969554,-0.0916582248,-5.4512183373,3.8592799397,-
0.2664924411,3.7419670453,-6.109875206,-0.2281730321,4.3018969969,-4.4
494115368,2.5951561921,-0.8172911178,-6.1050714369,0.0087724508,6.1111
673229,-2.9726505798,-2.6992202319,7.9606622623,-3.7412972418,-0.05474
38275,7.9619001121,0.9138327227,0.2673563126,4.0383605674,3.1104593195
,1.0771662467,-4.8513174043,-3.7811107839,-0.2846282147,-7.1693671533,
0.2038236003,-0.4212705949,0.8392631532,5.0313138099,0.1867248376,-3.1
794233161,7.2576686889,-0.104187124,-7.2258917701,4.8764995394,-0.4040
776527\PG=C01 [X(C14H12)]\NImag=0\

1,4-diethynylbenzene

1\1\GINC-SAW289\Mixed\G4MP2\G4MP2\C10H6\KFOREST\19-Jan-2011\0\#\# G4MP2
\name\0,1\C,0,3.6560876514,2.1636449916,0.1284317461\C,0,4.374542968
1,3.3710095132,0.1405568398\C,0,4.3702859278,0.954378018,0.0878300702\
C,0,2.2331801448,2.1655343371,0.1567144755\C,0,5.7594013422,3.36917073
6,0.1130307368\C,0,6.4735997642,2.159903902,0.072428991\C,0,5.75514464
86,0.9525391725,0.0603039401\C,0,7.8965073104,2.1580143629,0.044147265
8\C,0,1.0288637633,2.167135074,0.1806546288\C,0,9.1008238074,2.1564168
168,0.0202114028\H,0,3.8316903567,4.3085465694,0.1718193728\H,0,3.8241
330522,0.0182867203,0.0782132298\H,0,6.305554366,4.3052617604,0.122647
8112\H,0,6.2979972599,0.0150019409,0.029041652\H,0,-0.0327693557,2.168
5454153,0.201760902\H,0,10.1624569927,2.1550106695,-0.0008930646\Vers
ion=EM64L-G09RevB.01\State=1-A\MP2/GTbas1=-383.3003456\CCSD(T)/GTbas1=
-383.4046583\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-382.1690592\
MP2/GTMP2LargeXP=-383.7023491\HF/GFHFB3=-382.1737215\HF/GFHFB4=-382.19
92819\G4MP2=-383.9448492\FreqCoord=6.909004379,4.0886964828,0.24270082
69,8.2666881662,6.3702847713,0.2656139332,8.2586435259,1.8035130813,0.
1659747789,4.220098879,4.0922668285,0.2961474398,10.8836912262,6.36680
99859,0.2135971372,12.2333306483,4.0816268482,0.136870957,10.875647241
,1.8000381669,0.1139579315,14.922236223,4.0780561367,0.0834262418,1.94
42707407,4.0952917827,0.3413877731,17.1980645796,4.0750372122,0.038194
0161,7.2408454002,8.141973047,0.3246915589,7.2265641643,0.0345568933,0
.1478015842,11.9157708677,8.1357656576,0.231770774,11.9014900069,0.028
3495598,0.0548807688,-0.0619251078,4.0979569417,0.381272849,19.2042605
535,4.0723799787,-0.0016876475\PG=C01 [X(C10H6)]\NImag=0\

1,4-dihydro-1,4-ethenoanthracene

1\1\GINC-SAW61\Mixed\G4MP2\G4MP2\C16H12\KFOREST\27-Jan-2011\0\#\ G4MP2
\name\0,1\C,0,0.5102918485,0.9184240982,0.2636295516\C,0,1.001394856
8,-0.2077197294,-0.4570871332\C,0,2.4448923361,0.0027607704,-0.9268158
93\C,0,0.2143275667,-1.3025375414,-0.6598377919\C,0,1.5614741431,2.028
5683144,0.369780898\C,0,-0.7572258843,0.9253800927,0.7661825864\C,0,3.
234027931,0.3080497996,0.3515928106\C,0,2.4054425314,1.2937692069,-1.7
52944485\C,0,-1.1175405169,-1.3326060386,-0.1492942081\C,0,1.946935392
6,2.3451850989,-1.0799978407\C,0,2.7755625807,1.3595290767,1.024514879
\C,0,-1.6106918237,-0.201713637,0.574634413\C,0,-1.9695743731,-2.44665
43053,-0.3353717595\C,0,-2.932358021,-0.2387534166,1.0781382396\C,0,-3
.2507536706,-2.4524484706,0.1667827283\C,0,-3.7369277179,-1.3375111731
,0.8806271089\H,0,2.8315981004,-0.8527723506,-1.4799209303\H,0,0.58486
48084,-2.1639257159,-1.2092364114\H,0,1.1968304172,2.8959582965,0.9193
916924\H,0,-1.1360831826,1.7824589093,1.3166433215\H,0,4.0632710495,-0
.3187601405,0.6542470182\H,0,2.706147883,1.2955760464,-2.7929948537\H,
0,1.8142316691,3.340863516,-1.4839070109\H,0,3.171586894,1.7262371652,
1.9630392493\H,0,-1.5920215096,-3.3037213555,-0.8857036169\H,0,-3.3037
235045,0.6216676391,1.6274457286\H,0,-3.8909468203,-3.315266267,0.0149
017562\H,0,-4.748202984,-1.3492878887,1.2737599529\Version=EM64L-G09R
evB.01\State=1-A\MP2/GTBas1=-614.8783857\CCSD(T)/GTBas1=-615.0517847\M
P2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-613.019552\MP2/GTMP2LargeX
P=-615.5428874\HF/GFHFB3=-613.0254668\HF/GFHFB4=-613.0673622\G4MP2=-61
5.9100078\FreqCoord=0.9643118415,1.7355700194,0.4981876531,1.892362030
2,-0.392533401,-0.8637695006,4.6201769397,0.0052171,-1.7514282134,0.40
50204038,-2.461439231,-1.2469127187,2.9507584941,3.833438556,0.6987846
264,-1.4309495421,1.7487149441,1.447875256,6.1114270957,0.5821297565,0
.6644141223,4.5456276128,2.4448694802,-3.3125850028,-2.1118455193,-2.5
18260456,-0.2821251664,3.6791746904,4.4317575679,-2.040900143,5.245053
1423,2.5691376247,1.9360525405,-3.0437664314,-0.3811835312,1.085901667
1,-3.7219561634,-4.6235065788,-0.6337607783,-5.5413535832,-0.451178570
6,2.0373860062,-6.1430341628,-4.6344559645,0.3151736803,-7.0617699652,
-2.5275298169,1.664144061,5.3509449281,-1.6115061964,-2.7966452566,1.1
052343126,-4.089226975,-2.2851256474,2.2616817159,5.4725680726,1.73739
85075,-2.1468860793,3.3683591817,2.4880952923,7.6784694872,-0.60236936
77,1.2363476876,5.1138783739,2.448283912,-5.277995364,3.4284009962,6.3
133170926,-2.8041778572,5.9934306364,3.2621154827,3.7096065693,-3.0084
846509,-6.2431285812,-1.6737372708,-6.2431326424,1.1747815835,3.075426
7232,-7.352823888,-6.2649453022,0.028160238,-8.9728032631,-2.549784584
1,2.40705747\PG=C01 [X(C16H12)]\NImag=0\

1,4-dihydro-1,4-ethenonaphthalene

1\1\GINC-SAW329\Mixed\G4MP2\G4MP2\C12H10\KFOREST\22-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,3.3044162481,3.2388351602,1.6765278508\C,0,3.53177827
77,1.9368333785,2.1428686765\C,0,4.5804094001,4.089208472,1.6918185926
\C,0,2.0415583266,3.6273028727,1.2690467009\C,0,4.9952625458,1.7135329
587,2.5427171857\C,0,2.4964556911,1.0223063982,2.2020834026\C,0,5.5945
820186,3.3031164783,0.8484486069\C,0,5.0793418629,4.0349801081,3.14298
57606\C,0,0.9893242944,2.7027589335,1.3276591788\C,0,5.2949377544,2.80
03687286,3.5851878276\C,0,5.8101751286,2.0685041697,1.2906499957\C,0,1
.2146221835,1.412576943,1.7897661103\H,0,4.4119441312,5.1034674251,1.3
304828607\H,0,1.8645816908,4.6360644503,0.9075522479\H,0,5.1803631946,
0.7030821032,2.9065746435\H,0,2.6718521439,0.0131829549,2.5633383344\H
,0,6.0501256525,3.7472755773,-0.0274292589\H,0,5.2088231534,4.94228762
36,3.7191688029\H,0,-0.0046975315,2.9997171592,1.0097335271\H,0,5.6288
635716,2.5369204405,4.580701868\H,0,6.4701615424,1.3419084033,0.834101
8866\H,0,0.3967384273,0.7008696763,1.8331165005\Version=EM64L-G09RevB
.01\State=1-A\MP2/GTbas1=-461.7187945\CCSD(T)/GTbas1=-461.8546343\MP2/
GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-460.3230651\MP2/GTMP2LargeXP=
-462.2272256\HF/GFHFB3=-460.3266395\HF/GFHFB4=-460.3588045\G4MP2=-462.
5030792\FreqCoord=6.244441738,6.1205114424,3.1681784921,6.6740937069,3
.6600846504,4.0494349373,8.6557193427,7.7274841123,3.1970738065,3.8579
861216,6.8546090304,2.3981507145,9.4396781734,3.2381080115,4.805039114
4,4.7176175591,1.9318791165,4.1613345527,10.5722278431,6.2419855291,1.
6033355048,9.5985650562,7.6250073559,5.9393823272,1.8695519729,5.10747
41875,2.5089122457,10.0059822465,5.2919299682,6.7750231292,10.97963977
71,3.9089063855,2.4389750253,2.2953032817,2.6693835639,3.3821677905,8.
3373661215,9.6441557616,2.5142482313,3.523548748,8.7608921455,1.715025
1998,9.7894677067,1.3286326239,5.4926300611,5.0490688195,0.0249121744,
4.844007438,11.4330805527,7.0813245855,-0.0518337873,9.8432492345,9.33
95700786,7.0282104795,-0.0088770481,5.6686439071,1.9081198335,10.63701
05896,4.7940848534,8.6562720269,12.2268333506,2.5358393777,1.576224132
7,0.749726974,1.324451743,3.4640881556\PG=C01 [X(C12H10)]\NImag=0\

1, 4-dihydro-1, 4-methanonaphthalene

1\1\GINC-SAW94\Mixed\G4MP2\G4MP2\C11H10\KFOREST\20-Jan-2011\0\#\# G4MP2
\name\0,1\C,0,3.8151523254,1.9283221715,1.875051759\C,0,3.2696053846
,3.0962691777,2.4378037204\C,0,4.4598368724,3.9875373585,2.8121755014\
C,0,1.9042320534,3.2554963519,2.5559805621\C,0,5.3375549371,2.10845362
81,1.9067760582\C,0,2.9998165026,0.9099883427,1.4258444381\C,0,5.45221
91885,2.8710719862,3.2632663237\C,0,5.1375393735,4.3825253195,1.488317
0929\C,0,1.0703529693,2.2219473441,2.0992563312\C,0,5.6549077934,3.274
9027422,0.9546305868\C,0,1.6093456297,1.0680321591,1.5432654131\H,0,4.
2505273582,4.7979049191,3.5098443629\H,0,1.4765162724,4.1514298284,2.9
957183778\H,0,5.9297234535,1.2029587085,1.7776896004\H,0,3.414354291,0
.002763346,0.9967661568\H,0,6.4597107344,3.2496685197,3.4542088752\H,0
,5.0898295848,2.2905606544,4.1167614075\H,0,5.1053907468,5.3755872266,
1.060214635\H,0,-0.0065132554,2.3261107997,2.1843482883\H,0,6.13921955
8,3.1622859991,-0.0062214396\H,0,0.9499782265,0.2783834171,1.197691948
9\Version=EM64L-G09RevB.01\State=1-A\MP2/GTbas1=-423.7353399\CCSD(T)/
GTbas1=-423.8614354\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-422.4
533864\MP2/GTMP2LargeXP=-424.2089747\HF/GFHFB3=-422.4563677\HF/GFHFB4=
-422.4861756\G4MP2=-424.457502\FreqCoord=7.2095930503,3.6440008,3.5433
343095,6.1786587396,5.8511007796,4.6067813973,8.4278702862,7.535353552
2,5.3142415352,3.5984770743,6.1519965317,4.8301032633,10.0865170503,3.
9843999209,3.6032845467,5.6688316387,1.7196287518,2.6944554961,10.3032
010827,5.4255397616,6.1666796505,9.7085424127,8.2817726243,2.812511704
6,2.0226739776,4.1988719621,3.9670195486,10.6862270362,6.1886692946,1.
8039903672,3.0412224932,2.0182882818,2.9163489811,8.0323326274,9.06672
63087,6.6326446149,2.7902113855,7.8450654355,5.6610873053,11.205553370
9,2.2732625082,3.3593464941,6.4521945307,0.0052219672,1.8836150549,12.
2070841856,6.140983525,6.5275087798,9.6183839783,4.3285323275,7.779551
6146,9.6477903128,10.1583876618,2.0035153021,-0.012308269,4.3957123662
,4.1278200438,11.6014436343,5.9758544922,-0.011756817,1.7951986802,0.5
260684182,2.2633097749\PG=C01 [X(C11H10)]\NImag=0\

1,8-dihydro-as-indacene

1\1\GINC-SAW262\Mixed\G4MP2\G4MP2\C12H10\KFOREST\26-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,-1.6419377113,1.2576067423,0.0171921181\C,0,-0.390719
4965,2.0889554662,0.022216483\C,0,0.8690330387,1.2904904675,0.01286764
15\C,0,0.896929554,-0.0712678942,0.0008361504\C,0,2.299272076,-0.51785
18739,-0.0056765353\C,0,3.1074953657,0.5549669487,0.0022571795\C,0,2.2
784043653,1.8167874058,0.0148929298\C,0,-0.3205067416,-0.8320951061,-0
.0036167321\C,0,-1.6032982907,-0.086369302,0.0052968093\C,0,-2.6665274
469,-1.0828497166,-0.0015269987\C,0,-2.0748736074,-2.3071522847,-0.013
3612584\C,0,-0.6212786477,-2.1607752097,-0.014739273\H,0,-2.5899314972
,1.7899651453,0.023608083\H,0,-0.4239341387,2.7795174501,-0.8379709326
\H,0,-0.4207575031,2.7642361104,0.8945690175\H,0,2.6083851413,-1.55544
66218,-0.0153695857\H,0,4.1893471792,0.55141371,0.0002249232\H,0,2.492
2488207,2.4540901331,-0.8561550763\H,0,2.4954923126,2.4386736599,0.896
2213062\H,0,-3.7250777683,-0.864736701,0.0023220466\H,0,-2.588509688,-
3.2604925222,-0.0207971439\H,0,0.0802046839,-2.9843760071,-0.023261152
\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-461.6967897\CCSD(T)/G
TBas1=-461.8382013\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-460.31
29238\MP2/GTMP2LargeXP=-462.2047218\HF/GFHFB3=-460.3175367\HF/GFHFB4=-
460.3496721\G4MP2=-462.4891443\FreqCoord=-3.1028126016,2.3765323259,0.
0324883948,-0.7383528432,3.9475537349,0.0419830686,1.6422344435,2.4386
735606,0.0243163184,1.6949512176,-0.1346768021,0.0015800953,4.34499452
87,-0.978598219,-0.0107270971,5.8723152004,1.0487355458,0.004265451,4.
3055602704,3.4332306386,0.0281435587,-0.6056699654,-1.5724318671,-0.00
68346331,-3.0297946788,-0.163214327,0.0100095189,-5.0390066004,-2.0462
894074,-0.0028856094,-3.9209428783,-4.3598859649,-0.0252491193,-1.1740
464963,-4.0832733811,-0.0278531893,-4.8942612327,3.382543912,0.0446128
114,-0.8011194205,5.2525267623,-1.5835355699,-0.7951164492,5.223649215
3,1.69049045,4.9291335662,-2.9393681295,-0.0290443077,7.9167188443,1.0
420208978,0.0004250433,4.7096677261,4.6375582569,-1.6178986215,4.71579
70375,4.6084253447,1.6936128231,-7.0393768058,-1.634115542,0.004388032
1,-4.8915744026,-6.1614379253,-0.0393009063,0.1515648871,-5.639653331,
-0.0439572069\PG=C01 [X(C12H10)]\NImag=0\

1H-benz[e]indene

1\1\GINC-N050\Mixed\G4MP2\G4MP2\C13H10\KFOREST\12-May-2011\0\#\ G4MP2\
\name\0,1\C,0,-0.1767933858,0.6318968149,-0.0007300439\C,0,-1.4075187
808,-0.1090401921,0.000212053\C,0,-0.2354042189,2.0501331289,-0.001320
0337\C,0,-2.6317586624,0.6058417677,0.0005153221\C,0,-1.4410311745,2.7
072083879,-0.00100105\C,0,-2.6530493195,1.9789860307,-0.0000736603\C,0
,1.0284578541,-1.4936446036,-0.0004079122\C,0,-0.1830550766,-2.2186749
219,0.0005172946\C,0,1.0282562733,-0.1030869552,-0.0010148697\C,0,-1.3
713258523,-1.5294621386,0.0008138222\C,0,2.4170917814,-1.9608415438,-0
.0009018896\C,0,3.2479312349,-0.9045176861,-0.0017794223\C,0,2.4579068
198,0.3823927685,-0.00194686\H,0,0.6919406133,2.6140374463,-0.00203252
97\H,0,-3.5605334464,0.0425345877,0.0012282899\H,0,-1.4679874203,3.792
0585707,-0.0014614979\H,0,-3.599036752,2.5101416891,0.0001699659\H,0,-
0.1736069229,-3.3040334233,0.0009861971\H,0,-2.3149060089,-2.067209124
,0.0015229006\H,0,2.706189244,-3.004849393,-0.0005919176\H,0,4.3295951
105,-0.935994779,-0.0023084324\H,0,2.6905257041,1.0032337009,0.8744727
662\H,0,2.6896423857,1.0024598672,-0.8791484923\Version=EM64L-G09RevB
.01\State=1-A\MP2\GTBas1=-499.758096\CCSD(T)/GTBas1=-499.8992972\MP2/G
TBas2=0.\MP2\GTBas3=0.\HF/GTMP2LargeXP=-498.2577699\MP2/GTMP2LargeXP=-
500.2994724\HF/GFHFB3=-498.2634727\HF/GFHFB4=-498.2977228\G4MP2=-500.5
987058\FreqCoord=-0.3340910813,1.1941119245,-0.001379583,-2.6598250226
, -0.2060561006,0.000400722,-0.4448495042,3.8741901495,-0.0024945022,-4
.9733031198,1.1448750208,0.0009738176,-2.7231542687,5.1158824377,-0.00
18917103,-5.0135366309,3.7397416187,-0.0001391978,1.9435036834,-2.8225
792406,-0.0007708423,-0.3459239619,-4.1926879802,0.0009775452,1.943122
751,-0.1948061131,-0.0019178258,-2.5914302999,-2.8902645725,0.00153790
1,4.567641505,-3.7054535078,-0.0017043243,6.1377005324,-1.709290709,-0
.0033626209,4.6447707496,0.7226176077,-0.0036790322,1.3075782594,4.939
8148746,-0.0038409245,-6.7284331007,0.0803787219,0.0023211316,-2.77409
41909,7.1659521786,-0.0027618307,-6.8011938034,4.743480347,0.000321189
1,-0.3280695391,-6.243718304,0.0018636423,-4.3745383801,-3.9064591037,
0.002877865,5.113956535,-5.6783424234,-0.0011185621,8.1817490252,-1.76
87737941,-0.0043623051,5.0843567342,1.8958369421,1.6525140387,5.082687
5043,1.8943746083,-1.6613498805\PG=C01 [X(C13H10)]\NImag=0\

1H-benz[f]indene

1\1\GINC-N050\Mixed\G4MP2\G4MP2\C13H10\KFOREST\12-May-2011\0\#\ G4MP2\
\name\0,1\C,0,-0.9231968755,-0.7176601765,-0.0000634578\C,0,-0.931692
924,0.7180786053,-0.0010808069\C,0,-2.165284502,-1.4024273216,0.001030
5617\C,0,-2.178052664,1.3911065102,-0.0009507239\C,0,-3.3558975956,-0.
7172995453,0.0011249689\C,0,-3.3631882315,0.6952206465,0.0001233235\C,
0,1.491829966,-0.6969336611,-0.0012573968\C,0,1.4824727742,0.733267616
8,-0.0022705216\C,0,0.3170741046,-1.4079800003,-0.0001782315\C,0,0.304
8702153,1.4237163348,-0.0021864505\C,0,2.8879366811,-1.1329414409,-0.0
016270334\C,0,3.703892885,-0.0657090485,-0.0027868815\C,0,2.9144391137
,1.2237433249,-0.0033208563\H,0,-2.1570467765,-2.4886075668,0.00179966
44\H,0,-2.179831611,2.4773970272,-0.0017228437\H,0,-4.2954239969,-1.26
01771676,0.0019703236\H,0,-4.3077915112,1.229029719,0.000205159\H,0,0.
3170324841,-2.4943210576,0.0005952843\H,0,0.2860483621,2.5104949612,-0
.0029502573\H,0,3.196620488,-2.1713901568,-0.0010378001\H,0,4.78628089
39,-0.0926286261,-0.0032962484\H,0,3.1435247122,1.8452661113,0.8731089
533\H,0,3.1426640081,1.8440049118,-0.8808687289\\Version=EM64L-G09RevB
.01\State=1-A\MP2/GTbas1=-499.7576548\CCSD(T)/GTbas1=-499.8998554\MP2/
GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-498.2597945\MP2/GTMP2LargeXP=
-500.2986273\HF/GFHFB3=-498.2655599\HF/GFHFB4=-498.2997867\G4MP2=-500.
5987752\FreqCoord=-1.7445892615,-1.35618119,-0.0001199179,-1.760644466
4,1.3569719059,-0.002042429,-4.0917947085,-2.6502035591,0.0019474794,-
4.115923038,2.6288103259,-0.0017966079,-6.3417273856,-1.3554996958,0.0
021258831,-6.3555046909,1.3137766238,0.0002330476,2.8191500726,-1.3170
137522,-0.0023761355,2.8014675427,1.3856749779,-0.0042906639,0.5991832
216,-2.6606966011,-0.0003368088,0.5761212131,2.6904339637,-0.004131792
7,5.4574094164,-2.140949048,-0.0030746475,6.9993431783,-0.124172106,-0
.0052664428,5.5074917558,2.3125397411,-0.0062755089,-4.0762276633,-4.7
027867535,0.0034008728,-4.1192847606,4.6816019038,-0.0032557027,-8.117
1749788,-2.3813897257,0.0037233721,-8.1405461938,2.3225295782,0.000387
6943,0.5991045701,-4.7135836864,0.0011249244,0.540553065,4.7441479346,
-0.0055751783,6.0407372731,-4.103332724,-0.001961158,9.0447600845,-0.1
750427354,-0.0062290068,5.940400798,3.4870475927,1.6499368059,5.938774
3029,3.484664271,-1.6646006566\PG=C01 [X(C13H10)]\NImag=0\

1H-cyclopenta [1]phenanthrene

1\1\GINC-N111\Mixed\G4MP2\G4MP2\C17H12\KFOREST\17-May-2011\0\#\ G4MP2\
\name\0,1\C,0,-3.0338792382,-0.4167629148,0.0141759831\C,0,-1.8125001
667,-2.4103019599,0.0098540047\C,0,-3.0655622794,-1.924171478,0.014133
346\C,0,-0.8558302001,-1.2973227832,0.0067098398\C,0,-1.555846726,-0.1
145461959,0.0091779246\C,0,0.5268173304,1.1789158467,0.0021652482\C,0,
-0.901916792,1.1511463415,0.007020841\C,0,-1.6217282427,2.3670790471,0
.0094833838\C,0,-0.9717023163,3.5811350539,0.0072582186\C,0,0.43186423
87,3.6166812049,0.0024256532\C,0,1.156604308,2.4423298957,-0.000039675
\C,0,0.5778349159,-1.3190102707,0.0019078978\C,0,1.2750127397,-0.07317
85295,-0.0003352387\C,0,2.6866490427,-0.1136877529,-0.0049471363\C,0,3
.3795523507,-1.3068170726,-0.0072991132\C,0,2.6865142284,-2.5268734415
, -0.0051230812\C,0,1.3086041273,-2.5259758717,-0.0005813596\H,0,-3.544
0399383,0.0018408761,0.8929010695\H,0,-3.5501263234,0.0021023302,-0.86
08505133\H,0,-1.5419677455,-3.4581603828,0.0088468823\H,0,-3.980754205
3,-2.5011770139,0.0171766792\H,0,-2.7062618133,2.3325079405,0.01318545
28\H,0,-1.5398809989,4.5054211722,0.0092059594\H,0,0.9504268605,4.5696
008632,0.000602101\H,0,2.2377230729,2.5047369125,-0.0038167622\H,0,3.2
517846787,0.8101042371,-0.0066735713\H,0,4.4644874994,-1.2991792257,-0
.0108314649\H,0,3.2323760729,-3.4644002164,-0.0069877502\H,0,0.7693455
196,-3.4668766121,0.0011451811\Version=EM64L-G09RevB.01\State=1-A\MP2
/GTBas1=-652.9190998\CCSD(T)/GTBas1=-653.0960796\MP2/GTBas2=0.\MP2/GTB
as3=0.\HF/GTMP2LargeXP=-650.9516539\MP2/GTMP2LargeXP=-653.6175385\HF/G
FHF3=-650.9595242\HF/GFHF4=-651.0036033\G4MP2=-654.0061458\FreqCoord
=-5.7332008805,-0.7875677714,0.0267887257,-3.4251289308,-4.5548106018,
0.0186213702,-5.7930731513,-3.6361571262,0.0267081532,-1.6172846945,-2
.4515847661,0.0126797596,-2.9401242169,-0.2164609399,0.017343764,0.995
5404766,2.2278280839,0.0040917262,-1.7043757316,2.1753513242,0.0132674
668,-3.0646222406,4.4731311339,0.0179209982,-1.8362512605,6.7673644968
,0.0137160453,0.8161051377,6.8345369873,0.0045838202,2.1856653862,4.61
53346291,-0.0000749749,1.0919497411,-2.4925681782,0.0036054044,2.40942
4894,-0.1382873796,-0.0006335092,5.077030906,-0.2148387176,-0.00934873
28,6.3864283945,-2.469526373,-0.013793325,5.0767761438,-4.7750987769,-
0.0096812204,2.4729034169,-4.7734026158,-0.0010986104,-6.6972648874,0.
0034787516,1.6873384851,-6.7087664883,0.0039728284,-1.6267717116,-2.91
38967448,-6.5349760471,0.0167181847,-7.5225352504,-4.7265395661,0.0324
592195,-5.114093671,4.4078012104,0.0249168947,-2.9099533651,8.51401212
88,0.0173967421,1.7960464758,8.635294168,0.001137806,4.228683769,4.733
2667996,-0.0072126353,6.1449824859,1.5308751472,-0.0126112221,8.436658
6976,-2.4550929341,-0.0204685023,6.1083055363,-6.5467676237,-0.0132049
342,1.4538523336,-6.5514473333,0.0021640787\PG=C01 [X(C17H12)]\NImag=0
\

1H-cyclopent [b] anthracene

1\1\GINC-N111\Mixed\G4MP2\G4MP2\C17H12\KFOREST\17-May-2011\0\#\ G4MP2\
\name\0,1\C,0,4.1668335241,-0.8395019455,0.0052369321\C,0,4.918355617
9,0.274382537,0.0141617794\C,0,4.0586735368,1.5180107573,0.0214001398\
C,0,2.7486390616,-0.4894806043,0.0053749142\C,0,2.6562966933,0.9479481
416,0.0151749578\C,0,1.4476127196,1.5685050723,0.0174935402\C,0,1.6243
368396,-1.2671061937,-0.0018313312\C,0,0.335429566,-0.6521470129,0.000
3249229\C,0,0.2430685133,0.7922776285,0.0101620891\C,0,-1.018101705,1.
3892977815,0.0122357814\C,0,-0.8438399242,-1.4020674139,-0.0067878179\
C,0,-2.1064946525,-0.8022209016,-0.0046991949\C,0,-2.1972254067,0.6367
080087,0.0051108524\C,0,-3.4897547466,1.2393928266,0.007176668\C,0,-4.
623482746,0.4755499346,0.0000385193\C,0,-4.5343398582,-0.9446144972,-0
.009651432\C,0,-3.3145718691,-1.5613852649,-0.0119284668\H,0,4.5373515
804,-1.8574220087,-0.0012071506\H,0,6.0006285564,0.3089366119,0.016138
2058\H,0,4.2540794085,2.1569427143,-0.8508154183\H,0,4.2512250058,2.14
46747943,0.9031069084\H,0,1.3654339477,2.6521651314,0.0248474989\H,0,1
.688130079,-2.3514013454,-0.0092255784\H,0,-1.0868948715,2.474221753,0
.0196329058\H,0,-0.7766705927,-2.4870093727,-0.0141812875\H,0,-3.55377
24212,2.3235767017,0.0145809665\H,0,-5.6001794968,0.9480934802,0.00171
69976\H,0,-5.4444835915,-1.5353094962,-0.0152310332\H,0,-3.243052768,-
2.6450678177,-0.0193158688\Version=EM64L-G09RevB.01\State=1-A\MP2/GTB
as1=-652.9087846\CCSD(T)/GTBas1=-653.0887354\MP2/GTBas2=0.\MP2/GTBas3=
0.\HF/GTMP2LargeXP=-650.9452355\MP2/GTMP2LargeXP=-653.6063721\HF/GFHF
B3=-650.9532384\HF/GFHF4=-650.9972283\G4MP2=-653.9981991\FreqCoord=7.8
741742018,-1.586428765,0.0098963675,9.294345142,0.5185078505,0.0267618
846,7.6697814473,2.8686245982,0.0404404035,5.1941750645,-0.9249842895,
0.0101571159,5.019673278,1.7913623758,0.0286765143,2.7355915865,2.9640
450246,0.0330580002,3.0695517744,-2.3944836874,-0.0034607145,0.6338700
166,-1.2323792528,0.0006140153,0.4593329217,1.4971877391,0.0192035653,
-1.9239333979,2.6253923241,0.0231222758,-1.5946263568,-2.6495234321,-0
.0128271168,-3.9806979936,-1.5159778021,-0.0088801913,-4.1521542709,1.
203203763,0.0096581113,-6.5946807421,2.3421130134,0.0135619371,-8.7371
1617,0.8986591388,0.000072791,-8.5686605254,-1.7850627008,-0.018238563
3,-6.2636330804,-2.9505905386,-0.0225415355,8.5743518555,-3.5100189097
, -0.002281184,11.3395445968,0.5838055889,0.0304967892,8.0390450296,4.0
760310144,-1.6078081303,8.0336509903,4.0528480053,1.7066247256,2.58029
62137,5.0118657576,0.046954968,3.190103526,-4.4435045713,-0.0174338166
, -2.0539336423,4.6756015053,0.0371008151,-1.4676947157,-4.6997666044,-
0.0267987496,-6.7156566146,4.3909236149,0.0275540335,-10.5828055439,1.
791637026,0.0032446552,-10.2885829229,-2.9013144771,-0.0287824815,-6.1
284815661,-4.9984537784,-0.0365017021\PG=C01 [X(C17H12)]\NImag=0\

1a, 9b-dihydro-1H-cyclopropa [1]phenanthrene

1\1\GINC-SAW258\Mixed\G4MP2\G4MP2\C15H12\KFOREST\23-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,5.233508878,1.4230093018,2.1893807064\C,0,3.858291132
9,1.2712528777,1.568646672\C,0,5.0976134702,1.0489455715,0.7296100721\
C,0,3.0453429216,2.4933599485,1.3631012321\C,0,5.6885188542,2.78503511
3,2.5561646304\C,0,3.582118337,3.7773849276,1.6064836945\C,0,4.9286165
837,3.9259715077,2.2142650189\C,0,5.4617552711,5.1846798876,2.53852009
53\C,0,2.7691212148,4.8875468121,1.323108723\C,0,1.7301507635,2.362402
5414,0.9098160419\C,0,6.8969271998,2.9325567711,3.2419738477\C,0,6.677
8543949,5.3199720631,3.1932182975\C,0,7.3993977799,4.1867273045,3.5607
224414\C,0,0.9418402678,3.4741351347,0.6459254521\C,0,1.474288074,4.74
57574406,0.8444297209\H,0,5.5716262614,0.6323765093,2.8519260361\H,0,3
.2918607486,0.3808045113,1.8229064263\H,0,5.3372617838,0.029889466,0.4
478170744\H,0,5.3476900163,1.8025518865,-0.0086707441\H,0,4.9152596455
,6.0847679655,2.2863731\H,0,3.1453639999,5.8894589428,1.4874487733\H,0
,1.3316877458,1.3650064281,0.7478587559\H,0,7.4551592791,2.0407318174,
3.5118388892\H,0,7.0560072091,6.3100409935,3.4252311317\H,0,8.34500979
48,4.2800435744,4.0841488244\H,0,-0.0734891483,3.3510615062,0.28422915
73\H,0,0.8784775204,5.6283491961,0.6368059291\\Version=EM64L-G09RevB.0
1\State=1-A\MP2\GTBas1=-576.9110492\CCSD(T)/GTBas1=-577.0720072\MP2/GT
Bas2=0.\MP2\GTBas3=0.\HF/GTMP2LargeXP=-575.1705691\MP2/GTMP2LargeXP=-5
77.5407447\HF/GFHF3=-575.176011\HF/GFHF4=-575.2160456\G4MP2=-577.878
9337\FreqCoord=9.8898984935,2.6890978649,4.1373299357,7.2911135821,2.4
023197844,2.9643126093,9.6330933901,1.9822198584,1.3787632201,5.754864
1026,4.7117674534,2.5758880201,10.7497427361,5.262953634,4.830451102,6
.7692226324,7.1382230117,3.0358142195,9.3137355572,7.419010955,4.18435
44714,10.3212216672,9.7976250742,4.7971077629,5.2328807248,9.236124936
5,2.5003131305,3.2695111116,4.4642938189,1.7193031505,13.0333035661,5.
5417291666,6.1264427021,12.6193159617,10.0532902338,6.0343080648,13.98
28353523,7.9117679986,6.7287902495,1.7798201671,6.5651639533,1.2206222
067,2.7860007009,8.9681818558,1.595740911,10.5288477488,1.1950184154,5
.3893591595,6.2207152824,0.7196162366,3.4447939116,10.0859630709,0.056
482905,0.8462516283,10.1056695744,3.4063294059,-0.0163853316,9.2884946
02,11.4985450369,4.3206189967,5.9438765481,11.1294644727,2.8108708183,
2.516525134,2.5794883187,1.4132482347,14.0882093145,3.8564242456,6.636
4137234,13.333921217,11.924249365,6.4727487807,15.7697830884,8.0881101
925,7.7179227641,-0.138874364,6.3325885013,0.5371152663,1.6600819275,1
0.6360385608,1.2033888058\PG=C01 [X(C15H12)]\NImag=0\

1-methylene-1H-indene

```
1\1\GINC-SAW330\Mixed\G4MP2\G4MP2\C10H8\KFOREST\23-Jan-2011\0\#\# G4MP2
\name\0,1\C,0,1.8615740541,2.2437607302,0.\C,0,1.4223829123,0.978783
0855,0.\C,0,0.0206349865,0.5034920239,0.\C,0,2.2506549589,-0.237570470
4,0.\C,0,0.0504900212,-0.9107737628,0.\C,0,-1.1874020432,1.1814484225,
0.\C,0,1.4564051902,-1.3296577202,0.\C,0,-1.1309238178,-1.6411744049,0
.\C,0,-2.3757402387,0.4432832366,0.\C,0,-2.3463549354,-0.9507875966,0.
\H,0,1.1796747591,3.087266697,0.\H,0,2.921814401,2.473348064,0.\H,0,3.
3324857875,-0.2229378833,0.\H,0,-1.2209432818,2.2667270916,0.\H,0,1.78
44926999,-2.3615886498,0.\H,0,-1.114228478,-2.7265257767,0.\H,0,-3.329
1282635,0.9609234323,0.\H,0,-3.2786487122,-1.5061565188,0.\Version=EM
64L-G09RevB.01\State=1-A'\MP2/GTBas1=-384.5736945\CCSD(T)/GTBas1=-384.
6883129\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-383.4299244\MP2/G
TMP2LargeXP=-384.9945045\HF/GFHFB3=-383.434137\HF/GFHFB4=-383.4607874\
G4MP2=-385.230705\FreqCoord=3.5178651384,4.2400932878,0.,2.6879141603,
1.8496319751,0.,0.0389944732,0.9514620352,0.,4.2531214919,-0.448943126
3,0.,0.0954123125,-1.7211129807,0.,-2.2438646713,2.2326139586,0.,2.752
2069479,-2.5126889417,0.,-2.1371362927,-3.1013701616,0.,-4.4894984141,
0.8376839165,0.,-4.4339682384,-1.7967281681,0.,2.2292622205,5.83408855
64,0.,5.5214290289,4.6739504722,0.,6.2974854801,-0.4212915441,0.,-2.30
72484265,4.283493421,0.,3.372202489,-4.4627557866,0.,-2.1055866728,-5.
1523870122,0.,-6.2911406792,1.8158821218,0.,-6.195748152,-2.8462233337
,0.\PG=CS [SG(C10H8)]\NImag=0\
```

1H-phenalene

1\1\GINC-N111\Mixed\G4MP2\G4MP2\C13H10\KFOREST\12-May-2011\0\#\ G4MP2\
\name\0,1\C,0,3.3668665807,3.2560249317,1.1124382325\C,0,1.9942352441
,3.6237970711,1.057041271\C,0,3.7596873349,1.9293112919,0.7554502504\C
,0,4.3672792582,4.196066355,1.5216462408\C,0,1.5577004227,5.0270346259
,1.4318111326\C,0,1.0626854071,2.6864021176,0.6572437311\C,0,5.1357411
784,1.578543898,0.8164170232\C,0,2.7674688359,1.0049381181,0.352155206
8\C,0,5.6907840995,3.8064066692,1.5643406425\C,0,3.9526925361,5.546197
8301,1.8833346177\C,0,2.6757693151,5.9377912295,1.846838352\C,0,1.4455
58858,1.3784308651,0.3047834942\C,0,6.0761856805,2.4955594835,1.211206
246\H,0,1.0142748922,5.4821476363,0.5894508561\H,0,0.811782341,4.97838
94486,2.2400295368\H,0,0.0126170514,2.9625164144,0.613316291\H,0,5.427
5555788,0.5689241212,0.5438527514\H,0,3.0687215033,-0.0024255967,0.081
4538556\H,0,6.4455260145,4.5226577132,1.8752276644\H,0,4.73147446,6.23
91990907,2.1902474364\H,0,2.4047304796,6.952577981,2.1236870349\H,0,0.
6879238644,0.6659604387,-0.005154717\H,0,7.1243390636,2.2180482661,1.2
544928495\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-499.7641528\
CCSD(T)/GTBas1=-499.9067342\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeX
P=-498.2660329\MP2/GTMP2LargeXP=-500.3054992\HF/GFHFB3=-498.271696\HF/
GFHFB4=-498.3060129\G4MP2=-500.6053041\FreqCoord=6.3624557634,6.152995
4028,2.1022035992,3.7685584559,6.8479840255,1.9975185133,7.1047794083,
3.6458699668,1.4275940803,8.2529617439,7.9294162463,2.8754946662,2.943
6271961,9.4997187035,2.7057309147,2.0081843847,5.0765642851,1.24201065
43,9.7051443165,2.9830156559,1.542804584,5.2297581811,1.8990578237,0.6
654768971,10.7540234294,7.1930661552,2.9561753929,7.4695063808,10.4807
949776,3.558986644,5.0564712003,11.2207992581,3.4900186969,2.731710350
6,2.6048568281,0.5759573338,11.4823268687,4.7159239721,2.2888480954,1.
9167017697,10.3597576526,1.1139006869,1.5340463041,9.4077926407,4.2330
423541,0.0238427717,5.5983446874,1.1589998229,10.256593615,1.075110779
4,1.0277327568,5.7990432194,-0.0045837135,0.1539254796,12.1802789498,8
.5465844707,3.5436667226,8.9411909341,11.79037757,4.1389678181,4.54428
20299,13.1384683017,4.013186888,1.299987704,1.2584828444,-0.0097410035
,13.463049708,4.1915037725,2.3706479213\PG=C01 [X(C13H10)]\NImag=0\

1-methylacenaphthylene

1\1\GINC-N109\Mixed\G4MP2\G4MP2\C13H10\KFOREST\12-May-2011\0\#\ G4MP2\
\name\0,1\C,0,-0.6719541576,-1.2544168353,0.0554524242\C,0,-2.0428638
123,-0.7256406471,0.0702592023\C,0,-2.0111188713,0.6363410484,0.025669
2532\C,0,-0.5936570833,1.0600268013,-0.0209440057\C,0,0.1773838501,-0.
1239719985,-0.0007340335\C,0,1.5699873827,-0.1706321561,-0.0311277691\
C,0,2.1506505728,-1.4714075674,-0.0023712578\C,0,1.3379280048,-2.58573
52726,0.0524183086\C,0,-0.0834966055,-2.4988298082,0.0823265559\C,0,0.
0729459223,2.2637561494,-0.0748371155\C,0,1.4957383784,2.2563345845,-0
.1073736524\C,0,2.232368276,1.0879695336,-0.0867998313\C,0,-3.17585208
73,1.5735300492,0.0226689129\H,0,-2.9408677979,-1.3293919517,0.1105187
539\H,0,3.2301929067,-1.5849148882,-0.0235383913\H,0,1.7938009944,-3.5
705576519,0.0738574648\H,0,-0.6708859888,-3.4110171977,0.1255396963\H,
0,-0.4538621271,3.2131634933,-0.0930185166\H,0,2.0162341178,3.20779909
76,-0.1498604025\H,0,3.317112977,1.1293718116,-0.1131095385\H,0,-3.141
8013345,2.2568434869,0.8804343061\H,0,-4.1233660697,1.0299545648,0.062
4057308\H,0,-3.1829974475,2.2002353542,-0.8778860948\Version=EM64L-GO
9RevB.01\State=1-A\MP2/GTBas1=-499.761242\CCSD(T)/GTBas1=-499.9006808\
MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-498.257098\MP2/GTMP2Large
XP=-500.3025078\HF/GFHFB3=-498.2627731\HF/GFHFB4=-498.296921\G4MP2=-50
0.600126\FreqCoord=-1.2698093317,-2.3705042752,0.1047898952,-3.8604531
32,-1.3712620939,0.1327706506,-3.8004638875,1.2025103086,0.0485078585,
-1.1218493043,2.0031603479,-0.0395784348,0.335206897,-0.2342731253,-0.
0013871224,2.9668461853,-0.3224480444,-0.0588229586,4.0641405901,-2.78
05573322,-0.0044810278,2.5283175145,-4.8863315174,0.0990562475,-0.1577
857175,-4.7221039902,0.1555746442,0.1378478157,4.277879154,-0.14142165
29,2.8265359016,4.2638544289,-0.2029067969,4.2185646694,2.0559644595,-
0.1640279096,-6.0014906836,2.9735408548,0.0428380371,-5.557434731,-2.5
12186712,0.2088501774,6.1041799501,-2.9950550827,-0.0444811131,3.38979
26163,-6.7473761039,0.1395703814,-1.2677907853,-6.4458883382,0.2372356
447,-0.8576751223,6.0719990225,-0.1757795217,3.8101303025,6.0618617837
, -0.2831951189,6.2684350784,2.1342034262,-0.2137460508,-5.9371440861,4
.264816115,1.6637797165,-7.7920326174,1.9463320568,0.1179297404,-6.014
9934575,4.1578422472,-1.658964295\PG=C01 [X(C13H10)]\NImag=0\

2,3-benzofluorene

1\1\GINC-SAW313\Mixed\G4MP2\G4MP2\C17H12\KFOREST\28-Jan-2011\0\#\ G4MP2\name\0,1\C,0,4.6472243014,4.5800343785,1.0749442113\C,0,3.3647647308,5.2847883579,1.1625095931\C,0,5.6847117767,5.5534816635,0.938815611\C,0,4.9453400607,3.2392221991,1.1043707632\C,0,3.6000094367,6.6706169353,1.0823617267\C,0,2.065712287,4.7981242107,1.3019854628\C,0,5.0828565863,6.9445448318,0.9350676543\C,0,6.9922774459,5.1696622025,0.8353730927\C,0,6.2929517436,2.8109443562,0.9991444235\C,0,2.5430920603,7.5671636591,1.1411674903\C,0,1.0085278126,5.7026759649,1.3604778516\C,0,7.334451903,3.7895563776,0.862428246\C,0,6.6502439724,1.4381948909,1.0245049785\C,0,1.2433728786,7.0767664878,1.2808612573\C,0,8.6759336872,3.345736538,0.7584192866\C,0,7.9614293748,1.0434944742,0.9211914981\C,0,8.9859553493,2.0074888224,0.7866471952\H,0,4.1644922601,2.4911479885,1.2074793561\H,0,1.8766525925,3.7312556357,1.3644168076\H,0,5.4697907365,7.5618490495,1.7559092642\H,0,5.3099182541,7.4879832693,0.0089582859\H,0,7.7876266934,5.9031331328,0.7315554377\H,0,2.7191385909,8.636949136,1.0798048798\H,0,-0.0071655273,5.3365693223,1.4689203574\H,0,5.8607157776,0.6995232157,1.1280104843\H,0,0.4091435934,7.7688767556,1.327933488\H,0,9.4611203824,4.0891328956,0.6551115723\H,0,8.2151459332,-0.0112370376,0.9425808904\H,0,10.019275306,1.6867102863,0.7056388338\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-652.9334454\CCSD(T)/GTBas1=-653.1100718\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-650.9694726\MP2/GTMP2LargeXP=-653.6300557\HF/GFHFB3=-650.9775143\HF/GFHFB4=-651.0214875\G4MP2=-654.0179112\FreqCoord=8.7819812077,8.6550106545,2.0313501676,6.3584838428,9.9868026668,2.1968247578,10.7425484023,10.494559428,1.7741043942,9.3453383487,6.1212428399,2.0869582916,6.8030319113,12.6056391451,2.0453672402,3.9036304919,9.0671407098,2.4603959537,9.6052069208,13.1232878496,1.7670217823,13.2134894179,9.7692457622,1.578626364,11.8919553628,5.3119150079,1.8881093277,4.8057475247,14.2998669184,2.1564940284,1.9058413632,10.7764957983,2.5709305495,13.8601054314,7.1612237187,1.6297531943,12.5671398248,2.7177944695,1.9360338312,2.3496342216,13.3731505683,2.4204769906,16.3951386158,6.3225257696,1.4332047455,15.0449211447,1.9719187774,1.7407996473,16.9809946526,3.7936040892,1.4865477622,7.869749854,4.7075874548,2.2818052942,3.5463594463,7.0510512833,2.5783740976,10.3364064963,14.2898237618,3.3181876236,10.0342912882,14.1502376665,0.016928707,14.7164816758,11.155304947,1.3824394284,5.1384272541,16.3214684908,2.0405354997,-0.0135408842,10.0846545082,2.7758571864,11.0751477623,1.3219073013,2.1316308904,0.7731693406,14.6810494281,2.5094306151,17.8789264329,7.7273412936,1.2379814581,15.5243759554,-0.0212349235,1.7812197409,18.9336863783,3.1874205065,1.3334641446\PG=C01 [X(C17H12)]\NImag=0\

2,5-etheno[4.2.2]propella-3,7,9-triene

1\1\GINC-SAW314\Mixed\G4MP2\G4MP2\C12H10\KFOREST\26-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,3.0714463869,0.4710236642,1.0901078888\C,0,3.84850250
39,0.5392323565,2.1744988742\C,0,2.8492166666,1.3792069633,2.980870592
7\C,0,1.9369782609,1.2991378117,1.7078238599\C,0,1.6199522751,2.749833
1502,1.2065567761\C,0,0.9552442583,0.5312354971,2.6027482117\C,0,0.983
6339023,3.4590330186,2.4011440279\C,0,2.9818374182,3.4021800077,0.9728
515125\C,0,1.7323004297,0.5994352461,3.6871397929\C,0,3.1339963568,2.8
827251213,3.3194367107\C,0,1.7579573321,3.5269948166,3.4817316778\C,0,
3.7561607499,3.4701471504,2.0534389649\H,0,3.1640256568,-0.0211654739,
0.1284012946\H,0,4.8159559749,0.1238364604,2.4336906398\H,0,0.98524257
08,2.7630210287,0.3180621937\H,0,-0.0026285464,0.0689354877,2.39189477
54\H,0,-0.0329869182,3.8308156298,2.3510230688\H,0,3.2767872051,3.7366
463267,-0.0147669168\H,0,1.6493011035,0.2139212933,4.6971846033\H,0,3.
7672031149,3.0072019429,4.2003493429\H,0,1.4546144409,3.9613815779,4.4
270067389\H,0,4.7643892622,3.8672209112,2.0612150797\Version=EM64L-G0
9RevB.01\State=1-A\MP2/GTbas1=-461.5904377\CCSD(T)/GTbas1=-461.7297103
\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-460.1785386\MP2/GTMP2Lar
geXP=-462.1010969\HF/GFHFB3=-460.1807579\HF/GFHFB4=-460.212704\G4MP2=-
462.3813926\FreqCoord=5.8041925031,0.8901057274,2.0600053652,7.2726157
542,1.0190014759,4.1092073486,5.3842391932,2.6063234413,5.6330290577,3
.6603584385,2.4550146731,3.2273193785,3.0612661483,5.1964315649,2.2800
618705,1.8051500381,1.0038896015,4.918481313,1.8587986903,6.5366250897
,4.5375046184,5.6348560933,6.4291884693,1.8384229266,3.273573392,1.132
7684495,6.9676844222,5.9223948157,5.4475609957,6.2728262986,3.32205791
09,6.6650542755,6.5795193393,7.0981151284,6.5576277552,3.8804372742,5.
9791419688,-0.0399969492,0.2426432818,9.1008378606,0.2340169953,4.5990
088014,1.8618386333,5.2213530437,0.6010504394,-0.0049672329,0.13026919
26,4.5200260642,-0.0623362414,7.2391924058,4.4427897322,6.1922304134,7
.0612382129,-0.0279054286,3.1167273963,0.4042526584,8.8763924958,7.118
982174,5.6827880983,7.9375099206,2.7488229222,7.4859262902,8.365830324
9,9.003390896,7.3079884175,3.8951320015\PG=C01 [X(C12H10)]\NImag=0\

2-methylchrysene

1\1\GINC-SAW97\Mixed\G4MP2\G4MP2\C19H14\KFOREST\31-Jan-2011\0\#\ G4MP2
\name\0,1\C,0,8.4307023004,1.9675664002,1.0735112854\C,0,8.192808518
4,3.2734425476,1.5928136032\C,0,9.6822950468,1.6560539397,0.4958583102
\C,0,7.3932103838,0.9947459158,1.1479189363\C,0,9.2464544653,4.2143424
701,1.5015725056\C,0,6.9034922733,3.5778330803,2.1825538584\C,0,10.458
5789779,3.8871364916,0.9337180201\C,0,10.6840168357,2.5955797759,0.423
9717554\C,0,6.1865382357,1.2886478149,1.7025840648\C,0,5.8984104592,2.
582245795,2.2369871565\C,0,4.6107496724,2.8871238874,2.8260108162\C,0,
6.61370283,4.8701349419,2.7174923801\C,0,4.3695661725,4.1899841995,3.3
458405167\C,0,3.5528814057,1.9503662537,2.9196066905\C,0,5.4061105933,
5.1632516066,3.2723604002\C,0,3.1170292302,4.5003199656,3.9232978055\C
,0,2.3446849372,2.2816367571,3.4870900136\C,0,2.1001068538,3.574176975
,4.0048296152\C,0,0.7649767074,3.9058805157,4.6206003045\H,0,9.8369793
977,0.6536014979,0.1078562941\H,0,7.5847822146,0.002917695,0.749394511
5\H,0,9.1107239701,5.2184303602,1.882740083\H,0,11.244867683,4.6329368
36,0.8799396488\H,0,11.6411404318,2.3460325268,-0.0214954027\H,0,5.428
7031672,0.5165761253,1.7367020399\H,0,7.3702965658,5.6434431457,2.6846
404402\H,0,3.6826151719,0.9447954371,2.5397508319\H,0,5.2145806711,6.1
549633019,3.6712036458\H,0,2.9662852718,5.5046813269,4.3106710959\H,0,
1.5581683311,1.5340915071,3.5398620479\H,0,-0.0500982152,3.7701112116,
3.9002409559\H,0,0.7329262413,4.9401613313,4.9727384866\H,0,0.54710319
89,3.2528883635,5.4737272831\Version=EM64L-G09RevB.01\State=1-A\MP2/G
TBas1=-730.1054476\CCSD(T)/GTBas1=-730.3033026\MP2/GTBas2=0.\MP2/GTBas
3=0.\HF/GTMP2LargeXP=-727.9045946\MP2/GTMP2LargeXP=-730.8920909\HF/GFH
FB3=-727.9131951\HF/GFHFB4=-727.9628519\G4MP2=-731.3231253\FreqCoord=1
5.9317184556,3.7181616447,2.02864233,15.482164359,6.1859099267,3.00998
14907,18.2968859763,3.1294884073,0.9370364069,13.9711428683,1.87979735
28,2.1692524124,17.4732666395,7.9639530988,2.8375608042,13.0457097571,
6.761124671,4.1244290627,19.7638500074,7.3456234103,1.7644713433,20.18
98658187,4.9049349325,0.8011905057,11.6908629762,2.4351914519,3.217417
6007,11.1463803872,4.8797373603,4.2272930886,8.713054148,5.4558734589,
5.3403864912,12.4980870731,9.2032212705,5.1353163665,8.2572833855,7.91
79226382,6.3227222608,6.7139728393,3.6856580784,5.5172570608,10.216068
4653,9.7571314916,6.1838649645,5.8903315932,8.5043722454,7.4139583902,
4.4308123992,4.3116686056,6.5896451264,3.9686268035,6.7542156332,7.568
0311815,1.445596475,7.3810444824,8.7316691451,18.5891970365,1.23512783
11,0.2038188575,14.3331611632,0.0055136444,1.4161503923,17.2167731758,
9.8614042243,3.5578631362,21.2497203215,8.754981811,1.6628449496,21.99
85672905,4.4333589746,-0.0406204243,10.2587622427,0.9761874036,3.28189
12298,13.9278420275,10.6645619918,5.0732351972,6.9591341276,1.78540462
77,4.799433518,9.8541293662,11.6311949985,6.9375694687,5.6054667957,10
.4023401566,8.1459878202,2.9445114147,2.8990128112,6.6893698186,-0.094
6719064,7.1244776805,7.3703872589,1.3850298716,9.3355519685,9.39711387
01,1.0338752124,6.1470681479,10.3438454911\PG=C01 [X(C19H14)]\NImag=0\
\

2a, 3, 8, 8a-tetrahydro- (2 α , 3 α , 8 α , 8a α)-3, 8-methanocyclobuta [b] naphthalene

1\1\GINC-SAW98\Mixed\G4MP2\G4MP2\C13H12\KFOREST\26-Jan-2011\0\#\ G4MP2
\name\0,1\C,0,1.4494131974,3.5687326844,2.477789967\C,0,1.2905371549
,2.0338333897,2.19751316\C,0,2.6662511036,1.4146264,2.0819430074\C,0,0
.9044062608,1.5637048383,3.6326287706\C,0,2.0916689257,3.6030267166,3.
9198891585\C,0,2.6812709857,4.3466644359,2.0423462784\C,0,2.2206373497
,2.0835006249,4.2861043185\C,0,3.2257507897,4.3756365433,3.2647652267\
C,0,3.2380091624,1.4451367588,3.3658844403\C,0,4.5203019915,0.97133966
97,3.5809440706\C,0,3.3729363858,0.9101179298,1.0044098073\C,0,4.66343
2561,0.4123967734,1.2238405962\C,0,5.2296501924,0.4426093417,2.4953451
14\H,0,0.4904687286,4.0845376875,2.3680339734\H,0,0.5934689728,1.79235
86499,1.3937886119\H,0,0.776029789,0.4810055515,3.7155434825\H,0,0.010
3151411,2.0653986294,4.0188596609\H,0,1.5224814243,4.1396750205,4.6852
083031\H,0,2.9921795759,4.7321065065,1.0779111627\H,0,2.355533801,1.88
64568665,5.3506055396\H,0,4.1435439705,4.7933933157,3.6628855751\H,0,4
.968464009,0.9943875641,4.569814895\H,0,2.937805424,0.8860264248,0.009
7606053\H,0,5.2255745217,-0.005454631,0.3948251262\H,0,6.2290685817,0.
0480923081,2.6482791488\\Version=EM64L-G09RevB.01\State=1-A\MP2\GTBas1
=-500.8720252\CCSD(T)/GTBas1=-501.0204282\MP2\GTBas2=0.\MP2\GTBas3=0.\
HF/GTMP2LargeXP=-499.3479657\MP2/GTMP2LargeXP=-501.4333964\HF/GFHFB3=-
499.3509176\HF/GFHFB4=-499.3861448\G4MP2=-501.7244235\FreqCoord=2.7389
939965,6.743927415,4.6823444525,2.438761787,3.8433881064,4.1526980458,
5.0384843873,2.6732564764,3.9343021083,1.7090801457,2.9549738971,6.864
6735188,3.9526814303,6.8087337438,7.4075169808,5.066867851,8.214005375
4,3.8594751347,4.1963964315,3.9372455788,8.0995633389,6.0957855654,8.2
687547238,6.1695121666,6.1189505328,2.7309126987,6.3605997871,8.542132
8019,1.8355659577,6.7670035906,6.3739260329,1.7198736359,1.898059461,8
.8126103795,0.7793169598,2.312723557,9.8826066343,0.8364104398,4.71551
88726,0.9268515738,7.7186576087,4.4749356831,1.121493827,3.3870669802,
2.6338787635,1.4664837721,0.9089687608,7.0213596168,0.0194927917,3.903
0377648,7.5945441256,2.8770729343,7.822852068,8.8537605684,5.654399938
8,8.9423853289,2.036956893,4.4513137806,3.5648868392,10.111179115,7.83
01633238,9.0582006139,6.921850593,9.389036278,1.8791201661,8.635698629
6,5.5516476831,1.6743472894,0.018444871,9.8749047329,-0.0103077587,0.7
461113589,11.7712336824,0.0908812915,5.0045223146\PG=C01 [X(C13H12)]\N
Imag=0\\

2a, 3, 8, 8a-tetrahydro- (2 α , 3 β , 8 β , 8 α)-3, 8-methanocyclobuta [b] naphthalene

1\1\GINC-SAW326\Mixed\G4MP2\G4MP2\C13H12\KFOREST\20-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,3.3305163926,2.5914807645,1.7726074295\C,0,3.33902915
99,2.2502174874,3.1387357019\C,0,4.794826023,2.2300570881,3.5757986832
\C,0,2.159535277,1.9721836704,3.8055463695\C,0,4.7810208572,2.78348048
4,1.3603603244\C,0,2.1424721707,2.6562148899,1.0672667096\C,0,5.350907
8253,3.3700329448,2.6802174116\C,0,5.3745745116,1.3408704076,1.3565176
186\C,0,5.3841544787,0.9568406854,2.893848765\C,0,0.9537519543,2.05452
16275,3.0962085525\C,0,0.9453389411,2.3917854029,1.746090881\C,0,6.883
0387199,1.1582421385,1.428439408\C,0,6.8911296417,0.8339071181,2.72680
57825\H,0,4.9734955284,2.3073060857,4.6493938442\H,0,2.1588851281,1.70
87539823,4.8590166838\H,0,4.9473101115,3.3570302077,0.4471870963\H,0,2
.1286926522,2.919116132,0.0137542998\H,0,6.4391417139,3.4474218196,2.6
927682676\H,0,4.9133633285,4.3404440328,2.9253555639\H,0,4.8348129272,
0.670154091,0.6830172426\H,0,4.8503680158,0.0466208222,3.1791163532\H,
0,0.0167941917,1.8571272427,3.607066178\H,0,0.0018788318,2.4550610955,
1.2134473433\H,0,7.6612080365,1.2749196138,0.681720369\H,0,7.678343581
2,0.5880201656,3.431493121\Version=EM64L-G09RevB.01\State=1-A\MP2/GTB
as1=-500.8769256\CCSD(T)/GTBas1=-501.0257185\MP2/GTBas2=0.\MP2/GTBas3=
0.\HF/GTMP2LargeXP=-499.3539212\MP2/GTMP2LargeXP=-501.4375282\HF/GFHFB
3=-499.3569365\HF/GFHFB4=-499.39219\G4MP2=-501.728788\FreqCoord=6.2937
638632,4.8971889235,3.3497425829,6.3098506619,4.2522947906,5.931350880
1,9.0609080383,4.2141971572,6.7572802176,4.0809302478,3.7268870208,7.1
914404244,9.0348200558,5.260015811,2.5707084551,4.04868565,5.019518692
,2.016841792,10.1117503521,6.3684393245,5.0648768845,10.1564739078,2.5
3387785,2.5634467936,10.1745774218,1.8081668482,5.4685816358,1.8023299
924,3.88248321,5.8509862145,1.7864317015,4.5198193802,3.2996335682,13.
0070581427,2.1887604374,2.6993592786,13.0223477691,1.5758560736,5.1529
161465,9.3985444717,4.3601766067,8.7860810495,4.0797016444,3.229077055
1,9.1822108076,9.3490612052,6.3438677124,0.8450611421,4.0226461338,5.5
163300395,0.0259918597,12.1682143701,6.5146831035,5.0885945651,9.28491
10822,8.2022505172,5.5281208571,9.1364723362,1.2664076989,1.2907155325
,9.1658671936,0.0881005861,6.0076592521,0.031736423,3.5094618826,6.816
3672196,0.0035504776,4.63939311,2.2930831555,14.4775850361,2.409248911
5,1.2882647967,14.5099665227,1.1111970735,6.4845822255\PG=C01 [X(C13H1
2)]\NImag=0\

3-methyl-1, 2-benzanthracene

1\1\GINC-SAW99\Mixed\G4MP2\G4MP2\C19H14\KFOREST\30-Jan-2011\0\#\ G4MP2
\name\0,1\C,0,3.0492697266,2.0896053785,2.4125168231\C,0,2.099320531
4,0.9258874657,2.5338774618\C,0,2.6413591843,3.4159320648,2.8460593369
\C,0,4.29171559,1.9116538494,1.8986744929\C,0,3.539781725,4.5156611303
,2.7311308895\C,0,1.3580851945,3.6396357607,3.3850760307\C,0,5.2414126
894,2.9787181958,1.7572175633\C,0,4.875670985,4.3051959076,2.174646953
6\C,0,3.1006781483,5.7816056392,3.1640609232\C,0,0.9558581191,4.893926
2283,3.8014105618\C,0,6.5037487677,2.7430662913,1.2236766927\C,0,5.814
2794841,5.3195777513,2.0264502776\C,0,1.8369324156,5.9745147202,3.6891
682387\C,0,7.4510322706,3.7656391015,1.0738615156\C,0,7.0924358095,5.0
92474762,1.4886273892\C,0,8.7473181352,3.5435201074,0.5301226195\C,0,8
.048809617,6.1357367118,1.3396477678\C,0,9.6411133145,4.5729531877,0.4
022634252\C,0,9.287558626,5.8855045648,0.8121110793\H,0,1.1795797577,1
.0907805764,1.9601690027\H,0,1.7985258521,0.7538365205,3.5741488914\H,
0,2.5648100442,0.0093478388,2.1640207773\H,0,4.6015375222,0.9220230668
,1.5731034094\H,0,0.6704244664,2.8075280714,3.475028143\H,0,3.76403727
8,6.6343465859,3.0877317752\H,0,-0.0376087075,5.0382872049,4.212674779
5\H,0,6.7635577315,1.7342886029,0.9132571648\H,0,5.5784187244,6.333591
6451,2.3287701933\H,0,1.5322251961,6.9641815212,4.012823525\H,0,9.0133
214603,2.5379143384,0.217988494\H,0,7.7754313623,7.1387797681,1.654075
9062\H,0,10.6265272661,4.3909851542,-0.0138174509\H,0,10.0070317123,6.
6904002872,0.7042253468\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1
=-730.1004358\CCSD(T)/GTBas1=-730.2991924\MP2/GTBas2=0.\MP2/GTBas3=0.\
HF/GTMP2LargeXP=-727.8987085\MP2/GTMP2LargeXP=-730.8870093\HF/GFHFB3=-
727.907297\HF/GFHFB4=-727.9569457\G4MP2=-731.3184725\FreqCoord=5.76228
46886,3.9487818912,4.5589960866,3.9671408696,1.74967374,4.788334457,4.
9914454769,6.455176091,5.3782727047,8.1101671053,3.6125022362,3.587974
8071,6.6892180304,8.5333628452,5.1610894142,2.5664090828,6.8779148112,
6.396866637,9.9048345325,5.6289616171,3.3206599505,9.2136828757,8.1356
412138,4.109487178,5.8594325266,10.9256512664,5.9792086126,1.806310067
,9.248180286,7.1836248805,12.290304008,5.183644055,2.3124138243,10.987
395885,10.0525450925,3.8294360466,3.4712991901,11.2901965981,6.9715176
293,14.0804103987,7.1160266171,2.029304169,13.402761295,9.6233826388,2
.8130980795,16.5300356728,6.6962825493,1.0017865678,15.2100458719,11.5
948620088,2.5315673956,18.2190637805,8.6416291432,0.7601677068,17.5509
422463,11.1219917813,1.5346675293,2.229082694,2.0612765604,3.704182589
2,3.3987213034,1.4245445726,6.7541625629,4.8467885664,0.0176648552,4.0
894066149,8.6956457072,1.7423710845,2.9727346225,1.2669186342,5.305459
1654,6.5668514943,7.1129996093,12.5370981181,5.834967427,-0.0710701573
,9.5209829961,7.9608016202,12.7812717964,3.2773304949,1.7258059303,10.
5416836437,11.9687536468,4.4007378918,2.8954859945,13.1603958148,7.583
1374819,17.0327091077,4.7959630483,0.4119385538,14.6934358398,13.49033
86846,3.1257504656,20.0812262766,8.2977593951,-0.026111198,18.91054933
94,12.6430242621,1.3307930413\PG=C01 [X(C19H14)]\NImag=0\

4, 5, 6-trihydrobenz [de] anthracene

1\1\GINC-SAW100\Mixed\G4MP2\G4MP2\C17H14\KFOREST\29-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,-0.2260177759,-0.9023223701,-0.0498218127\C,0,-0.2182
541849,-2.4192093899,-0.084864471\C,0,1.0881251511,-3.0206998144,0.442
7621721\C,0,2.2858317499,-2.3788559787,-0.2578844437\C,0,2.265432104,-
0.8787145893,-0.093429676\C,0,0.9966236329,-0.2005680471,-0.0236742772
\C,0,0.9965844557,1.2406001209,0.068737339\C,0,3.4279611775,-0.1569243
, -0.0348893424\C,0,3.4227825034,1.2591774582,0.0736428321\C,0,2.240576
3244,1.937893257,0.1184974676\C,0,-1.4376185408,1.2478482482,0.0386944
67\C,0,-1.4474550859,-0.1927353232,-0.0433327786\C,0,-0.2181366551,1.9
224318875,0.104204036\C,0,-3.8699903444,1.2938729085,-0.020026321\C,0,
-3.8881587023,-0.1232658566,-0.1152467674\C,0,-2.7214821362,-0.8372312
251,-0.1241480745\C,0,-2.6772673648,1.954420128,0.0539190404\H,0,-1.05
49858819,-2.8097100186,0.5014631325\H,0,-0.3853912159,-2.7644730257,-1
.1163950789\H,0,1.0872939343,-4.1053485618,0.2931835165\H,0,1.16107819
02,-2.8441684862,1.5228378352\H,0,2.2461466905,-2.6295952967,-1.328662
1831\H,0,3.2310481891,-2.7836451654,0.118280435\H,0,4.379241829,-0.679
6493455,-0.0796470157\H,0,4.3663476898,1.7933972068,0.1156224172\H,0,2
.2215527998,3.020907159,0.192399374\H,0,-0.2153605062,3.0066753348,0.1
765359627\H,0,-4.8049751939,1.8441461396,-0.0098877871\H,0,-4.83928381
96,-0.6412407694,-0.1830358644\H,0,-2.7663605699,-1.9156158057,-0.2111
225333\H,0,-2.6471684438,3.0378835211,0.1219183998\Version=EM64L-G09R
evB.01\State=1-A\MP2/GTBas1=-654.1097529\CCSD(T)/GTBas1=-654.29428\MP2
/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-652.129434\MP2/GTMP2LargeXP=
-654.8256536\HF/GFHFB3=-652.1360452\HF/GFHFB4=-652.1813255\G4MP2=-655.
2073252\FreqCoord=-0.4271116976,-1.705142163,-0.0941495814,-0.41244063
69,-4.571643205,-0.1603706086,2.0562585339,-5.7082953789,0.8366992473,
4.3195959932,-4.4953863094,-0.4873309726,4.2810462492,-1.6605299228,-0
.1765565004,1.8833457238,-0.37901868,-0.0447379002,1.8832716896,2.3443
944689,0.1298947458,6.4779078196,-0.2965439506,-0.0659313022,6.4681215
438,2.3795005487,0.1391647844,4.234075633,3.6620875305,0.2239277611,-2
.7167053257,2.3580914444,0.0731219455,-2.735293702,-0.364216977,-0.081
8870841,-0.4122185377,3.6328697764,0.1969170901,-7.3132218879,2.445065
4478,-0.0378442621,-7.3475551086,-0.2329387105,-0.2177848281,-5.142855
913,-1.5821377253,-0.2346058607,-5.0593021039,3.6933187904,0.101892219
7,-1.9936343908,-5.309582448,0.9476279862,-0.7282838521,-5.2240969204,
-2.1096809552,2.0546877618,-7.7579844618,0.5540365528,2.1941197984,-5.
3746995147,2.8777464533,4.2446020994,-4.9692149511,-2.5108076491,6.105
7961995,-5.2603270137,0.2235176291,8.2755677264,-1.2843511294,-0.15051
1047,8.2512013346,3.3890295684,0.2184947033,4.1981263813,5.7086872034,
0.3635821249,-0.4069723766,5.6817929532,0.3336046222,-9.0800871918,3.4
849311528,-0.0186852097,-9.1449210983,-1.2117694394,-0.3458876562,-5.2
27663862,-3.6199892485,-0.3989637685,-5.0024233864,5.7407678784,0.2303
923862\PG=C01 [X(C17H14)]\NImag=0\

4, 5-dihydroacephenanthrylene

1\1\GINC-SAW233\Mixed\G4MP2\G4MP2\C16H12\KFOREST\27-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,1.9398985482,-3.1876042999,-0.0023821784\C,0,3.101128
7602,-2.3979831414,-0.0051713844\C,0,0.6968637558,-2.5882648348,-0.000
1851467\C,0,0.5546477444,-1.1857079293,-0.0006743741\C,0,2.9956063477,
-1.0235777247,-0.0057214085\C,0,-2.0101505008,-1.1390883192,0.00482449
37\C,0,-0.7379899297,-0.5257799154,0.0017898639\C,0,-3.1634469324,-0.3
705913529,0.0072348043\C,0,1.738367018,-0.3803555633,-0.0035448732\C,0
, -3.1261601104,1.0396694394,0.0071559934\C,0,-0.7332447769,0.879211801
2,0.0012319311\C,0,1.660715133,1.0583278908,-0.004495563\C,0,-1.897432
1658,1.6647864681,0.0042727476\C,0,0.4504899566,1.6723766849,-0.002377
6024\C,0,-1.5134012485,3.1322230558,0.004932259\C,0,0.0526383592,3.136
7917415,-0.0043189452\H,0,2.0195333121,-4.2695793097,-0.0019413031\H,0
,4.0784347158,-2.8693235688,-0.0068937099\H,0,-0.1904004151,-3.2114994
236,0.0020011711\H,0,3.8904028116,-0.4078552864,-0.007894319\H,0,-2.10
03490937,-2.2194533023,0.0052564793\H,0,-4.127532432,-0.8695060998,0.0
094204136\H,0,-4.052735562,1.6052082629,0.009460988\H,0,2.5906042363,1
.6204277755,-0.0071847983\H,0,-1.9105195427,3.6492356191,0.8853940307\
H,0,-1.9217275239,3.6544247206,-0.8672083578\H,0,0.4453106315,3.655270
2517,-0.8854618607\H,0,0.4566789032,3.6622563603,0.867400649\Version=
EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-614.944159\CCSD(T)/GTBas1=-615.
1124972\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-613.0896628\MP2/G
TMP2LargeXP=-615.6058481\HF/GFHFB3=-613.096738\HF/GFHFB4=-613.1385638\
G4MP2=-615.9680303\FreqCoord=3.6658769818,-6.0236991469,-0.0045016647,
5.8602840595,-4.5315314086,-0.0097725003,1.3168816504,-4.8911116972,-0
.0003498765,1.0481323372,-2.24066326,-0.0012743823,5.6608755991,-1.934
2815754,-0.0108118951,-3.7986339324,-2.1525649644,0.0091169718,-1.3945
988559,-0.9935800462,0.0033823526,-5.9780483381,-0.7003161643,0.013671
7988,3.2850375825,-0.7187678478,-0.0066988395,-5.9075864563,1.96469050
92,0.0135228678,-1.3856318166,1.6614695171,0.0023280123,3.1382967862,1
.9999498724,-0.0084953828,-3.5856271491,3.1459904944,0.0080743228,0.85
13026437,3.1603339254,-0.0044930173,-2.8599138889,5.9190437626,0.00932
06187,0.0994720831,5.9276773273,-0.0081616236,3.8163648761,-8.06833559
8,-0.0036685313,7.7071246637,-5.4222357317,-0.0130272237,-0.3598046401
, -6.0688543865,0.0037816653,7.3517958605,-0.7707347932,-0.0149181009,-
3.9690845705,-4.194158906,0.0099333063,-7.7999059011,-1.6431283996,0.0
178020017,-7.6585603011,3.0334040031,0.0178786763,4.8955325252,3.06216
47138,-0.0135773012,-3.6103587072,6.8960559146,1.6731522377,-3.6315387
221,6.9058618952,-1.6387862963,0.8415151376,6.9074597174,-1.6732804179
,0.8629980577,6.9206615493,1.6391496741\PG=C01 [X(C16H12)]\NImag=0\

5, 6-dihydro-4H-benz [de] anthracene

1\1\GINC-SAW249\Mixed\G4MP2\G4MP2\C17H14\KFOREST\28-Jan-2011\0\#\# G4MP
2\name\0,1\C,0,-2.6536719948,-1.9530444582,0.0323557122\C,0,-3.86596
49442,-1.3019673492,0.086075893\C,0,-1.4398052342,-1.2325656907,-0.007
1037429\C,0,-3.8970033936,0.1022310502,0.1023548027\C,0,-1.4635787651,
0.1890634778,0.0125498884\C,0,-0.1858830901,-1.9146020676,-0.067784904
4\C,0,-2.7228003932,0.8261774428,0.0667234437\C,0,-0.2018849933,0.9126
98063,-0.0183597918\C,0,1.02583252,0.1867110271,-0.0815025916\C,0,-0.1
449043574,2.3217887851,0.0142884182\C,0,1.0037033339,-1.2578776862,-0.
1166525284\C,0,2.262158503,0.8904311387,-0.0954666715\C,0,2.307049954,
-2.0182620254,-0.2196355678\C,0,1.0607998558,2.9892859117,-0.003373017
\C,0,2.2623710898,2.2719628493,-0.0519171982\C,0,3.5721628203,0.133387
5189,-0.1594585466\C,0,3.4595316209,-1.2660440883,0.45097185\H,0,-2.61
22338425,-3.0382108084,0.0177396343\H,0,-4.7914416509,-1.8673875289,0.
1151132932\H,0,-4.8484642562,0.6220782027,0.1437053829\H,0,-0.19967660
97,-3.0017855419,-0.0799883248\H,0,-2.7817057873,1.9074902495,0.080526
7114\H,0,-1.0597322432,2.898961072,0.0596877111\H,0,2.5578079098,-2.16
57016298,-1.2809397333\H,0,2.1839911542,-3.0188136927,0.2076395789\H,0
,1.0798405121,4.0737750107,0.0285832141\H,0,3.2090430414,2.8045882918,
-0.0522861815\H,0,4.3552339977,0.7166815415,0.3366325503\H,0,3.8854349
65,0.0354856975,-1.2097351503\H,0,4.3989335818,-1.8144237851,0.3263428
351\H,0,3.2711066958,-1.1856209779,1.5285430306\Version=EM64L-G09RevB
.01\State=1-A\MP2/GTBas1=-654.1210339\CCSD(T)/GTBas1=-654.3047465\MP2/
GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-652.1434858\MP2/GTMP2LargeXP=
-654.8364749\HF/GFHFB3=-652.1501543\HF/GFHFB4=-652.1954322\G4MP2=-655.
2173461\FreqCoord=-5.0147133166,-3.6907191513,0.0611434348,-7.30561498
39,-2.4603617239,0.1626598645,-2.7208375773,-2.3292115963,-0.013424128
7,-7.3642691528,0.1931886872,0.1934225455,-2.7657630399,0.3572781947,0.
.0237158521,-0.3512681331,-3.6180735612,-0.1280949053,-5.1453470576,1.
561249104,0.1260890352,-0.3815073477,1.7247493811,-0.0346949784,1.9385
42521,0.3528327073,-0.1540175772,-0.273829551,4.3875449422,0.027001197
3,1.8967244198,-2.3770443355,-0.2204413313,4.2748600398,1.6826709923,-
0.1804058639,4.359692588,-3.8139624923,-0.4150510721,2.0046212092,5.64
89317061,-0.0063740784,4.2752617707,4.2933875693,-0.0981092862,6.75040
94324,0.2520658802,-0.3013329827,6.5375673116,-2.3924765991,0.85221329
01,-4.9364065573,-5.7413863619,0.0335230506,-9.0545125018,-3.528851013
7,0.2175325985,-9.1622696093,1.1755574362,0.2715638175,-0.3773341075,-
5.6725525838,-0.1511560277,-5.2566621203,3.6046341728,0.1521734309,-2.
0026037139,5.478242496,0.1127934275,4.8335564501,-4.0925829659,-2.4206
252887,4.127145158,-5.7047311255,0.3923819384,2.0406028351,7.698319097
3,0.0540144466,6.0642124969,5.299903787,-0.0988065635,8.2301995003,1.3
54331838,0.6361433275,7.342407991,0.06705825,-2.2860681274,8.312779746
4,-3.4287640429,0.6166985837,6.1814958064,-2.2404989457,2.8885277103\P
G=C01 [X(C17H14)]\NImag=0\

4H-cyclopenta[def]phenanthrene

1\1\GINC-SAW269\Mixed\G4MP2\G4MP2\C15H10\KFOREST\27-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,0.9908992487,1.5742435243,2.0290775436\C,0,1.09190316
02,1.3355201898,3.4229147386\C,0,2.3498326089,1.2140811851,3.977890964
3\C,0,3.4454036729,1.3372176432,3.1123799137\C,0,3.3965136718,1.571820
9627,1.7361651059\C,0,4.6557851765,1.1918685608,3.8143168804\C,0,4.417
2972383,0.9658089776,5.1768762165\C,0,5.9027339169,1.2708608035,3.1895
980421\C,0,2.8973352415,0.9626731298,5.3894558972\C,0,5.5200881643,0.8
037601032,5.9909543798\C,0,6.8079520345,0.8757012002,5.4025617815\C,0,
7.0130714923,1.1013378932,4.0467534\C,0,5.8622864471,1.513065539,1.767
5151847\C,0,4.6801437803,1.6550239758,1.0819540951\C,0,2.0966382066,1.
6917290937,1.195565425\H,0,0.0003070791,1.6693227047,1.5952957472\H,0,
0.1871145685,1.2542919242,4.0171090504\H,0,2.5436689952,0.0098424662,5
.802000732\H,0,2.5811675294,1.7401722007,6.0956376409\H,0,5.4303270806
,0.6246592181,7.0578059514\H,0,7.6734872675,0.747886329,6.0452063908\H
,0,8.0246841709,1.1459250643,3.6548268408\H,0,6.7997659237,1.585078027
4,1.2234439808\H,0,4.7095172344,1.8360870389,0.0112441993\H,0,1.954856
0899,1.8748222446,0.134749898\Version=EM64L-G09RevB.01\State=1-A\MP2/
GTBas1=-575.7715009\CCSD(T)/GTBas1=-575.9235351\MP2/GTBas2=0.\MP2/GTBa
s3=0.\HF/GTMP2LargeXP=-574.0356999\MP2/GTMP2LargeXP=-576.3802092\HF/GF
HFB3=-574.0430117\HF/GFHFB4=-574.081345\G4MP2=-576.7216623\FreqCoord=1
.8725282054,2.9748891274,3.8344008598,2.0633979365,2.5237674036,6.4683
714322,4.4405400889,2.294280943,7.5171245091,6.510869359,2.5269751258,
5.8815456584,6.4184806463,2.9703111494,3.2808765717,8.7981589171,2.252
3051664,7.208014288,8.3474820279,1.8251144643,9.782878273,11.154550538
2,2.4015788717,6.0274667735,5.4751701216,1.8191885709,10.184595651,10.
4314548599,1.5188864715,11.3212630524,12.865164871,1.6548354425,10.209
362183,13.2527844709,2.0812269979,7.6472556533,11.0781158975,2.8592794
898,3.3401196348,8.8441900073,3.1275420576,2.0445969282,3.9620720102,3
.1969046782,2.2592912272,0.0005802953,3.1545627393,3.0146720632,0.3535
952899,2.3702682274,7.5912359512,4.8068377737,0.0185995655,10.96419240
64,4.8776997336,3.2884488835,11.5190857466,10.2618309943,1.1804348486,
13.3373203473,14.5007894199,1.4133003403,11.4237844953,15.164455386,2.
1654845403,6.9066217923,12.8496953636,2.9953633711,2.3119740627,8.8996
977912,3.4697016596,0.0212484572,3.6941426392,3.5429005902,0.254640403
7\PG=C01 [X(C15H10)]\NImag=0\

5H-dibenzo [a, d] cycloheptene

1\1\GINC-SAW320\Mixed\G4MP2\G4MP2\C15H12\KFOREST\22-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,2.1492006862,3.8932513121,1.8510785782\C,0,3.24697017
39,4.7745361722,1.7589730188\C,0,0.9305150716,4.3849312069,2.347877934
9\C,0,2.2263294282,2.4855527705,1.4671994051\C,0,3.1105955111,6.084803
2462,2.2171238733\C,0,4.5284180503,4.311438863,1.1042992782\C,0,1.9056
568915,6.5475966712,2.736772054\C,0,0.8059844163,5.693454491,2.7929067
525\C,0,5.2374610315,3.2220548778,1.8760933155\C,0,4.6422318172,1.9488
142338,1.9977680241\C,0,6.5049463823,3.4373826895,2.4168472998\C,0,5.3
753470709,0.9181889657,2.609410854\C,0,3.2892986774,1.6564910264,1.529
7442537\C,0,7.2051256207,2.4142813115,3.0485922197\C,0,6.6392500944,1.
1438047555,3.1361350431\H,0,0.0786012436,3.7132613695,2.3991462339\H,0
,1.2731320674,2.0353623927,1.196672849\H,0,3.9596225992,6.7581581119,2
.1440727804\H,0,4.2888494108,3.928668566,0.1020431834\H,0,5.200938143,
5.163687919,0.9715777176\H,0,1.8203756474,7.5741719586,3.0772797673\H,
0,-0.1432233919,6.0467407493,3.1816695223\H,0,6.9574604718,4.419997470
5,2.320465607\H,0,4.9267495491,-0.0680470035,2.6844098724\H,0,3.102941
239,0.6082046669,1.3043383263\H,0,8.194334376,2.6028091656,3.452322952
2\H,0,7.1814077222,0.3339020393,3.6126492835\Version=EM64L-G09RevB.01
\State=1-A\MP2\GTBas1=-576.9198789\CCSD(T)/GTBas1=-577.0844407\MP2\GTB
as2=0.\MP2\GTBas3=0.\HF/GTMP2LargeXP=-575.1850983\MP2\GTMP2LargeXP=-57
7.5489815\HF/GFHFB3=-575.1910055\HF/GFHFB4=-575.2309205\G4MP2=-577.891
1101\FreqCoord=4.0614007016,7.3571787464,3.4980315632,6.1358843903,9.0
225657771,3.3239772806,1.7584186478,8.2863190926,4.4368462904,4.207152
9009,4.697014025,2.772605058,5.8781736261,11.4986117079,4.1897569231,8
.5574699303,8.1474386897,2.0868232045,3.6011696282,12.3731645372,5.171
7496702,1.5230898141,10.759069738,5.2778288769,9.8973669812,6.08880130
42,3.545302566,8.7725467798,3.6827251858,3.7752344425,12.2925671717,6.
4957118972,4.5671795016,10.1579338332,1.7351256833,4.9310718821,6.2158
736696,3.1303143816,2.8907976928,13.6157141762,4.5623304865,5.76100438
6,12.5463644062,2.1614777374,5.9264363473,0.1485348241,7.0170470481,4.
5337293347,2.4058709383,3.8462775034,2.2613839553,7.482602302,12.77106
79942,4.0517103639,8.1047508116,7.4241076567,0.1928336703,9.8283487244
,9.7579560026,1.8360158031,3.4400114325,14.3131106852,5.8152159945,-0.
2706529864,11.4266840127,6.0124840425,13.1476948721,8.3525847272,4.385
0444979,9.3102073731,-0.1285902007,5.0727994873,5.8637091482,1.1493402
532,2.4648422214,15.4850478119,4.9185964992,6.523944902,13.5708938435,
0.6309834094,6.82691776\PG=C01 [X(C15H12)]\NImag=0\

6b, 8a-dihydrocyclobut [a] acenaphthylene

1\1\GINC-SAW238\Mixed\G4MP2\G4MP2\C14H10\KFOREST\01-Feb-2011\0\#\ G4MP
2\name\0,1\C,0,4.9679815737,3.3260037742,1.3088853295\C,0,5.61797780
89,4.5826382439,1.4269461726\C,0,4.9063868065,5.6996102961,1.811573932
4\C,0,4.7858455226,0.9430164896,0.8861627009\C,0,5.5547232088,2.086568
0948,0.9413307182\C,0,3.5165217036,5.6510054243,2.1011553516\C,0,3.588
0132655,3.303413982,1.6047451267\C,0,3.3973197305,0.9473507316,1.18603
19037\C,0,2.8581222632,4.4500705165,1.9951432701\C,0,2.7993529114,2.13
11099689,1.5439734036\C,0,1.4137144905,4.0545171167,2.199814392\C,0,1.
3740797319,2.4911501497,1.8955876892\C,0,0.4881736979,4.1820692649,0.9
888745643\C,0,0.4550603996,2.8720712679,0.7338770068\H,0,6.6809436794,
4.6582528913,1.218621963\H,0,5.4218284118,6.6510351321,1.8997224823\H,
0,5.2533764219,0.0039409236,0.6064999734\H,0,6.6146621768,2.0427363632
,0.7097682816\H,0,3.0003918793,6.5578909203,2.4004245507\H,0,2.8347215
343,0.0207579028,1.1285670406\H,0,0.9916616028,4.3791236892,3.15627027
78\H,0,0.9275664942,1.8527765933,2.6646221642\H,0,0.0548408499,5.05342
41645,0.5116530384\H,0,-0.0156561651,2.2653560987,-0.0310413334\Versi
on=EM64L-G09RevB.01\State=1-A\MP2\GTBas1=-537.7081785\CCSD(T)/GTBas1=-
537.8575876\MP2\GTBas2=0.\MP2\GTBas3=0.\HF/GTMP2LargeXP=-536.0884936\M
P2/GTMP2LargeXP=-538.2831986\HF/GFHFB3=-536.0941699\HF/GFHFB4=-536.130
3867\G4MP2=-538.606005\FreqCoord=9.3881246075,6.2852362501,2.473434812
,10.6164394795,8.6599312471,2.6965374726,9.2717273662,10.7707025239,3.
4233786016,9.043937352,1.782042904,1.6746048139,10.4969056087,3.943042
2568,1.7788572578,6.6452629602,10.6788526274,3.9706081772,6.780362433,
6.2425477295,3.0325288025,6.4200038765,1.7902334345,2.2412754828,5.401
0683318,8.4094145482,3.7702743763,5.2900103519,4.0272142003,2.91768688
93,2.6715332171,7.6619269517,4.157046744,2.5966343779,4.7075915389,3.5
821415934,0.9225145942,7.9029655794,1.8687021063,0.8599395292,5.427428
1304,1.386826558,12.6251538634,8.8028222223,2.3028617696,10.2457708379
,12.5686348999,3.58995522,9.9274427104,0.0074472664,1.1461188494,12.49
98999758,3.8602122881,1.34126767,5.6699189432,12.3926178487,4.53614500
34,5.3568473628,0.0392267513,2.1326826293,1.8739688458,8.2753444746,5.
9644864263,1.7528466441,3.5012403467,5.035406138,0.1036341871,9.549587
7042,0.9668841177,-0.0295858644,4.28090262,-0.058659619\PG=C01 [X(C14H
10)]\NImag=0\

9,10-dihydro-9,10[1',2']-benzenoanthracene

1\1\GINC-SAW306\Mixed\G4MP2\G4MP2\C20H14\KFOREST\01-Feb-2011\0\#\ G4MP
2\name\0,1\C,0,4.0855733223,2.1347214732,5.3501886889\C,0,2.90651289
23,3.0292990213,5.728886675\C,0,4.1208081958,2.1168010472,3.8229334179
\C,0,5.3392338388,2.8909280451,5.7868317678\C,0,2.9928719438,4.3132507
255,5.1691992474\C,0,1.8295650624,2.6868560887,6.5305570659\C,0,4.2071
671133,3.4007525016,3.2632460808\C,0,4.0759014479,0.9990785551,3.00531
17879\C,0,5.4255933271,4.1748866688,5.2271413007\C,0,6.3304847073,2.43
13859268,6.6388427222\C,0,4.2451526636,4.5072837344,4.3159649632\C,0,2
.0019980705,5.2505205713,5.4130300269\C,0,0.8291902855,3.6327551277,6.
7768946242\C,0,4.2483340351,3.5627401347,1.8877859236\C,0,4.1174637729
,1.1622996477,1.6168931899\C,0,6.5029108479,4.9949490851,5.5213598406\
C,0,7.4181236937,3.2589710734,6.9360971572\C,0,0.9147725841,4.90515854
07,6.2222411984\C,0,4.2030446688,2.4346838648,1.0622481258\C,0,7.50370
68613,4.5313879199,6.3814379235\H,0,4.0183787343,1.1361985445,5.785436
2188\H,0,1.7622198476,1.6934103314,6.9636543186\H,0,4.0089319859,0.005
3570944,3.4378360786\H,0,6.2638863499,1.4380341669,7.0722697678\H,0,4.
312279452,5.5057968394,3.8806844262\H,0,2.0682981003,6.2440578467,4.97
99814674\H,0,-0.0165414756,3.3703011194,7.4038504591\H,0,4.3150097717,
4.5560028233,1.4541638567\H,0,4.0826729622,0.290741555,0.9716124747\H,
0,6.569957631,5.9885795699,5.0886413906\H,0,8.1972537661,2.9044706929,
7.6028045851\H,0,0.135779067,5.6349422482,6.4166705714\H,0,4.234989649
4,2.5553286534,-0.0155438198\H,0,8.349584824,5.1692687617,6.615556477\
\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-768.0865344\CCSD(T)/GT
Bas1=-768.2890188\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-765.756
7712\MP2/GTMP2LargeXP=-768.9063104\HF/GFHF3=-765.7647854\HF/GFHF4=-7
65.816356\G4MP2=-769.3545494\FreqCoord=7.7206146751,4.0340389543,10.11
03913813,5.4925133681,5.724545525,10.8260268621,7.7871989362,4.0001742
57,7.224297184,10.0896897149,5.4630622751,10.9355272183,5.6557083246,8
.1508626137,9.7683709039,3.4573769102,5.0774221661,12.3409643497,7.950
3936395,6.4264908738,6.1666413969,7.7023374812,1.8879848543,5.67921622
3,10.2528854966,7.8893924398,9.8778655162,11.9628823852,4.5946535251,1
2.5455945843,8.0221759264,8.5175318612,8.1559917797,3.7832280718,9.922
0459349,10.2291443,1.5669425517,6.8649122992,12.8064748711,8.028187847
3,6.7326031373,3.5673983932,7.7808788929,2.1964280185,3.0554853151,12.
288720569,9.4390858185,10.4338579798,14.0182222009,6.1585628037,13.107
3240582,1.7286696578,9.2694062802,11.7583317977,7.9426033483,4.6008857
247,2.007358043,14.1799509493,8.5630821704,12.0591700093,7.593635306,2
.1471040817,10.9328900128,3.3301128979,3.200081757,13.1593995463,7.575
7835387,0.0101234413,6.4965686784,11.8370297288,2.7174907451,13.364652
999,8.1490271727,10.4044481698,7.3334307737,3.9085169708,11.7995592881
,9.4108011202,-0.0312588586,6.368946101,13.9912496965,8.1541867291,8.6
095975966,2.7479714415,7.7151337887,0.5494219144,1.8360814844,12.41542
06272,11.316775312,9.6161386166,15.4905646597,5.4886541706,14.36721850
77,0.2565852513,10.6484976237,12.1257500649,8.0029706129,4.8288713344,
-0.0293735625,15.7784286407,9.7685022669,12.5015899582\PG=C01 [X(C20H1
4)]\NImag=0\

9, 10-dehydrophenanthrene

```
1\1\GINC-SAW307\Mixed\G4MP2\G4MP2\C14H8\KFOREST\26-Jan-2011\0\#\# G4MP2
\name\0,1\C,0,0.4481755601,-2.016794515,0.\C,0,1.5118496201,-1.40482
11855,0.\C,0,0.4510901658,0.68474087,0.\C,0,1.7246462487,-0.0075079538
,0.\C,0,2.9353656905,0.6970702949,0.\C,0,2.9351074774,2.0783010395,0.\
C,0,1.7184417591,2.7728987259,0.\C,0,0.5138537882,2.0928841617,0.\C,0,
-0.866573861,-1.4977480746,0.\C,0,-0.8246784061,-0.0488571244,0.\C,0,-
2.0734925137,0.6050133627,0.\C,0,-3.2670496143,-0.0941440149,0.\C,0,-3
.2783554888,-1.4950501238,0.\C,0,-2.0845482364,-2.1897679077,0.\H,0,3.
8640391544,0.1381408768,0.\H,0,3.872964088,2.6231501712,0.\H,0,1.71713
07816,3.8577195683,0.\H,0,-0.4019669819,2.6718595874,0.\H,0,-2.1134222
84,1.6878089307,0.\H,0,-4.2040020477,0.4526103779,0.\H,0,-4.22083459,-
2.0318598383,0.\H,0,-2.0686003101,-3.2735572291,0.\Version=EM64L-G09R
evB.01\State=1-A'\MP2/GTBas1=-536.4840866\CCSD(T)/GTBas1=-536.6205174\
MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-534.8540813\MP2/GTMP2Larg
eXP=-537.043803\HF/GFHFB3=-534.8615604\HF/GFHFB4=-534.8968519\G4MP2=-5
37.3685748\FreqCoord=0.8469290681,-3.8111892996,0.,2.8569817361,-2.654
7273064,0.,0.8524368745,1.2939727162,0.,3.2591090862,-0.0141879766,0.,
5.5470372548,1.3172719527,0.,5.5465493029,3.9274197864,0.,3.2473843001
,5.2400191863,0.,0.9710429321,3.9549778936,0.,-1.6375872711,-2.8303336
77,0.,-1.5584163352,-0.0923265848,0.,-3.9183329895,1.1433095622,0.,-6.
1738290335,-0.1779064053,0.,-6.1951940402,-2.8252352889,0.,-3.93922527
75,-4.1380616401,0.,7.3019757686,0.2610484248,0.,7.3188414488,4.957035
429,0.,3.2449069115,7.2900334816,0.,-0.7596075103,5.0490828857,0.,-3.9
937893198,3.1894966436,0.,-7.9444125323,0.8553096592,0.,-7.9762214272,
-3.8396586347,0.,-3.9090880645,-6.1861266433,0.\PG=CS [SG(C14H8)]\NIma
g=0\
```

9-ethylidene fluorene

1\1\GINC-SAW335\Mixed\G4MP2\G4MP2\C15H12\KFOREST\23-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,-3.3586555578,0.8867388607,0.0379945093\C,0,-3.413671
758,-0.5085091245,0.0077800823\C,0,-2.2420532458,-1.2635833667,-0.0164
1744\C,0,-2.1319759974,1.5506260841,0.0445157058\C,0,-0.9583806101,0.8
05406208,0.0204863118\C,0,-1.0167468354,-0.6046931337,-0.0099964639\C,
0,0.4607825995,1.2321032928,0.0205051033\C,0,1.2495553485,-0.018608251
6,-0.0118979078\C,0,0.3556355511,-1.1184860822,-0.030171177\C,0,0.8326
161772,-2.42335666,-0.0618022808\C,0,2.2101355097,-2.6410395485,-0.075
4700327\C,0,3.0958005411,-1.5639490434,-0.0576443362\C,0,2.6235992356,
-0.2504700624,-0.0258647224\C,0,0.8762219358,2.5104512288,0.0455601044
\C,0,2.2925650877,3.0095712525,0.0472284906\H,0,-4.2794695811,1.460303
3052,0.0565930724\H,0,-4.3767492601,-1.0082790954,0.0031209467\H,0,-2.
2902440292,-2.347613972,-0.0398316659\H,0,-2.1050897593,2.6355264058,0
.0681381025\H,0,0.1459343956,-3.2637716235,-0.0757623748\H,0,2.5954837
749,-3.6550768222,-0.10013164\H,0,4.1652470011,-1.7466302425,-0.068561
5069\H,0,3.3319155109,0.5673730989,-0.012606721\H,0,0.1053872928,3.277
2789399,0.0672256321\H,0,2.852173872,2.644084183,0.9168262772\H,0,2.32
22885174,4.1012064286,0.0708949795\H,0,2.8407142834,2.6825877402,-0.84
47110487\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-576.9183736\C
CSD(T)/GTBas1=-577.0824585\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP
=-575.1849625\MP2/GTMP2LargeXP=-577.5479067\HF/GFHFB3=-575.1912376\HF/
GFHFB4=-575.2310388\G4MP2=-577.8917193\FreqCoord=-6.346939179,1.675693
5981,0.0717992172,-6.4509047301,-0.9609429814,0.0147022248,-4.23686660
98,-2.3878265091,-0.0310244654,-4.028850757,2.9302586335,0.0841224926,
-1.8110768842,1.5219971588,0.0387135188,-1.9213730655,-1.1427044171,-0
.0188905791,0.8707529199,2.3283377909,0.0387490296,2.3613173965,-0.035
1644993,-0.0224837873,0.6720537947,-2.1136323788,-0.0570152616,1.57341
65487,-4.5794804096,-0.1167893852,4.17655083,-4.9908414528,-0.14261769
31,5.8502151847,-2.9554353778,-0.1089320085,4.9578840377,-0.4733198224
, -0.0488772418,1.6558194902,4.7440652924,0.0860961199,4.3323201576,5.6
872654445,0.0892489129,-8.0870255023,2.7595733177,0.1069454079,-8.2708
574538,-1.9053713558,0.0058977345,-4.3279339926,-4.4363474729,-0.07527
094,-3.9780431302,4.9804231229,0.128762353,0.275776041,-6.1676345286,-
0.1431701395,4.9047535169,-6.9070941885,-0.1892213768,7.8711761078,-3.
3006528138,-0.1295624713,6.2964078134,1.0721797721,-0.02382325,0.19915
31212,6.1931596574,0.1270380338,5.3898275015,4.9965949781,1.7325505754
,4.3884892995,7.7501569645,0.1339720955,5.3681720174,5.0693561564,-1.5
962725436\PG=C01 [X(C15H12)]\NImag=0\

2-methyl-9H-fluorene

1\1\GINC-SAW329\Mixed\G4MP2\G4MP2\C14H12\KFOREST\21-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,6.4132223963,6.1066046269,0.7136366343\C,0,7.40384016
8,7.2456707389,0.7043261916\C,0,5.0405014968,6.3523774375,0.8431554279
\C,0,6.8536353714,4.7798342138,0.6149508429\C,0,4.1459280927,5.2941888
332,0.8783338663\C,0,5.9643023048,3.709869355,0.6487890165\C,0,4.60128
69536,3.9666001354,0.7820317804\C,0,2.6371639363,5.3152124569,1.008114
5107\C,0,3.4449903049,3.0668104086,0.8424137607\C,0,2.2779695093,3.844
207411,0.976718743\C,0,3.3615624779,1.6766936255,0.7900010479\C,0,1.03
38955019,3.237472176,1.0586431041\C,0,2.1085774825,1.0722920365,0.8726
420201\C,0,0.9531921971,1.8440304747,1.0058736703\H,0,8.2374461848,7.0
457551314,0.0240476485\H,0,6.9319504062,8.1831065062,0.3964670646\H,0,
7.8337339581,7.4094195529,1.700589625\H,0,4.6845754192,7.377039883,0.9
143232791\H,0,7.9170793823,4.5853826896,0.5078657445\H,0,6.3343244967,
2.6926658676,0.5671662433\H,0,2.3105645948,5.7986867241,1.937950727\H,
0,2.1616734545,5.8720963976,0.1903239407\H,0,4.2557420502,1.070205013,
0.6867620894\H,0,0.1316133051,3.8329489743,1.1623418926\H,0,2.03017636
06,-0.009338658,0.833093548\H,0,-0.0148378061,1.3580679886,1.068917580
5\Version=EM64L-G09RevB.01\State=1-A\MP2/GTbas1=-538.9465559\CCSD(T)/
GTbas1=-539.1009266\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-537.3
245248\MP2/GTMP2LargeXP=-539.5398364\HF/GFHFB3=-537.3300808\HF/GFHFB4=
-537.3676731\G4MP2=-539.8572731\FreqCoord=12.1192339583,11.5398103466,
1.3485777972,13.9912302491,13.6923333455,1.3309836104,9.5251674014,12.
0042536496,1.5933328462,12.9514938667,9.0325776246,1.1620886784,7.8346
686618,10.0045669905,1.6598104606,11.2708979299,7.0106370697,1.2260335
592,8.6951722012,7.4957879345,1.4778258921,4.9835176072,10.0442958817,
1.9050603358,6.5100882066,5.7954317738,1.5919312984,4.3047385116,7.264
4992048,1.8457309332,6.3524324618,3.1684917609,1.4928856252,1.95377934
86,6.1179357756,2.0005455391,3.9846339719,2.0263382834,1.6490544301,1.
8012722046,3.4847125779,1.9008257612,15.5665173237,13.3145475978,0.045
4434699,13.0994878345,15.4638302129,0.7492141728,14.8036117787,14.0017
737586,3.2136486557,8.8525645911,13.9405850502,1.7278205945,14.9611118
049,8.6651174977,0.9597271694,11.9701385356,5.0884010572,1.0717888717,
4.3663342965,10.957929839,3.662196133,4.0849708178,11.0966540173,0.359
6601244,8.042186967,2.0223943806,1.2977922674,0.2487131021,7.243223842
7,2.1965078498,3.8364773229,-0.017647506,1.5743186489,-0.0280393899,2.
5663765683,2.0199614857\PG=C01 [X(C14H12)]\NImag=0\

9,9-dimethyl-9H-fluorene

1\1\GINC-SAW161\Mixed\G4MP2\G4MP2\C15H14\KFOREST\27-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,3.9969045481,5.3625581494,0.9057002656\C,0,4.34793535
44,4.3751548072,2.0390026164\C,0,4.747168069,5.1524871324,3.3113704387
\C,0,3.1957079471,3.412658931,2.3142951665\C,0,5.4474107282,3.40653687
25,1.6115152655\C,0,3.5852465738,2.0818687664,2.0765861418\C,0,1.90727
12419,3.6981900701,2.7410615239\C,0,4.9852278251,2.078062527,1.6396375
093\C,0,6.7512557202,3.6850202011,1.2292035717\C,0,2.6839508129,1.0365
593468,2.2663851359\C,0,1.0036801936,2.649711578,2.9313003198\C,0,5.82
92835125,1.0280076786,1.2846942322\C,0,7.5974335352,2.6317845145,0.873
3214053\C,0,1.3907032015,1.330036628,2.6953451368\C,0,7.1383721882,1.3
144098284,0.9014380083\H,0,3.7110876306,4.8299415659,-0.0054157014\H,0
,4.8530571861,6.0042050273,0.6728107731\H,0,3.1634669408,6.0087988357,
1.200149461\H,0,4.999771416,4.4691179947,4.1266633519\H,0,3.9260998185
,5.7952658885,3.6454785774\H,0,5.6156886357,5.7906720415,3.1181403508\
H,0,1.5965566159,4.7220310924,2.9273823785\H,0,7.1178583089,4.70701980
2,1.2041267474\H,0,2.9798312776,0.008239339,2.0843006403\H,0,-0.006436
2246,2.8633017403,3.2649838134\H,0,5.4772685543,0.0014492306,1.3048245
909\H,0,8.6190696768,2.8398503549,0.5728737577\H,0,0.6785029194,0.5255
248613,2.8472006436\H,0,7.8065157922,0.5061451945,0.6224738778\Versio
n=EM64L-G09RevB.01\State=1-A\MP2\GTBas1=-578.1184583\CCSD(T)/GTBas1=-5
78.2867867\MP2\GTBas2=0.\MP2\GTBas3=0.\HF/GTMP2LargeXP=-576.369228\MP2
/GTMP2LargeXP=-578.7668333\HF/GFHFB3=-576.3739154\HF/GFHFB4=-576.41491
76\G4MP2=-579.1019308\FreqCoord=7.5530549751,10.1337662741,1.711525460
4,8.2164070634,8.2678443746,3.8531565293,8.9708475573,9.7367895834,6.2
575832536,6.0390128207,6.4489907645,4.3733840554,10.2941144096,6.43742
17506,3.0453225108,6.7751341434,3.9341618132,3.9241790993,3.6042203084
,6.9885664199,5.1798555935,9.4207152995,3.926969063,3.0984658498,12.75
80243642,6.9636789742,2.322858112,5.0719319905,1.9588132859,4.28284721
85,1.896680691,5.0072292136,5.5393548177,11.0157493897,1.942652975,2.4
277202634,14.3570686944,4.9733519731,1.6503382821,2.6280481829,2.51340
49736,5.0934641421,13.4895684703,2.4838746021,1.7034709614,7.012939277
,9.1272667974,-0.0102341925,9.170948989,11.3463031473,1.2714281005,5.9
780861485,11.3549841871,2.2679537997,9.4481987033,8.4454090655,7.79826
35777,7.4192534274,10.9514653966,6.8889561345,10.612113569,10.94278428
38,5.8924313069,3.0170547597,8.9233455555,5.5319509816,13.4508028566,8
.8949783278,2.2754697818,5.6310650369,0.0155700942,3.9387573888,-0.012
1627018,5.410856125,6.1699252355,10.3505375238,0.0027386489,2.46576112
83,16.2876812093,5.3665394291,1.0825745107,1.2821846981,0.9930980639,5
.3804294619,14.7521768992,0.9564758011,1.1763051539\PG=C01 [X(C15H14)]
\Nimag=0\

9-methyl-9H-fluorene

1\1\GINC-SAW313\Mixed\G4MP2\G4MP2\C14H12\KFOREST\23-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,2.9448450657,4.1200910229,4.8956068453\C,0,3.66385970
42,2.914654392,4.2627389795\C,0,4.7757902393,3.2990922929,3.3018746419
\C,0,2.7683455277,2.0588602116,3.3834725126\C,0,4.5451088894,2.7376712
584,2.0316095985\C,0,5.8988485211,4.0804925694,3.5294864101\C,0,3.2979
957839,1.9671843816,2.0823034758\C,0,1.5831388054,1.4141743705,3.70491
28174\C,0,5.4422492618,2.9585670435,0.9887397129\C,0,6.7966794374,4.30
24585573,2.4827149428\C,0,2.6394874887,1.2269685238,1.1026675063\C,0,0
.9231390068,0.6736822146,2.7214672506\C,0,6.5687154402,3.7446434834,1.
2237482141\C,0,1.4490232371,0.5816039408,1.4318567225\H,0,2.5153524244
,4.7644711802,4.1228949\H,0,3.6397046792,4.7184596389,5.4927428431\H,0
,2.1356890765,3.789269368,5.5538399507\H,0,4.0763364977,2.3005708128,5
.0766580054\H,0,6.0841223338,4.5161779229,4.5068651705\H,0,1.168828606
7,1.4794298047,4.706664464\H,0,5.2712661582,2.5268373704,0.0076938906\
H,0,7.6782945427,4.9124111047,2.6499150664\H,0,3.0436834056,1.15059547
63,0.0982427329\H,0,-0.0048490771,0.1656277966,2.9622208994\H,0,7.2753
778959,3.9252385783,0.4202671788\H,0,0.925487048,0.0021566838,0.678385
2679\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-538.946046\CCSD(T
)\GTBas1=-539.1002121\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-537
.3232397\MP2/GTMP2LargeXP=-539.5401185\HF/GFHFB3=-537.3285031\HF/GFHFB
4=-537.3661441\G4MP2=-539.8562171\FreqCoord=5.5649506779,7.7858436759,
9.251356192,6.9236914303,5.5078985728,8.0554092473,9.0249356203,6.2343
809207,6.2396387984,5.2314148885,3.8906819457,6.393836427,8.5890110451
,5.1734489203,3.8391857502,11.1472082043,7.7110134434,6.6697627048,6.2
32308819,3.717439734,3.9349832948,2.9916987725,2.6724022643,7.00127057
11,10.2843606517,5.5908814579,1.868447274,12.8438627498,8.1304683715,4
.6916513079,4.9879084848,2.3186344837,2.0837396025,1.7444799054,1.2730
748862,5.1428277832,12.4130732268,7.0763506489,2.3125489802,2.73825707
83,1.0990721659,2.7058170671,4.7533272098,9.0035456985,7.7911422357,6.
8780450484,8.9165964867,10.3797796918,4.0358674595,7.1606813492,10.495
2364926,7.7031596062,4.3474487855,9.5934933006,11.4973249698,8.5343394
416,8.51674089,2.2087659629,2.7957171636,8.8943068363,9.9612494125,4.7
750306124,0.0145393462,14.5098738533,9.2831116399,5.0076137509,5.75172
80718,2.1743103399,0.1856518597,-0.0091634278,0.3129911755,5.597786245
,13.7484717364,7.4176259192,0.7941898706,1.7489170602,0.0040755417,1.2
819623689\PG=C01 [X(C14H12)]\NImag=0\

1,9-dimethyl-9H-fluorene

1\1\GINC-SAW166\Mixed\G4MP2\G4MP2\C15H14\KFOREST\27-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,-0.2128250655,2.6364340544,-0.7578582319\C,0,-0.14451
8394,1.5311158865,0.3158701807\C,0,1.0072985502,0.5510235537,0.1334432
164\C,0,-1.3543820861,0.6142945948,0.267257846\C,0,0.5066717212,-0.751
4906365,-0.0605015081\C,0,2.3818231923,0.7914013159,0.1602190855\C,0,-
0.95647536,-0.7121749955,0.0238487763\C,0,-2.6978012646,0.9295002807,0
.4085061886\C,0,1.3674111568,-1.82719206,-0.2619899995\C,0,2.961958980
1,2.1645204067,0.4016937967\C,0,3.233004643,-0.3040415855,-0.039436208
6\C,0,-1.9060380302,-1.7266011663,-0.08026073\C,0,-3.6489861016,-0.088
2670503,0.3068886754\C,0,2.738758811,-1.5892166591,-0.255235873\C,0,-3
.2543620576,-1.4047487013,0.0630078589\H,0,0.6550578056,3.298277517,-0
.7071800673\H,0,-1.1093906034,3.248690534,-0.620225171\H,0,-0.25288198
19,2.1966916174,-1.7587602725\H,0,-0.0760005678,2.0160154698,1.3007632
165\H,0,-3.0124268399,1.9513551617,0.5989602169\H,0,0.9820518352,-2.83
05179509,-0.4110403998\H,0,2.3857825164,2.7238996514,1.1456122079\H,0,
2.976256719,2.7670970313,-0.5144088744\H,0,3.9931169119,2.0938117065,0
.7586781816\H,0,4.3071007161,-0.1435076304,-0.0179027361\H,0,-1.605385
8481,-2.7527202375,-0.266604409\H,0,-4.7025082805,0.1459602347,0.41895
69977\H,0,3.4318616587,-2.4105908111,-0.4058367504\H,0,-4.0048227362,-
2.1847295322,-0.0145652136\Version=EM64L-G09RevB.01\State=1-A\MP2/GTB
as1=-578.1169297\CCSD(T)/GTBas1=-578.2859784\MP2/GTBas2=0.\MP2/GTBas3=
0.\HF/GTMP2LargeXP=-576.3698736\MP2/GTMP2LargeXP=-578.7648234\HF/GFHF
B3=-576.3748173\HF/GFHF4=-576.4158374\G4MP2=-579.1008966\FreqCoord=-0.
402181088,4.9821383302,-1.4321445059,-0.2731001859,2.8933897032,0.5969
08135,1.9035183939,1.0412836093,0.2521711333,-2.559411222,1.1608485491
,0.5050441358,0.9574707924,-1.4201114945,-0.1143312809,4.5009935303,1.
4955317482,0.3027701928,-1.8074764833,-1.3458157002,0.0450676557,-5.09
81055511,1.756500971,0.77196482,2.5840325973,-3.4528925855,-0.49508934
85,5.5972912892,4.0903507777,0.759091265,6.1094933617,-0.5745553295,-0
.0745236339,-3.601889876,-3.2628033451,-0.151670799,-6.8955843947,-0.1
668005516,0.5799355498,5.1755040968,-3.0031842515,-0.4823258993,-6.149
8530261,-2.6545903311,0.1190675976,1.2378798537,6.2328412173,-1.336376
6538,-2.0964444148,6.1391353998,-1.1720557139,-0.4778776898,4.15114555
52,-3.3235752484,-0.1436202591,3.8097171176,2.458086243,-5.6926617227,
3.6875268437,1.1318707744,1.8558090168,-5.3489037413,-0.7767537851,4.5
084755687,5.1474243547,2.1648933274,5.6243101001,5.2290555722,-0.97209
18928,7.54589738,3.9567306991,1.4336939862,8.1392407802,-0.2711901193,
-0.0338312682,-3.0337395905,-5.2018873694,-0.5038093189,-8.8864527877,
0.2758248699,0.7917139872,6.4852786609,-4.5553564514,-0.7669203129,-7.
5680181821,-4.1285404904,-0.0275242647\PG=C01 [X(C15H14)]\NImag=0\

1-methyl-9H-fluorene

1\1\GINC-SAW32\Mixed\G4MP2\G4MP2\C14H12\KFOREST\26-Jan-2011\0\#\# G4MP2
\name\0,1\C,0,1.3119366107,4.4896184122,1.0319584855\C,0,1.894487168
,3.2404344215,1.6429859113\C,0,3.2694388834,3.0120782789,1.6515202342\
C,0,1.0771957767,2.2638173823,2.224249274\C,0,3.8148192337,1.847185262
,2.2211891528\C,0,4.3772464022,3.8849710039,1.1013741928\C,0,1.6119006
212,1.1059684841,2.7911064215\C,0,5.2738889388,1.8933442128,2.07813738
92\C,0,2.9860842784,0.8852969928,2.7956407391\C,0,5.6238845078,3.08801
74401,1.4199469945\C,0,6.2607658604,0.992160227,2.4728543368\C,0,6.952
9721479,3.3831885984,1.1561952057\C,0,7.5946749286,1.293534651,2.20544
71078\C,0,7.9400214194,2.4782995414,1.5528417911\H,0,1.5690759316,4.57
48422308,-0.0306865496\H,0,1.6945278824,5.3928785971,1.5222062535\H,0,
0.2221115172,4.5012050051,1.1139027907\H,0,0.0015440626,2.4138022324,2
.2326742339\H,0,4.3927223727,4.8782975998,1.5703514173\H,0,4.266832477
4,4.0628778054,0.0229407191\H,0,0.9456892625,0.371652996,3.2323610732\
H,0,3.3979962863,-0.0161780046,3.2373116885\H,0,5.9995296231,0.0691925
188,2.9806216811\H,0,7.2274627955,4.3032831407,0.6488730894\H,0,8.3733
517314,0.6006170254,2.5073254111\H,0,8.9835292799,2.6976939448,1.35227
09553\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-538.9479942\CCSD
(T)/GTBas1=-539.1022297\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-5
37.3252495\MP2/GTMP2LargeXP=-539.5415715\HF/GFHFB3=-537.3307483\HF/GFH
FB4=-537.3683647\G4MP2=-539.8586971\FreqCoord=2.4792008979,8.484149240
3,1.9501189182,3.5800619099,6.1235336082,3.1047934126,6.1783440978,5.6
920030379,3.1209209455,2.0356050095,4.2779948674,4.2032219791,7.208963
5982,3.4906742619,4.197439188,8.2717969164,7.3415312316,2.0812955942,3
.0460507275,2.0899775465,5.2744267443,9.9662057496,3.5779020375,3.9271
105322,5.6428814959,1.6729688626,5.2829953629,10.6276015227,5.83550725
53,2.6833109428,11.8311328583,1.874911109,4.6730174632,13.1392131691,6
.3932999069,2.1848922949,14.3518556834,2.4444262338,4.1676910342,15.00
44659719,4.6833074085,2.9344457128,2.9651237925,8.6451989175,-0.057989
1746,3.2021936222,10.1910636165,2.876552937,0.4197299385,8.5060447276,
2.1049712131,0.0029178555,4.5614251582,4.2191428461,8.3010422623,9.218
6464583,2.9675341111,8.0631448372,7.6777263636,0.0433516765,1.78709371
29,0.7023223789,6.108277191,6.4212823818,-0.0305719981,6.1176324981,11
.3374679138,0.130754911,5.632558683,13.6579253192,8.1320266081,1.22619
2434,15.8233415866,1.1350016887,4.738158353,16.9764100458,5.097902746,
2.555421763\PG=C01 [X(C14H12)]\NImag=0\

2,3-dimethyl-9H-fluorene

1\1\GINC-SAW46\Mixed\G4MP2\G4MP2\C15H14\KFOREST\27-Jan-2011\0\#\ G4MP2
\name\0,1\C,0,2.46329951,-1.0360714299,-0.0402002426\C,0,3.473853002
5,-2.1563435282,-0.0830838038\C,0,1.0989937786,-1.3301085478,-0.048957
0617\C,0,2.8867218405,0.3102394055,0.0088885894\C,0,0.1571850854,-0.30
5193426,-0.009648495\C,0,4.3563065235,0.6521932266,0.0192777254\C,0,1.
9324407199,1.3327296481,0.0480732529\C,0,-1.3087932717,-0.3369423485,-
0.0084749017\C,0,0.5794228145,1.0328471928,0.039073745\C,0,-1.78534132
28,0.9882971693,0.0411266368\C,0,-2.2031531277,-1.4048574373,-0.046386
4383\C,0,-0.620187699,1.9557229103,0.0750578576\C,0,-3.1476706097,1.24
57818175,0.0528547286\C,0,-3.5712907655,-1.1399451574,-0.0344006564\C,
0,-4.0418019143,0.1732255494,0.0147892017\H,0,2.9785379479,-3.12995104
83,-0.1182689198\H,0,4.1298702179,-2.1473424456,0.79576589\H,0,4.12721
48574,-2.0825130034,-0.9608535115\H,0,0.7806967293,-2.3681366945,-0.08
68342248\H,0,4.8712463481,0.2115624155,0.8816799013\H,0,4.5078080921,1
.73389279,0.0587184061\H,0,4.8687343925,0.275888963,-0.8745151328\H,0,
2.266270488,2.3664800573,0.0857075365\H,0,-1.844682958,-2.4285865533,-
0.084727991\H,0,-0.6353991449,2.6468267658,-0.777878668\H,0,-0.6326822
788,2.5821199758,0.9766272447\H,0,-3.5195306614,2.2654084052,0.0910915
241\H,0,-4.2783774817,-1.9626729849,-0.0635705874\H,0,-5.1101911124,0.
3623083131,0.0235383951\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1
=-578.1177457\CCSD(T)/GTBas1=-578.2869238\MP2/GTBas2=0.\MP2/GTBas3=0.\
HF/GTMP2LargeXP=-576.3715032\MP2/GTMP2LargeXP=-578.7643106\HF/GFHFB3=-
576.3768408\HF/GFHFB4=-576.4178122\G4MP2=-579.1015313\FreqCoord=4.6549
614571,-1.9578912567,-0.0759674491,6.5646308005,-4.0748987167,-0.15700
56353,2.0767972633,-2.5135408823,-0.0925154388,5.4551137003,0.58626751
2,0.0167969996,0.2970367636,-0.5767319926,-0.0182330131,8.2322262804,1
.2324665839,0.0364296215,3.6517837286,2.5184940441,0.0908452823,-2.473
2608481,-0.6367287612,-0.0160152432,1.0949504345,1.9517983315,0.073838
677,-3.3738061539,1.8676109879,0.0777180803,-4.1633560402,-2.654795812
2,-0.0876576647,-1.1719849021,3.6957806924,0.1418387949,-5.948235409,2
.3541864564,0.0998809618,-6.7487614877,-2.1541841541,-0.0650078194,-7.
6378987013,0.3273488476,0.0279475408,5.628620998,-5.9147502906,-0.2234
958684,7.8043236762,-4.0578891358,1.5037795979,7.7993057721,-3.9353792
446,-1.8157499905,1.4753030112,-4.4751297979,-0.1640929039,9.205321523
8,0.3997950253,1.6661335503,8.5185227536,3.2765825169,0.1109617065,9.2
005746157,0.5213545832,-1.6525941001,4.2826305653,4.4719992071,0.16196
37715,-3.4859455927,-4.5893634758,-0.1601126988,-1.2007303689,5.001777
7086,-1.4699776472,-1.195596236,4.8794995964,1.8455580263,-6.650949066
3,4.2810014649,0.1721380337,-8.0849617336,-3.7089144299,-0.1201310003,
-9.6568616891,0.6846634875,0.0444811203\PG=C01 [X(C15H14)]\NImag=0\

4-methyl-9H-fluorene

1\1\GINC-SAW31\Mixed\G4MP2\G4MP2\C14H12\KFOREST\26-Jan-2011\0\#\# G4MP2
\name\0,1\C,0,1.6078637783,-1.2603235258,0.0309628958\C,0,1.22839208
84,-2.7195586119,0.0278592333\C,0,0.6559148968,-0.2268997822,0.0107812
501\C,0,2.9561302178,-0.8920555298,0.0545138571\C,0,-0.8173922651,-0.2
561044093,-0.0161240181\C,0,1.0688422125,1.1213062828,0.0145248718\C,0
,3.3599892493,0.4420000387,0.0581414147\C,0,-1.2920913254,1.0731051634
, -0.0285650644\C,0,-1.7332478462,-1.3112507976,-0.0298818843\C,0,-0.13
15212711,2.0390073717,-0.0097089646\C,0,2.411948175,1.4631093794,0.038
0245112\C,0,-2.6501945607,1.3467487849,-0.0543829308\C,0,-3.0985323817
, -1.0297523136,-0.0558049065\C,0,-3.5580982972,0.2863015558,-0.0680923
77\H,0,0.6175099109,-2.9818427486,0.8992538453\H,0,2.1200921134,-3.351
5139539,0.0450009238\H,0,0.6483824073,-2.9860216014,-0.8631495716\H,0,
3.7093044738,-1.6745256771,0.0703633038\H,0,4.4179130783,0.6825172819,
0.076756399\H,0,-1.4027518658,-2.3414154822,-0.0207138139\H,0,-0.12803
69058,2.6965139056,-0.888907584\H,0,-0.1601403822,2.7000191175,0.86645
95284\H,0,2.7206853259,2.5039131106,0.0406552572\H,0,-3.0064865243,2.3
725839178,-0.06386425\H,0,-3.8114361618,-1.8479122709,-0.0665437664\H,
0,-4.6241081402,0.4872107943,-0.0883881598\\Version=EM64L-G09RevB.01\S
tate=1-A\MP2/GTBas1=-538.9464074\CCSD(T)/GTBas1=-539.1005962\MP2/GTBas
2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-537.3227672\MP2/GTMP2LargeXP=-539.
5406538\HF/GFHFB3=-537.3282073\HF/GFHFB4=-537.3658374\G4MP2=-539.85717
93\FreqCoord=3.0384222,-2.3816663026,0.0585113933,2.3213246308,-5.1392
209789,0.0526463212,1.2394995215,-0.4287784479,0.02037361,5.5862765247
, -1.6857406467,0.1030162604,-1.5446475242,-0.4839671951,-0.0304699784,
2.0198190609,2.1189617856,0.0274480299,6.3494594906,0.8352590238,0.109
8713508,-2.4416987437,2.0278748706,-0.0539801486,-3.2753637497,-2.4779
04899,-0.0564685776,-0.248539183,3.8531655154,-0.0183472841,4.55792149
75,2.7648760295,0.0718559125,-5.0081419186,2.5449863733,-0.1027688454,
-5.8553776154,-1.9459498575,-0.1054559902,-6.7238313356,0.5410315319,-
0.1286759442,1.1669246159,-5.6348661661,1.6993434915,4.0063934709,-6.3
334435035,0.0850394216,1.2252651792,-5.6427630536,-1.6311163021,7.0095
695989,-3.1643949322,0.132967374,8.3486457969,1.2897707438,0.145048573
, -2.6508168587,-4.4246340247,-0.0391434355,-0.2419546869,5.0956727951,
-1.6797918911,-0.3026214653,5.1022966856,1.6373712139,5.1413501596,4.7
317100396,0.076827302,-5.6814361532,4.4835338319,-0.1206859421,-7.2025
705188,-3.4920481096,-0.1257494944,-8.7382979939,0.9206949703,-0.16702
94155\PG=C01 [X(C14H12)]\NImag=0\

9-methylene-9H-fluorene

```
1\1\GINC-SAW330\Mixed\G4MP2\G4MP2\C14H10\KFOREST\22-Jan-2011\0\#\# G4MP
2\name\0,1\C,0,0.0289837998,2.9238210094,0.\C,0,0.017382567,1.586223
5778,0.\C,0,1.1872580477,0.679982058,0.\C,0,-1.1682819622,0.7009096144
,0.\C,0,0.7319629041,-0.6574525678,0.\C,0,2.5483225249,0.9580403682,0.
\C,0,-0.7368581633,-0.64435135,0.\C,0,-2.5241856925,1.0032073824,0.\C,
0,1.6401714204,-1.7104371739,0.\C,0,3.4560418138,-0.1016065573,0.\C,0,
-1.6637577409,-1.6809688649,0.\C,0,-3.450664392,-0.0400880268,0.\C,0,3
.0052588139,-1.4232143547,0.\C,0,-3.0235056248,-1.3695021903,0.\H,0,0.
9558842168,3.4865522471,0.\H,0,-0.888214768,3.5021941341,0.\H,0,2.9075
406228,1.9823350101,0.\H,0,-2.8650432514,2.0338205321,0.\H,0,1.2981963
773,-2.74041416,0.\H,0,4.5214374281,0.1030373051,0.\H,0,-1.3402774562,
-2.7169153253,0.\H,0,-4.5122440435,0.1834872181,0.\H,0,3.724836797,-2.
2353778718,0.\H,0,-3.7574542387,-2.1687020141,0.\Version=EM64L-G09Rev
B.01\State=1-A'\MP2/GTbas1=-537.7490565\CCSD(T)/GTbas1=-537.8982452\MP
2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-536.1391452\MP2/GTMP2LargeX
P=-538.3256001\HF/GFHFB3=-536.1456378\HF/GFHFB4=-536.1820245\G4MP2=-53
8.6496884\FreqCoord=0.0547714439,5.5252209694,0.,0.0328482911,2.997528
1476,0.,2.2435925592,1.284979865,0.,-2.2077329545,1.3245272152,0.,1.38
32094282,-1.2424052985,0.,4.8156316704,1.8104339202,0.,-1.3924601274,-
1.2176475848,0.,-4.7700196674,1.8957872072,0.,3.0994747955,-3.23225782
62,0.,6.5309725318,-0.1920085666,0.,-3.1440464818,-3.1765707926,0.,-6.
5208106775,-0.0757553918,0.,5.6791161167,-2.6894853589,0.,-5.713597592
,-2.5879840781,0.,1.8063593844,6.588628895,0.,-1.6784826587,6.61818777
77,0.,5.4944554974,3.7460702728,0.,-5.4141471041,3.843363809,0.,2.4532
356198,-5.178632253,0.,8.5442784661,0.1947122881,0.,-2.5327573343,-5.1
342258911,0.,-8.526905487,0.346740591,0.,7.0389214361,-4.2242519811,0.
,-7.100559468,-4.0982528705,0.\PG=CS [SG(C14H10)]\NImag=0\
```

10, 11-dihydro-5H-dibenzo (a, d) cycloheptene

1\1\GINC-SAW216\Mixed\G4MP2\G4MP2\C15H14\KFOREST\27-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,5.7937100423,2.4635079987,1.8527074968\C,0,5.80770198
64,3.9793209682,2.0230020378\C,0,4.6212184706,1.8000203758,1.108757642
1\C,0,4.7574519637,4.8615895218,1.7078508877\C,0,6.9854920951,4.513910
4028,2.5628255598\C,0,3.4325944533,4.4271484426,1.0919933598\C,0,2.727
0135858,3.2953275131,1.8056373047\C,0,3.2940543222,2.0110603989,1.7927
809097\C,0,1.5131470476,3.5005622861,2.4601227482\C,0,2.6300786299,0.9
656748009,2.4343937691\C,0,4.9335271701,6.2302271859,1.9507957229\C,0,
6.1074069002,6.7431326843,2.486396162\C,0,7.147639019,5.8725376762,2.7
958317175\C,0,1.4176970091,1.178266184,3.0870108854\C,0,0.8575105108,2
.4513414956,3.1007665589\H,0,5.8532778363,2.0127387142,2.8529617065\H,
0,6.7245699529,2.1768330334,1.347243832\H,0,4.8314076801,0.7276070738,
1.0404794326\H,0,4.5837266579,2.1714342866,0.0768243648\H,0,7.79714771
01,3.8326382766,2.8054314208\H,0,2.7703870853,5.2968448337,1.061661665
6\H,0,3.5973987798,4.1438258428,0.0429086193\H,0,1.0747303578,4.494404
736,2.4655198925\H,0,3.0679938588,-0.0285145389,2.41946708\H,0,4.11975
20888,6.9076468423,1.708241661\H,0,6.2067602321,7.8094134211,2.6601218
628\H,0,8.0761005391,6.2462180299,3.214777853\H,0,0.9143054338,0.35274
55624,3.5793468368\H,0,-0.0866014189,2.629155951,3.6050510099\Version
=EM64L-G09RevB.01\State=1-A\MP2\GTBas1=-578.1028216\CCSD(T)/GTBas1=-57
8.274653\MP2\GTBas2=0.\MP2\GTBas3=0.\HF/GTMP2LargeXP=-576.3586885\MP2/
GTMP2LargeXP=-578.7508119\HF/GFHFB3=-576.3634909\HF/GFHFB4=-576.404649
9\G4MP2=-579.0872806\FreqCoord=10.9485252733,4.6553554437,3.5011097732
,10.9749662158,7.5198268248,3.8229198176,8.7328373097,3.4015455438,2.0
952482913,8.9902813017,9.1870727667,3.2273704536,13.2006669633,8.53005
44497,4.8430384344,6.486663442,8.3660981062,2.0635683889,5.1533088377,
6.227266518,3.4121600012,6.2248605358,3.8003533907,3.3878649356,2.8594
335188,6.6151040318,4.6489582474,4.9701283186,1.8248609071,4.600337523
3,9.3230152206,11.7734231269,3.6864696575,11.5413264235,12.742674051,4
.698607804,13.5070802427,11.0974879131,5.2833562598,2.6790590866,2.226
6003994,5.8336051426,1.6204600214,4.6323640849,5.8595995984,11.0610920
903,3.8035249469,5.3913162929,12.7075955724,4.1136182702,2.5459218766,
9.1300373518,1.3749781019,1.9662211745,8.6619880514,4.1034161173,0.145
1770098,14.7344737898,7.2426367092,5.30149707,5.2352728733,10.00958610
41,2.0062497937,6.7980984845,7.8306959852,0.0810855392,2.0309460429,8.
4931940814,4.6591573721,5.7976681705,-0.0538846694,4.5721301688,7.7852
031833,13.0535607547,3.228108908,11.7290770111,14.7576526244,5.0269018
008,15.2616182405,11.8036414428,6.0750497202,1.7277868716,0.6665925075
,6.7639852561,-0.1636529644,4.968384708,6.8125591038\PG=C01 [X(C15H14)
]\Nimag=0\

17H-cyclopenta [a]phenanthrene

1\1\GINC-SAW307\Mixed\G4MP2\G4MP2\C17H12\KFOREST\29-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,3.4761877247,0.2168928982,0.0085746273\C,0,4.25445539
09,1.3133416357,0.0148374375\C,0,3.4066601465,2.5607978026,0.02103836\
C,0,2.0640596705,0.6114187786,0.0098927184\C,0,2.0037920647,2.00575848
66,0.0172832664\C,0,0.7723697896,2.6591152035,0.0201030575\C,0,-0.3912
79524,1.9096134252,0.0154525948\C,0,0.8877355159,-0.1732657691,0.00507
39133\C,0,-0.3741759829,0.4963129151,0.0079091292\C,0,-0.2073746386,-2
.3426988057,-0.0069384486\C,0,0.9304028117,-1.6040736584,-0.0024367445
\C,0,-1.4968869985,-1.7215459194,-0.0044334296\C,0,-1.5936816117,-0.30
00592521,0.0029498037\C,0,-2.8870059318,0.2676516186,0.0050672853\C,0,
-4.0220246088,-0.5171493916,0.0002554882\C,0,-3.918377022,-1.91762734,
-0.0069616865\C,0,-2.672041906,-2.5034657658,-0.0092410744\H,0,3.83140
75374,-0.8055175647,0.0033354697\H,0,5.3365139677,1.329785358,0.015510
8845\H,0,3.6052101515,3.1976151921,-0.8522287095\H,0,3.6041865696,3.18
80781756,0.9014232511\H,0,0.7183574878,3.7435214323,0.0258742214\H,0,-
1.3387013238,2.4335976589,0.0177727402\H,0,-0.1605001498,-3.4276311168
, -0.0125944948\H,0,1.8965186116,-2.0967466032,-0.0044882265\H,0,-3.003
6054273,1.3442716572,0.0105518761\H,0,-5.0000638341,-0.0472440227,0.00
2059243\H,0,-4.8134118683,-2.5305857476,-0.0107127714\H,0,-2.572556612
5,-3.5849912811,-0.0148297817\Version=EM64L-G09RevB.01\State=1-A\MP2/
GTBas1=-652.918459\CCSD(T)/GTBas1=-653.0960688\MP2/GTBas2=0.\MP2/GTBas
3=0.\HF/GTMP2LargeXP=-650.9528313\MP2/GTMP2LargeXP=-653.6166382\HF/GFH
FB3=-650.9607574\HF/GFHFB4=-651.0048071\G4MP2=-654.006063\FreqCoord=6.
5690427862,0.4098681779,0.0162036972,8.0397555334,2.4818560105,0.02803
86933,6.4376547048,4.8392065285,0.0397567387,3.9005074991,1.155414044,
0.0186945285,3.7866182296,3.7903342284,0.0326606402,1.4595673756,5.024
9994905,0.0379892731,-0.7394111417,3.6086463933,0.0292011722,1.6775770
034,-0.3274248519,0.0095883065,-0.7070901331,0.9378954857,0.0149460882
, -0.3918812739,-4.4270591545,-0.0131117676,1.7582065074,-3.0312599114,
-0.0046047799,-2.828706479,-3.2532503129,-0.0083779677,-3.011621789,-0
.5670298101,0.0055743212,-5.4556505552,0.5057882582,0.0095757814,-7.60
05250103,-0.97727072,0.0004828028,-7.404659457,-3.6237904976,-0.013155
681,-5.049427418,-4.7308646804,-0.0174630999,7.2403109492,-1.522207592
5,0.0063031242,10.0845499032,2.5129301422,0.0293113238,6.8128598377,6.
0426169914,-1.6104788636,6.8109255483,6.0245946422,1.7034430743,1.3574
989174,7.0742302796,0.0488951923,-2.5297788758,4.598833093,0.033585611
6,-0.3033013274,-6.4772840953,-0.0238001459,3.5839007818,-3.9622768502
, -0.0084815188,-5.6759916689,2.5403052803,0.0199401561,-9.4487512933,-
0.0892782642,0.0038914052,-9.0960301958,-4.7821140187,-0.020244204,-4.
8614274589,-6.7746517101,-0.028024226\PG=C01 [X(C17H12)]\NImag=0\

17-methyl-16, 17-dihydro-15H-cyclopenta (a) phenanthrene

1\1\GINC-SAW314\Mixed\G4MP2\G4MP2\C18H16\KFOREST\29-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,-2.5038601007,0.7962150222,0.0366165192\C,0,-1.340723
9915,1.4897985454,-0.0456039548\C,0,-0.0372528332,-0.6094119596,-0.083
4447185\C,0,1.2222659794,-1.2454255456,-0.157898643\C,0,2.3978914014,-
0.526368046,-0.2485955693\C,0,-0.0764693645,0.8178777974,-0.1050734403
\C,0,-2.5164531795,-0.6347160572,0.0706523092\C,0,-3.7344139003,-1.342
6337044,0.1618743955\C,0,-3.7578494629,-2.7191496606,0.1963942525\C,0,
-2.5487379297,-3.4316792201,0.1401521741\C,0,-1.3461165731,-2.76138292
01,0.0503465089\C,0,-1.2859824746,-1.3505474518,0.0122183838\C,0,1.139
1551323,1.5302866288,-0.1840510341\C,0,2.3555003636,0.8739438846,-0.25
701199\C,0,3.5081155397,1.8543782581,-0.3734217511\C,0,2.8497301719,3.
1861566579,0.0706830696\C,0,1.3410636034,3.0303458403,-0.2334410556\C,
0,4.7655810042,1.4880099081,0.4189251595\H,0,-3.4551685902,1.318365620
3,0.0798665572\H,0,-1.3545048218,2.5738854979,-0.0722377326\H,0,1.2791
193724,-2.3268019445,-0.1462820413\H,0,3.3464984274,-1.0510335861,-0.3
062016098\H,0,-4.6598537075,-0.7758268817,0.2052701371\H,0,-4.70091943
81,-3.2506658236,0.266880639\H,0,-2.5585788192,-4.5163584866,0.1676449
995\H,0,-0.4323429312,-3.3414003108,0.0103582084\H,0,3.7879474726,1.93
23653869,-1.4357992364\H,0,3.2963108546,4.060078967,-0.4113418089\H,0,
2.9899882638,3.3031127502,1.1520066739\H,0,1.094236172,3.4197297842,-1
.2313014507\H,0,0.714972832,3.5785362186,0.4777138492\H,0,5.526821891,
2.2694244198,0.3229572937\H,0,5.2090620228,0.5522174866,0.0635198438\H
,0,4.5353576135,1.3679429244,1.4830950625\Version=EM64L-G09RevB.01\St
ate=1-A\MP2/GTBas1=-693.2827562\CCSD(T)/GTBas1=-693.4819286\MP2/GTBas2
=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-691.1847358\MP2/GTMP2LargeXP=-694.0
519438\HF/GFHFB3=-691.1911077\HF/GFHFB4=-691.2397941\G4MP2=-694.453914
7\FreqCoord=-4.7316098653,1.5046283348,0.0691951931,-2.5336011637,2.81
53112439,-0.0861789852,-0.0703976523,-1.1516217057,-0.1576876652,2.309
7479626,-2.3535132,-0.2983851921,4.5313580451,-0.9946914521,-0.4697775
439,-0.1445061564,1.5455650473,-0.1985600261,-4.7554073356,-1.19943952
03,0.1335135151,-7.0570195383,-2.537209998,0.3058982754,-7.1013063335,
-5.1384481728,0.3711313514,-4.8164166717,-6.4849339019,0.2648492259,-2
.543791666,-5.218257467,0.0951411135,-2.4301546887,-2.5521648135,0.023
0893991,2.1526912229,2.8918226332,-0.347806049,4.4512505931,1.65151459
73,-0.4856822739,6.6293776126,3.5042670547,-0.7056648416,5.3852095775,
6.0209634999,0.1335716437,2.5342429372,5.726523726,-0.4411396632,9.005
642962,2.8119312093,0.7916538217,-6.5293223785,2.4913499654,0.15092592
02,-2.5596431589,4.8639386884,-0.136509531,2.4171853052,-4.3970184406,
-0.2764329963,6.3239655319,-1.9861656342,-0.578637184,-8.8058473265,-1
.4661003329,0.3879043424,-8.8834503108,-6.142868156,0.5043313178,-4.83
50132578,-8.5346806577,0.3168031365,-0.8170097355,-6.3143314878,0.0195
741771,7.158183329,3.6516413699,-2.7132673385,6.229124764,7.6724373256
, -0.7773233658,5.6502589591,6.241978484,2.1769771169,2.0678066898,6.46
23527406,-2.3268225289,1.351102845,6.7624534097,0.9027483449,10.444179
7593,4.2885906326,0.6103008377,9.8437006323,1.0435398155,0.1200351087,
8.5705838043,2.5850374926,2.8026434971\PG=C01 [X(C18H16)]\NImag=0\

aceanthrylene

1\1\GINC-N265\Mixed\G4MP2\G4MP2\C16H10\KFOREST\13-May-2011\0\#\ G4MP2\
\name\0,1\C,0,-3.7802936321,0.3912628683,0.\C,0,-3.7976871206,-1.0299
257412,0.\C,0,-2.6255989671,-1.7323265261,0.\C,0,-2.5943719502,1.07335
96353,0.\C,0,-1.3483954374,0.3851324224,0.\C,0,-1.3598993129,-1.071118
2471,0.\C,0,-0.1645080617,-1.8119859366,0.\C,0,-0.0963618965,1.0214609
828,0.\C,0,1.0570591804,0.2338923268,0.\C,0,1.0821728059,-1.1695267145
,0.\C,0,2.379442006,-1.7730023158,0.\C,0,3.5056195646,-0.9837041549,0.
\C,0,3.4442319266,0.4456953025,0.\C,0,2.2171444684,1.0601160214,0.\C,0
,0.3622727102,2.417781346,0.\C,0,1.7250998405,2.4412519902,0.\H,0,-4.7
192995201,0.9351801331,0.\H,0,-4.7482847723,-1.5525380823,0.\H,0,-2.63
56300464,-2.8183209964,0.\H,0,-2.5874649989,2.158278529,0.\H,0,-0.2232
74238,-2.8970953458,0.\H,0,2.470344476,-2.85487515,0.\H,0,4.4830227237
, -1.4553466857,0.\H,0,4.3697193439,1.0139452979,0.\H,0,-0.2816072059,3
.2871770577,0.\H,0,2.3485981137,3.325061983,0.\Version=EM64L-G09RevB.
01\State=1-A'\MP2/GTbas1=-613.7405561\CCSD(T)/GTbas1=-613.9012104\MP2/
GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-611.8899856\MP2/GTMP2LargeXP=
-614.386106\HF/GFHFB3=-611.8981226\HF/GFHFB4=-611.9386513\G4MP2=-614.7
535936\FreqCoord=-7.1437196665,0.739379667,0.,-7.1765885964,-1.9462775
881,0.,-4.9616629826,-3.273622707,0.,-4.9026524727,2.0283557529,0.,-2.
5480980955,0.7277948032,0.,-2.5698372696,-2.024120143,0.,-0.3108751832
, -3.4241571769,0.,-0.1820975939,1.9302815129,0.,1.9975523572,0.4419924
422,0.,2.0450102316,-2.2100851956,0.,4.4964937404,-3.3504888098,0.,6.6
246609032,-1.8589314486,0.,6.5086550794,0.8422420605,0.,4.1897958423,2
.0033289495,0.,0.6845962078,4.5689445932,0.,3.2599662505,4.6132976829,
0.,-8.918183632,1.7672343365,0.,-8.9729578205,-2.9338717864,0.,-4.9806
189753,-5.3258548378,0.,-4.8896002263,4.0785553383,0.,-0.4219271624,-5
.4747167844,0.,4.6682745136,-5.394932177,0.,8.4716851952,-2.7502066644
,0.,8.2575728375,1.9160789268,0.,-0.5321604962,6.2118643894,0.,4.43820
72312,6.2834565227,0.\PG=CS [SG(C16H10)]\NImag=0\

acenaphthene

1\1\GINC-SAW301\Mixed\G4MP2\G4MP2\C12H10\KFOREST\23-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,3.3011023895,3.0052416034,1.7352087428\C,0,4.07794589
63,3.9768509231,2.3981755557\C,0,1.940414529,3.3628000439,1.6473712413
\C,0,3.8290652823,1.8032927472,1.2151270929\C,0,3.1746971013,5.1234900
687,2.8137896116\C,0,5.4245580795,3.7544331779,2.5536189284\C,0,1.7467
874616,4.7132841207,2.3122591317\C,0,1.0690709046,2.5032311736,1.02375
38035\C,0,2.9039956491,0.9366414769,0.5769918695\C,0,5.2228887806,1.60
27892475,1.3915059612\C,0,5.983347573,2.55355404,2.0403095946\C,0,1.57
22799356,1.2863874488,0.4909175929\H,0,3.1897848245,5.2733576477,3.898
8066145\H,0,3.4980882384,6.0707789062,2.368803464\H,0,6.0666882662,4.4
709174833,3.0564639607\H,0,1.3416861759,5.4513129407,1.6114337403\H,0,
1.0334038551,4.6538436255,3.1414161092\H,0,0.0119247332,2.7315632421,0
.9297298567\H,0,3.2494980173,-0.0030590372,0.1568283655\H,0,5.68785022
16,0.6974051989,1.0133037805\H,0,7.0481735355,2.3827055984,2.165845921
7\H,0,0.8793487048,0.6105887229,-0.000961707\Version=EM64L-G09RevB.01
\State=1-A\MP2/GTbas1=-461.7810609\CCSD(T)/GTbas1=-461.9131478\MP2/GTB
as2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-460.391892\MP2/GTMP2LargeXP=-462
.2864423\HF/GFHFB3=-460.3967048\HF/GFHFB4=-460.4287552\G4MP2=-462.5586
546\FreqCoord=6.2381794527,5.6790835936,3.2790693073,7.7062009287,7.51
5159116,4.5318950189,3.6668520442,6.3547711226,3.1130804852,7.23588472
85,3.4077294297,2.2962574223,5.9993080763,9.6819930744,5.3172917615,10
.2509291622,7.0948504905,4.8256404223,3.3009499148,8.9068161746,4.3695
365071,2.0202512263,4.7304213653,1.9346143161,5.4877564678,1.769995876
,1.0903566143,9.8698294178,3.0288327266,2.6295651789,11.3068882709,4.8
255178012,3.8556263601,2.9711784824,2.430919979,0.9276998044,6.0278197
411,9.965201755,7.3676767465,6.6104287593,11.4721095461,4.4763898096,1
1.4643793568,8.4488096062,5.7758798207,2.5354194287,10.3014885225,3.04
51684504,1.9528502709,8.7944899176,5.9364161159,0.0225344799,5.1619064
423,1.7569348067,6.140661322,-0.0057807426,0.2963626606,10.7484792036,
1.3179048295,1.9148666345,13.3191177191,4.5026610362,4.092855638,1.661
7282274,1.1538454662,-0.0018173628\PG=C01 [X(C12H10)]\NImag=0\

acenaphthylene

1\1\GINC-SAW321\Mixed\G4MP2\G4MP2\C12H8\KFOREST\22-Jan-2011\0\#\# G4MP2
\name\0,1\C,0,3.7515260976,3.3048772618,0.8728675177\C,0,3.262316415
9,4.6052011969,0.6054156025\C,0,5.156603217,3.2698851967,0.710902191\C
,0,2.9633385979,2.2159437153,1.2424198572\C,0,4.4402306684,5.415333024
1,0.2586018758\C,0,1.9060536107,4.8189088164,0.7165148558\C,0,5.551153
0731,4.6322172675,0.3204446603\C,0,5.8012912176,2.0730895454,0.9334339
633\C,0,3.6570498567,0.9929223538,1.4655857029\C,0,1.5660391908,2.4669
112256,1.3491405407\C,0,1.0701619198,3.7301036091,1.0918322235\C,0,5.0
286973892,0.9396648545,1.3122769991\H,0,4.4152667942,6.4651752824,-0.0
022904983\H,0,1.460499956,5.7907052772,0.5263520122\H,0,6.5655730344,4
.9493744639,0.1174169745\H,0,6.8773000665,1.9723088717,0.8279989022\H,
0,3.1076028834,0.1026290948,1.7561846893\H,0,0.8908345049,1.6652666615
,1.6327361188\H,0,0.0025257406,3.9053711524,1.1775210932\H,0,5.5429358
567,-0.0001585166,1.4860559572\\Version=EM64L-G09RevB.01\State=1-A\MP2
/GTBas1=-460.5876246\CCSD(T)/GTBas1=-460.7120073\MP2/GTBas2=0.\MP2/GTB
as3=0.\HF/GTMP2LargeXP=-459.2052234\MP2/GTMP2LargeXP=-461.07615\HF/GFH
FB3=-459.2111384\HF/GFHFB4=-459.2418844\G4MP2=-461.353377\FreqCoord=7.
0893569048,6.2453129276,1.6494805587,6.1648845848,8.7025690489,1.14406
96852,9.7445678561,6.1791875078,1.3434104482,5.5998983891,4.1875267477
,2.3478332721,8.3908199301,10.2334963339,0.4886867228,3.6019193188,9.1
064179223,1.3540168476,10.4901590299,8.7536220236,0.6055526487,10.9628
516184,3.9175714897,1.7639345538,6.9108226834,1.8763513198,2.769555602
8,2.9593851839,4.6617866105,2.5495061367,2.0223129463,7.0488742686,2.0
632638855,9.5028608707,1.7757092316,2.4798441388,8.3436450447,12.21741
06848,-0.0043284145,2.7599449339,10.9428470902,0.9946611525,12.4071349
404,9.3529622658,0.2218859251,12.9962136594,3.727123617,1.5646911634,5
.8725183795,0.1939408824,3.3187081015,1.6834332439,3.1468979284,3.0854
241119,0.004772958,7.3800819253,2.2251923819,10.4746307413,-0.00029955
29,2.8082387773\PG=C01 [X(C12H8)]\NImag=0\

anthracene

1\1\GINC-SAW321\Mixed\G4MP2\G4MP2\C14H10\KFOREST\23-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,3.4071737629,2.118861094,1.1956946093\C,0,3.567054794
9,3.4627797686,0.694987144\C,0,4.5433689546,1.3330951864,1.4054613315\
C,0,2.0880632003,1.6412930324,1.4588132586\C,0,4.8536394234,3.94114835
01,0.4337718598\C,0,2.3991131966,4.2559000388,0.484681955\C,0,5.829953
4779,1.8114636246,1.1442460882\C,0,0.9962655463,2.433860328,1.24357085
18\C,0,5.989834607,3.1553823209,0.6435386622\C,0,1.1540116206,3.759833
7039,0.7495492861\C,0,6.997894989,1.0183432962,1.3545513308\C,0,7.3089
453545,3.6329503487,0.380420144\C,0,8.2429965808,1.5144094579,1.089684
0787\C,0,8.4007428842,2.8403828633,0.5956626256\H,0,4.422939203,0.3207
940082,1.7826171553\H,0,1.9714802576,0.6294449683,1.8355442451\H,0,4.9
740691257,4.9534496078,0.0566160237\H,0,2.5231690139,5.266799988,0.107
7922072\H,0,-0.0004924366,2.0572632509,1.448126128\H,0,0.2751690273,4.
3744031866,0.5848229649\H,0,6.8738390037,0.0074433924,1.7314410085\H,0
,7.4255283732,4.6447984283,0.0036891283\H,0,9.1218391143,0.8998399326,
1.2544104132\H,0,9.3975009127,3.2169797806,0.3911073825\Version=EM64L
-G09RevB.01\State=1-A\MP2/GTBas1=-537.7651707\CCSD(T)/GTBas1=-537.9130
036\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-536.1519903\MP2/GTMP2
LargeXP=-538.3415969\HF/GFHFB3=-536.1586356\HF/GFHFB4=-536.1950857\G4M
P2=-538.6634916\FreqCoord=6.4386252991,4.0040671812,2.2595353501,6.740
7566634,6.5437054211,1.3133353679,8.5857230449,2.5191848113,2.65593700
69,3.9458675967,3.1015943351,2.7567575378,9.172049258,7.4476910308,0.8
197100191,4.5336669034,8.0424855223,0.9159161566,11.0170154408,3.42317
01503,2.1623117354,1.8826690382,4.5993294655,2.3500083368,11.319146988
4,5.9628084311,1.2161118274,2.1807659172,7.1050560056,1.4164428738,13.
2241050358,1.9243899391,2.5597310482,13.8119050402,6.8652812135,0.7188
898875,15.577006052,2.8618191284,2.0592044802,15.8751033639,5.36754572
42,1.1256392299,8.358143796,0.6062128206,3.3686582234,3.7255577633,1.1
894786057,3.468675928,9.3996284137,9.3606631719,0.1069887796,4.7680984
233,9.9528095739,0.2036977509,-0.0009305703,3.8876641275,2.7365617877,
0.5199941018,8.2664240175,1.1051552399,12.9896731985,0.0140659731,3.27
19493213,14.0322150174,8.777396972,0.0069714422,17.2377777542,1.700451
0361,2.3704921391,17.7587030586,6.0792107604,0.7390858415\PG=C01 [X(C1
4H10)]\NImag=0\

1-methylantracene

1\1\GINC-SAW254\Mixed\G4MP2\G4MP2\C15H12\KFOREST\27-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,4.5718823953,7.2797717261,0.8606223609\C,0,5.46432534
,6.1467208592,1.2976408244\C,0,4.8968612541,4.8857465956,1.7028867979\
C,0,6.8260240443,6.2988877663,1.3158529049\C,0,5.7798952163,3.81965808
3,2.1163185027\C,0,3.5191797748,4.6484271507,1.713049872\C,0,7.6957991
407,5.2500178007,1.7225948512\C,0,5.2374337351,2.5943040402,2.51062899
95\C,0,7.1889368663,4.0452125183,2.1116915841\C,0,2.9759543317,3.42098
82331,2.1080059603\C,0,3.8600556885,2.3610586631,2.5194543553\C,0,1.56
99818567,3.1783880081,2.1185232369\C,0,3.2944694134,1.1137938239,2.920
1138736\C,0,1.0671416164,1.9690757088,2.5093559631\C,0,1.9414421056,0.
9221340595,2.9158316435\H,0,5.1641642314,8.1571122079,0.5899815935\H,0
,3.9637062651,7.0044633839,-0.0091819657\H,0,3.8758413108,7.5768296909
,1.6540166566\H,0,7.2577254124,7.2477224749,1.0111961025\H,0,2.8363135
092,5.4335363293,1.4067815207\H,0,8.7674438538,5.4202708406,1.71951220
86\H,0,5.9097240413,1.7982248275,2.8200400499\H,0,7.8444849178,3.23809
1428,2.4240050332\H,0,0.9050798085,3.9789491793,1.8078990486\H,0,3.965
3093751,0.3178142973,3.229468739\H,0,-0.0044371941,1.7987833567,2.5123
428416\H,0,1.5237916894,-0.0310630529,3.2227864414\Version=EM64L-G09R
evB.01\State=1-A\MP2/GTBas1=-576.9366298\CCSD(T)/GTBas1=-577.0992782\M
P2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-575.1999655\MP2/GTMP2Large
XP=-577.5667298\HF/GFHFB3=-575.206316\HF/GFHFB4=-575.2461745\G4MP2=-57
7.9084798\FreqCoord=8.6396056388,13.7567748722,1.626340566,10.32607839
36,11.6156190393,2.4521857771,9.2537266811,9.2327230205,3.2179896833,1
2.8993160203,11.90317282,2.4866016214,10.9224190356,7.2181076982,3.999
26238,6.6502859869,8.7842542634,3.2371951101,14.5429527497,9.921095836
2,3.2552325067,9.8973153984,4.9025241413,4.7444012303,13.5851218639,7.
644343809,3.9905187711,5.623738671,6.4647308643,3.9835539515,7.2944481
089,4.461754257,4.7610787358,2.9668357427,6.0062828793,4.0034287238,6.
2256449445,2.1047652957,5.5182154979,2.0166054,3.7210138246,4.74199554
01,3.6687938824,1.7425808303,5.5101232558,9.7588561026,15.4147081082,1
.1149036351,7.4903193121,13.2365175034,-0.0173514006,7.324278612,14.31
81330713,3.1256385001,13.7151133772,13.6962105647,1.9108837004,5.35985
57594,10.2678955955,2.6584318029,16.5680677691,10.2428274548,3.2494071
563,11.1677599589,3.3981524493,5.3291033782,14.8239281482,6.1191059922
,4.5807056575,1.7103529665,7.5191242455,3.4164340778,7.4933487512,0.60
0581983,6.1028114714,-0.0083850816,3.3992079165,4.7476399226,2.8795489
766,-0.0587006628,6.090183759\PG=C01 [X(C15H12)]\NImag=0\

2-methylanthracene

1\1\GINC-SAW241\Mixed\G4MP2\G4MP2\C15H12\KFOREST\27-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,4.0228067526,1.4343774098,0.8310880275\C,0,3.29545373
99,1.2717136596,2.1404768442\C,0,3.8034378102,1.7509452155,3.317534780
3\C,0,2.0337696175,0.5962439172,2.1617844198\C,0,3.1142956798,1.596923
1579,4.5584624419\C,0,1.3383238223,0.4247600608,3.3223567496\C,0,1.844
758272,0.9144965921,4.5641778464\C,0,3.6260208384,2.0831402177,5.76384
43213\C,0,1.1599499267,0.7567400956,5.770501354\C,0,2.9419810391,1.926
3338795,6.9732436365\C,0,1.6716654442,1.243187324,6.9773086249\C,0,3.4
547702759,2.4187242567,8.2106571552\C,0,0.9829606668,1.0892420749,8.21
74848508\C,0,2.7628960279,2.2501809487,9.3770796643\C,0,1.5094675738,1
.5760632814,9.3808263729\H,0,3.4174932486,1.993184031,0.1073363212\H,0
,4.2421516577,0.4615010569,0.3751446427\H,0,4.9685211747,1.9663823384,
0.9616905715\H,0,4.7599275963,2.2671310843,3.3248925335\H,0,1.63077532
7,0.2159666112,1.2273963033\H,0,0.3821377861,-0.0902942538,3.320474834
2\H,0,4.5832069354,2.5981562515,5.7623136799\H,0,0.2027473277,0.241704
4061,5.7719897784\H,0,4.4114081362,2.9327238957,8.204936778\H,0,0.0267
856231,0.5743102241,8.2164271958\H,0,3.1657600034,2.6301853012,10.3101
551248\H,0,0.9745076968,1.4516569621,10.3165351472\Version=EM64L-G09R
evB.01\State=1-A\MP2/GTBas1=-576.9369448\CCSD(T)/GTBas1=-577.0998312\M
P2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-575.2018522\MP2/GTMP2Large
XP=-577.5665554\HF/GFHFB3=-575.2082598\HF/GFHFB4=-575.2480814\G4MP2=-5
77.9090075\FreqCoord=7.6020030479,2.7105804758,1.5705287642,6.22750505
2,2.4031905361,4.0449150294,7.1874558247,3.3088069311,6.2692321712,3.8
432675945,1.1267377119,4.0851805117,5.8851659316,3.0177474237,8.614245
6023,2.5290655012,0.8026801871,6.2783443725,3.4860879155,1.7281481085,
8.6250461515,6.8521863368,3.9365645079,10.8920872398,2.1919876893,1.43
00315345,10.9046672085,5.559538452,3.6402434727,13.1775207308,3.158989
8754,2.3492835742,13.1852024457,6.5285696735,4.5707264361,15.515893394
3,1.8575264596,2.0583692139,15.5287958692,5.2211168263,4.2522257426,17
.7201124918,2.8524803209,2.9783279699,17.7271927449,6.4581263009,3.766
571951,0.2028362512,8.0165048472,0.8721106075,0.7089206348,9.389144305
5,3.715924092,1.8173318047,8.9949595693,4.2842568566,6.2831363095,3.08
17187524,0.408117749,2.3194428698,0.7221357608,-0.1706314111,6.2747880
678,8.6610059183,4.9098037659,10.8891947467,0.3831369235,0.4567551326,
10.9074799229,8.3363532378,5.5420449862,15.505083448,0.050617492,1.085
2890389,15.5267971908,5.9824194089,4.9703298979,19.4833695735,1.841552
6614,2.7432340973,19.4954260685\PG=C01 [X(C15H12)]\NImag=0\

9,10-dihydroanthracene

1\1\GINC-SAW227\Mixed\G4MP2\G4MP2\C14H12\KFOREST\27-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,3.3764977943,3.1852423505,0.691060953\C,0,3.376649640
7,1.7837106067,0.6878530693\C,0,4.6392306684,3.911876711,0.2793825251\
C,0,2.2216467315,3.8705875845,1.0667669644\C,0,4.639540062,1.059242383
8,0.272853634\C,0,2.22194743,1.096402454,1.0604174598\C,0,5.8859965598
,3.185408484,0.7374106117\C,0,1.0692196949,3.1786864133,1.4297700736\C
,0,5.8861484965,1.7838767337,0.7342032525\C,0,1.0693706668,1.786384864
1,1.4265835135\C,0,7.0260957012,3.8709055773,1.1555035481\C,0,7.026396
3639,1.0967204481,1.1491550185\C,0,8.1644236013,3.1791560017,1.5608166
074\C,0,8.164574476,1.7868544624,1.5576304683\H,0,4.6595198636,3.99753
82775,-0.8194376511\H,0,4.6321610413,4.9386475857,0.6584744799\H,0,2.2
269795233,4.9568972007,1.0781871952\H,0,4.632693196,0.0307453156,0.647
2411989\H,0,4.6598475723,0.9786163307,-0.8263471612\H,0,2.2275157214,0
.0100531274,1.066864932\H,0,0.1782101157,3.7249173042,1.7212952898\H,0
,0.1784796911,1.238632031,1.7156048196\H,0,7.0202012768,4.9572144553,1
.1667160475\H,0,7.0207373884,0.0103703829,1.1553954808\H,0,9.043988182
2,3.7255041037,1.8850435478\H,0,9.044257548,1.23921881,1.8793541031\\V
ersion=EM64L-G09RevB.01\State=1-A\MP2\GTBas1=-538.9437106\CCSD(T)/GTBa
s1=-539.0995411\MP2\GTBas2=0.\MP2\GTBas3=0.\HF/GTMP2LargeXP=-537.32233
61\MP2/GTMP2LargeXP=-539.5369187\HF/GFHF3=-537.3276933\HF/GFHF4=-537
.3654177\G4MP2=-539.8540142\FreqCoord=6.3806561195,6.0192357093,1.3059
159422,6.3809430676,3.370724547,1.2998539207,8.7668754305,7.3923756494
,0.5279564587,4.1983038866,7.314350508,2.0158974104,8.7674600997,2.001
6780138,0.5156186426,4.1988721243,2.0719003694,2.0038985856,11.1229215
172,6.0195496562,1.3935041036,2.0205323992,6.0068467834,2.7018738721,1
1.1232086358,3.3710384814,1.3874430731,2.0208176949,3.3757781611,2.695
8521462,13.2773966588,7.3149514273,2.1835852514,13.2779648288,2.072501
2913,2.1715882691,15.4285246392,6.007734177,2.9495159317,15.4288097512
,3.3766655733,2.9434950014,8.805216453,7.5542525501,-1.5485127435,8.75
35157714,9.3326914039,1.2443364324,4.2083814027,9.3671781781,2.0374785
189,8.7545213981,0.0581002263,1.2231086079,8.8058357326,1.8493168541,-
1.5615698254,4.2093946702,0.0189976577,2.0160825423,0.3367683128,7.039
0735727,3.2527766916,0.3372777364,2.340675318,3.2420232614,13.26625781
08,9.3677777026,2.2047738046,13.2672709149,0.0195971836,2.1833810339,1
7.0906608134,7.040182463,3.562216054,17.0911698411,2.3417841696,3.5514
645616\PG=C01 [X(C14H12)]\NImag=0\

azulene

1\1\GINC-SAW314\Mixed\G4MP2\G4MP2\C10H8\KFOREST\23-Jan-2011\0\#\# G4MP2
\name\0,1\C,0,2.6467714675,1.9250043563,2.3196354665\C,0,3.914331153
8,2.7172513755,2.2106694698\C,0,4.8927464729,2.0029358094,2.9177803013
\C,0,4.0983001073,3.9212463753,1.5449843561\C,0,2.9510038115,0.7892951
303,3.0846836092\C,0,1.4091018755,2.2403606724,1.7762119403\C,0,4.3057
943589,0.8424344469,3.4418333481\C,0,3.1750480631,4.6801043895,0.82714
46304\C,0,1.0395463157,3.3453418318,1.0107416544\C,0,1.8254186153,4.41
92280599,0.5954555848\H,0,5.924166774,2.3071164863,3.0323076531\H,0,5.
1076813813,4.3276084143,1.5922015742\H,0,2.2489888135,0.0100806637,3.3
481800904\H,0,0.6172024444,1.5204888141,1.9785030835\H,0,4.8223682238,
0.097565342,4.0346007286\H,0,3.5585615979,5.5977582274,0.3896093576\H,
0,0.0001160787,3.3736370776,0.6955198916\H,0,1.3065523376,5.1674327507
,0.0000376346\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-384.5569
119\CCSD(T)/GTBas1=-384.665381\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2Lar
geXP=-383.3979308\MP2/GTMP2LargeXP=-384.9793958\HF/GFHFB3=-383.402039\
HF/GFHFB4=-383.4287691\G4MP2=-385.208864\FreqCoord=5.0016732099,3.6377
310379,4.3834757598,7.3970138741,5.134860934,4.1775598683,9.2459508714
,3.7850001415,5.5138056853,7.7446648131,7.4100817489,2.9195973126,5.57
65890209,1.4915516344,5.8292072279,2.662816638,4.2336681098,3.35655412
12,8.1367721228,1.5919703895,6.5041224229,5.999971298,8.8441155694,1.5
630768237,1.964457839,6.3217798831,1.9100249179,3.4495412608,8.3511307
519,1.1252479795,11.1950527683,4.3598183158,5.730231015,9.6521189847,8
.1779947135,3.0088249235,4.2499729334,0.0190496937,6.3271434145,1.1663
435885,2.8733074467,3.7388289809,9.1129552549,0.1843717765,7.624290432
6,6.7247068471,10.5782300079,0.7362549847,0.0002193569,6.3752501483,1.
3143421151,2.4690260964,9.765032709,0.0000711191\PG=C01 [X(C10H8)]\NIm
ag=0\

benz[a]anthracene

1\1\GINC-SAW192\Mixed\G4MP2\G4MP2\C18H12\KFOREST\29-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,4.1970360111,1.5253215326,5.0853487372\C,0,4.61883975
44,1.4279197406,3.6879704586\C,0,5.0899770372,1.0578687366,6.115195269
8\C,0,2.9696133802,2.0496499808,5.4744194753\C,0,5.8942704012,0.876422
9435,3.3853770148\C,0,3.8163348795,1.8577901891,2.6134071446\C,0,4.709
8610648,1.1406827061,7.4501958877\C,0,6.3671212684,0.5099953457,5.7455
672137\C,0,2.5773316198,2.1371827589,6.8205779837\C,0,6.7483994249,0.4
239989287,4.4512090632\C,0,6.310564268,0.7778449841,2.0436333618\C,0,4
.243951498,1.7521063267,1.3027103367\C,0,3.4719571385,1.6695735957,7.8
412860558\C,0,1.3186738093,2.6754488798,7.2104728498\C,0,5.5017772114,
1.2077755674,1.0111125496\C,0,3.0676284726,1.7614945745,9.2028356948\C
,0,0.9627409228,2.748397617,8.530710766\C,0,1.8483748797,2.2856032062,
9.5394053213\H,0,2.2697188987,2.4119490009,4.7297238306\H,0,2.83886661
63,2.282997111,2.8063857348\H,0,5.3951203483,0.7836439811,8.2146704526
\H,0,7.0219357979,0.1646313114,6.5400100029\H,0,7.7159526562,0.0079238
735,4.1866204027\H,0,7.2882012822,0.3536353424,1.8342667975\H,0,3.6005
336098,2.0930099478,0.4984108692\H,0,0.6434323267,3.0286185888,6.43655
86603\H,0,5.8360814928,1.125415516,-0.0175683763\H,0,3.7478891229,1.40
64310233,9.9713372121\H,0,0.0001080049,3.1610557536,8.8138338072\H,0,1
.5513968781,2.350401107,10.5809454332\Version=EM64L-G09RevB.01\State=
1-A\MP2/GTBas1=-690.9291088\CCSD(T)/GTBas1=-691.1130716\MP2/GTBas2=0.\
MP2/GTBas3=0.\HF/GTMP2LargeXP=-688.8511066\MP2/GTMP2LargeXP=-691.66212
37\HF/GFHF3=-688.8599794\HF/GFHF4=-688.9062158\G4MP2=-692.0737553\Fr
eqCoord=7.9312486308,2.8824399612,9.6099164035,8.7283421874,2.69837724
94,6.9692541528,9.618662623,1.9990821966,11.556044309,5.6117560091,3.8
73277132,10.3451535448,11.1385568115,1.6561993399,6.3974354145,7.21182
77537,3.5107146699,4.938623777,8.9003475365,2.155577919,14.0788298641,
12.0321154522,0.9637515324,10.857548512,4.870450915,4.0386901102,12.88
90244572,12.7526267484,0.8012418558,8.4115660897,11.9252382105,1.46991
39939,3.8619073698,8.0199060525,3.3110011133,2.4617657669,6.561048137,
3.1550368546,14.817883175,2.4919323581,5.0558656653,13.6258189748,10.3
968521737,2.2823650523,1.9107258083,5.7969776907,3.3287423304,17.39083
91091,1.819316681,5.1937188004,16.1207070667,3.4929223135,4.3191641081
,18.0268635278,4.2891471172,4.5579230582,8.9378827241,5.3646804326,4.3
142393019,5.303300462,10.1952999122,1.48087251,15.5234774274,13.269535
5806,0.3111080914,12.3588278118,14.5810373746,0.0149739508,7.911565983
5,13.7727044247,0.6682739481,3.466261902,6.8040224548,3.9552155947,0.9
418600444,1.2159108825,5.7232596938,12.1633331062,11.0285957106,2.1267
271109,-0.0331994199,7.0824840186,2.6577694589,18.8430965095,0.0002040
996,5.973529665,16.6557320764,2.931715223,4.4416143946,19.9950890958\ P
G=C01 [X(C18H12)]\NImag=0\

2-methylbenz[a]anthracene

1\1\GINC-SAW241\Mixed\G4MP2\G4MP2\C19H14\KFOREST\01-Feb-2011\0\#\ G4MP
2\name\0,1\C,0,8.2571020719,2.2389936168,2.3582011944\C,0,9.60041684
22,2.7505007334,2.8157351966\C,0,7.0905509922,2.5882201734,3.019447115
5\C,0,8.166692231,1.3890131307,1.2393771621\C,0,5.8219438252,2.1265298
854,2.6159558049\C,0,6.9428520321,0.9185846808,0.816742955\C,0,4.58566
49145,2.4901021936,3.3080007435\C,0,5.753862951,1.2703868897,1.4852111
05\C,0,3.3351464761,1.9661225479,2.8184116794\C,0,4.5525445043,3.32124
74503,4.4223133262\C,0,4.4817486206,0.7735460171,1.0354585163\C,0,2.14
68855371,2.2982608747,3.4604644505\C,0,3.3329625326,1.1036267076,1.668
191211\C,0,3.3569983591,3.6616619845,5.0766334572\C,0,2.1154528553,3.1
362167786,4.5835768712\C,0,3.3323326486,4.5134039447,6.2170050336\C,0,
0.9081158883,3.4855676894,5.2517887214\C,0,2.1517859365,4.8283973557,6
.8348983318\C,0,0.924225304,4.3079541589,6.3461724339\H,0,10.272622296
9,1.9252699226,3.0778240178\H,0,10.0969602688,3.3269297029,2.026605996
7\H,0,9.5057106596,3.3962579288,3.692596777\H,0,7.1722069214,3.2431034
305,3.8794621864\H,0,9.0708286677,1.1048635856,0.708861775\H,0,6.87894
12845,0.2631447872,-0.0469711151\H,0,5.4712036186,3.7359258305,4.82166
42168\H,0,4.4668969789,0.1210278018,0.1674912597\H,0,1.2130421211,1.89
44424148,3.0781353565\H,0,2.3783062978,0.7220350398,1.3190398132\H,0,4
.2724973442,4.9101095993,6.5887873312\H,0,-0.0280251939,3.0850804046,4
.8742920897\H,0,2.1473288786,5.4788102859,7.7033112667\H,0,-0.00244466
71,4.5673624525,6.8474037188\Version=EM64L-G09RevB.01\State=1-A\MP2/G
TBas1=-730.1005463\CCSD(T)/GTBas1=-730.2994683\MP2/GTBas2=0.\MP2/GTBas
3=0.\HF/GTMP2LargeXP=-727.8998993\MP2/GTMP2LargeXP=-730.8865733\HF/GFH
FB3=-727.9085741\HF/GFHFB4=-727.958173\G4MP2=-731.3187766\FreqCoord=15
.6036615671,4.2310847491,4.4563544236,18.1421585934,5.1976931145,5.320
9683844,13.3991995064,4.8910272994,5.7059281209,15.4328117281,2.624854
412,2.3420834118,11.0018793907,4.0185590967,4.9434400469,13.1200889219
,1.7358734767,1.5434205059,8.6656508256,4.7056111888,6.2512154526,10.8
732251836,2.4006833043,2.806642238,6.3025134528,3.7154331592,5.3260262
039,8.6030623209,6.2762481007,8.3569610603,8.4692774894,1.4617901234,1
.9567330178,4.0570257038,4.3430836351,6.5393301041,6.2983863979,2.0855
522303,3.1524245262,6.3438075273,6.9195383418,9.5934469112,3.997626543
6,5.926590805,8.6617049956,6.2971960896,8.5290973827,11.7484368803,1.7
160903259,6.5867683506,9.9244423912,4.0662861166,9.1243486631,12.91608
59931,1.7465327097,8.1408535533,11.9925278921,19.4124428078,3.63823288
57,5.8162444788,19.0804896827,6.2869860018,3.829730313,17.9631898451,6
.4179973621,6.9779966277,13.5535068499,6.1285773042,7.3311210753,17.14
13819803,2.0878895909,1.3395546209,12.9993151118,0.4972715811,-0.08876
25436,10.3390764564,7.0598766724,9.1116248745,8.4412119539,0.228709399
8,0.3165126104,2.2923173965,3.5799773385,5.8168328238,4.4943475629,1.3
644484836,2.4926240054,8.0738498839,9.2787624251,12.4510036037,-0.0529
599413,5.8299570626,9.2110771412,4.0578634979,10.3534509743,14.5571486
105,-0.0046197512,8.6310641849,12.9397177498\PG=C01 [X(C19H14)]\NImag=
0\

6-methylbenz [a] anthracene

1\1\GINC-SAW199\Mixed\G4MP2\G4MP2\C19H14\KFOREST\31-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,5.7971633116,0.6799359815,2.437763077\C,0,6.090971809
8,2.1098380175,2.8114435138\C,0,5.1421314191,3.1604288997,2.4861503711
\C,0,7.2413976879,2.4315083261,3.4539319996\C,0,5.4326456954,4.5275669
583,2.8485010241\C,0,3.9497275282,2.8750703928,1.8275499464\C,0,7.5779
003612,3.7745873321,3.8360813197\C,0,6.6832476432,4.8355852515,3.54043
00882\C,0,4.5030229101,5.5081353925,2.5223587209\C,0,3.0126734346,3.86
67189529,1.4992556828\C,0,8.7888109429,4.0472084605,4.5020033412\C,0,7
.0511270043,6.1372731601,3.9323364109\C,0,3.2991425899,5.2238709775,1.
8580812165\C,0,1.7927129939,3.5781592824,0.8259772838\C,0,9.1238079436
,5.3333538198,4.8745519509\C,0,8.2445217082,6.3853555688,4.5854309137\
C,0,2.3529779836,6.2344042134,1.5280946302\C,0,0.9047948368,4.57609785
78,0.5240226418\C,0,1.1883145797,5.9209959839,0.8794433332\H,0,5.67268
52167,0.5614065896,1.3548757465\H,0,6.6109321007,0.023883013,2.7553870
197\H,0,4.8730703641,0.3204133862,2.9056925219\H,0,7.9546781403,1.6490
467124,3.6996466967\H,0,3.722322362,1.8516533527,1.5511031073\H,0,4.69
26876733,6.5435729809,2.7812117859\H,0,9.4595602667,3.2210652045,4.718
8801538\H,0,6.393467165,6.972168229,3.7235447467\H,0,1.5791687387,2.54
82115639,0.5556353673\H,0,10.0597300182,5.5292817261,5.3869396467\H,0,
8.4984679449,7.3999248094,4.8740074009\H,0,2.5734313431,7.262044936,1.
8016344762\H,0,-0.02237412,4.3441907082,0.0103736817\H,0,0.4744104021,
6.6999519587,0.633030183\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas
1=-730.1007061\CCSD(T)/GTBas1=-730.2994904\MP2/GTBas2=0.\MP2/GTBas3=0.
\HF/GTMP2LargeXP=-727.8989863\MP2/GTMP2LargeXP=-730.8873222\HF/GFHFB3=
-727.9075763\HF/GFHFB4=-727.9572302\G4MP2=-731.3187294\FreqCoord=10.95
50510066,1.284892793,4.6067045924,11.5102686036,3.9870160378,5.3128582
792,9.7172201215,5.9723450829,4.6981433265,13.6842584494,4.5948848262,
6.5269855608,10.2662125413,8.5558615995,5.3828868248,7.4639033278,5.43
30956551,3.4535688928,14.320156345,7.1329363224,7.2491431177,12.629507
724,9.1379318176,6.6904432593,8.5094800701,10.4088673948,4.7665671915,
5.6931277193,7.3070398538,2.8331826438,16.6084457157,7.6481155931,8.50
75533642,13.3246989664,11.5977654753,7.4310388789,6.2344759683,9.87168
55011,3.5112646319,3.3877365933,6.7617411036,1.5608708583,17.241498302
5,10.0785780893,9.2115682078,15.5798881251,12.0665732861,8.6652086281,
4.4464839857,11.7813165651,2.8876803562,1.709814448,8.6475717085,0.990
2592804,2.2455891153,11.1890608435,1.6619070492,10.7198214977,1.060904
7036,2.5603441049,12.4928511535,0.0451323538,5.2069268574,9.2087684145
,0.6054935493,5.4909630927,15.0321631605,3.1162466667,6.9913190451,7.0
341698425,3.4991177296,2.9311600767,8.8678945296,12.3655608645,5.25572
85929,17.8759782415,6.0869310926,8.9173911446,12.0819019814,13.1754885
052,7.0364798148,2.9841964338,4.8154219845,1.049998674,19.0101347051,1
0.448828174,10.1798406267,16.059776965,13.9838312938,9.2105391573,4.86
30804603,13.7232760938,3.4045957516,-0.0422809593,8.2093307075,0.01960
34174,0.8965057346,12.6610743054,1.1962536798\PG=C01 [X(C19H14)]\NImag
=0\

8-methylbenz [a] anthracene

1\1\GINC-SAW250\Mixed\G4MP2\G4MP2\C19H14\KFOREST\01-Feb-2011\0\#\ G4MP
2\name\0,1\C,0,0.6390188331,1.0291754137,2.1797477076\C,0,1.87036938
65,1.8962821615,2.1165993581\C,0,2.7603984351,1.9834216792,3.240550217
9\C,0,2.1608483347,2.6164934722,0.9840944452\C,0,2.5476941213,1.285901
7791,4.4387234875\C,0,3.9270876113,2.8181202611,3.1522634472\C,0,3.311
5335193,3.4407918797,0.8947935263\C,0,3.4175093626,1.3781005658,5.5218
858214\C,0,4.7989659345,2.9050511129,4.2498532637\C,0,4.1734103407,3.5
400492301,1.950897579\C,0,4.5859338969,2.2127518714,5.4361739894\C,0,3
.1624250265,0.6460285461,6.73247486\C,0,5.4848465027,2.2936656374,6.58
66646477\C,0,3.9981360468,0.7255817529,7.7927398611\C,0,5.1795181926,1
.545854444,7.7572648995\C,0,6.6512209865,3.0832774751,6.5954754557\C,0
,6.0373424203,1.615283943,8.872059106\C,0,7.4801241371,3.1374106306,7.
7007636397\C,0,7.1737994168,2.3981944514,8.8512816052\H,0,0.8921858455
, -0.0220355609,2.3612522664\H,0, -0.0336826062,1.3384554842,2.988397574
3\H,0,0.080326117,1.0811257718,1.2422527112\H,0,1.4918971763,2.5549417
501,0.1307600633\H,0,1.6768871818,0.6468790106,4.5394216256\H,0,3.4999
008795,3.991500564, -0.0209484187\H,0,5.6665173914,3.5461038343,4.14004
5416\H,0,5.0569105288,4.1685163803,1.8919088396\H,0,2.2741745041,0.022
6291799,6.7735655829\H,0,3.7930790154,0.1669590231,8.7011564239\H,0,6.
9147688254,3.6659955897,5.7210736658\H,0,5.7861131761,1.0365030026,9.7
560676913\H,0,8.371169409,3.7558524013,7.6744965844\H,0,7.8251600502,2
.4417372621,9.7176530559\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas
1=-730.1005964\CCSD(T)/GTBas1=-730.29934\MP2/GTBas2=0.\MP2/GTBas3=0.\HF
F/GTMP2LargeXP=-727.8989621\MP2/GTMP2LargeXP=-730.8871719\HF/GFHFB3=-7
27.9075692\HF/GFHFB4=-727.9572094\G4MP2=-731.3186685\FreqCoord=1.20757
05883,1.9448596747,4.1191262061,3.5344859078,3.5834539559,3.9997931198
,5.2163970599,3.7481237798,6.1237524317,4.0834115673,4.9444560909,1.85
96689903,4.8144441597,2.4300021963,8.3879717709,7.4211200852,5.3254755
03,5.9569146139,6.2578914314,6.5021543329,1.6909147103,6.4581567519,2.
604232653,10.4348519396,9.0687313373,5.4897510054,8.0310587733,7.88660
25841,6.6897235418,3.6866621376,8.6661591287,4.1814950369,10.272880050
7,5.9761172159,1.2208170261,12.7225336819,10.364857771,4.3343998951,12
.4469923133,7.5553821705,1.3711508,14.7261441623,9.7878708844,2.921241
5405,14.6591062003,12.5689861138,5.8265500195,12.4636423274,11.4089237
448,3.0524442791,16.7657619452,14.135386059,5.9288468582,14.552334293,
13.5565162301,4.5319307265,16.7264981588,1.6859869077, -0.0416411754,4.
4621201142, -0.0636509011,2.5293143062,5.6472529916,0.1517943624,2.0430
316238,2.347517412,2.8192770816,4.8281401931,0.2471007088,3.1688575294
,1.2224241712,8.5782636741,6.6138541545,7.5428429252, -0.0395867742,10.
708165997,6.7011650857,7.8235520139,9.556175978,7.8773543393,3.5751895
753,4.2975669912,0.0427629526,12.8001838948,7.1678805396,0.315506829,1
6.4428026806,13.0670193523,6.9277276688,10.8112624145,10.9341692767,1.
9587068108,18.4362960705,15.8192175951,7.097532434,14.5026967522,14.78
74094409,4.6142147138,18.36370293\PG=C01 [X(C19H14)]\NImag=0\

9-methylbenz [a] anthracene

1\1\GINC-SAW206\Mixed\G4MP2\G4MP2\C19H14\KFOREST\02-Feb-2011\0\#\ G4MP
2\name\0,1\C,0,9.6397831723,1.05265733,6.4509424818\C,0,8.5460316956
,1.6527065805,5.6055562764\C,0,7.3189395307,1.0540812392,5.4746722616\
C,0,8.7845358022,2.8799897541,4.9168938998\C,0,6.2867124271,1.62246469
02,4.6755793391\C,0,7.8207817622,3.4590238898,4.1397247793\C,0,5.02624
26006,1.0279661278,4.5279626256\C,0,6.5398389228,2.8556335208,3.989329
1117\C,0,4.0278348967,1.5965567996,3.742955571\C,0,5.5283610039,3.4236
854404,3.1992061342\C,0,4.2765687836,2.8350934446,3.0515354612\C,0,2.7
444371657,0.9618259525,3.6113784626\C,0,3.2118779029,3.4132339775,2.23
26473196\C,0,1.7653397142,1.5033214811,2.8517624377\C,0,1.9632169023,2
.7384400984,2.1413087677\C,0,3.3610422494,4.6194341569,1.5205580514\C,
0,0.9305601781,3.2860642504,1.355394636\C,0,2.3344583538,5.1399513067,
0.7546295967\C,0,1.106481263,4.4701876469,0.6686346228\H,0,9.947027342
4,1.7392168144,7.248753814\H,0,10.5341489557,0.8422788107,5.8525219975
\H,0,9.3183259527,0.1175856882,6.9164747185\H,0,7.1144300553,0.1190523
52,5.989743512\H,0,9.7556549335,3.3559413027,5.0190255662\H,0,8.019689
2536,4.3933475007,3.6227516797\H,0,4.8206159677,0.092904497,5.04247371
12\H,0,5.7562607045,4.3563744126,2.6954079631\H,0,2.5809613777,0.02875
41968,4.1422884608\H,0,0.8008078627,1.0125652536,2.7616277229\H,0,4.29
83084196,5.1606457967,1.5670069044\H,0,-0.0150946124,2.754916582,1.299
1066147\H,0,2.4830569278,6.0715453287,0.2186968529\H,0,0.3018925323,4.
8797737765,0.0672686459\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1
=-730.1008327\CCSD(T)/GTBas1=-730.2998382\MP2/GTBas2=0.\MP2/GTBas3=0.\
HF/GTMP2LargeXP=-727.9007798\MP2/GTMP2LargeXP=-730.8868982\HF/GFHF3=-
727.909437\HF/GFHF4=-727.9590459\G4MP2=-731.3191369\FreqCoord=18.2165
50176,1.9892340655,12.1905145896,16.1496594277,3.1231628152,10.5929661
849,13.8307912963,1.9919248639,10.3456312418,16.6003668706,5.442391900
8,9.291582895,11.8801647633,3.0660139247,8.8355644634,14.7791356756,6.
5366078388,7.8229460984,9.4982219925,1.9425744555,8.5566093023,12.3585
045172,5.3963652902,7.5387394751,7.6115048633,3.0170551069,7.073160956
8,10.4470882612,6.4698278474,6.0456234363,8.0815437895,5.3575501715,5.
7665663065,5.186234632,1.8175876377,6.8245162565,6.0695696088,6.450077
4449,4.2190919853,3.3360085913,2.8408658889,5.3890500033,3.7099422848,
5.1749018172,4.0464871368,6.3514493724,8.7294654454,2.8734382864,1.758
5038869,6.2097614883,2.5613246641,4.4114869572,9.7131003061,1.42604326
95,2.0909465582,8.4474304153,1.26353632,18.7971575135,3.286643465,13.6
981595131,19.9066565693,1.5916762797,11.0596637619,17.6090840675,0.222
2047479,13.070243023,13.4443243961,0.2249763408,11.318974844,18.435516
0713,6.3418099802,9.4845837741,15.1550163601,8.302223583,6.8460085221,
9.1096439708,0.1755640558,9.5288943464,10.8777562809,8.232354572,5.093
5828667,4.8773101634,0.054337557,7.8277907543,1.5133075456,1.913471020
9,5.2187200773,8.1226257478,9.7522072246,2.9612138977,-0.0285246836,5.
2060378589,2.4549557192,4.692297566,11.4735578746,0.413277158,0.570494
2077,9.2214360281,0.127119318\PG=C01 [X(C19H14)]\NImag=0\

10-methylbenz [a] anthracene

1\1\GINC-SAW185\Mixed\G4MP2\G4MP2\C19H14\KFOREST\01-Feb-2011\0\#\ G4MP
2\name\0,1\C,0,1.8940096706,2.5766058097,9.5171149441\C,0,2.00905115
88,2.1076892696,8.0894784294\C,0,3.1526037008,2.2920081975,7.354620143
5\C,0,0.9000884084,1.451310526,7.4754978241\C,0,3.2609403508,1.8489098
279,6.005785142\C,0,0.9607353379,1.0099686341,6.183584057\C,0,4.429208
6541,2.0349464246,5.2487686445\C,0,2.1379396729,1.1912950837,5.4036999
981\C,0,4.5432238222,1.6051109395,3.930602249\C,0,2.249191254,0.757235
1287,4.0767963009\C,0,5.7529136881,1.7917186721,3.1299939344\C,0,3.410
3622452,0.9455150006,3.33370739\C,0,5.7768331793,1.3183008676,1.788929
8623\C,0,6.9103083088,2.4242152373,3.6249354505\C,0,3.49557788,0.48917
7418,1.9732702195\C,0,4.6180151359,0.6658381488,1.2401359422\C,0,6.936
415945,1.4925854934,1.0087007864\C,0,8.0384381231,2.5852153296,2.84210
46597\C,0,8.0555830996,2.1165188255,1.5215166769\H,0,1.6827669087,1.74
01813425,10.1938486342\H,0,2.8141831876,3.0594993594,9.8555787434\H,0,
1.0731404405,3.2939831943,9.6343795723\H,0,4.0090414368,2.7894582949,7
.8024764465\H,0,-0.0063665867,1.3044584034,8.0558854298\H,0,0.10830188
81,0.5122597135,5.730644996\H,0,5.2599475152,2.5354872136,5.7332753386
\H,0,1.4031066824,0.2577681697,3.6120013292\H,0,6.9282550438,2.7973272
909,4.6417625842\H,0,2.6278838706,-0.00503737,1.5466325513\H,0,4.66842
28689,0.3159600658,0.2133688277\H,0,6.9339039279,1.1238424571,-0.01280
39754\H,0,8.9131017204,3.0770836925,3.2546901577\H,0,8.9415914602,2.24
36533383,0.9086067101\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-
730.100831\CCSD(T)/GTBas1=-730.299821\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/G
TMP2LargeXP=-727.9007294\MP2/GTMP2LargeXP=-730.886915\HF/GFHFB3=-727.9
093899\HF/GFHFB4=-727.9589987\G4MP2=-731.3190803\FreqCoord=3.579159570
5,4.8690793327,17.9847408195,3.7965564771,3.9829554927,15.2868987894,5
.9575576,4.3312677877,13.8982178827,1.7009205873,2.7425794279,14.12664
35945,6.1622841987,3.4939332191,11.3492891313,1.8155266748,1.908564121
3,11.6852803874,8.3699913416,3.8454914376,9.9187352729,4.0401204703,2.
2512214516,10.2115131006,8.5854487843,3.0332200886,7.4277617879,4.2503
554906,1.4309670115,7.7040285082,10.8714313367,3.3858575975,5.91483133
37,6.4446506573,1.7867644056,6.2997939743,10.9166326242,2.4912276006,3
.3805875107,13.0585901975,4.5811028856,6.8501352509,6.6056848693,0.924
4113504,3.7289403011,8.7267838843,1.25825175,2.3435172983,13.107926479
9,2.8205778124,1.9061682363,15.1904465888,4.8853489675,5.3707994478,15
.2228458989,3.9996409353,2.875249826,3.1799686029,3.2884661588,19.2635
821587,5.3180355124,5.781615893,18.6243447062,2.0279415348,6.224726123
5,18.206338852,7.5759903708,5.2713122365,14.7445436422,-0.0120311052,2
.4650691341,15.2234172202,0.2046609082,0.9680305674,10.8293496073,9.93
9860277,4.7913764472,10.8343202344,2.6514873649,0.4871112465,6.8256933
038,13.0925046116,5.2861824838,8.7716600581,4.9659808245,-0.0095192496
,2.9227119502,8.8220406948,0.5970779933,0.4032086496,13.1031794555,2.1
237544604,-0.0241960069,16.8433212461,5.8148454668,6.1504730454,16.897
159052,4.2398903464,1.7170178445\PG=C01 [X(C19H14)]\NImag=0\

11-methylbenz [a] anthracene

1\1\GINC-SAW46\Mixed\G4MP2\G4MP2\C19H14\KFOREST\02-Feb-2011\0\#\# G4MP2
\name\0,1\C,0,1.9600878439,4.7082803358,1.3187541375\C,0,1.468922634
7,3.3204366386,0.9932142644\C,0,3.3669043694,4.9972912663,1.3645779293
\C,0,1.0659168766,5.7183843736,1.5767977889\C,0,4.3464546418,4.0207949
419,1.1132315898\C,0,3.7959461362,6.3327968322,1.6785743808\C,0,1.4899
661516,7.0357985786,1.8865465906\C,0,5.7117185806,4.2896079488,1.15489
49202\C,0,5.1698172618,6.6045807736,1.7207948311\C,0,2.821785891,7.337
317772,1.9366172607\C,0,6.7338089577,3.2763896168,0.8940023513\C,0,6.1
285997975,5.6298081756,1.4701981262\C,0,8.1064846003,3.6441525831,0.95
93271111\C,0,6.4265389742,1.9384500498,0.5774065939\C,0,7.5310008376,5
.9416031483,1.5215603029\C,0,8.4695572611,4.9990571408,1.2790652341\C,
0,9.1001792489,2.6777270756,0.7101648875\C,0,7.417589405,1.005107995,0
.3362462782\C,0,8.7679291953,1.3740803025,0.4022372024\H,0,1.805164106
3,2.9921764173,0.002586828\H,0,0.3769602153,3.2851791994,1.002799262\H
,0,1.8334886694,2.5803966333,1.715434864\H,0,0.0017120399,5.5045280682
,1.5432753886\H,0,4.0117184921,3.0194900176,0.8780647917\H,0,0.7457359
609,7.8005747034,2.0830521077\H,0,5.4966779914,7.613772377,1.958016537
8\H,0,3.1590610543,8.3419794514,2.1725864868\H,0,5.3924302891,1.621246
4651,0.518538135\H,0,7.8180428047,6.9609176132,1.761871512\H,0,9.52600
99275,5.246934407,1.3208817357\H,0,10.1419103493,2.9798466382,0.765276
3623\H,0,7.1457225253,-0.0171786599,0.0949690698\H,0,9.5442769095,0.64
05011202,0.2127351377\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-
730.1004617\CCSD(T)/GTBas1=-730.2992209\MP2/GTBas2=0.\MP2/GTBas3=0.\HF
/GIMP2LargeXP=-727.8987117\MP2/GIMP2LargeXP=-730.8872263\HF/GFHFB3=-72
7.9072916\HF/GFHFB4=-727.9569363\G4MP2=-731.3186619\FreqCoord=3.704029
2214,8.8973603914,2.4920841564,2.77586149,6.2747158885,1.876902951,6.3
625271738,9.4435118995,2.5786785734,2.0142909773,10.8061803887,2.97971
5988,8.2136089221,7.5982012767,2.1037028272,7.1732986126,11.9672516681
,3.1720458735,2.8156279738,13.2957324398,3.5650563932,10.7935838654,8.
1061842406,2.1824351115,9.7695387819,12.4808488847,3.2518309617,5.3324
025395,13.865521139,3.659676247,12.7250547613,6.1914790803,1.689419606
,11.5813751953,10.6387956325,2.7782718196,15.319035795,6.8864503684,1.
8128655117,12.1443986436,3.6631397164,1.0911403298,14.2315290895,11.22
80027406,2.8753322671,16.0051436902,9.4468489188,2.4170829985,17.19684
65406,5.0601708314,1.3420171466,14.0172125416,1.8993788446,0.635413378
9,16.5689849317,2.5966354562,0.7601181531,3.4112657858,5.65439397,0.00
48883965,0.7123515698,6.2080889843,1.8950159714,3.464791453,4.87624295
11,3.2417020919,0.0032352865,10.4020505397,2.9163678321,7.5810492722,5
.7060091942,1.6593019832,1.4092367335,14.7409498685,3.936398004,10.387
2160445,14.3879446306,3.7001150201,5.9697602296,15.7640565693,4.105593
4601,10.1902164371,3.063711813,0.9798950647,14.773959796,13.1542279225
,3.329454639,18.0015499021,9.9152690664,2.4961047343,19.1654330245,5.6
310940642,1.4461627407,13.5034585944,-0.0324629626,0.179465533,18.0360
694953,1.2103717049,0.402011149\PG=C01 [X(C19H14)]\NImag=0\

5-methylbenzo [c]phenanthrene

1\1\GINC-SAW42\Mixed\G4MP2\G4MP2\C19H14\KFOREST\03-Feb-2011\0\#\ G4MP2
\name\0,1\C,0,2.8022170121,-0.3923846813,0.1559672\C,0,4.2911681339,
-0.4841347799,0.3712455719\C,0,2.1402710946,0.8830012203,0.0709708502\
C,0,2.0577556496,-1.5186935797,-0.0250912777\C,0,0.7195926424,0.946261
0308,-0.1110834902\C,0,2.8851712298,2.0851635541,0.0970775951\C,0,0.63
86168511,-1.4958513419,-0.156202753\C,0,-0.0662410696,-0.2751322844,-0
.0731359317\C,0,0.1661988818,2.2143690999,-0.4197851154\C,0,2.29432750
78,3.3083719239,-0.1265973648\C,0,-0.0595903051,-2.7227929261,-0.36631
94413\C,0,-1.5130505163,-0.3355464834,0.0442985878\C,0,0.925612244,3.3
64625698,-0.4272024248\C,0,-1.4139790245,-2.7528080766,-0.4616027057\
,0,-2.1796437405,-1.5753886906,-0.2177432102\C,0,-2.3226701165,0.73545
77085,0.5028248796\C,0,-3.5902108985,-1.6442845187,-0.1638601505\C,0,-
3.6952051373,0.6313184166,0.5810243773\C,0,-4.3455988205,-0.5572978835
,0.2087710852\H,0,4.8520247801,0.0126920558,-0.428984911\H,0,4.6102811
991,-1.5285613709,0.4039102382\H,0,4.5929905287,-0.0121800928,1.313449
1251\H,0,2.5467638618,-2.4891717215,-0.0398314332\H,0,3.9534168734,2.0
358628953,0.2706069209\H,0,-0.8711306582,2.2802059854,-0.7131623772\H,
0,2.8902193591,4.2148011524,-0.1110547264\H,0,0.5242600388,-3.63159359
17,-0.4762629777\H,0,0.4623540737,4.3120156203,-0.6823673464\H,0,-1.93
89541611,-3.6818380502,-0.6617114961\H,0,-1.8552308895,1.6433793583,0.
8551037387\H,0,-4.0667182618,-2.5920335599,-0.3966345809\H,0,-4.273957
5122,1.471720341,0.9500948924\H,0,-5.4270808501,-0.6273724275,0.255258
652\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-730.0988506\CCSD(T
.8909614\MP2/GTMP2LargeXP=-730.8855301\HF/GFHFB3=-727.8990874\HF/GFHFB
4=-727.948751\G4MP2=-731.3137532\FreqCoord=5.2954227177,-0.7414995864,
0.2947352938,8.1091325633,-0.9148821454,0.701552459,4.0445262189,1.668
6304814,0.1341154702,3.8885946261,-2.8699149454,-0.0474156432,1.359833
0214,1.7881741985,-0.2099173744,5.4521834707,3.9403880596,0.1834500684

6-methylbenzo [c]phenanthrene

1\1\GINC-SAW47\Mixed\G4MP2\G4MP2\C19H14\KFOREST\04-Feb-2011\0\#\# G4MP2
\\name\0,1\C,0,2.9106344589,-2.7332649187,0.1781807839\C,0,2.16378342
58,-1.4228854613,0.135290952\C,0,0.7355178237,-1.3933526958,-0.0636121
635\C,0,2.8319433575,-0.249311469,0.3143425031\C,0,0.0234680941,-0.167
7952165,-0.0311358297\C,0,0.0264860774,-2.6127123649,-0.2933162146\C,0
,2.1908767967,1.0135949156,0.173316395\C,0,0.7847518067,1.0687857357,-
0.0664553648\C,0,-1.4272764985,-0.2227604689,0.0351735662\C,0,-1.32402
49441,-2.635716881,-0.4449111087\C,0,2.95036028,2.204952384,0.20082826
38\C,0,0.246885299,2.3311301046,-0.4243964506\C,0,-2.0943251891,-1.457
5396034,-0.2390636372\C,0,-2.2433411561,0.8588857037,0.4568987893\C,0,
2.3751672837,3.4238853006,-0.0739703038\C,0,1.0161352106,3.4757382436,
-0.4265631725\C,0,-3.5067169778,-1.5168242601,-0.235166154\C,0,-3.6182
491557,0.7657121104,0.4882193049\C,0,-4.265199888,-0.4210562406,0.1022
169986\H,0,2.5127301889,-3.408269651,0.9443106993\H,0,3.9670161043,-2.
5625216337,0.3985018875\H,0,2.8534545457,-3.2659292644,-0.7784937728\H
,0,3.901610087,-0.259480075,0.5055664445\H,0,0.5879310345,-3.534663669
, -0.3780532564\H,0,-1.8414809672,-3.5653199262,-0.661787184\H,0,4.0124
859457,2.1330724565,0.4157112214\H,0,-0.7781399651,2.3985401293,-0.758
7798315\H,0,-1.7802480962,1.7653360318,0.8183928612\H,0,2.9715841281,4
.329927404,-0.0594946875\H,0,0.5688446238,4.4196867338,-0.720170583\H,
0,-3.9816395512,-2.4631113383,-0.47687639\H,0,-4.202981111,1.612979972
7,0.8311963232\H,0,-5.3482230724,-0.4817720886,0.1115491104\Version=E
M64L-G09RevB.01\State=1-A\MP2/GTBas1=-730.0983692\CCSD(T)/GTBas1=-730.
2950159\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-727.8900728\MP2/G
TMP2LargeXP=-730.8850274\HF/GFHF3=-727.8981924\HF/GFHF4=-727.9478489
\G4MP2=-731.3132405\FreqCoord=5.5003020002,-5.165122145,0.3367128838,4
.0889580856,-2.6888638403,0.2556628475,1.3899272527,-2.6330550016,-0.1
202095677,5.3515973695,-0.4711303982,0.5940212429,0.0443482707,-0.3170
870056,-0.0588381911,0.0500514327,-4.9373108337,-0.5542873158,4.140157
1367,1.9154168001,0.3275205209,1.4829659969,2.0197123351,-0.1255824396
, -2.6971616981,-0.4209562795,0.0664684072,-2.5020445375,-4.9807830689,
-0.840760149,5.5753729226,4.1667561417,0.3795104184,0.4665456014,4.405
1974778,-0.8019930635,-3.9577010406,-2.7543506782,-0.4517648025,-4.239
3004077,1.6230587595,0.8634135822,4.4884156859,6.4702055286,-0.1397836
161,1.9202172621,6.56819339,-0.8060875745,-6.6267347136,-2.8663824434,
-0.4443996268,-6.8374999848,1.4469861853,0.922600779,-8.0600596903,-0.
7956809812,0.1931621335,4.7483719029,-6.4406962273,1.7844886061,7.4965
74002,-4.8424640973,0.7530594308,5.3922476241,-6.171711879,-1.47114002
67,7.3729745417,-0.4903462787,0.9553821221,1.1110286403,-6.6795463062,
-0.7144171182,-3.4798947069,-6.7374782366,-1.2505965361,7.5824995495,4
.0309227644,0.7855803588,-1.470471427,4.532583963,-1.4338860768,-3.364
1813504,3.3360016326,1.5465383768,5.615480183,8.1823769689,-0.11242866
57,1.0749605511,8.3519975201,-1.3609251707,-7.5242083116,-4.6546058642
, -0.9011657763,-7.9424832414,3.0480904063,1.5707334136,-10.1066769044,
-0.9104173058,0.210797269\PG=C01 [X(C19H14)]\NImag=0\

benzo[ghi]fluoranthene

1\1\GINC-SAW16\Mixed\G4MP2\G4MP2\C18H10\KFOREST\02-Feb-2011\0\#\ G4MP2
\name\0,1\C,0,-1.1515922236,0.0244523054,0.\C,0,-0.7761313438,1.3950
820609,0.\C,0,-2.4299284078,-0.5193107753,0.\C,0,-0.0166539844,-0.7878
695542,0.\C,0,-1.8209817501,2.2971207831,0.\C,0,0.7272939784,1.4004385
843,0.\C,0,-3.1544343696,1.7953179705,0.\C,0,-3.4732768991,0.443750868
1,0.\C,0,-2.4711625356,-1.9639748813,0.\C,0,-1.3315319289,-2.747892914
9,0.\C,0,-0.0117679624,-2.1650807636,0.\C,0,1.3120915238,-2.7384949605
,0.\C,0,1.1124856197,0.0324962914,0.\C,0,2.4461327635,-1.9464902224,0.
\C,0,2.3946432779,-0.5021651905,0.\C,0,3.4311411247,0.4682998365,0.\C,
0,3.1027104723,1.8175560275,0.\C,0,1.7657066537,2.3098748972,0.\H,0,-1
.6632317039,3.3709898251,0.\H,0,-3.9652838491,2.5169790007,0.\H,0,-4.5
150961573,0.1379115639,0.\H,0,-3.4391922807,-2.4569583613,0.\H,0,-1.44
19727668,-3.8283853193,0.\H,0,1.4302104698,-3.8181745056,0.\H,0,3.4176
383329,-2.432584929,0.\H,0,4.4751011617,0.1698522561,0.\H,0,3.90839098
88,2.5449860316,0.\H,0,1.6003717957,3.3826040755,0.\Version=EM64L-G09
RevB.01\State=1-A'\MP2/GTBas1=-689.7541411\CCSD(T)/GTBas1=-689.9256103
\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-687.6688549\MP2/GTMP2Lar
geXP=-690.4665847\HF/GFHFB3=-687.6786154\HF/GFHFB4=-687.7231683\G4MP2=
-690.8762729\FreqCoord=-2.1761939194,0.0462081605,0.,-1.4666756828,2.6
36323028,0.,-4.5918992133,-0.9813551432,0.,-0.0314714696,-1.4888576858
,0.,-3.4411568006,4.3409291742,0.,1.3743864373,2.6464453903,0.,-5.9610
170626,3.3926592858,0.,-6.563542123,0.8385676119,0.,-4.6698204222,-3.7
113746575,0.,-2.5162306828,-5.1927650516,0.,-0.0222382261,-4.091409698
8,0.,2.4794936413,-5.1750054916,0.,2.102293148,0.061409091,0.,4.622521
0077,-3.6783334407,0.,4.5252199812,-0.9489546835,0.,6.483917049,0.8849
584391,0.,5.8632730622,3.4346831231,0.,3.3367020065,4.3650309569,0.,-3
.1430524159,6.3702475663,0.,-7.4933005139,4.7564009935,0.,-8.532295200
8,0.2606150863,0.,-6.4991315289,-4.6429784228,0.,-2.7249336203,-7.2345
997846,0.,2.7027061003,-7.2153041431,0.,6.4584004704,-4.5969193107,0.,
8.4567156126,0.3209742471,0.,7.3857885892,4.8093266117,0.,3.0242644047
,6.3921953187,0.\PG=CS [SG(C18H10)]\NImag=0\

bicyclo[4.4.1]undeca-1,3,5,7,9-pentaene

```
1\1\GINC-SAW321\Mixed\G4MP2\G4MP2\C11H10\KFOREST\21-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,2.550819802,2.4794788554,3.4765820174\C,0,1.566434188
1,1.3665441686,3.3408098795\C,0,1.0984848645,0.7987033352,4.540071165\
C,0,1.3311416309,0.8982100078,2.0346826342\C,0,3.808680451,1.681614018
5,3.5618663617\C,0,4.1751622441,1.2310245553,4.8433922338\C,0,4.408516
8597,1.3306287414,2.3380731547\C,0,3.2460222483,1.0041878589,5.8502970
308\C,0,1.8435090355,0.8071129547,5.7120273551\C,0,2.2794956353,0.9931
318025,1.0244055873\C,0,3.6820355953,1.1902097915,1.1626784537\H,0,2.5
454907258,3.1308641673,2.6022291318\H,0,2.3798365989,3.0598592478,4.38
37096406\H,0,0.1725515572,0.2276934533,4.5272470773\H,0,0.4227058613,0
.3354564263,1.8311410752\H,0,5.2064288488,0.9350332203,5.0235236528\H,
0,5.4575607047,1.0429270977,2.3275135754\H,0,3.6459777128,0.7394437566
,6.8261297266\H,0,1.3518176068,0.4170779476,6.5999549067\H,0,1.9623960
798,0.6776470556,0.0333210399\H,0,4.2569317492,1.0000615378,0.25953430
07\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-423.7105023\CCSD(T)
/GTBas1=-423.831501\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-422.4
127974\MP2/GTMP2LargeXP=-424.1879413\HF/GFHFB3=-422.4159154\HF/GFHFB4=
-422.4460486\G4MP2=-424.4332762\FreqCoord=4.8203508401,4.685535989,6.5
697878913,2.9601316206,2.5823942272,6.3132157342,2.075835555,1.5093305
649,8.5794911256,2.5154931265,1.6973709246,3.844992946,7.1973629802,3.
1777899562,6.7309519455,7.8899132017,2.3262992723,9.1526848759,8.33088
9517,2.5145239058,4.418317941,6.1340930706,1.8976400393,11.0554591843,
3.4837272006,1.5252224427,10.7941673647,4.3076224718,1.8767471206,1.93
5846009,6.9580388867,2.2491705467,2.1971438581,4.8102803456,5.91647583
54,4.9175003942,4.497239413,5.7822959836,8.2840106668,0.3260751869,0.4
302782689,8.5552571119,0.7987983126,0.6339207752,3.4603551427,9.838724
6545,1.7669567116,9.4930839258,10.3132950855,1.9708465912,4.3983632281
,6.8898993637,1.3973461906,12.8995157308,2.5545650585,0.788163097,12.4
72107263,3.708391155,1.2805673498,0.0629676398,8.0444351723,1.88984242
24,0.4904487505\PG=C01 [X(C11H10)]\NImag=0\
```

biphenyl

1\1\GINC-SAW199\Mixed\G4MP2\G4MP2\C12H10\KFOREST\01-Feb-2011\0\#\ G4MP
2\name\0,1\C,0,2.4573548411,0.4201445199,3.8725184134\C,0,3.59386479
43,0.9701256897,3.2626920606\C,0,1.4348116265,-0.065514773,3.045140666
3\C,0,2.3403038777,0.3540480333,5.3488994536\C,0,3.704100139,1.0326045
422,1.877517861\C,0,1.544247463,-0.0039739739,1.6598568436\C,0,1.11378
94593,0.588326914,5.9867084053\C,0,3.4528763578,0.0554554942,6.1482969
455\C,0,2.679644178,0.5456349824,1.0690689387\C,0,1.0034725147,0.52669
03372,7.3719145172\C,0,3.3435514156,-0.0069191483,7.5335515587\C,0,2.1
180470544,0.2285664402,8.1523519158\H,0,4.3861312181,1.3756785616,3.88
29476942\H,0,0.5577341373,-0.5189693359,3.4945723679\H,0,4.5900723725,
1.4702109293,1.4288605775\H,0,0.7429673175,-0.3937742563,1.0403850979\
H,0,0.2453205448,0.8466755365,5.3901412669\H,0,4.406157167,-0.15499498
82,5.6751767115\H,0,2.7653117524,0.5939983775,-0.0112879432\H,0,0.0451
129612,0.7198112361,7.843073345\H,0,4.2172332432,-0.2478438456,8.13052
29753\H,0,2.0323961695,0.1802087948,9.2327103783\Version=EM64L-G09Rev
B.01\State=1-A\MP2/GTbas1=-461.768716\CCSD(T)/GTbas1=-461.9022832\MP2/
GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-460.3892327\MP2/GTMP2LargeXP=
-462.2758686\HF/GFHFB3=-460.3939398\HF/GFHFB4=-460.4262881\G4MP2=-462.
5506746\FreqCoord=4.6437276611,0.7939580788,7.3179992459,6.7914202199,
1.833271868,6.1655944505,2.7114010264,-0.1238049786,5.7544818954,4.422
5333965,0.6690538208,10.1079550796,6.9997348315,1.9513397884,3.5479945
669,2.9182047865,-0.0075097224,3.1366748541,2.1047570478,1.1117767441,
11.3132393235,6.5249906869,0.1047956965,11.6185974107,5.06379363,1.031
1006853,2.0202475112,1.8962882346,0.9953004942,13.9308995125,6.3183964
867,-0.0130752954,14.2363492539,4.0025288693,0.4319279752,15.405712459
8,8.2885867851,2.5996557283,7.3377077304,1.0539647745,-0.9807099163,6.
603784727,8.6739797142,2.778296014,2.7001551735,1.4040047557,-0.744125
5027,1.9660429077,0.4635886445,1.5999848874,10.185890812,8.326430344,-
0.2928980797,10.7245297405,5.225681884,1.1224942569,-0.0213311213,0.08
52511418,1.3602461035,14.8212606622,7.9694158681,-0.4683569919,15.3644
617405,3.8406721538,0.340545269,17.4472940793\PG=C01 [X(C12H10)]\NImag
=0\

biphenylene

1\1\GINC-SAW51\Mixed\G4MP2\G4MP2\C12H8\KFOREST\01-Feb-2011\0\#\ G4MP2\
\name\0,1\C,0,3.3196472055,3.2653196482,0.6112693394\C,0,4.8227164045
,3.3572366356,0.661872583\C,0,3.4135428471,1.8675323892,0.3609039528\C
,0,2.1163388458,3.9129723661,0.701037599\C,0,4.9166360517,1.9594509613
,0.4115085114\C,0,5.9295115035,4.1461584998,0.8294162261\C,0,2.3067428
178,1.0786252377,0.1933612046\C,0,0.9652287125,3.103378427,0.528757458
8\C,0,6.1199473866,1.3118126974,0.3217434639\C,0,7.179538519,3.4834002
064,0.7379771054\C,0,1.0567191788,1.741393785,0.2848035161\C,0,7.27105
26273,2.1214167999,0.4940246308\H,0,2.0241009616,4.9765164329,0.891064
3041\H,0,5.8786752881,5.2122344199,1.0208365494\H,0,2.3575710364,0.012
5470513,0.0019392559\H,0,-0.0157296205,3.5633956406,0.5896623168\H,0,6
.2121933744,0.2482671444,0.1317169421\H,0,8.0909116126,4.059138572,0.8
625925165\H,0,0.1453394491,1.1656690704,0.1601903934\H,0,8.2520157978,
1.6614140122,0.4331221462\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBa
s1=-460.5266472\CCSD(T)/GTBas1=-460.6527917\MP2/GTBas2=0.\MP2/GTBas3=0
.\HF/GTMP2LargeXP=-459.145897\MP2/GTMP2LargeXP=-461.0139743\HF/GFHFB3=
-459.1518951\HF/GFHFB4=-459.1825102\G4MP2=-461.2939609\FreqCoord=6.273
2240762,6.1705598715,1.1551316449,9.1136132211,6.3442578045,1.25075791
67,6.4506611238,3.5291247598,0.6820096312,3.9993008229,7.3944461374,1.
3247690709,9.2910956329,3.7028256876,0.7776383879,11.2051528433,7.8351
040682,1.5673695175,4.3591121846,2.0383062992,0.3653997213,1.824017922
3,5.8645353137,0.9992067878,11.5650245083,2.4789667357,0.6080070318,13
.5673615614,6.5826724013,1.3945746215,1.9969098474,3.2907573432,0.5382
006472,13.7402981635,4.0088967656,0.9335712551,3.8249964828,9.40425315
4,1.6838675015,11.1090863187,9.8496955941,1.9291015047,4.4551635975,0.
0237104907,0.0036646625,-0.0297246749,6.7338418638,1.1143002896,11.739
3441622,0.4691569108,0.2489089476,15.2896071132,7.6706602364,1.6300636
204,0.2746517552,2.2027953047,0.3027159727,15.5940499022,3.1396174764,
0.8184822384\PG=C01 [X(C12H8)]\NImag=0\

3,4-dihydrocyclopenta (cd) pyrene

```
1\1\GINC-SAW121\Mixed\G4MP2\G4MP2\C18H12\KFOREST\04-Feb-2011\0\#\ G4MP
2\name\0,1\C,0,-0.8651550766,-1.6523627207,-0.0084583762\C,0,-0.9862
796537,-0.2263055329,-0.0024934122\C,0,-2.0503433932,-2.4015936494,-0.
0050592257\C,0,0.4465785017,-2.2637590081,-0.0175619709\C,0,-2.2566089
547,0.4135337889,0.0065467736\C,0,0.1807809007,0.5733483449,-0.0056541
81\C,0,-3.4064612161,-0.3871493579,0.0095772224\C,0,-2.2856827668,1.85
33713116,0.0120622729\C,0,-3.2946959204,-1.7747992385,0.0038014358\C,0
,0.1471248447,1.9922980168,-0.0002392501\C,0,1.4229963415,-0.068986476
1,-0.0145863869\C,0,-1.1502490238,2.607703166,0.0088882346\C,0,1.37627
91207,2.678569313,-0.0042226382\C,0,2.6343360794,0.6144314007,-0.01860
81186\C,0,1.5634017224,-1.4857543193,-0.0204840753\C,0,2.6062413301,2.
0082343224,-0.0132967465\C,0,3.765958818,-0.3969860468,-0.028788221\C,
0,3.0514096879,-1.7976163936,-0.0290461924\H,0,-1.9919955971,-3.485934
47,-0.0094197702\H,0,0.503468286,-3.348925554,-0.0218401727\H,0,-4.385
6741706,0.0818042898,0.0164566623\H,0,-3.2571117332,2.3395219016,0.018
9803945\H,0,-4.194527142,-2.3817821993,0.0062429607\H,0,-1.2165662787,
3.6918106624,0.0132610542\H,0,1.3672075038,3.7647925892,-0.0001408425\
H,0,3.5255991773,2.5860715772,-0.0161001344\H,0,4.4190914266,-0.282477
2399,0.843690113\H,0,4.4080393193,-0.2767004194,-0.9086841149\H,0,3.33
25564539,-2.3864255918,-0.9084881312\H,0,3.3413214126,-2.3909624666,0.
8445048368\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-690.9526027
\CCSD(T)/GTBas1=-691.1328887\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2Large
XP=-688.8619239\MP2/GTMP2LargeXP=-691.6828097\HF/GFHFB3=-688.8706034\H
F/GFHFB4=-688.916539\G4MP2=-692.0889994\FreqCoord=-1.6349061572,-3.122
5130143,-0.0159840145,-1.8637984359,-0.4276554795,-0.0047118662,-3.874
5874916,-4.5383542799,-0.009560551,0.8439110651,-4.2778845561,-0.03318
73153,-4.2643729133,0.7814656077,0.0123716092,0.3416263925,1.083471350
6,-0.0106848536,-6.4372787808,-0.731606259,0.0180983275,-4.3193144559,
3.5023642014,0.0227943924,-6.2260729808,-3.3538845017,0.0071836725,0.2
780256638,3.7648976268,-0.0004521171,2.6890733736,-0.1303655467,-0.027
5642765,-2.1736556396,4.9278448197,0.0167963292,2.6007906206,5.0617624
295,-0.0079796297,4.978173732,1.1611070747,-0.0351642481,2.954401091,-
2.8076687643,-0.0387092923,4.9250823501,3.79501288,-0.0251272093,7.116
6307937,-0.750194907,-0.0544018536,5.7663286293,-3.3970026759,-0.05488
93488,-3.7643261363,-6.5874614656,-0.0178007858,0.9514171771,-6.328552
1365,-0.0412719451,-8.2877230906,0.1545877042,0.0310985847,-6.15504915
99,4.4210556759,0.0358677475,-7.9265075553,-4.5009160648,0.011797486,-
2.2989770892,6.9765110864,0.0250597607,2.583647749,7.1144269407,-0.000
2661538,6.6624168995,4.886967041,-0.0304248447,8.3508725526,-0.5338046
223,1.5943432545,8.3299870965,-0.5228880136,-1.7171641185,6.2976190203
,-4.509690805,-1.716793763,6.3141823918,-4.5182642559,1.5958828595\PG=
C01 [X(C18H12)]\NImag=0\
```

cyclopenta[cd]pyrene

1\1\GINC-SAW288\Mixed\G4MP2\G4MP2\C18H10\KFOREST\04-Feb-2011\0\#\ G4MP
2\name\0,1\C,0,-1.2257552007,-0.5980928796,0.\C,0,0.1547910564,-0.57
81119232,0.\C,0,0.8010752852,0.6813316203,0.\C,0,0.8541910716,-1.81646
44625,0.\C,0,-2.0508661525,0.5706114615,0.\C,0,-1.9976396921,-1.762373
7534,0.\C,0,0.0108072382,1.8737735298,0.\C,0,2.2178985788,0.7204995616
,0.\C,0,2.2887136316,-1.7390126131,0.\C,0,0.085691403,-2.9982052548,0.
\C,0,-1.4356129189,1.7921809588,0.\C,0,-3.4287336999,0.0606757248,0.\C
,0,-3.3962251233,-1.3035380302,0.\C,0,-1.3177712727,-2.9841471597,0.\C
,0,0.6937620891,3.0993608813,0.\C,0,2.929631861,-0.534113672,0.\C,0,2.
8450467652,1.9743134138,0.\C,0,2.0867783282,3.1431136556,0.\H,0,2.8652
020036,-2.6595333502,0.\H,0,0.6003906952,-3.9545733887,0.\H,0,-1.99857
11067,2.722006563,0.\H,0,-4.3199748334,0.6736825463,0.\H,0,-4.26241349
88,-1.9528745343,0.\H,0,-1.854878221,-3.9279507434,0.\H,0,0.1251422217
,4.0246255089,0.\H,0,4.015223237,-0.500161855,0.\H,0,3.9295303002,2.03
09883414,0.\H,0,2.5888459542,4.1049698532,0.\Version=EM64L-G09RevB.01
\State=1-A'\MP2/GTbas1=-689.7592999\CCSD(T)/GTbas1=-689.9314961\MP2/GT
Bas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-687.6748682\MP2/GTMP2LargeXP=-6
90.4728525\HF/GFHFB3=-687.6846451\HF/GFHFB4=-687.7292796\G4MP2=-690.88
36157\FreqCoord=-2.3163416353,-1.1302317445,0.,0.2925127045,-1.0924732
09,0.,1.5138129008,1.287530168,0.,1.6141871904,-3.4326203642,0.,-3.875
5753635,1.0782993906,0.,-3.7749919303,-3.3304037377,0.,0.0204227204,3.
5409188064,0.,4.1912209044,1.3615468503,0.,4.3250419604,-3.2862575805,
0.,0.1619332836,-5.6657868217,0.,-2.7129152496,3.3867311926,0.,-6.4793
676754,0.1146605027,0.,-6.4179353687,-2.4633298809,0.,-2.4902268113,-5
.6392208721,0.,1.3110203497,5.8569432526,0.,5.5362018875,-1.0093285639
,0.,5.3763592214,3.7309116526,0.,3.9434395404,5.9396240136,0.,5.414447
1022,-5.0257896731,0.,1.1345739867,-7.473060677,0.,-3.7767520487,5.143
8469359,0.,-8.1635693361,1.273075513,0.,-8.0547941779,-3.6903980416,0.
, -3.5052118475,-7.4227511686,0.,0.2364845267,7.6054399992,0.,7.5876722
803,-0.945168928,0.,7.4257360983,3.8380117444,0.,4.8922098537,7.757268
8062,0.\PG=CS [SG(C18H10)]\NImag=0\

dibenzo[a,e]cyclooctene

1\1\GINC-SAW74\Mixed\G4MP2\G4MP2\C16H12\KFOREST\04-Feb-2011\0\#\ G4MP2
\name\0,1\C,0,3.1908639371,1.7173452364,3.3668731996\C,0,2.960955021
3,2.0428244292,2.0172020041\C,0,4.4599231413,1.1592968575,3.8794729553
\C,0,2.1337475482,1.8435263469,4.2813265178\C,0,3.9594634214,1.8677889
182,0.9415479832\C,0,1.6832408815,2.4813037456,1.6366444852\C,0,5.1977
555452,2.3621228643,0.8498212468\C,0,5.9304741743,3.2282742258,1.79723
48434\C,0,6.1603816457,2.9027974417,3.1469071182\C,0,6.4975979889,4.40
32218336,1.2800211126\C,0,5.6982146812,1.6536321607,3.7877470322\C,0,6
.9481006784,3.7654504211,3.924705102\C,0,0.6583423718,2.6354028614,2.5
59480378\C,0,0.8860142406,2.3130899232,3.8960197964\C,0,7.4718192215,4
.9421869083,3.4081781349\C,0,7.2441495158,5.2644964278,2.0716376565\H,
0,4.3373149421,0.2653469264,4.4898427589\H,0,2.308872302,1.5672386782,
5.3168575157\H,0,3.5845696619,1.330993342,0.070895494\H,0,1.5036322399
,2.7072081948,0.5897271276\H,0,5.7237345248,2.1849617805,-0.0875637412
\H,0,6.3383830199,4.6372647798,0.2315925012\H,0,7.1436161899,3.4973057
864,4.9587264539\H,0,-0.3152481766,2.9886883465,2.2365964973\H,0,0.092
27548,2.4117606022,4.6289495746\H,0,8.066478,5.5951161526,4.0382634554
\H,0,7.6589583772,6.1720375367,1.6459077787\H,0,6.4764794246,1.1193172
721,4.331385018\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-614.87
49851\CCSD(T)/GTBas1=-615.0513179\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2
LargeXP=-613.0321988\MP2/GTMP2LargeXP=-615.5385813\HF/GFHFB3=-613.0386
421\HF/GFHFB4=-613.0808126\G4MP2=-615.9104499\FreqCoord=6.0298589684,3
.2453121724,6.3624682713,5.5953940821,3.8603787087,3.8119593424,8.4280
333108,2.1907535674,7.3311414255,4.0321985029,3.4837599144,8.090534604
1,7.4823014996,3.5296095294,1.7792678291,3.1808642818,4.6889845317,3.0
92809854,9.8223344862,4.4637653058,1.6059294183,11.2069720276,6.100554
1686,3.3962816505,11.6414341845,5.4854921841,5.946792619,12.2786807206
,8.3208833679,2.4188893472,10.7680651938,3.1249119083,7.1578045514,13.
1300074259,7.1156700629,7.4166177951,1.2440867845,4.9801896579,4.83671
69569,1.6743242645,4.3711064756,7.3624104234,14.1196920431,9.339379754
2,6.440523287,13.6894586506,9.948456476,3.9148278174,8.1963373926,0.50
14330211,8.484573194,4.3631363266,2.9616518866,10.0474045923,6.7738549
652,2.5152129011,0.1339730677,2.8414531379,5.115882073,1.1144227643,10
.8162907092,4.1289793759,-0.1654714901,11.9778080329,8.7631604395,0.43
76464017,13.4994781973,6.6089501393,9.3706349658,-0.5957327176,5.64780
24713,4.2265548496,0.174375386,4.5575670363,8.7474469789,15.243434277,
10.5732372101,7.6312119832,14.473333796,11.6634606263,3.1103149417,12.
2387724178,2.1152031002,8.18513146\PG=C01 [X(C16H12)]\NImag=0\

fluoranthene

1\1\GINC-SAW292\Mixed\G4MP2\G4MP2\C16H10\KFOREST\03-Feb-2011\0\#\ G4MP
2\name\0,1\C,0,4.2976216022,0.819031582,1.7218340138\C,0,5.553200479
4,1.0082434718,1.0846087139\C,0,6.7396740519,1.0760994396,1.7882810507
\C,0,4.2619140405,0.6986970511,3.0929983385\C,0,3.2085842785,0.4994970
619,4.1038836067\C,0,5.4843355938,0.7697691887,3.8043345421\C,0,6.7367
227322,0.9554430138,3.2047128023\C,0,5.2803387872,0.6293663098,5.19861
84789\C,0,7.8510901283,1.0004368354,4.0861791837\C,0,7.6635003556,0.86
45790492,5.4477401839\C,0,6.3795956883,0.6772970071,6.0263830421\C,0,3
.8291210604,0.4572518819,5.3868765081\C,0,1.8323462124,0.3611961872,3.
9890842698\C,0,3.0606007066,0.2775796832,6.5285520888\C,0,1.6759382952
,0.1395024411,6.4004528679\C,0,1.0690115009,0.1808203846,5.1456076228\
H,0,3.3960455668,0.7732492135,1.1190966883\H,0,5.5748852935,1.10242063
39,0.0035693295\H,0,7.6772974733,1.2217995752,1.2605968239\H,0,8.85058
23272,1.1419248537,3.6864133084\H,0,8.526138605,0.9015089923,6.1053708
909\H,0,6.2904699261,0.5762027124,7.1034459078\H,0,1.3507579425,0.3919
905617,3.016815478\H,0,3.5237776637,0.2440557944,7.5096351334\H,0,1.06
69619823,-0.00135403,7.2872738165\H,0,-0.007502468,0.0717927228,5.0657
75447\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-613.7649377\CCSD
(T)/GTBas1=-613.9239791\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-6
11.9172257\MP2/GTMP2LargeXP=-614.4088043\HF/GFHFB3=-611.9254135\HF/GFH
FB4=-611.9659031\G4MP2=-614.7739762\FreqCoord=8.1213278509,1.547745384
2,3.2537947323,10.4940280672,1.905304037,2.0496134307,12.7361381831,2.
0335332326,3.3793614345,8.0538503385,1.3203460765,5.8449197892,6.06334
55607,0.9439126512,7.7552160979,10.363892293,1.4546529521,7.1891504024
,12.7305609971,1.8055256316,6.0560295309,9.9783941967,1.1893299627,9.8
239651944,14.8364101871,1.8905516321,7.7217595871,14.4819168914,1.6338
17623,10.2947369907,12.0556886894,1.279905854,11.3882135214,7.23599013
38,0.8640808306,10.1797213121,3.4626325221,0.6825618741,7.538276791,5.
7836971376,0.5245495813,12.3371754922,3.1670643935,0.2636214086,12.095
1030467,2.0201389696,0.3417010061,9.7237891943,6.4175960561,1.46122924
61,2.114786257,10.5350064269,2.0832730813,0.0067450552,14.5079896653,2
.3088665863,2.3821827612,16.725176715,2.1579252378,6.9663115654,16.112
0669345,1.7036051017,11.5374789236,11.8872654075,1.0888653235,13.42356
73655,2.5525625832,0.7407548084,5.7009550468,6.6589747376,0.4611986125
,14.19115376,2.0162659408,-0.0025587458,13.7709517685,-0.0141776099,0.
1356685845,9.5729282455\PG=C01 [X(C16H10)]\NImag=0\

fluorene

```
1\1\GINC-SAW319\Mixed\G4MP2\G4MP2\C13H10\KFOREST\21-Jan-2011\0\#\ G4MP
2\name\0,1\C,0,3.2935527497,1.4265135193,2.7786054367\C,0,4.42656882
45,1.4643672403,3.7097026767\C,0,2.3025641825,2.3145103346,3.239946294
6\C,0,3.0934610916,0.6945601154,1.6096827407\C,0,4.1301406246,2.375568
494,4.7418234069\C,0,5.6403594279,0.7796506444,3.7026886125\C,0,2.7606
353157,2.9819152728,4.5195375942\C,0,1.1167966906,2.4718091866,2.53822
35061\C,0,1.9001811844,0.8565239157,0.9085948187\C,0,5.0406834028,2.60
29041216,5.7628198697\C,0,6.5515433955,1.0119234363,4.731020139\C,0,0.
9188851,1.7371080014,1.3671858997\C,0,6.2562355455,1.9154261819,5.7533
475738\H,0,3.8520590283,0.0081295537,1.2472868559\H,0,5.8765993721,0.0
757687708,2.9110261107\H,0,2.0798336572,2.7783025912,5.3562565769\H,0,
2.8054990025,4.0742678207,4.420535693\H,0,0.3499181848,3.155394486,2.8
902570156\H,0,1.7317342694,0.2925885845,-0.0030831207\H,0,4.8163129003
,3.3046143136,6.5606793244\H,0,7.5003297641,0.4853146319,4.7374695654\
H,0,-0.0047498872,1.8516574814,0.8095433935\H,0,6.9766369195,2.0849013
266,6.5467506293\Version=EM64L-G09RevB.01\State=1-A\MP2/GTbas1=-499.7
757632\CCSD(T)/GTbas1=-499.9151244\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP
2LargeXP=-498.2763508\MP2/GTMP2LargeXP=-500.3161866\HF/GFHFB3=-498.282
0859\HF/GFHFB4=-498.3163229\G4MP2=-500.6129336\FreqCoord=6.2239127012,
2.6957198764,5.2508033067,8.3650027866,2.7672530422,7.0103220934,4.351
2157083,4.3737906642,6.122611182,5.8457942659,1.3125284009,3.041859540
8,7.8048346707,4.4891738635,8.9607476095,10.6587346097,1.4733261973,6.
997067433,5.2168446995,5.6350032171,8.5406883003,2.1104398913,4.671042
4154,4.7965472906,3.5908220413,1.618595627,1.7169953731,9.5255111539,4
.91877594,10.8901513068,12.3806227652,1.9122581621,8.9403323919,1.7364
411866,3.2826583859,2.5836069232,11.8225718039,3.6196309115,10.8722512
618,7.2793366112,0.0153626301,2.3570305667,11.1051634059,0.1431822262,
5.501042115,3.9303160141,5.2502310117,10.1218580278,5.3016247808,7.699
2503732,8.3536018204,0.6612495382,5.9628314198,5.4617942132,3.27250350
41,0.5529122943,-0.0058262538,9.1015123518,6.2448160275,12.3978871687,
14.1735691604,0.9171117426,8.9525200414,-0.008975986,3.4991255317,1.52
98153064,13.1839331064,3.9398925214,12.3715657496\PG=C01 [X(C13H10)]\N
Imag=0\
```


naphthalene

1\1\GINC-SAW46\Mixed\G4MP2\G4MP2\C10H8\KFOREST\02-Feb-2011\0\#\ G4MP2\
\name\0,1\C,0,3.4121388133,1.8165466081,2.137949407\C,0,2.8377043998,
3.0839655466,2.4730929929\C,0,3.5303037481,3.9313690806,3.3749794066\C
,0,1.59641085,3.447188314,1.8913324642\C,0,2.7195395028,0.9691430711,1
.2360629983\C,0,4.6534323473,1.4533238359,2.7197099055\C,0,4.730921226
4,3.5495182956,3.9208917825\C,0,0.9513618009,2.603245606,1.0212835439\
C,0,1.5189220012,1.350993827,0.6901506384\C,0,5.2984814202,2.297266497
,3.5897588326\H,0,3.0913637744,4.8923191818,3.626938627\H,0,1.16359038
52,4.4096705323,2.1479864498\H,0,3.1584794796,0.0081929877,0.984103777
7\H,0,5.0862528014,0.4908416252,2.4630559079\H,0,5.2501119859,4.207807
9133,4.6096435089\H,0,0.002087797,2.8938817367,0.5834562558\H,0,0.9997
312832,0.6927041446,0.0013989325\H,0,6.2477553935,2.0066303357,4.02758
6128\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-384.6144386\CCSD(
T)/GTBas1=-384.7246459\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-38
3.4672868\MP2/GTMP2LargeXP=-385.0342505\HF/GFHFB3=-383.4716791\HF/GFHFB
B4=-383.4983748\G4MP2=-385.2645882\FreqCoord=6.4480078858,3.4327755979
,4.0401388634,5.3624841627,5.8278502871,4.6734684562,6.6713072509,7.42
92108905,6.3777867808,3.0167793021,6.5142418419,3.5741003836,5.1391848
679,1.831414988,2.3358205498,8.7937127159,2.7463840336,5.1395068799,8.
9401454742,6.7076174823,7.4094116655,1.7978132573,4.9194212522,1.92994
62014,2.8703465995,2.5530083403,1.304195697,10.0126788061,4.3412045351
,6.7836610739,5.8418309117,9.2451434091,6.8539207043,2.1988671589,8.33
30696423,4.0591061273,5.9686612127,0.015482503,1.8596866263,9.61162483
9,0.9275562478,4.6545011131,9.921273822,7.9516045774,8.7109637994,0.00
39453645,5.4686439434,1.102572534,1.8892183318,1.3090211244,0.00264359
92,11.806546641,3.7919817863,7.6110347552\PG=C01 [X(C10H8)]\NImag=0\

1-methylnaphthalene

1\1\GINC-SAW222\Mixed\G4MP2\G4MP2\C11H10\KFOREST\02-Feb-2011\0\#\ G4MP
2\name\0,1\C,0,2.0653292286,1.2134578421,3.7100093355\C,0,0.62526388
54,0.8377451757,3.4639794161\C,0,2.7474670941,2.1133208537,2.830583788
4\C,0,2.7450881329,0.6931550629,4.7887201808\C,0,4.115060448,2.4487090
987,3.0938011212\C,0,2.1228001002,2.6949150176,1.6966195228\C,0,4.0937
884455,1.0233816427,5.0490532752\C,0,4.7655657265,1.8828596916,4.21981
90673\C,0,4.7876269958,3.3402856457,2.2207120865\C,0,2.8035469865,3.55
63689066,0.8694462486\C,0,4.151043448,3.8840601738,1.132582558\H,0,-0.
0316667507,1.715303286,3.4764094931\H,0,0.4920950003,0.3541775167,2.48
91792743\H,0,0.2698562137,0.1449671287,4.230585486\H,0,2.2313933052,0.
0099412622,5.4586410857\H,0,1.0885014094,2.4538253649,1.4802674264\H,0
,4.5917232643,0.5905543129,5.9105540875\H,0,5.8022939118,2.1437281838,
4.4102244595\H,0,5.8243271059,3.5861857036,2.4317359857\H,0,2.30407259
5,3.98833186,0.008375461\H,0,4.6793034535,4.5650262699,0.4734706407\|V
ersion=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-423.7853202\CCSD(T)/GTBa
s1=-423.9103443\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-422.51470
81\MP2/GTMP2LargeXP=-424.2589017\HF/GFHFB3=-422.5187945\HF/GFHFB4=-422
.5488938\G4MP2=-424.509088\FreqCoord=3.9029066164,2.2931029954,7.01090
15945,1.1815775042,1.5831089512,6.5459724264,5.1919603669,3.9935976445
,5.3490281562,5.1874647819,1.3098732365,9.0493696687,7.776337267,4.627
3895757,5.8464368286,4.0115108242,5.0926513347,3.2061462498,7.73613900
79,1.9339110341,9.5413279205,9.0056140914,3.5580891638,7.9743023675,9.
0473038485,6.312225076,4.1965376634,5.2979360051,6.7205632609,1.643015
2971,7.8443352824,7.3398100122,2.1402708575,-0.0598414864,3.2414534454
,6.5694618677,0.929924782,0.669298509,4.703867124,0.5099543392,0.27394
81716,7.9946479502,4.2167222416,0.018786263,10.3153367096,2.0569695591
,4.6370579176,2.7973000393,8.6770994475,1.115985918,11.169328519,10.96
47464358,4.0510591708,8.3341164129,11.0063831385,6.7769088415,4.595315
0404,4.3540661948,7.5368549425,0.0158273275,8.8426020198,8.6266494395,
0.8947298429\PG=C01 [X(C11H10)]\NImag=0\

2-methylnaphthalene

1\1\GINC-SAW16\Mixed\G4MP2\G4MP2\C11H10\KFOREST\03-Feb-2011\0\#\# G4MP2
\name\0,1\C,0,4.6414649925,1.1236666467,1.9806468411\C,0,5.227294411
2,0.8548537279,0.6176215554\C,0,3.3790111442,0.6986390786,2.3236643245
\C,0,5.4034994807,1.8346296766,2.9472235875\C,0,2.8250814364,0.9500797
829,3.6052912393\C,0,4.902998571,2.0969147493,4.1958501713\C,0,3.60319
17339,1.666266484,4.5670610032\C,0,1.5250637201,0.5160563598,3.9680204
516\C,0,3.0514241952,1.9181995954,5.8476032392\C,0,1.0176525192,0.7757
836413,5.2180250758\C,0,1.7880145857,1.4840387905,6.1681675762\H,0,4.5
295915546,0.3005782624,-0.0153698814\H,0,5.4808485361,1.7887506004,0.1
023814864\H,0,6.1526519868,0.271458974,0.6904390169\H,0,2.7776723646,0
.153109551,1.6008891755\H,0,6.4013341551,2.1732080409,2.6828689803\H,0
,5.4993055028,2.6416192885,4.9221864683\H,0,0.9344924788,-0.0280277575
,3.2367120934\H,0,3.6478385145,2.4628734381,6.5737547974\H,0,0.0209052
738,0.4373262349,5.4814860919\H,0,1.3762728429,1.6830548343,7.15208670
62\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-423.7858904\CCSD(T)
/GTBas1=-423.9111359\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-422.
51666\MP2/GTMP2LargeXP=-424.2587926\HF/GFHFB3=-422.5208251\HF/GFHFB4=-
422.550886\G4MP2=-424.5096167\FreqCoord=8.7710976911,2.1234222269,3.74
28800956,9.8781548532,1.6154394294,1.1671355935,6.3854056626,1.3202365
242,4.391089198,10.2111341777,3.466947644,5.5694454328,5.338630218,1.7
953905942,6.8130130716,9.265324529,3.9625946002,7.9290077183,6.8090455
813,3.1487873191,8.6304945283,2.8819527662,0.9752051891,7.4984719431,5
.7663560441,3.6248719034,11.0503686559,1.9230845597,1.4660186205,9.860
6383479,3.3788578886,2.8044268847,11.6561474608,8.559687532,0.56801059
75,-0.0290448665,10.3573027091,3.3802487548,0.1934729703,11.6268272459
,0.5129831171,1.3047406534,5.249040056,0.2893351197,3.0252421108,12.09
67684382,4.106768027,5.0698876232,10.3921813214,4.9919370026,9.3015844
,1.7659348582,-0.0529647858,6.1164994275,6.8934157693,4.654156298,12.4
225962317,0.0395052422,0.8264268148,10.3585075149,2.6007787571,3.18051
27034,13.5154851534\PG=C01 [X(C11H10)]\NImag=0\

phenanthrene

1\1\GINC-SAW26\Mixed\G4MP2\G4MP2\C14H10\KFOREST\03-Feb-2011\0\#\ G4MP2
\name\0,1\C,0,4.2654168289,4.2087903308,6.0264645337\C,0,3.401545062
6,3.360977863,5.3638661179\C,0,3.4331541117,3.224590931,3.9588914516\C
,0,5.2074835027,4.9647756996,5.3099171585\C,0,5.263975437,4.8544550228
,3.9380815711\C,0,4.3910674662,3.9942052142,3.2380821231\C,0,4.4580551
174,3.88678264,1.8111025892\C,0,2.5387662029,2.3413687181,3.2262642214
\C,0,2.6445218533,2.2694634159,1.8074231926\C,0,1.5594160752,1.5418477
958,3.8549122208\C,0,3.6245155203,3.0636485983,1.1283190552\C,0,1.7822
33631,1.4161792394,1.0860587136\C,0,0.8367813905,0.6486382098,1.729713
8653\C,0,0.727361009,0.714905593,3.1283143995\H,0,4.2153482334,4.29073
92746,7.1071917936\H,0,2.6863510555,2.7913652169,5.9446748589\H,0,5.88
47304615,5.6300721031,5.8348306414\H,0,5.9868116265,5.4323300503,3.369
6460644\H,0,5.1973902937,4.484471027,1.2862362818\H,0,1.4503321063,1.5
707796485,4.9322067011\H,0,3.6839065606,2.9898810106,0.0464857948\H,0,
1.8793598101,1.3761551094,0.0050800628\H,0,0.1806180268,-0.0028286106,
1.1623885427\H,0,-0.0151212926,0.113085797,3.6418580568\\Version=EM64L
-G09RevB.01\State=1-A\MP2/GTBas1=-537.7753602\CCSD(T)/GTBas1=-537.9219
389\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-536.1630249\MP2/GTMP2
LargeXP=-538.351885\HF/GFHFB3=-536.1696292\HF/GFHFB4=-536.2061208\G4MP
2=-538.6722418\FreqCoord=8.0604696492,7.953461076,11.3883675183,6.4279
88597,6.3513276997,10.1362379763,6.4877210432,6.0935937502,7.481220633
4,9.8407176617,9.3820663834,10.0342892179,9.9474719462,9.1735905175,7.
4418956584,8.2979149422,7.5479539733,6.1190884085,8.4245032572,7.34495
47276,3.4224878921,4.7975728389,4.4245456534,6.0967558107,4.9974220552
,4.2886643246,3.4155348403,2.9468693093,2.9136700727,7.2847283636,6.84
93416978,5.7894568183,2.1322140048,3.3679334675,2.6761909176,2.0523535
33,1.5812876611,1.2257485758,3.2686854936,1.3745131068,1.3509757816,5.
9116574726,7.9658537158,8.1083221367,13.4306460637,5.0764677918,5.2749
157968,11.2338074324,11.1205289381,10.6392943833,11.0262319441,11.3134
343832,10.2656160586,6.3677082265,9.8216442607,8.4744220918,2.43063431
48,2.7407304825,2.9683433508,9.3205198959,6.9615744986,5.65005628,0.08
78454213,3.5514753462,2.6005562732,0.0095999275,0.3413186053,-0.005345
2994,2.1965960056,-0.0285751018,0.2137011859,6.8821143421\PG=C01 [X(C1
4H10)]\NImag=0\

1-methylphenanthrene

1\1\GINC-N098\Mixed\G4MP2\G4MP2\C15H12\KFOREST\14-May-2011\0\#\ G4MP2\
\name\0,1\C,0,3.3250925965,4.5530766898,1.7316279798\C,0,4.3177008158
,5.0980074887,0.7326441053\C,0,3.7445480505,3.6995333343,2.792672099\C
,0,1.9877751757,4.8823275577,1.6223034049\C,0,2.7902213669,3.195675090
8,3.7256413593\C,0,5.1223474045,3.3316768638,2.9446513777\C,0,1.043691
2292,4.3908107861,2.5358470174\C,0,3.2343998989,2.3246792286,4.8041750
651\C,0,1.4369807782,3.5653775039,3.5650375077\C,0,5.5360286879,2.5197
817184,3.9501836215\C,0,4.6148263705,1.9919728755,4.9073707151\C,0,2.3
564304335,1.7827876689,5.7695635518\C,0,5.0575804606,1.1481788251,5.94
90654323\C,0,2.8114225894,0.960087395,6.7792652342\C,0,4.1752252494,0.
6367447173,6.8739146936\H,0,3.8145462629,5.7293596976,-0.0035745904\H,
0,5.092884335,5.7039224315,1.2157225291\H,0,4.8311233385,4.2971375769,
0.1882246472\H,0,1.6637647667,5.5324594963,0.815265565\H,0,5.847201653
8,3.7142054408,2.2363591234\H,0,-0.0010701037,4.663640384,2.4291052571
\H,0,0.6886442293,3.1995665566,4.2566034295\H,0,6.5848043832,2.2542729
41,4.0460569057\H,0,1.2988504973,2.0112603466,5.7266078997\H,0,6.11547
48247,0.9091113114,6.0063932272\H,0,2.1097493258,0.5609881654,7.504300
6704\H,0,4.527645379,-0.0106220918,7.6698621716\\Version=EM64L-G09RevB
.01\State=1-A\MP2/GTbas1=-576.9456142\CCSD(T)/GTbas1=-577.1069868\MP2/
GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-575.2094382\MP2/GTMP2LargeXP=
-577.5758651\HF/GFHFB3=-575.2157484\HF/GFHFB4=-575.2556399\G4MP2=-577.
9160591\FreqCoord=6.2835143739,8.6040680058,3.2723026459,8.1592720657,
9.6338379771,1.3844967118,7.0761703068,6.9911048212,5.277385446,3.7563
506958,9.226261975,3.0657091398,5.2727542335,6.0389507312,7.0404418385
,9.6798337519,6.2959568358,5.5645846606,1.9722905905,8.297429887,4.792
0563778,6.1121300131,4.3930070888,9.0785751675,2.7155001289,6.73758704
28,6.736944543,10.461578084,4.7616973625,7.4647652193,8.7207579911,3.7
642831989,9.273586684,4.4530081704,3.3689804472,10.9028950192,9.557441
9657,2.1697435309,11.2421044136,5.3128187377,1.8143022401,12.810954674
7,7.8900322645,1.2032731323,12.9898162317,7.2084477581,10.8269207453,-
0.0067549969,9.6241566196,10.7788512787,2.2973826335,9.129500024,8.120
4131757,0.3556930346,3.1440597586,10.4548332892,1.5406286435,11.049609
7694,7.0188310845,4.226106278,-0.0020222029,8.813003108,4.5903436839,1
.3013489964,6.0463045358,8.043814738,12.4434769229,4.2599584872,7.6459
394699,2.4544717275,3.8007312371,10.8217206009,11.5565725913,1.7179714
029,11.3504382457,3.9868484349,1.0601139963,14.1810730858,8.5560097932
, -0.0200728445,14.4939389813\PG=C01 [X(C15H12)]\NImag=0\

2-methylphenanthrene

1\1\GINC-N100\Mixed\G4MP2\G4MP2\C15H12\KFOREST\14-May-2011\0\#\ G4MP2\
\name\0,1\C,0,4.639248949,1.5581586932,1.8138763417\C,0,5.3392289101,
0.9752912767,0.6124242901\C,0,5.0612188721,2.7323967968,2.4037314163\C
,0,3.5186613257,0.9072795275,2.3727910333\C,0,4.4108227002,3.284188303
6,3.5288167505\C,0,2.8639447238,1.421664553,3.4699933619\C,0,3.2820762
121,2.6219622224,4.086147466\C,0,4.8756240512,4.505194966,4.1161170956
\C,0,2.6196777543,3.1981722543,5.2442808285\C,0,4.2586591367,5.0445986
597,5.1970845549\C,0,3.1189128699,4.4145412294,5.7931281106\C,0,1.4942
660667,2.6098660335,5.8620279205\C,0,2.4845104946,4.9845609529,6.91791
30499\C,0,0.8910066741,3.1860441511,6.9610103839\C,0,1.3880018392,4.38
53834232,7.497397825\H,0,6.1841162123,1.595822198,0.3029423644\H,0,4.6
572598983,0.8854191718,-0.2410561241\H,0,5.7198988229,-0.0309377653,0.
8226079306\H,0,5.9211534624,3.2596372729,1.9987089451\H,0,3.1667944116
, -0.0186639876,1.9267423903\H,0,2.0087060609,0.8835108151,3.8608722351
\H,0,5.7391564816,4.9920405113,3.6727166368\H,0,4.619615793,5.97087050
84,5.6342443483\H,0,1.0877923809,1.6848242709,5.4714660443\H,0,2.88075
2374,5.9120303135,7.320829788\H,0,0.0275612054,2.7086966064,7.41259060
98\H,0,0.9102123174,4.8345270414,8.3615944027\Version=EM64L-G09RevB.0
1\State=1-A\MP2\GTBas1=-576.9468635\CCSD(T)/GTBas1=-577.1084521\MP2\GT
Bas2=0.\MP2\GTBas3=0.\HF/GTMP2LargeXP=-575.2122521\MP2\GTMP2LargeXP=-5
77.5764232\HF/GFHFB3=-575.2186476\HF/GFHFB4=-575.2584965\G4MP2=-577.91
73304\FreqCoord=8.7669099759,2.9444932018,3.4277295248,10.0896804009,1
.8430334127,1.1573141855,9.5643175668,5.1634816323,4.5423940738,6.6493
062599,1.714509833,4.4839252234,8.335246924,6.2062164626,6.6684972315,
5.4120711877,2.686556658,6.5573371369,6.2022251881,4.9547905311,7.7216
996494,9.2135941837,8.5135846609,7.7783340416,4.9504735121,6.043669686
4,9.9102545298,8.0476994617,9.5329099172,9.8210664983,5.8938911565,8.3
422739259,10.9474255817,2.8237536357,4.9319320469,11.0776273531,4.6950
44409,9.4194550936,13.0729610754,1.6837585966,6.0207508928,13.15440323
37,2.6229433481,8.2871736575,14.1680285986,11.6862860152,3.015666911,0
.5724781028,8.8009457374,1.6731997475,-0.4555300573,10.8090422831,-0.0
584639035,1.5545037036,11.1893584347,6.1598217383,3.7770125256,5.98437
4157,-0.0352698251,3.6410154464,3.7959043365,1.6695934759,7.2959911584
,10.8454339839,9.4335894107,6.9404286072,8.7298086879,11.2833100358,10
.647178784,2.0556296893,3.1838564541,10.3395723691,5.4438330436,11.172
1181818,13.8343633647,0.0520831301,5.1186947632,14.0077661878,1.720052
0027,9.1359320902,15.8011234554\PG=C01 [X(C15H12)]\NImag=0\

3-methylphenanthrene

1\1\GINC-N100\Mixed\G4MP2\G4MP2\C15H12\KFOREST\14-May-2011\0\#\ G4MP2\
\name\0,1\C,0,8.3753956713,3.514528762,1.0402482341\C,0,6.9717872814,
2.97781237,1.1691308114\C,0,5.8848365291,3.8253238397,1.2796696358\C,0
,6.7452297952,1.5848729667,1.1787837722\C,0,4.5600364018,3.3509342742,
1.4015401589\C,0,5.469763288,1.0852558245,1.2957776997\C,0,3.409020819
7,4.2327355517,1.5184720894\C,0,4.3543986605,1.9435502814,1.4091362782
\C,0,2.1083323985,3.6626104876,1.6373682781\C,0,3.5129402035,5.6410696
02,1.5204875639\C,0,3.0287164937,1.4173162579,1.5307564297\C,0,1.95470
2087,2.2387625354,1.6398955517\C,0,0.9839666963,4.5088239846,1.7514932
008\C,0,2.3991460931,6.4474823174,1.6332584326\C,0,1.1199058335,5.8793
025124,1.7501568179\H,0,8.3883177679,4.6075496595,1.0485471735\H,0,8.8
458344776,3.1801376873,0.1082480738\H,0,9.0125628553,3.1648492226,1.86
09114558\H,0,6.0705914977,4.8932743645,1.271144122\H,0,7.5890903894,0.
9064599874,1.0927646459\H,0,5.301638527,0.0122032761,1.3026361598\H,0,
4.4855757144,6.1093813056,1.4318989126\H,0,2.9026280864,0.3386581335,1
.5335825141\H,0,0.9526387406,1.8306679262,1.7317455617\H,0,0.001667982
7,4.0542961331,1.841091379\H,0,2.513668999,7.5264407695,1.6314748539\H
,0,0.2467967095,6.5170799673,1.8386201938\\Version=EM64L-G09RevB.01\St
ate=1-A\MP2\GTBas1=-576.9468062\CCSD(T)/GTBas1=-577.1083661\MP2\GTBas2
=0.\MP2\GTBas3=0.\HF/GTMP2LargeXP=-575.2119677\MP2/GTMP2LargeXP=-577.5
764116\HF/GFHF3=-575.2183497\HF/GFHF4=-575.258202\G4MP2=-577.9172454
\FreqCoord=15.8272040733,6.6414968463,1.9657842727,13.1747686186,5.627
2498544,2.2093370471,11.1207293767,7.2288144267,2.4182251522,12.746637
0163,2.9949758625,2.2275784993,8.6172199555,6.3323480675,2.6485270645,
10.336354626,2.0508362923,2.4486649815,6.4421157306,7.9987109856,2.869
4963893,8.2286209417,3.6727777574,2.6628816498,3.9841708303,6.92133075
29,3.0941776242,6.6384949059,10.6600766442,2.8733050842,5.7234447072,2
.6783395711,2.8927104282,3.6938516158,4.2306480685,3.0989534792,1.8594
275798,8.5204425122,3.3098424731,4.5337290688,12.1839758265,3.08641114
18,2.11631532,11.1102716007,3.3073170755,15.851623297,8.7070070001,1.9
814669953,16.7162045795,6.0095892938,0.2045592139,17.0312755519,5.9806
982826,3.516613009,11.4717553952,9.2469484419,2.4021142661,14.34130243
36,1.7129611267,2.0650259084,10.0186448715,0.0230608498,2.4616255928,8
.4765096485,11.5450575089,2.7058967948,5.4851721489,0.639971125,2.8980
509539,1.8002263233,3.4594610208,3.2725248435,0.0031520305,7.661509353
3,3.4791584918,4.7501459969,14.2229118097,3.0830406666,0.4663781914,12
.3154963242,3.4744886286\PG=C01 [X(C15H12)]\NImag=0\

4-methylphenanthrene

1\1\GINC-N100\Mixed\G4MP2\G4MP2\C15H12\KFOREST\14-May-2011\0\#\ G4MP2\
\name\0,1\C,0,4.2317436234,3.6325977912,6.0281656465\C,0,3.098656228,
2.7870910314,5.4865847631\C,0,3.0287865372,2.2348028861,4.1644341916\C
,0,2.0792254242,2.5190844736,6.3918425548\C,0,3.9961281299,2.459427165
8,3.0837110267\C,0,1.9192404383,1.3712771802,3.8826368741\C,0,0.977661
6131,1.7163983165,6.0826973673\C,0,3.8542527775,1.7360834164,1.8557135
592\C,0,5.074114114,3.3772228434,3.1381683078\C,0,1.8130032765,0.69867
42989,2.6231221212\C,0,0.9112325475,1.1382990593,4.8396707614\C,0,2.75
01046184,0.8501828235,1.6615275147\C,0,4.7842384776,1.9092928846,0.809
087273\C,0,5.9653690818,3.5389448843,2.0949150779\C,0,5.8352868501,2.7
90766332,0.9185250743\H,0,4.1084190625,3.7599337296,7.1062842223\H,0,4
.2573107721,4.6365401696,5.589616744\H,0,5.2104445711,3.1732736773,5.8
614758068\H,0,2.1515186455,2.9473578169,7.3867587491\H,0,0.2049666206,
1.5409510163,6.823496015\H,0,5.2163243301,3.9992152349,4.0026230221\H,
0,0.9598253303,0.0452204967,2.46895205\H,0,0.0865787583,0.4849769143,4
.5722511221\H,0,2.6719303289,0.3223834715,0.7160146562\H,0,4.643037936
,1.331807408,-0.0997200634\H,0,6.7703268612,4.2599608996,2.1936960449\
H,0,6.5409630457,2.915013778,0.1041495174\Version=EM64L-G09RevB.01\St
ate=1-A\MP2\GTBas1=-576.9366551\CCSD(T)/GTBas1=-577.0979235\MP2\GTBas2
=0.\MP2\GTBas3=0.\HF/GTMP2LargeXP=-575.1982407\MP2/GTMP2LargeXP=-577.5
677023\HF/GFHFB3=-575.2044741\HF/GFHFB4=-575.2443547\G4MP2=-577.907085
4\FreqCoord=7.9968365129,6.8646149762,11.3915821555,5.855611651,5.2668
387567,10.3681426071,5.7235770702,4.2231654157,7.8696401206,3.92916662
03,4.7603797606,12.0788319131,7.5515877574,4.6476437872,5.8273693135,3
.6268388116,2.5913383229,7.3371203655,1.8475126995,3.2435227531,11.494
6321735,7.2834821963,3.2807222008,3.506790408,9.5886860425,6.382026263
7,5.9302786607,3.4260796707,1.3203030809,4.9569824221,1.7219799582,2.1
510734795,9.1456523124,5.1969445655,1.6066126994,3.139831965,9.0409004
771,3.6080406594,1.5289533636,11.2729138462,6.6876366307,3.9588157689,
11.0270940536,5.2737840684,1.7357608365,7.7637868673,7.1052450267,13.4
289310026,8.0451514218,8.7617911247,10.5628448339,9.8463132699,5.99661
81948,11.0765840094,4.0657810097,5.5696990896,13.9589510454,0.38733077
93,2.911975405,12.8945387372,9.8574244043,7.5574215405,7.5638613249,1.
8138070097,0.0854543544,4.6656432098,0.1636101421,0.9164735487,8.64030
24315,5.0492165678,0.6092164708,1.3530716074,8.7740701236,2.5167512629
, -0.1884436098,12.7940635979,8.050159437,4.1454847436,12.3606288017,5.
508577714,0.1968140647\PG=C01 [X(C15H12)]\NImag=0\

9, 10-dihydrophenanthrene

1\1\GINC-N100\Mixed\G4MP2\G4MP2\C14H12\KFOREST\12-May-2011\0\#\ G4MP2\
\name\0,1\C,0,2.8660770971,2.6003842904,4.6964802775\C,0,2.3445886502
,2.0942356216,3.4058227806\C,0,4.1230986514,3.2392383343,4.725806908\C
,0,2.1504427954,2.4729119644,5.894525649\C,0,2.8544406562,2.6264192276
,2.2033551055\C,0,1.3629042454,1.0967702724,3.3347365049\C,0,4.8889594
915,3.3967680302,3.432857916\C,0,4.6331562512,3.7018423325,5.936781126
2\C,0,2.6696440259,2.9388025466,7.0968050951\C,0,3.927550221,3.6877094
776,2.2752937949\C,0,2.3578022049,2.1727111639,0.9834702051\C,0,0.8753
0713,0.6518278987,2.111472108\C,0,3.9195438663,3.551599702,7.122423319
5\C,0,1.3689528675,1.194608037,0.9282017238\H,0,1.1632046556,2.0246588
993,5.8836652737\H,0,0.9915920987,0.6446109785,4.2476258687\H,0,5.6343
690559,4.1924995581,3.5291101575\H,0,5.4409665323,2.4709905487,3.21399
91768\H,0,5.6030132218,4.1913995863,5.9474809658\H,0,2.0940115366,2.83
17207252,8.0102939149\H,0,4.4681150092,3.7442865665,1.32520053\H,0,3.4
646240012,4.6725273428,2.4350059117\H,0,2.7572403347,2.5906872077,0.06
36070331\H,0,0.1179082816,-0.1245878254,2.0830688371\H,0,4.330534893,3
.921966627,8.0556477184\H,0,0.9971422256,0.8502108861,-0.0310379015\\V
ersion=EM64L-G09RevB.01\State=1-A\MP2\GTBas1=-538.9487308\CCSD(T)/GTBa
s1=-539.1036156\MP2\GTBas2=0.\MP2\GTBas3=0.\HF/GTMP2LargeXP=-537.32559
94\MP2/GTMP2LargeXP=-539.5423409\HF/GFHFB3=-537.3308076\HF/GFHFB4=-537
.3685119\G4MP2=-539.8577186\FreqCoord=5.4161007892,4.9140141491,8.8750
615129,4.4306304431,3.9575317825,6.4360723125,7.7915272699,6.121273330
9,8.930480813,4.0637479477,4.6731263634,11.1390391599,5.3941111027,4.9
632130504,4.1637377228,2.5755157691,2.0725954455,6.3017387196,9.238794
5137,6.418961314,6.4871613144,8.7553964456,6.9954681955,11.2188904393,
5.0448960812,5.5535319717,13.4110180482,7.4219942908,6.9687609703,4.29
96821442,4.4556004427,4.1058290656,1.8584893475,1.6540907578,1.2317762
142,3.9901040213,7.4068644732,6.7115507705,13.4594294763,2.5869460084,
2.2574820262,1.754047054,2.1981382355,3.8260508322,11.1185160249,1.873
8375022,1.2181382116,8.0268496068,10.6474144472,7.9226759771,6.6690516
905,10.2819366443,4.669495414,6.0735782354,10.5881605082,7.9205973315,
11.2391102058,3.9571083233,5.3511766554,15.1372617431,8.4435136977,7.0
756761738,2.5042660728,6.5471905157,8.8297970264,4.6014943051,5.210429
1151,4.8956893186,0.1201998727,0.222814361,-0.2354368694,3.936429618,8
.1835249567,7.4114428273,15.2229680107,1.8843257218,1.60666573,-0.0586
531336\PG=C01 [X(C14H12)]\NImag=0\

9,10-dihydro-1-methylphenanthrene

1\1\GINC-N149\Mixed\G4MP2\G4MP2\C15H14\KFOREST\15-May-2011\0\#\ G4MP2\
\name\0,1\C,0,0.8886904389,1.9331214881,-0.5584789446\C,0,-0.40536611
57,1.9838758913,0.2626013816\C,0,1.6765141146,0.6893354477,-0.23116744
5\C,0,-1.2105313555,0.7146787558,0.0784763624\C,0,-0.509961236,-0.5015
026337,-0.0640235015\C,0,-2.6149699495,0.7268292998,0.062556037\C,0,0.
9700410034,-0.5041951023,0.0164883342\C,0,-1.2317757134,-1.6843377106,
-0.2712673372\C,0,1.6975859239,-1.6570930484,0.3415496927\C,0,3.068297
0354,0.6943617409,-0.1766070334\C,0,-2.6183292758,-1.6707855434,-0.305
29999\C,0,-3.3029638841,-0.4732631961,-0.128921078\C,0,-3.3952691093,2
.0078627889,0.2501780516\C,0,3.7789943024,-0.4633136178,0.1273016723\C
,0,3.0866983377,-1.6415674014,0.3932662908\H,0,1.4952895633,2.82635312
58,-0.3782793676\H,0,0.6299496878,1.9374352424,-1.6275688415\H,0,-0.99
15314441,2.8604697178,-0.023123417\H,0,-0.152193447,2.1123523821,1.325
8617676\H,0,-0.7029240913,-2.6171632553,-0.4294352619\H,0,1.1706125084
, -2.5738427965,0.581009341\H,0,3.6006712155,1.6212499357,-0.3710390913
\H,0,-3.166994816,-2.5920888566,-0.4712593667\H,0,-4.3886352221,-0.463
5227117,-0.148778672\H,0,-3.127488095,2.5183247102,1.1818698781\H,0,-4
.4687081429,1.804671192,0.2799452554\H,0,-3.2176499561,2.7200189045,-0
.5646486441\H,0,4.8629049517,-0.4415947558,0.1694985984\H,0,3.62648277
07,-2.5468899936,0.6508053286\Version=EM64L-G09RevB.01\State=1-A\MP2/
GTBas1=-578.1186505\CCSD(T)/GTBas1=-578.2884674\MP2/GTBas2=0.\MP2/GTBa
s3=0.\HF/GTMP2LargeXP=-576.3714355\MP2/GTMP2LargeXP=-578.7657076\HF/GF
HFB3=-576.3763781\HF/GFHFB4=-576.4174648\G4MP2=-579.1011253\FreqCoord=
1.6793815465,3.6530701941,-1.0553722563,-0.7660309422,3.7489821162,0.4
962446934,3.1681525346,1.3026552099,-0.4368431619,-2.2875727372,1.3505
471215,0.1482988328,-0.9636870743,-0.9477026326,-0.1209868839,-4.94157
70503,1.373508322,0.1182137779,1.8331118341,-0.9527906608,0.0311584361
, -2.3277187556,-3.1829369884,-0.5126209761,3.2079724831,-3.1314520382,
0.64543538,5.7982410913,1.3121535275,-0.3337389263,-4.9479252569,-3.15
73271038,-0.5769333694,-6.2416971677,-0.8943378294,-0.2436255302,-6.41
6128764,3.7943107834,0.4727680019,7.1412642892,-0.8755358512,0.2405652
97,5.8330145131,-3.1021128172,0.7431655869,2.8256877639,5.3410333626,-
0.7148444065,1.1904323875,3.6612220084,-3.0756593728,-1.8737228814,5.4
055043781,-0.0436969254,-0.2876039341,3.9917674984,2.5055156308,-1.328
3340247,-4.9457217975,-0.8115150368,2.2121370486,-4.8638579945,1.09794
85352,6.8042824919,3.0637183714,-0.7011622672,-5.9847528665,-4.8983380
511,-0.8905511406,-8.2933186668,-0.8759309816,-0.2811509444,-5.9100959
834,4.7589440159,2.2334103943,-8.4446345579,3.4103343128,0.5290198649,
-6.0804772086,5.1400908059,-1.0670312986,9.1895585689,-0.8344931502,0.
320305931,6.8530592622,-4.8129245784,1.229843837\PG=C01 [X(C15H14)]\NI
mag=0\

9-methylphenanthrene

1\1\GINC-N208\Mixed\G4MP2\G4MP2\C15H12\KFOREST\13-May-2011\0\#\ G4MP2\
\name\0,1\C,0,5.1377274406,1.5044887576,5.9583662907\C,0,5.7233399242
,1.6487728707,7.3401198911\C,0,3.7451223403,1.8142198202,5.7163302049\
C,0,5.9114837678,1.0815099727,4.9230372165\C,0,3.1980893396,1.67512808
2,4.4056096193\C,0,2.9041436959,2.256860762,6.7617179407\C,0,5.4107206
124,0.9261226309,3.5922432552\C,0,4.0479956371,1.2206741072,3.31576802
85\C,0,1.8349200261,1.9885962589,4.2167351617\C,0,1.5758922749,2.55494
39452,6.5433358959\C,0,6.2551001455,0.4836419404,2.5514611295\C,0,3.59
26578789,1.0545400819,1.9899517138\C,0,1.0369541233,2.4188360431,5.256
4358313\C,0,5.7812294838,0.3311803111,1.2669345042\C,0,4.4359598652,0.
6204778986,0.9871246342\H,0,6.7807333073,1.3740560229,7.3402846769\H,0
,5.6440138403,2.6779550228,7.7095451564\H,0,5.2103179456,1.0088706409,
8.067654217\H,0,6.958540852,0.8468510735,5.0967325421\H,0,3.3144033287
,2.3641919388,7.7586703678\H,0,1.3946445349,1.8916953736,3.2320153785\
H,0,0.9516856402,2.8930381692,7.3637542828\H,0,7.2929406057,0.26412133
93,2.7844261266\H,0,2.5606259903,1.2691957988,1.7413405829\H,0,-0.0072
714743,2.6512122435,5.0756378571\H,0,6.4408044275,-0.0097367723,0.4759
501951\H,0,4.0556344465,0.5027556669,-0.0221727007\Version=EM64L-G09R
evB.01\State=1-A\MP2/GTBas1=-576.9465165\CCSD(T)/GTBas1=-577.1079121\M
P2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-575.2105029\MP2/GTMP2Large
XP=-577.5766257\HF/GFHFB3=-575.21682\HF/GFHFB4=-575.2567234\G4MP2=-577
.91672\FreqCoord=9.7088978081,2.8430717219,11.2596804888,10.8155450221
,3.1157291809,13.8708163767,7.0772555573,3.4283786051,10.8022985724,11
.1710853602,2.0437576583,9.3031920812,6.0435130003,3.1655333125,8.3253
956289,5.4880362357,4.2648487602,12.7777950957,10.2247801389,1.7501181
379,6.7883559551,7.6496031413,2.30673976,6.265893494,3.467496325,3.757
9023182,7.9684746304,2.9780048144,4.8281443414,12.3651128388,11.820426
2088,0.9139508137,4.8215627735,6.7891394804,1.9927919509,3.7604637568,
1.9595593053,4.5709376817,9.9332241563,10.9249404358,0.6258400885,2.39
41592413,8.3827492817,1.1725332998,1.8653952176,12.8137289309,2.596589
5744,13.8711277767,10.6656404483,5.0606015892,14.5689289547,9.84607398
24,1.9064892147,15.2456570049,13.1497364948,1.6003166042,9.6314286771,
6.2633145852,4.46767529,14.6617621505,2.6354962236,3.5747861829,6.1076
239227,1.7984252245,5.4670498318,13.9154789044,13.7816604483,0.4991169
972,5.2618028166,4.8388818504,2.3984324687,3.2906568058,-0.013741095,5
.0100650603,9.5915654996,12.1713564435,-0.0183998332,0.8994155217,7.66
40383989,0.9500705221,-0.0419003319\PG=C01 [X(C15H12)]\NImag=0\

pyrene

1\1\GINC-N287\Mixed\G4MP2\G4MP2\C16H10\KFOREST\14-May-2011\0\#\ G4MP2\
\name\0,1\C,0,3.4612745939,3.8101690098,1.3944841618\C,0,4.7283493794
,3.409318477,1.9050756092\C,0,5.6863638485,4.3923480791,2.2932614692\C
,0,5.0431606879,2.0236187908,2.0297987887\C,0,2.5032611175,2.827139308
1,1.0062987417\C,0,3.1464624506,5.1958690572,1.2697608722\C,0,5.339781
9409,5.7779371255,2.1557189405\C,0,6.9261915138,3.9725559316,2.7928275
639\C,0,4.05845955,1.0591931131,1.630875936\C,0,6.2967727943,1.6545872
136,2.5350111246\C,0,2.8498421357,1.4415505569,1.1438408401\C,0,1.2634
322678,3.2469306582,0.5067325605\C,0,4.1311645493,6.1602944233,1.66868
40788\C,0,1.8928506752,5.5648993568,0.7645491011\C,0,7.2248282175,2.61
95333481,2.9110786407\C,0,0.9647952297,4.5999521198,0.3884816328\H,0,6
.0726795972,6.5223584632,2.4526750781\H,0,7.6559869283,4.7201462786,3.
088537272\H,0,4.3031036957,0.0055177555,1.7278383552\H,0,6.5372184948,
0.6000509722,2.630278236\H,0,2.1169446413,0.6971294737,0.8468846659\H,
0,0.533638567,2.4993385548,0.2110235136\H,0,3.8865202797,7.2139699809,
1.5717214726\H,0,1.6524029195,6.6194351232,0.6692813374\H,0,8.19058119
98,2.3140093461,3.3002469708\H,0,-0.0009575574,4.9054774819,-0.0006862
644\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-613.7869747\CCSD(T
)\GTBas1=-613.9455582\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-611
.939039\MP2/GTMP2LargeXP=-614.4318793\HF/GFHFB3=-611.9472538\HF/GFHFB4
=-611.9878502\G4MP2=-614.7962542\FreqCoord=6.5408610532,7.2001759484,2
.6351931625,8.9352853876,6.4426782213,3.6000711639,10.7456703657,8.300
3349499,4.3336361278,9.5301925442,3.8240853119,3.8357638155,4.73047795
13,5.3425190319,1.9016290298,5.9459523191,9.8187695404,2.3995003027,10
.0907254777,10.9187187802,4.073718417,13.0886051051,7.5070427584,5.277
6792321,7.6693770709,2.0015849056,3.0819088757,11.8991761022,3.1267166
967,4.7904767694,5.3854211584,2.7241357593,2.1615459274,2.3875409736,6
.1358097164,0.9575857619,7.806769608,11.641269358,3.1533559112,3.57696
93865,10.5161357414,1.4447884163,13.6529466882,4.9502006239,5.50114138
22,1.8231987585,8.6926497308,0.7341238937,11.4757013315,12.325471236,4
.6348841906,14.4677185715,8.9197837738,5.8364895953,8.1316875062,0.010
4270467,3.2651412933,12.3535526261,1.1339320032,4.9705055193,4.0004456
105,1.3173837845,1.6003800847,1.0084307456,4.7230653819,0.3987766483,7
.3444589385,13.6324275947,2.9701231404,3.122588979,12.5089195372,1.264
7584335,15.4779553368,4.3728439331,6.2365629457,-0.0018095212,9.270008
9918,-0.0012968517\PG=C01 [X(C16H10)]\NImag=0\

4, 5-dihydropyrene

1\1\GINC-N067\Mixed\G4MP2\G4MP2\C16H12\KFOREST\14-May-2011\0\#\ G4MP2\
\name\0,1\C,0,0.6228875789,0.3775826881,-0.0137926404\C,0,-0.62828512
32,-0.346931617,0.0132732397\C,0,-1.8646203054,0.3388894902,-0.0745877
941\C,0,-0.6154951487,-1.7651570762,0.0875770722\C,0,1.8465881106,-0.3
394799856,-0.0874621893\C,0,0.6434415404,1.791287885,0.0734428113\C,0,
-1.8454786735,1.8270259014,-0.3401264913\C,0,-3.0453476706,-0.37770658
76,-0.0068828803\C,0,0.6430664584,-2.4505891828,0.0576792723\C,0,-1.84
06764546,-2.4612541414,0.1549333606\C,0,1.8146033404,-1.7722160402,-0.
0569332159\C,0,3.0601870809,0.3766186788,-0.1548274483\C,0,-0.65683725
78,2.5155380689,0.3383268823\C,0,1.8526917003,2.4586267673,0.005749333
2\C,0,-3.0366705417,-1.7765893775,0.1239684817\C,0,3.0616782219,1.7547
33951,-0.1244779753\H,0,-2.7878593024,2.2842220468,-0.0221263507\H,0,-
1.7743352776,1.984158924,-1.426723095\H,0,-3.9931718737,0.1492223972,-
0.069505355\H,0,0.6378648362,-3.5356158671,0.1044563959\H,0,-1.8266973
624,-3.5447431588,0.2244450629\H,0,2.7582643234,-2.3078082951,-0.10322
80233\H,0,3.9929720422,-0.1748554547,-0.223853363\H,0,-0.5842090961,3.
5603124768,0.0198847943\H,0,-0.8288128604,2.532528371,1.4248719904\H,0
,1.867453042,3.543000646,0.0678916408\H,0,-3.9762174141,-2.3164453238,
0.1808035894\H,0,3.9975860867,2.3008738155,-0.1813171053\Version=EM64
L-G09RevB.01\State=1-A\MP2/GTBas1=-614.9577725\CCSD(T)/GTBas1=-615.125
3644\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-613.1007165\MP2/GTMP
2LargeXP=-615.6194957\HF/GFHFB3=-613.1076051\HF/GFHFB4=-613.1494281\G4
MP2=-615.9798822\FreqCoord=1.1770869356,0.7135278731,-0.0260643129,-1.
1872868162,-0.655605743,0.0250827879,-3.523621719,0.6404083258,-0.1409
505037,-1.1631172671,-3.3356634555,0.165496682,3.4895458092,-0.6415242
003,-0.1652795847,1.2159282938,3.3850435279,0.1387867999,-3.4874492769
,3.4525785913,-0.6427459191,-5.7548730768,-0.7137620091,-0.0130067588,
1.2152194916,-4.6309424198,0.1089980283,-3.4783743984,-4.6510962707,0.
2927816205,3.4291033532,-3.3490029644,-0.1075881859,5.7829154982,0.711
7061594,-0.2925814751,-1.2412425312,4.753678027,0.639345151,3.50107992
22,4.6461312533,0.0108646652,-5.7384756797,-3.3572673741,0.2342664794,
5.7857333464,3.3159666034,-0.2352292828,-5.2682905785,4.3165540951,-0.
0418127431,-3.3530077425,3.7495169704,-2.696115917,-7.5460012429,0.281
9894635,-0.1313460857,1.2053898501,-6.6813457,0.1973939811,-3.45195774
27,-6.6985937815,0.4241397007,5.2123641733,-4.361125645,-0.1950726933,
7.5456236159,-0.3304289223,-0.42302155,-1.103995196,6.7280155287,0.037
5768154,-1.5662293216,4.785785045,2.6926178362,3.5289748155,6.69530090
95,0.1282966078,-7.5139619574,-4.3774472638,0.3416692677,7.5543428965,
4.3480213776,-0.3426396722\PG=C01 [X(C16H12)]\NImag=0\

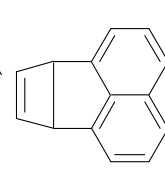
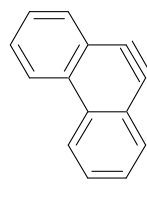
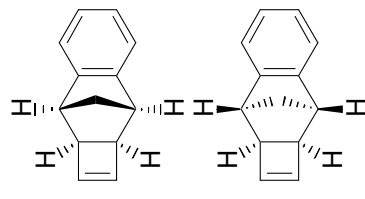
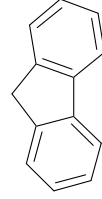
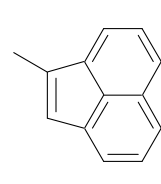
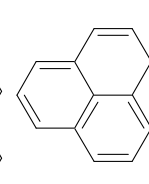
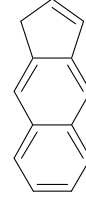
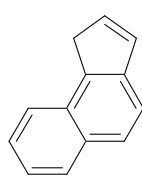
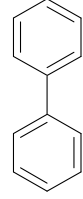
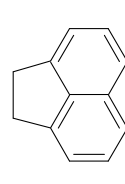
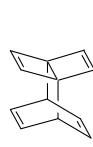
4-methylpyrene

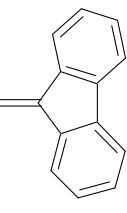
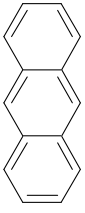
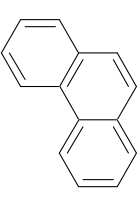
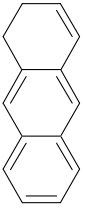
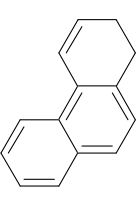
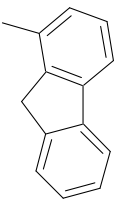
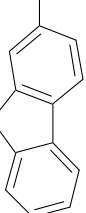
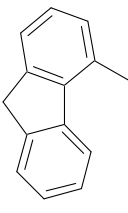
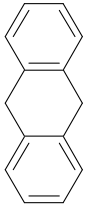
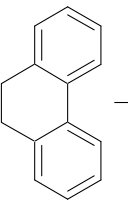
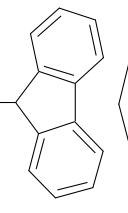
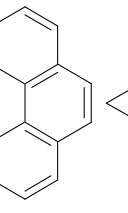
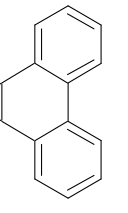
1\1\GINC-N065\Mixed\G4MP2\G4MP2\C17H12\KFOREST\16-May-2011\0\#\ G4MP2\
\name\0,1\C,0,1.6356538826,-1.6772576957,-0.012795433\C,0,2.918587647
4,-2.4682506835,-0.0142834661\C,0,1.6757395544,-0.2288718145,0.0146713
409\C,0,0.4308075703,-2.3114180944,-0.0373165318\C,0,0.4473908804,0.50
04189504,0.0155147663\C,0,2.8783694801,0.4913391894,0.0406931285\C,0,-
0.8186422048,-1.6097582919,-0.0373521458\C,0,-0.7992030916,-0.18675788
52,-0.0104403897\C,0,0.4637786679,1.9269223317,0.0424458329\C,0,2.8849
645616,1.8830466895,0.0669088891\C,0,-2.0521559749,-2.2732745684,-0.06
2744105\C,0,-2.0254506703,0.5398680464,-0.0096649112\C,0,-0.7860845074
,2.6321824436,0.0425744272\C,0,1.6941227738,2.5963239035,0.0678828284\
C,0,-3.2450639761,-1.5575089459,-0.0617838273\C,0,-1.9725840634,1.9728
882813,0.0177625556\C,0,-3.2351110608,-0.1674111905,-0.035601633\H,0,3
.5407600124,-2.2283435269,-0.8845719787\H,0,2.711884931,-3.5408292167,
-0.0354849919\H,0,3.5232662047,-2.2598008954,0.8762145687\H,0,0.398623
0465,-3.3977456712,-0.0580194322\H,0,3.8222221656,-0.0404800968,0.0405
492109\H,0,3.8314782386,2.4134475524,0.0867812824\H,0,-2.0674813843,-3
.3587828169,-0.0832779622\H,0,-0.7602348243,3.7176891613,0.0631862237\
H,0,1.704841682,3.6818271176,0.0884273898\H,0,-4.1910421842,-2.0888062
06,-0.0816381329\H,0,-2.9090055248,2.5228473942,0.0182091593\H,0,-4.16
96218323,0.3853365387,-0.0350466627\Version=EM64L-G09RevB.01\State=1-
A\MP2\GTBas1=-652.9586541\CCSD(T)/GTBas1=-653.1320661\MP2\GTBas2=0.\MP
2\GTBas3=0.\HF/GTMP2LargeXP=-650.987206\MP2/GTMP2LargeXP=-653.6570479\
HF/GFHF3=-650.9951478\HF/GFHF4=-651.0391477\G4MP2=-654.0412766\FreqC
oord=3.0909378863,-3.1695576992,-0.0241798642,5.5153313484,-4.66431781
91,-0.0269918391,3.1666888279,-0.432505049,0.0277248162,0.8141083238,-
4.367947177,-0.0705180253,0.8454462383,0.9456547679,0.0293186593,5.439
3300266,0.9284965063,0.0768988683,-1.5470095679,-3.0420023118,-0.07058
53261,-1.5102749676,-0.3529212561,-0.0197294772,0.8764146687,3.6413554
863,0.0802109997,5.4517929245,3.5584425386,0.1264394762,-3.8780127745,
-4.2958663591,-0.118569175,-3.8275470626,1.0202027556,-0.0182640352,-1
.4854844362,4.9741039502,0.0804540076,3.2014280779,4.90634113,0.128279
9549,-6.1322821986,-2.9432653573,-0.116754513,-3.7276436539,3.72821854
23,0.0335663655,-6.1134739144,-0.3163613015,-0.0672773363,6.6910667257
, -4.2109589959,-1.6715987845,5.1247198234,-6.6911975028,-0.0670569166,
6.6580082202,-4.2704048072,1.6558055684,0.7532883881,-6.4208087878,-0.
1096408373,7.2229531119,-0.0764962968,0.0766269034,7.2404445551,4.5607
549101,0.1639928572,-3.9069736013,-6.3471796637,-0.1573725414,-1.43663
56146,7.0254143621,0.1194046582,3.221683879,6.9576449208,0.1671035494,
-7.9199219396,-3.9472716741,-0.1542737131,-5.497223761,4.7674906501,0.
0344103242,-7.8794433408,0.7281805271,-0.0662285944\PG=C01 [X(C17H12)]
\Nimag=0\

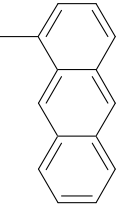
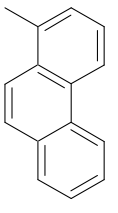
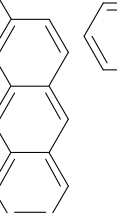
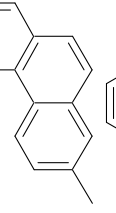
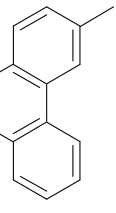
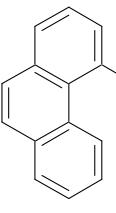
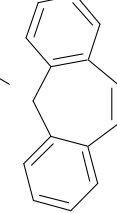
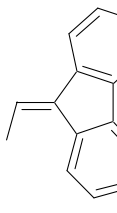
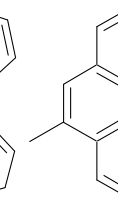
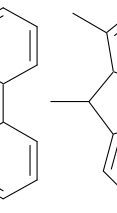
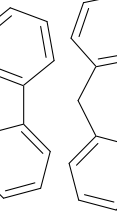
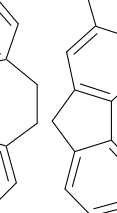
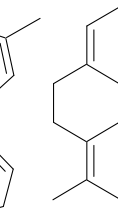
Table S1. Estimated gas phase (298.15 K, 1 atm) enthalpies of formation ($\Delta_f H_{(g),298K}$) for various polycyclic aromatic hydrocarbons (PAHs) and other C_{10} through C_{20} unsaturated hydrocarbons using the MNDO, MNDO-d, AM1, PM3, RM1, and PM6 semiempirical methods as implemented in MOPAC 2009 with the restricted (RHF) and unrestricted (UHF) Hartree-Fock Hamiltonians. Values are in kJ/mol. G4MP2 $\Delta_f H_{(g),298K}$ estimates are also shown for comparison.

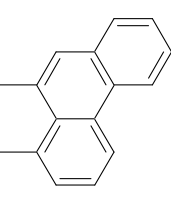
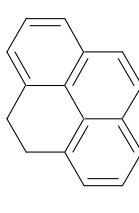
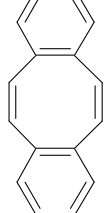
name	structure	CAS-RN	formula	MW (g/mol)	G4MP2 $\Delta_f H_{(g),298K}$ (kJ/mol)	MNDO		MNDO-d		AM1		PM3		RM1		PM6	
						RHF	UHF	RHF	UHF	RHF	UHF	RHF	UHF	RHF	UHF	RHF	UHF
1,4-diethynylbenzene		935-14-8	$C_{10}H_6$	126.15	546.9	528.5	515.2	529.0	515.7	547.7	547.7	526.1	526.1	489.6	489.6	555.4	555.3
[4.2.2]propella-2,4,7,9-tetraene		88090-34-0	$C_{10}H_8$	128.17	555.0	521.4	507.9	521.9	508.4	659.7	657.7	573.6	572.9	522.2	522.2	506.3	506.3
1-methylene-1H-indene		2471-84-3	$C_{10}H_8$	128.17	227.3	251.9	230.0	252.4	230.5	295.8	292.0	268.3	266.7	250.9	250.8	256.5	256.5
azulene		275-51-4	$C_{10}H_8$	128.17	284.2	301.2	236.4	301.7	236.9	352.6	314.7	339.8	308.1	334.3	312.0	318.8	301.8
naphthalene		91-20-3	$C_{10}H_8$	128.17	137.1	159.8	159.8	160.3	160.3	169.3	169.3	169.7	169.7	158.5	158.5	167.7	167.7
1,4-dihydro-1,4-methanonaphthalene		4453-90-1	$C_{11}H_{10}$	142.20	236.4	283.1	272.3	283.8	272.9	312.7	312.6	274.6	274.6	235.2	235.2	264.2	264.2
1-methylnaphthalene		90-12-0	$C_{11}H_{10}$	142.20	103.8	138.7	106.0	139.3	106.6	141.5	132.9	135.8	130.2	123.2	120.9	130.5	129.5
2-methylnaphthalene		91-57-6	$C_{11}H_{10}$	142.20	102.9	127.7	95.3	128.3	95.9	137.3	128.9	130.4	125.0	117.0	117.0	125.8	125.5
bicyclo[4.4.1]undeca-1,3,5,7,9-pentaene		2443-46-1	$C_{11}H_{10}$	142.20	301.4	334.0	267.4	334.6	268.0	338.6	304.5	350.5	324.6	310.1	302.5	300.2	297.1
acenaphthylene		208-96-8	$C_{12}H_8$	152.19	245.9	280.3	251.3	280.9	251.9	337.2	331.8	305.3	302.2	282.0	281.1	294.4	294.1
biphenylene		259-79-0	$C_{12}H_8$	152.19	403.1	395.8	351.4	396.4	352.0	503.0	489.3	458.9	449.8	437.4	437.4	411.4	411.4
1,4-dihydro-1,4-ethenonaphthalene		7322-47-6	$C_{12}H_{10}$	154.2078	288.3	309.2	297.5	309.9	298.2	314.8	314.8	294.7	294.7	246.2	246.2	277.9	277.9
1,8-dihydro-as-indacene		18837-46-2	$C_{12}H_{10}$	154.21	327.0	322.2	272.3	322.8	272.9	399.4	373.1	343.7	326.0	323.8	314.6	325.1	320.7

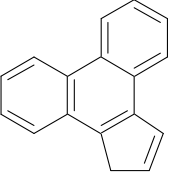
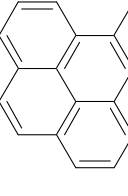
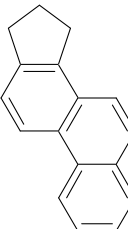
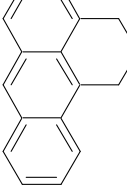
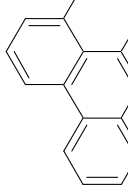
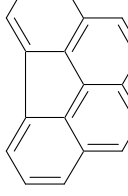
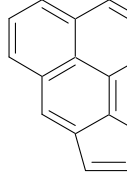
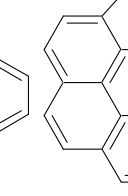
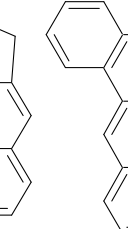
2,5-etheno[4.2.2]propella-3,7,9-triene	88090-38-4	C ₁₂ H ₁₀	154.21	607.9	653.6 650.4 654.3 651.0 759.5 759.5 660.0 660.0 560.2 560.2 581.5 581.5
acenaphthene	83-32-9	C ₁₂ H ₁₀	154.21	143.3	138.0 107.1 138.6 107.8 177.6 169.8 161.9 156.8 144.5 142.7 154.5 154.5
biphenyl	92-52-4	C ₁₂ H ₁₀	154.21	165.7	192.1 172.9 192.7 173.5 198.6 196.3 200.5 200.0 187.6 187.6 196.7 196.7
1H-benz[e]indene	232-54-2	C ₁₃ H ₁₀	166.22	209.8	236.7 190.0 237.4 190.7 272.8 256.9 244.0 234.0 225.6 220.5 237.9 234.5
1H-benz[f]indene	268-40-6	C ₁₃ H ₁₀	166.22	209.6	227.8 185.6 228.5 186.3 265.0 252.2 239.3 230.4 220.9 217.0 231.1 229.1
1H-phenalene	203-80-5	C ₁₃ H ₁₀	166.22	192.2	193.2 147.1 193.9 147.7 214.5 197.8 210.0 197.6 188.0 181.7 196.6 193.5
1-methylacenaphthylene	19345-99-4	C ₁₃ H ₁₀	166.22	207.2	238.7 n/c ^a 239.4 n/c 302.2 n/c 263.7 n/c 241.3 n/c 249.1 n/c
fluorene	86-73-7	C ₁₃ H ₁₀	166.22	172.2	187.4 157.9 188.1 158.6 226.8 222.3 204.4 204.4 190.2 190.2 199.8 199.8
2a,3,8,8a-tetrahydro-(2α,3α,8α,8α)-3,8-methanocyclobuta[b]naphthalene	54443-68-4	C ₁₃ H ₁₂	168.23	313.6	364.3 354.2 365.0 355.0 434.2 434.2 371.2 371.2 310.9 310.9 335.1 335.1
2a,3,8,8a-tetrahydro-(2α,3β,8β,8α)-3,8-methanocyclobuta[b]naphthalene	54483-73-7	C ₁₃ H ₁₂	168.23	302.1	361.0 351.2 361.7 351.9 424.1 423.8 360.4 360.4 304.0 304.0 327.8 327.8
9,10-dehydrophenanthrene	n/a	C ₁₄ H ₈	176.21	550.9	690.5 585.6 691.2 586.2 716.5 646.0 657.0 607.1 653.6 628.4 631.3 611.9
6b,8a-dihydrocyclobut[a]acenaphthylene	30736-79-9	C ₁₄ H ₁₀	178.23	361.1	357.1 326.3 357.8 327.0 454.5 446.9 394.3 389.6 356.4 354.8 361.7 361.2



9-methylene-9H-fluorene		4425-82-5	C ₁₄ H ₁₀	178.23	248.1	283.1 254.0 283.9 254.8 330.9 326.6 301.2 299.4 278.1 277.8 288.7 288.6
anthracene		120-12-7	C ₁₄ H ₁₀	178.23	210.8	245.5 176.9 246.2 177.7 262.5 231.4 257.3 232.3 236.2 219.1 248.9 239.7
phenanthrene		85-01-8	C ₁₄ H ₁₀	178.23	187.8	232.2 184.1 232.9 184.9 239.6 226.4 229.5 229.5 212.6 208.6 227.1 224.5
1,2-dihydroanthracene		58746-82-0	C ₁₄ H ₁₂	180.24	172.9	175.8 251.9 176.6 132.3 191.1 176.8 192.3 182.3 170.2 165.8 180.3 177.8
1,2-dihydrophenanthrene		56179-83-0	C ₁₄ H ₁₂	180.24	180.5	190.7 145.0 191.5 145.7 201.3 185.8 197.7 187.1 182.8 177.9 190.4 187.1
1-methyl-9H-fluorene		1730-37-6	C ₁₄ H ₁₂	180.24	136.1	159.0 128.5 159.8 129.2 196.5 191.6 166.4 166.4 151.4 151.4 161.1 161.0
2-methyl-9H-fluorene		1430-97-3	C ₁₄ H ₁₂	180.24	140.3	155.4 124.7 156.2 125.5 194.9 189.8 165.3 162.8 151.0 150.4 157.6 157.5
4-methyl-9H-fluorene		1556-99-6	C ₁₄ H ₁₂	180.24	139.6	167.5 136.7 168.2 137.4 198.4 193.4 166.7 164.3 157.5 157.0 161.0 161.0
9,10-dihydroanthracene		613-31-0	C ₁₄ H ₁₂	180.24	146.6	153.6 133.3 154.3 134.1 160.6 160.6 159.8 159.8 144.1 144.1 151.8 151.8
9,10-dihydrophenanthrene		776-35-2	C ₁₄ H ₁₂	180.24	136.6	159.5 129.4 160.3 130.2 160.7 156.1 158.9 156.6 141.3 141.1 153.6 153.6
9-methyl-9H-fluorene		2523-37-7	C ₁₄ H ₁₂	180.24	142.0	176.5 146.9 177.3 147.6 210.7 206.2 184.5 182.5 165.3 165.4 178.5 178.5
4H-cyclopenta[def]phenanthrene		203-64-5	C ₁₅ H ₁₀	190.24	228.1	258.7 210.7 259.5 211.5 319.4 305.8 285.4 285.4 256.1 252.0 271.3 271.3
1a,9b-dihydro-1H-cyclopropa[1]phenanthrene		949-41-7	C ₁₅ H ₁₂	192.26	252.3	278.8 248.1 279.7 248.9 311.0 306.1 287.1 286.9 268.6 268.6 256.1 256.1

1-methylanthracene		610-48-0	C ₁₅ H ₁₂	192.26	176.2	224.8	155.0	225.6	155.7	234.7	202.6	223.4	197.6	200.9	183.3	211.6	198.5
1-methylphenanthrene		832-69-9	C ₁₅ H ₁₂	192.26	156.4	213.3	163.7	214.1	164.5	212.8	198.6	196.4	187.0	178.1	173.5	190.7	188.0
2-methylanthracene		613-12-7	C ₁₅ H ₁₂	192.26	175.3	213.6	143.8	214.4	144.6	230.8	198.6	218.3	192.4	197.2	179.5	207.1	194.0
2-methylphenanthrene		2531-84-2	C ₁₅ H ₁₂	192.26	153.7	199.7	150.6	200.5	151.4	207.6	193.6	190.3	181.2	173.3	168.9	185.1	182.5
3-methylphenanthrene		832-71-3	C ₁₅ H ₁₂	192.26	153.9	200.5	151.5	201.4	152.3	207.7	193.7	190.1	181.0	173.2	168.8	185.2	182.6
4-methylphenanthrene		832-64-4	C ₁₅ H ₁₂	192.26	179.4	237.6	183.5	238.4	184.3	235.1	219.4	218.6	208.2	199.4	193.8	208.8	205.6
5H-dibenzo[a,d]cycloheptene		256-81-5	C ₁₅ H ₁₂	192.26	220.6	246.9	211.6	247.8	212.4	252.7	247.4	253.8	253.2	227.9	227.9	233.5	233.5
9-ethylidenefluorene		7151-64-6	C ₁₅ H ₁₂	192.26	221.6	253.3	224.0	254.1	224.7	294.1	289.9	260.2	258.4	249.4	249.1	251.8	251.8
9-methylphenanthrene		883-20-5	C ₁₅ H ₁₂	192.26	154.5	213.6	164.2	214.5	165.0	212.7	198.5	196.3	188.9	177.9	173.4	190.5	187.9
1,9-dimethyl-9H-fluorene		17057-98-6	C ₁₅ H ₁₄	194.27	108.4	155.1	124.1	155.9	124.9	181.9	176.9	144.8	142.4	129.3	128.8	141.0	141.0
10,11-dihydro-5H-dibenzo(a,d)cycloheptene		833-48-7	C ₁₅ H ₁₄	194.27	141.5	168.9	149.3	169.8	150.1	155.3	154.4	160.4	160.4	147.5	150.6	147.9	147.8
2,3-dimethyl-9H-fluorene		4612-63-9	C ₁₅ H ₁₄	194.27	107.1	137.1	105.3	137.9	106.0	168.7	163.1	132.9	130.0	117.5	116.8	125.4	125.2
9,10-dihydro-1-methylphenanthrene		95676-48-5	C ₁₅ H ₁₄	194.27	106.3	154.6	122.0	155.4	122.8	147.6	141.6	137.7	134.5	125.3	124.6	131.1	131.1

9,9-dimethyl-9H-fluorene	4569-45-3		C ₁₅ H ₁₄	194.27	105.3	181.3 151.5 182.1 152.3 202.1 197.7 162.7 160.8 132.7 132.7 151.6 151.6
aceanthrylene	202-03-9		C ₁₆ H ₁₀	202.25	316.3	366.8 298.8 367.6 299.6 430.9 401.1 392.2 368.4 359.3 342.9 376.2 363.0
fluoranthene	206-44-0		C ₁₆ H ₁₀	202.25	262.6	303.6 264.3 304.5 265.1 367.1 359.9 334.0 333.9 305.3 304.0 320.9 320.4
pyrene	129-00-0		C ₁₆ H ₁₀	202.25	203.4	253.1 179.6 253.9 180.5 281.0 250.5 267.6 243.8 235.1 219.3 257.2 245.0
1,4-dihydro-1,4-ethenoanthracene	27765-96-4		C ₁₆ H ₁₂	204.27	340.9	376.8 344.3 377.7 345.1 388.3 380.9 363.3 358.8 304.9 303.3 340.1 339.6
4,5-dihydroacephenanthrylene	6232-48-0		C ₁₆ H ₁₂	204.27	189.6	203.4 156.3 204.3 157.1 242.0 229.1 219.2 210.6 194.8 190.9 209.7 207.9
4,5-dihydropyrene	6628-98-4		C ₁₆ H ₁₂	204.27	157.4	178.6 128.3 179.4 129.2 200.2 185.2 193.1 183.0 161.9 156.9 180.5 177.4
dibenzo[a,e]cyclooctene	262-89-5		C ₁₆ H ₁₂	204.27	342.5	331.8 299.2 332.6 300.0 361.1 358.0 358.1 357.9 322.5 322.5 323.3 323.3
1,2-benzofluorene	238-84-6		C ₁₇ H ₁₂	216.28	228.3	265.8 209.1 266.7 210.0 309.5 292.1 280.1 268.9 255.6 249.6 271.4 267.2
17H-cyclopenta[a]phenanthrene	219-08-9		C ₁₇ H ₁₂	216.28	261.5	309.8 245.8 310.5 246.7 342.8 321.1 303.6 289.0 280.2 272.4 297.1 291.6
1H-cyclopent[b]anthracene	259-06-3		C ₁₇ H ₁₂	216.28	282.0	311.8 233.7 312.7 234.5 356.6 320.7 325.9 296.3 297.3 278.0 310.7 296.5

1H-cyclopenta[1]phenanthrene		235-92-7	C ₁₇ H ₁₂	216.28	261.3	317.0	251.1	318.0	252.0	347.6	323.6	306.3	290.6	282.0	273.1	300.7	294.1
2,3-benzofluorene		243-17-4	C ₁₇ H ₁₂	216.28	230.0	255.7	204.0	256.6	204.9	300.4	286.9	273.3	264.3	249.0	245.1	262.9	260.7
4-methylpyrene		3353-12-6	C ₁₇ H ₁₂	216.28	168.8	238.3	162.6	239.2	163.4	259.6	227.1	232.2	207.0	202.5	185.7	221.7	209.0
1,2-cyclopentenophenanthrene		482-66-6	C ₁₇ H ₁₄	218.29	161.9	177.5	126.7	178.4	127.6	199.4	184.1	181.3	171.3	161.3	156.2	180.9	177.2
4,5,6-trihydrobenz[de]anthracene		n/a	C ₁₇ H ₁₄	218.29	168.1	198.0	126.1	198.9	127.0	205.1	171.1	201.0	173.5	172.4	153.6	187.7	174.3
5,6-dihydro-4H-benz[de]anthracene		4389-09-7	C ₁₇ H ₁₄	218.29	141.9	171.2	120.5	172.1	121.4	176.4	161.2	170.1	160.0	143.3	138.3	160.7	158.1
benzo[ghi]fluoranthene		203-12-3	C ₁₈ H ₁₀	226.27	335.5	398.8	n/c	399.7	n/c	486.8	n/c	438.5	429.9	394.1	n/c	414.7	412.9
cyclopenta[cd]pyrene		27208-37-3	C ₁₈ H ₁₀	226.27	316.2	380.9	310.3	381.9	311.2	456.9	429.2	410.4	389.2	365.5	351.5	391.2	380.2
3,4-dihydrocyclopenta(cd)pyrene		25732-74-5	C ₁₈ H ₁₂	228.29	213.3	236.9	163.4	237.9	164.3	295.4	264.4	265.1	240.7	226.0	210.1	249.6	238.2
benz[a]anthracene		56-55-3	C ₁₈ H ₁₂	228.29	254.7	312.3	232.6	313.2	233.5	326.5	294.8	310.6	286.5	284.0	268.6	302.4	290.8
1,2,3,4-tetrahydrochrysene		2091-90-9	C ₁₈ H ₁₆	232.32	128.3	165.8	114.9	166.8	115.9	155.1	140.2	153.1	143.3	131.2	126.4	150.3	147.0

17-methyl-16,17-dihydro-15h-cyclopenta(a)phenanthrene

	n/a	C ₁₈ H ₁₆	232.32	129.9	167.7	117.0	168.6	117.9	180.4	165.5	159.3	m/c	135.9	130.9	157.1	153.6
---	-----	---------------------------------	--------	-------	-------	-------	-------	-------	-------	-------	-------	-----	-------	-------	-------	-------

10-methylbenz[a]anthracene

	2381-15-9	C ₁₉ H ₁₄	242.31	219.8	280.1	199.4	281.1	200.4	294.2	261.8	271.1	246.4	244.2	228.7	260.2	248.6
---	-----------	---------------------------------	--------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

11-methylbenz[a]anthracene

	6111-78-0	C ₁₉ H ₁₄	242.31	220.4	292.2	211.1	293.2	212.1	298.8	266.2	276.7	251.7	248.8	232.8	265.1	253.3
---	-----------	---------------------------------	--------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

2-methylbenz[a]anthracene

	2498-76-2	C ₁₉ H ₁₄	242.31	220.8	280.8	199.9	281.8	200.9	294.8	262.2	271.7	246.8	245.0	229.1	260.7	248.9
---	-----------	---------------------------------	--------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

2-methylchrysene

	3351-32-4	C ₁₉ H ₁₄	242.31	209.6	279.8	209.4	280.8	210.4	285.8	262.4	256.2	240.2	233.1	224.3	250.1	244.0
---	-----------	---------------------------------	--------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

3-methyl-1,2-benzanthracene

	2319-96-2	C ₁₉ H ₁₄	242.31	220.9	294.1	212.7	295.1	213.6	299.6	266.7	277.5	258.0	249.5	233.3	265.8	254.0
--	-----------	---------------------------------	--------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

5-methylbenzo[c]phenanthrene

	652-04-0	C ₁₉ H ₁₄	242.31	232.8	312.5	236.3	313.5	237.3	311.6	290.5	289.0	270.8	262.1	250.7	276.8	269.3
---	----------	---------------------------------	--------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

6-methylbenz[a]anthracene

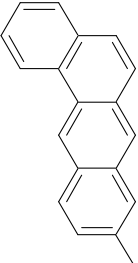
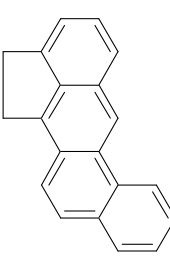
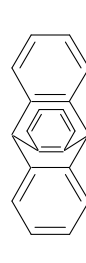
	316-14-3	C ₁₉ H ₁₄	242.31	220.1	294.3	213.2	295.3	214.2	299.6	267.1	277.5	252.7	249.5	233.6	266.0	254.4
---	----------	---------------------------------	--------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

6-methylbenzo[c]phenanthrene

	2381-34-2	C ₁₉ H ₁₄	242.31	234.2	313.3	236.3	314.3	237.3	312.3	291.4	290.5	272.1	262.6	251.1	277.9	270.3
---	-----------	---------------------------------	--------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

8-methylbenz[a]anthracene

	2381-31-9	C ₁₉ H ₁₄	242.31	220.4	291.1	210.1	292.2	211.1	298.5	265.8	276.7	251.7	248.7	232.6	265.0	253.2
---	-----------	---------------------------------	--------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

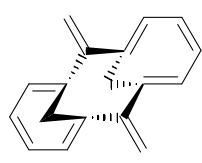
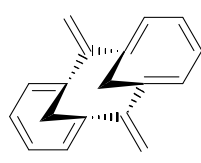
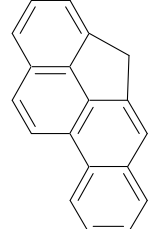
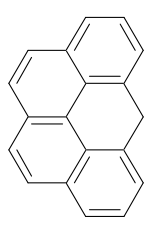
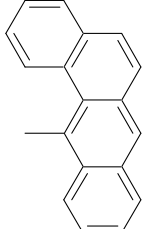
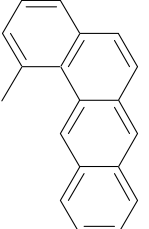
9-methylbenz[a]anthracene	2381-16-0	C ₁₉ H ₁₄	242.31	219.7	279.9	199.3	280.9	200.3	294.0	261.8	270.9	246.3	244.2	228.6	260.0	248.5
																
1,2-dihydrobenz[<i>h</i>]aceanthrylene	479-23-2	C ₂₀ H ₁₄	254.32	260.0	295.5	215.6	296.6	216.6	337.5	305.4	304.1	279.1	270.5	254.9	291.0	280.4
																
9,10-dihydro-9,10[1',2']-benzenoanthracene	477-75-8	C ₂₀ H ₁₄	254.32	294.6	364.2	332.9	365.3	334.0	383.4	383.3	354.9	296.9	296.9	334.9	334.9	334.9
																

^a UHF calculation converged on a structure having one or more cleaved bonds compared to RHF geometry.

Table S2. Estimated gas phase (298.15 K, 1 atm) enthalpies of formation ($\Delta_f H_{(g),298K}$) for various polycyclic aromatic hydrocarbons (PAHs) and other C_{11} through C_{42} unsaturated hydrocarbons using the MNDO, MNDO-d, AM1, PM3, RM1, and PM6 semiempirical methods as implemented in MOPAC 2009 with the restricted (RHF) and unrestricted (UHF) Hartree-Fock Hamiltonians. Values are in kJ/mol.

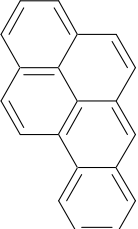
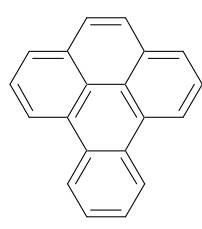
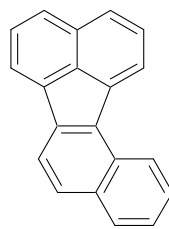
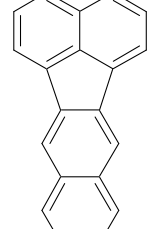
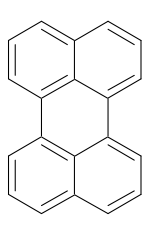
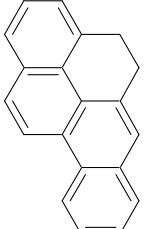
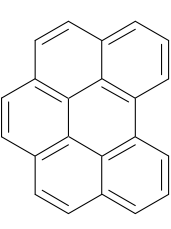
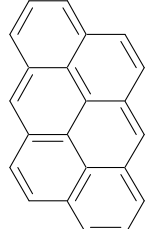
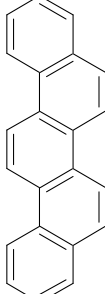
name	structure	CAS-RN	formula	MW (g/mol)	MNDO		MNDO-d		AM1		PM3		RM1		PM6	
					RHF	UHF	RHF	UHF	RHF	UHF	RHF	UHF	RHF	UHF	RHF	UHF
1-ethylidene-1H-indene		2471-83-2	$C_{11}H_{10}$	142.20	214.8	191.8	215.4	192.3	255.2	251.2	226.6	224.9	216.2	216.1	217.4	217.4
3,4-benzotropilidene		264-09-5	$C_{11}H_{10}$	142.20	197.5	174.0	198.1	174.6	211.4	208.3	220.3	220.3	198.3	198.3	198.4	198.4
3-methyl-9H-fluorene		2523-39-9	$C_{14}H_{12}$	180.24	155.7	125.1	156.5	125.9	195.3	190.3	165.6	163.2	151.3	150.8	159.2	159.1
9-methylanthracene		779-02-2	$C_{15}H_{12}$	192.26	245.0	173.0	245.8	173.8	245.7	212.5	226.4	199.7	209.7	191.4	219.4	205.6
[2.2]paracyclopentadiene		6572-60-7	$C_{16}H_{12}$	204.27	510.9	458.8	511.7	459.6	525.7	515.9	504.8	498.2	446.7	445.3	446.5	445.7
1-methylpyrene		2381-21-7	$C_{17}H_{12}$	216.28	236.4	161.2	237.4	162.1	257.6	225.8	230.8	205.9	201.3	184.7	221.0	208.3
2-methylfluoranthene		33543-31-6	$C_{17}H_{12}$	216.28	273.4	232.9	274.3	233.8	336.4	328.3	295.7	290.9	266.9	265.2	279.6	279.1
2-methylpyrene		3442-78-2	$C_{17}H_{12}$	216.28	221.7	147.2	222.6	148.1	249.5	218.2	228.8	204.3	196.1	179.8	215.2	203.2
7H-benzo[c]fluorene		205-12-9	$C_{17}H_{12}$	216.28	279.2	221.1	280.1	222.0	316.8	298.3	278.6	266.5	260.5	253.9	272.8	268.0

benz[a]anthracene		56-55-3	C ₁₈ H ₁₂	228.29	C ₁₈ H ₁₂	312.3 232.6 313.3 233.5 326.5 294.8 310.6 286.5 284.1 268.7 302.5 290.9
benzo[c]phenanthrene		195-19-7	C ₁₈ H ₁₂	228.29	C ₁₈ H ₁₂	332.6 258.1 333.5 259.0 338.9 314.2 323.6 306.7 294.7 284.2 312.0 304.8
chrysene		218-01-9	C ₁₈ H ₁₂	228.29	C ₁₈ H ₁₂	312.4 243.0 313.4 243.9 318.0 295.3 295.5 280.1 272.5 272.5 292.3 292.3
naphthacene		92-24-0	C ₁₈ H ₁₂	228.29	C ₁₈ H ₁₂	337.5 224.6 338.4 225.6 362.9 298.8 352.0 296.7 320.9 278.1 336.6 312.1
triphenylene		217-59-4	C ₁₈ H ₁₂	228.29	C ₁₈ H ₁₂	320.4 259.4 321.4 260.3 315.0 298.9 284.8 284.8 266.1 261.0 287.3 283.8
1,3-dimethylpyrene		64401-21-4	C ₁₈ H ₁₄	230.30	C ₁₈ H ₁₄	216.7 139.9 217.7 140.9 230.0 196.9 197.1 171.1 166.2 148.8 182.9 170.8
11-methylbenzo[a]fluorene		71265-25-3	C ₁₈ H ₁₄	230.30	C ₁₈ H ₁₄	261.8 204.5 262.7 205.5 296.1 278.6 259.4 248.2 234.7 228.6 251.1 246.9
2,7-dimethylpyrene		15679-24-0	C ₁₈ H ₁₄	230.30	C ₁₈ H ₁₄	190.3 114.9 191.3 115.8 218.1 186.0 190.0 164.9 157.1 140.4 173.8 161.6
5,12-dihydronaphthacene		959-02-4	C ₁₈ H ₁₄	230.30	C ₁₈ H ₁₄	225.9 181.7 226.9 182.7 237.8 227.8 229.9 223.7 203.9 201.5 217.1 215.9
9,10-dihydronaphthacene		n/a	C ₁₈ H ₁₄	230.30	C ₁₈ H ₁₄	261.4 179.6 262.4 180.5 284.0 245.1 279.6 248.1 247.6 226.6 260.7 245.0

dihydrochrysene		41593-31-1	C ₁₈ H ₁₄	230.30	C ₁₈ H ₁₄	246.3	190.7	247.3	191.6	246.4	230.2	234.0	223.3	209.9	204.8	226.6	223.2
anti-7,14-dihydro-7,14-dimethylene-1,6,8,13-bismethano[14]annulene		109281-33-6	C ₁₈ H ₁₆	232.32	C ₁₈ H ₁₆	529.6	488.7	530.6	489.6	515.5	493.4	517.0	505.6	437.7	437.7	422.3	422.3
syn-7,14-dihydro-7,14-dimethylene-1,6-8,13-bismethano[14]annulene		109216-46-8	C ₁₈ H ₁₆	232.32	C ₁₈ H ₁₆	517.5	472.3	518.5	473.2	535.2	525.5	524.5	521.1	455.0	455.0	429.5	457.0
4H-cyclopenta[def]chrysene		202-98-2	C ₁₉ H ₁₂	240.30	C ₁₉ H ₁₂	325.1	528.9	326.1	529.9	386.3	1710.7	346.2	331.0	308.9	301.0	328.5	323.4
6H-benzo[cd]pyrene		191-33-3	C ₁₉ H ₁₂	240.30	C ₁₉ H ₁₂	261.2	190.1	262.3	191.1	294.2	269.5	275.3	257.5	234.0	223.9	257.6	251.0
12-methylbenz[a]anthracene		2422-79-9	C ₁₉ H ₁₄	242.31	C ₁₉ H ₁₄	332.2	242.9	333.3	243.9	328.9	293.3	305.9	278.8	277.4	259.6	292.0	279.1
1-methylbenz[a]anthracene		2498-77-3	C ₁₉ H ₁₄	242.31	C ₁₉ H ₁₄	316.6	231.3	317.8	232.2	321.1	287.1	302.6	277.1	269.9	253.0	283.3	271.2
1-methylbenzo[c]phenanthrene		4076-39-5	C ₁₉ H ₁₄	242.31	C ₁₉ H ₁₄	333.3	251.5	334.3	252.4	334.7	306.5	316.9	296.0	274.0	261.4	338.5	330.3

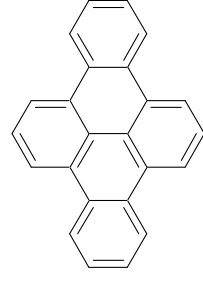
1-methylchrysene		3351-28-8	C ₁₉ H ₁₄	242.31	C ₁₉ H ₁₄	293.1	222.2	294.1	223.2	290.9	267.3	262.3	246.0	237.8	228.8	255.6	249.4
1-methyltriphenylene		2871-91-2	C ₁₉ H ₁₄	242.31	C ₁₉ H ₁₄	320.3	n/c ^a	321.3	252.9	309.8	291.2	280.4	268.4	252.9	246.4	270.4	266.2
2-methylbenzo[c]phenanthrene		2606-85-1	C ₁₉ H ₁₄	242.31	C ₁₉ H ₁₄	300.8	225.2	301.8	226.2	306.9	281.4	284.2	266.9	255.3	244.4	269.8	262.7
2-methyltriphenylene		1705-84-6	C ₁₉ H ₁₄	242.31	C ₁₉ H ₁₄	288.5	226.5	289.5	227.4	283.0	266.2	245.4	234.9	226.7	221.3	245.2	241.7
3-methylbenz[a]anthracene		2498-75-1	C ₁₉ H ₁₄	242.31	C ₁₉ H ₁₄	279.8	199.0	280.8	200.0	294.4	261.9	271.4	246.6	244.8	228.9	260.4	248.7
3-methylbenzo[c]phenanthrene		2381-19-3	C ₁₉ H ₁₄	242.31	C ₁₉ H ₁₄	299.8	224.4	300.8	225.4	306.6	281.2	284.0	266.6	255.1	244.3	269.6	262.5
3-methylchrysene		3351-31-3	C ₁₉ H ₁₄	242.31	C ₁₉ H ₁₄	280.9	210.5	281.9	211.5	286.0	262.6	256.1	240.1	233.0	224.3	250.3	244.2
4-methylbenz[a]anthracene		242.3145	C ₁₉ H ₁₄	242.31	C ₁₉ H ₁₄	293.7	212.2	294.7	213.2	299.7	266.9	277.7	258.2	249.8	233.6	266.2	254.3

4-methylbenzo[c]phenanthrene		4076-40-8	C ₁₉ H ₁₄	242.31	C ₁₉ H ₁₄	312.6 236.1 313.7 237.1 311.9 286.1 289.0 271.1 262.0 250.7 277.0 269.4
4-methylchrysene		3351-30-2	C ₁₉ H ₁₄	242.31	C ₁₉ H ₁₄	316.1 238.7 317.2 239.7 313.7 287.5 286.3 268.2 260.0 249.4 275.0 267.7
5-methylchrysene		3697-24-3	C ₁₉ H ₁₄	242.31	C ₁₉ H ₁₄	316.8 239.0 317.8 240.1 314.8 288.3 287.2 268.9 260.3 249.6 276.0 268.6
6-methylchrysene		1705-85-7	C ₁₉ H ₁₄	242.31	C ₁₉ H ₁₄	294.4 223.6 295.5 224.6 291.1 267.4 262.2 245.8 237.7 228.7 255.7 249.4
7-methylbenz[a]anthracene		2541-69-7	C ₁₉ H ₁₄	242.31	C ₁₉ H ₁₄	314.2 229.9 315.0 230.8 311.0 277.1 280.2 254.5 258.1 241.5 273.7 261.4
1,2-benzfluoranthene		203-33-8	C ₂₀ H ₁₂	252.31	C ₂₀ H ₁₂	401.1 322.1 402.2 323.2 465.0 432.4 418.9 393.3 386.2 368.6 404.1 390.3
benz[e]acephenanthrylene		205-99-2	C ₂₀ H ₁₂	252.31	C ₂₀ H ₁₂	368.7 313.1 369.8 314.2 431.0 418.6 390.7 383.1 354.9 351.7 375.7 373.7
benzo[a]acephenanthrylene		n/a	C ₂₀ H ₁₂	252.31	C ₂₀ H ₁₂	439.6 372.3 440.7 393.6 491.9 472.9 439.4 426.7 403.4 396.6 420.1 415.7

benzo[a]pyrene		50-32-8	C ₂₀ H ₁₂	252.31	C ₂₀ H ₁₂	337.7 237.4 338.8 238.5 365.2 318.8 340.7 312.5 301.6 275.6 328.3 307.4
benzo[e]pyrene		192-97-2	C ₂₀ H ₁₂	252.31	C ₂₀ H ₁₂	334.3 250.9 335.4 251.9 350.4 320.2 319.3 297.2 285.0 270.9 313.6 302.7
benzo[j]fluoranthene		205-82-3	C ₂₀ H ₁₂	252.31	C ₂₀ H ₁₂	392.5 708.5 393.6 709.6 455.4 437.2 409.1 395.8 376.2 369.3 395.8 731.6
benzo[k]fluoranthene		207-08-9	C ₂₀ H ₁₂	252.31	C ₂₀ H ₁₂	370.5 310.5 371.6 311.6 438.6 424.3 400.2 393.6 361.8 358.4 382.0 380.4
perylene		198-55-0	C ₂₀ H ₁₂	252.31	C ₂₀ H ₁₂	352.5 252.9 353.6 253.9 372.7 326.3 342.2 314.2 306.2 280.1 332.8 312.2
4,5-dihydrobenzo[a]pyrene		57652-66-1	C ₂₀ H ₁₄	254.32	C ₂₀ H ₁₄	257.3 185.7 258.4 186.8 276.9 252.4 259.0 241.8 221.2 211.7 244.7 238.1
benzo[ghi]perylene		191-24-2	C ₂₂ H ₁₂	276.33	C ₂₂ H ₁₂	344.2 241.9 345.3 243.1 381.0 338.7 347.9 315.4 297.9 275.9 335.0 316.9
dibenzo[def,mno]chrysene		191-26-4	C ₂₂ H ₁₂	276.33	C ₂₂ H ₁₂	365.9 233.5 367.1 234.6 414.9 342.3 387.4 325.3 332.2 284.6 365.9 326.3
1,2,7,8-dibenzphenanthrene		213-46-7	C ₂₂ H ₁₄	278.35	C ₂₂ H ₁₄	389.9 301.3 391.1 302.4 393.7 363.3 359.4 338.4 330.3 318.3 355.4 346.4

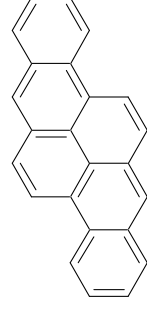
benzo[b]chrysene		214-17-5	C ₂₂ H ₁₄	278.35	C ₂₂ H ₁₄	395.4	291.6	396.6	292.7	407.7	363.7	379.4	345.6	346.6	324.2	370.3	352.6
dibenzo[c,g]phenanthrene		188-52-3	C ₂₂ H ₁₄	278.35	C ₂₂ H ₁₄	423.2	324.2	424.4	325.3	431.9	397.1	414.5	388.9	362.2	346.5	388.8	376.8
pentacene		135-48-8	C ₂₂ H ₁₄	278.35	C ₂₂ H ₁₄	433.0	272.2	434.2	273.4	466.9	365.5	450.3	360.4	409.4	336.0	428.0	365.5
coronene		191-07-1	C ₂₄ H ₁₂	300.35	C ₂₄ H ₁₂	346.2	233.1	347.5	234.4	401.5	354.5	364.9	328.8	299.8	275.3	346.9	325.9
dibenzo[de,qr]naphthacene		193-09-9	C ₂₄ H ₁₄	302.37	C ₂₄ H ₁₄	410.9	299.9	412.2	301.2	433.0	387.9	395.8	361.5	351.8	329.1	384.9	367.0
dibenzo(a,i)pyrene		189-55-9	C ₂₄ H ₁₄	302.37	C ₂₄ H ₁₄	417.5	295.0	418.8	296.2	444.2	386.3	408.9	362.3	363.3	330.6	394.8	368.3
naphtho[1,2,3,4-def]chrysene		192-65-4	C ₂₄ H ₁₄	302.37	C ₂₄ H ₁₄	418.9	311.0	420.2	311.8	433.2	389.8	389.9	357.2	349.3	327.4	383.0	365.4

dibenzo[fg,op]naphthacene



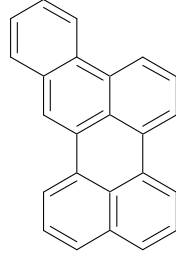
192-51-8 C₂₄H₁₄ 302.37 C₂₄H₁₄ 421.7 326.6 423.0 327.8 424.6 393.1 373.4 351.5 337.3 323.6 372.8 362.0

dibenzo[b,def]chrysene



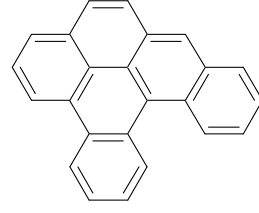
189-64-0 C₂₄H₁₄ 302.37 C₂₄H₁₄ 428.8 295.9 430.1 297.1 455.6 387.6 419.6 363.5 374.2 332.3 405.6 370.3

benzo[b]perylene



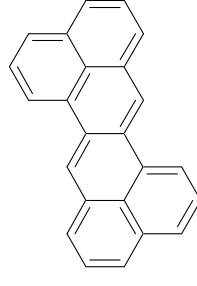
197-70-6 C₂₄H₁₄ 302.37 C₂₄H₁₄ 429.7 313.0 431.0 314.3 446.3 394.1 403.4 362.4 361.9 333.4 394.3 371.6

1,2:9,10-dibenzopyrene



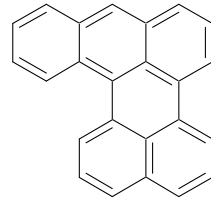
191-30-0 C₂₄H₁₄ 302.37 C₂₄H₁₄ 441.7 322.4 443.0 323.6 460.6 409.2 427.5 387.7 377.7 348.9 409.7 386.6

dibenzo[de,mn]naphthacene



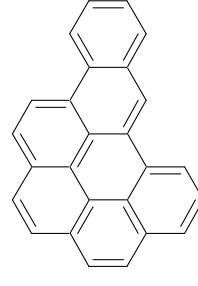
214-63-1 C₂₄H₁₄ 302.37 C₂₄H₁₄ 457.6 301.9 458.9 303.1 490.2 395.9 454.1 371.7 406.1 341.6 434.0 380.4

benzo[a]perylene



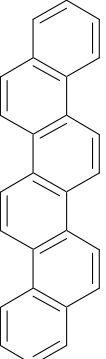
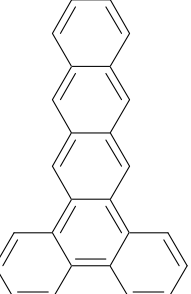
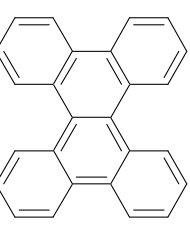
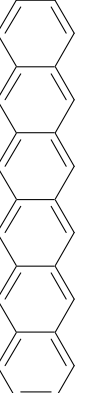
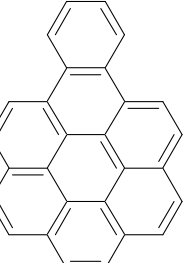
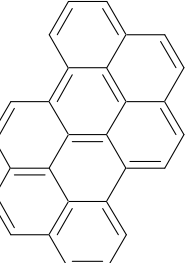
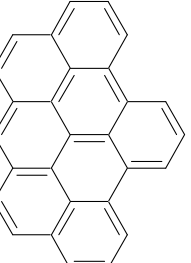
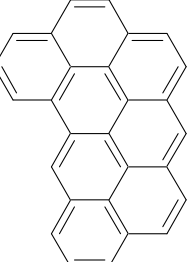
191-85-5 C₂₄H₁₄ 302.37 C₂₄H₁₄ 463.9 321.9 465.2 323.1 490.4 413.9 459.4 394.6 406.1 356.4 436.3 394.9

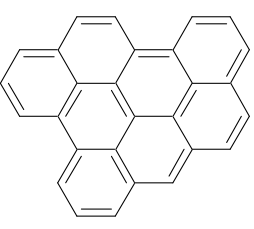
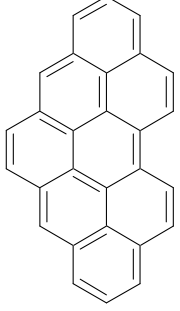
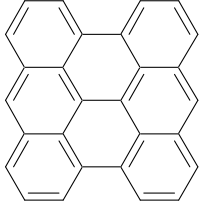
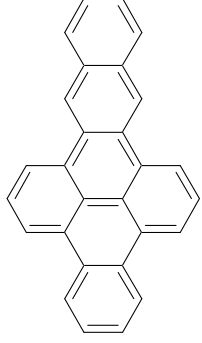
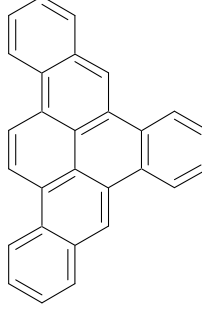
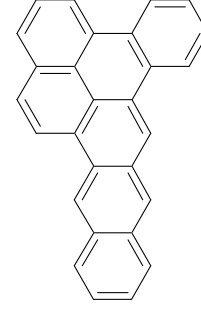
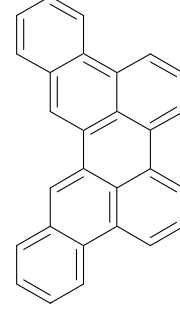
dibenzo[b,ghi]perylene

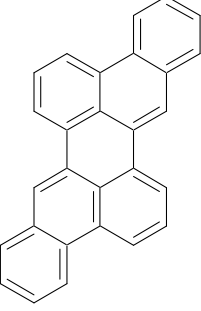
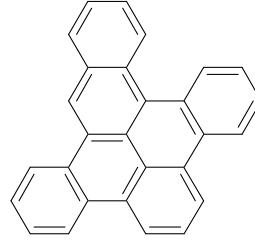
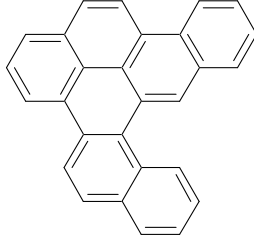
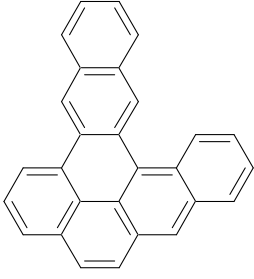
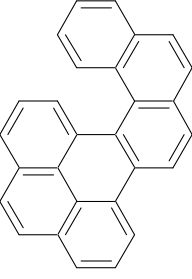
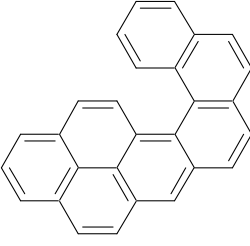


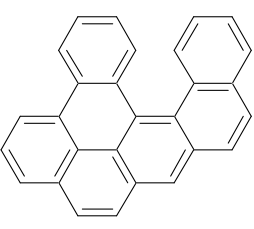
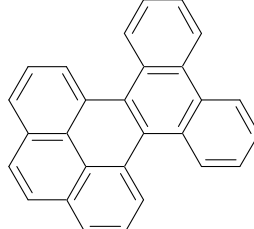
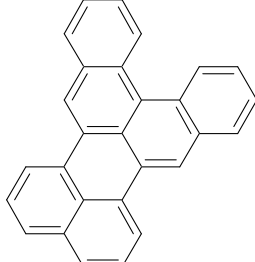
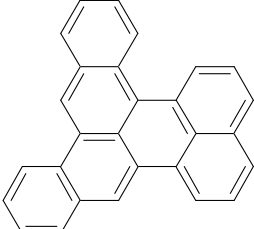
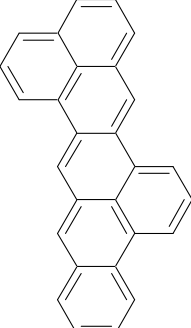
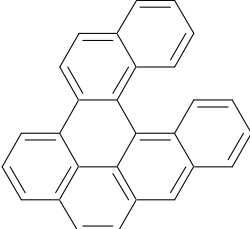
5869-30-7 C₂₆H₁₄ 326.39 C₂₆H₁₄ 425.7 301.5 427.1 302.8 460.6 407.4 415.6 374.5 359.4 331.3 403.4 378.4

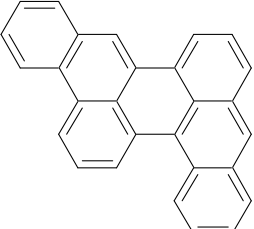
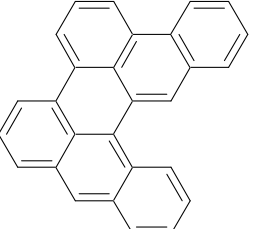
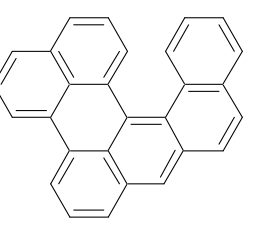
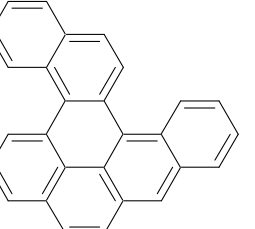
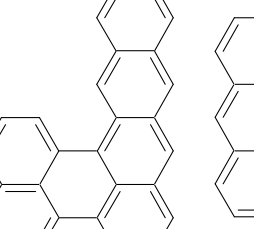
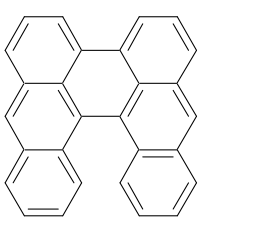
dibenzo[b,pqr]perylene		190-95-4	C ₂₆ H ₁₄	326.39	C ₂₆ H ₁₄	431.9	314.3	433.3	315.7	456.4	411.3	404.0	370.4	352.2	329.5	395.7	377.0
1,12-phenyleneperylene		190-84-1	C ₂₆ H ₁₄	326.39	C ₂₆ H ₁₄	439.3	315.8	440.7	317.2	465.5	412.8	413.2	372.6	360.5	332.3	403.4	379.9
benzo[f]naphtho[7,8,1,2,3-nopqr]tetrathene		n/a	C ₂₆ H ₁₄	326.39	C ₂₆ H ₁₄	445.0	305.5	446.4	307.0	481.3	412.7	435.7	379.2	379.0	336.9	419.7	384.6
naphtho[8,1,2-bcd]perylene		188-89-6	C ₂₆ H ₁₄	326.39	C ₂₆ H ₁₄	445.4	303.1	448.6	304.5	484.9	412.9	439.7	380.2	382.7	338.3	422.9	386.0
dibenzo[cd,lm]perylene		188-96-5	C ₂₆ H ₁₄	326.39	C ₂₆ H ₁₄	447.9	301.9	449.3	303.2	485.4	410.4	440.2	377.8	383.0	336.0	423.5	383.4
dibenzo[a,ghi]perylene		6596-37-8	C ₂₆ H ₁₄	326.39	C ₂₆ H ₁₄	457.3	316.6	458.7	318.0	495.2	428.7	458.1	404.9	393.9	353.9	433.9	400.6
anthra[2,1,9,8-opqra]naphthacene		92586-98-6	C ₂₆ H ₁₄	326.39	C ₂₆ H ₁₄	458.6	291.1	460.0	292.5	507.5	410.1	468.8	384.3	407.2	340.0	445.3	387.8

benzo(c)picene		217-37-8	C ₂₆ H ₁₆	328.40	C ₂₆ H ₁₆	468.2 359.3 469.6 360.6 470.2 431.2 424.0 396.8 388.8 372.8 419.3 406.9
dibenzo(a,c)naphthacene		216-00-2	C ₂₆ H ₁₆	328.40	C ₂₆ H ₁₆	486.3 356.4 487.7 357.7 494.4 435.0 452.4 405.0 414.5 380.1 443.3 415.4
dibenzo[g,p]chrysene		191-68-4	C ₂₆ H ₁₆	328.40	C ₂₆ H ₁₆	509.7 395.8 511.1 397.1 505.6 465.9 472.0 443.9 422.1 403.0 453.1 438.2
hexacene		258-31-1	C ₂₆ H ₁₆	328.40	C ₂₆ H ₁₆	530.5 319.8 531.9 321.1 573.1 432.3 550.8 423.9 500.2 393.7 521.3 429.4
benzo[a]coronene		190-70-5	C ₂₈ H ₁₄	350.41	C ₂₈ H ₁₄	435.6 305.5 437.2 306.9 480.1 426.6 425.3 384.7 357.9 330.2 410.9 387.0
benzo(pqr)naphtho(8,1,2-bcd)perylene		190-71-6	C ₂₈ H ₁₄	350.41	C ₂₈ H ₁₄	443.9 306.1 445.4 307.5 489.7 429.4 436.1 388.9 368.7 335.0 420.3 391.6
n/a		n/a	C ₂₈ H ₁₄	350.41	C ₂₈ H ₁₄	448.6 308.8 450.1 310.3 494.8 433.0 441.0 392.3 373.4 338.6 424.6 395.2
n/a		n/a	C ₂₈ H ₁₄	350.41	C ₂₈ H ₁₄	450.5 296.2 452.0 297.6 507.0 430.0 459.4 395.9 387.2 340.0 436.8 396.8

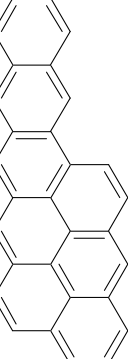
n/a		n/a	C ₂₈ H ₁₄	350.41	C ₂₈ H ₁₄	461.8 308.8 463.3 310.2 510.7 434.7 457.2 394.8 388.5 341.8 438.3 398.7
phenanthro[2,1,10,9,8,7-pqrstuv]pentaphene		4552-79-8	C ₂₈ H ₁₄	350.41	C ₂₈ H ₁₄	478.0 296.5 479.5 298.0 538.5 432.7 491.4 399.2 417.7 344.3 464.6 401.4
phenanthro(1,10,9,8-opqra)perylene		190-39-6	C ₂₈ H ₁₄	350.41	C ₂₈ H ₁₄	507.8 311.9 509.3 313.3 563.5 441.2 510.4 402.3 439.7 350.6 486.2 408.2
dibenzo(fg,st)pentacene		192-59-6	C ₂₈ H ₁₆	352.43	C ₂₈ H ₁₆	499.3 369.7 500.8 371.1 508.0 461.0 450.6 416.1 404.9 382.2 444.8 426.7
dibenzo[h,rst]pentaphene		192-47-2	C ₂₈ H ₁₆	352.43	C ₂₈ H ₁₆	499.9 370.2 501.5 371.6 512.1 458.7 456.9 416.3 410.0 382.7 449.0 426.9
benzo[a]naphtho[8,1,2-cde]naphthacene		192-70-1	C ₂₈ H ₁₆	352.43	C ₂₈ H ₁₆	503.5 359.4 505.0 360.8 524.6 457.4 475.4 421.6 425.1 386.2 462.6 430.5
dibenzo(fg,ij)pentaphene		197-69-3	C ₂₈ H ₁₆	352.43	C ₂₈ H ₁₆	506.6 368.4 502.1 369.8 519.8 461.9 464.6 419.8 417.5 386.6 455.6 430.9

dibenzo[fg,qr]pentacene		197-74-0	C ₂₈ H ₁₆	352.43	C ₂₈ H ₁₆	506.9	373.1	508.4	374.6	520.1	461.9	464.9	419.8	417.7	386.7	455.8	431.0
benzo[fg]naphtho[1,2,3-op]tetracene		n/a	C ₂₈ H ₁₆	352.43	C ₂₈ H ₁₆	517.4	390.1	518.9	391.5	528.6	479.3	479.1	442.5	426.1	400.5	465.7	445.2
benzo[a]naphtho[8,1,2-fgh]tetracene		n/a	C ₂₈ H ₁₆	352.43	C ₂₈ H ₁₆	518.0	377.8	519.5	379.3	536.0	475.6	491.9	445.9	434.9	402.1	472.8	446.1
n/a		n/a	C ₂₈ H ₁₆	352.43	C ₂₈ H ₁₆	518.4	370.4	519.9	371.8	543.8	476.0	505.4	451.8	445.1	406.0	481.7	450.1
naphtho[2,1,8-def]pentahelicene		n/a	C ₂₈ H ₁₆	352.43	C ₂₈ H ₁₆	522.6	384.4	524.1	385.8	544.7	489.4	508.4	466.5	436.8	408.5	478.0	454.8
naphtho[8,1,2-cde]pentahelicene		n/a	C ₂₈ H ₁₆	352.43	C ₂₈ H ₁₆	525.4	375.8	527.0	377.3	553.5	487.0	522.6	469.2	447.9	410.1	487.0	456.0

naphtho[8,1,2-fgh]pentahelicene		n/a	C ₂₈ H ₁₆	352.43	C ₂₈ H ₁₆	526.1 386.3 527.6 387.8 548.1 490.0 511.8 466.3 440.2 408.7 481.1 455.1
benzo(p)naphtho(1,8,7-ghi)chrysene		385-14-8	C ₂₈ H ₁₆	352.43	C ₂₈ H ₁₆	530.6 392.6 532.2 394.1 545.8 489.4 508.6 465.7 443.4 412.2 482.0 456.7
dibenzo[b,e]perylene		n/a	C ₂₈ H ₁₆	352.43	C ₂₈ H ₁₆	531.1 385.5 532.6 386.9 546.2 481.6 501.4 450.8 445.2 408.5 481.7 452.8
n/a		n/a	C ₂₈ H ₁₆	352.43	C ₂₈ H ₁₆	532.7 379.9 534.2 381.3 556.9 480.6 515.1 452.2 455.3 408.9 491.9 453.6
dibenzo[de,qr]pentacene		n/a	C ₂₈ H ₁₆	352.43	C ₂₈ H ₁₆	533.1 360.0 534.7 361.4 563.1 462.4 515.7 428.6 461.9 394.3 495.2 439.1
n/a		n/a	C ₂₈ H ₁₆	352.43	C ₂₈ H ₁₆	535.4 386.8 536.9 388.2 558.6 492.9 521.7 469.4 449.4 412.1 489.8 459.0

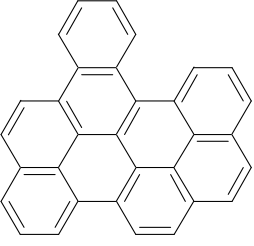
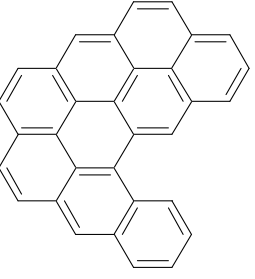
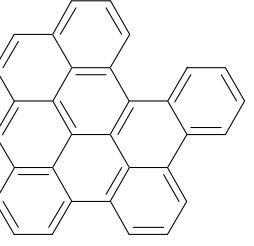
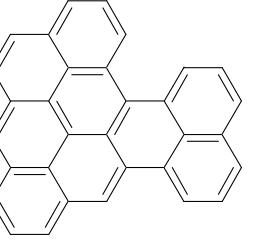
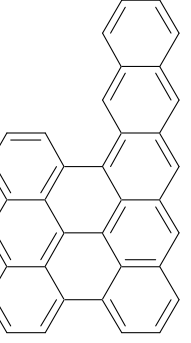
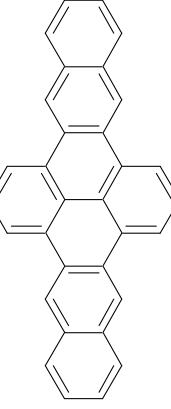
n/a	n/a		C ₂₈ H ₁₆	352.43	C ₂₈ H ₁₆	536.7	378.7	538.2	380.1	562.1	480.4	521.0	452.4	460.9	409.3	496.9	454.0
dibenzo[a,n]perylene	n/a		C ₂₈ H ₁₆	352.43	C ₂₈ H ₁₆	536.7	378.7	538.2	380.1	561.8	479.9	520.5	452.1	460.4	408.6	496.4	453.3
n/a	n/a		C ₂₈ H ₁₆	352.43	C ₂₈ H ₁₆	544.9	386.8	546.4	388.2	574.9	495.2	539.2	473.0	464.9	416.3	503.6	463.2
n/a	n/a		C ₂₈ H ₁₆	352.43	C ₂₈ H ₁₆	549.0	401.0	550.5	402.4	567.0	501.0	530.0	478.7	466.2	428.0	501.1	470.5
n/a	n/a		C ₂₈ H ₁₆	352.43	C ₂₈ H ₁₆	555.6	369.3	557.1	370.8	590.0	480.2	553.6	458.2	490.1	413.4	523.7	458.3
dibenzo[a,o]perylene	190-36-3		C ₂₈ H ₁₆	352.43	C ₂₈ H ₁₆	570.9	386.4	572.4	387.9	603.8	497.7	570.3	542.0	494.0	420.6	531.1	468.2

dibenzo[a,j]perylene		191-87-7	C ₂₈ H ₁₆	352.43	C ₂₈ H ₁₆	604.0 411.2 605.6 412.6 624.5 513.5 588.3 493.0 521.8 443.6 553.0 486.8
dibenzo[a,f]perylene		191-81-1	C ₂₈ H ₁₆	352.43	C ₂₈ H ₁₆	605.3 404.6 606.8 406.1 627.2 508.1 592.0 487.0 524.8 438.3 556.3 481.5
naphtho(8,1,2-abc)coronene		6596-38-9	C ₃₀ H ₁₄	374.43	C ₃₀ H ₁₄	455.4 298.6 457.1 300.1 521.5 448.6 465.2 406.6 382.2 339.2 442.5 405.2
dibenzo(bc,ef)coronene		190-31-8	C ₃₀ H ₁₄	374.43	C ₃₀ H ₁₄	483.5 301.6 485.2 303.1 554.0 454.4 498.0 413.1 413.5 346.8 471.3 413.4
dibenzo[bc,kl]coronene		190-55-6	C ₃₀ H ₁₄	374.43	C ₃₀ H ₁₄	510.2 292.9 511.8 294.4 593.3 456.8 543.2 421.5 452.9 353.3 506.6 420.4
tribenzo(b,n,pqr)perylene		190-81-8	C ₃₀ H ₁₆	376.45	C ₃₀ H ₁₆	515.0 385.6 516.7 387.1 531.5 484.4 459.5 425.5 405.8 383.1 456.1 437.2

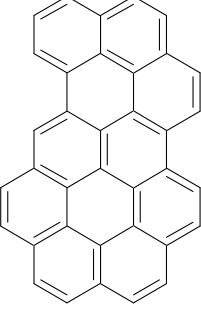
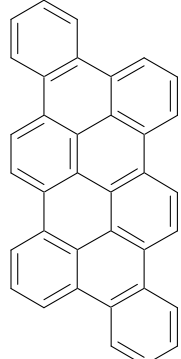
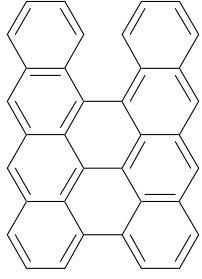
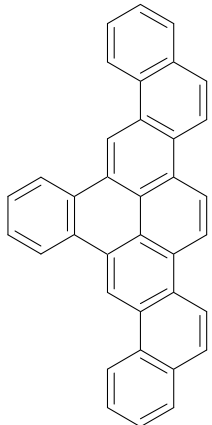
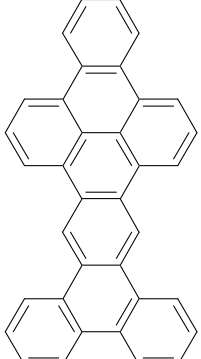
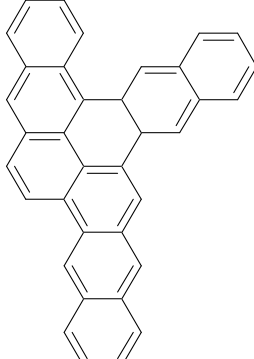
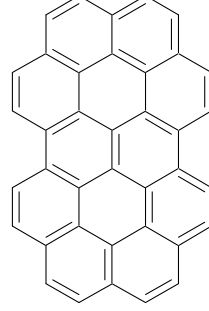
benzo(qr)naphtho(2,1,8,7-fghi)pentacene		190-87-4	C ₃₀ H ₁₆	376.45	C ₃₀ H ₁₆	515.3 376.3 516.9 377.8 537.7 480.6 473.1 429.9 414.9 385.4 463.7 439.1
1,2:7,8-dibenzanthanthrene		191-13-9	C ₃₀ H ₁₆	376.45	C ₃₀ H ₁₆	523.9 424.9 525.5 350.5 569.7 475.8 520.0 440.8 452.3 392.2 496.3 445.7
tribenzo[b,e,ghi]perylene		n/a	C ₃₀ H ₁₆	376.45	C ₃₀ H ₁₆	531.4 384.0 533.0 385.5 560.7 498.7 507.8 460.7 439.7 406.1 487.3 459.7
tribenzo[a,e,ghi]perylene		n/a	C ₃₀ H ₁₆	376.45	C ₃₀ H ₁₆	536.7 386.3 538.3 387.8 565.4 500.0 511.5 460.7 443.9 406.7 491.3 460.3
benzo[b]naphtho[1,2,3,4-pqr]perylene		n/a	C ₃₀ H ₁₆	376.45	C ₃₀ H ₁₆	539.0 393.3 540.6 394.9 562.3 501.7 505.0 459.0 438.9 405.8 487.6 460.0
n/a		n/a	C ₃₀ H ₁₆	376.45	C ₃₀ H ₁₆	547.3 339.2 548.9 340.8 603.5 476.9 559.0 447.8 487.7 397.6 529.2 451.5

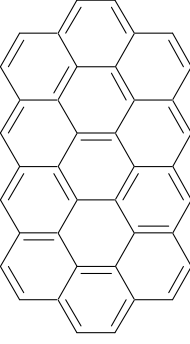
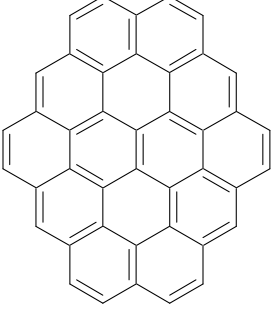
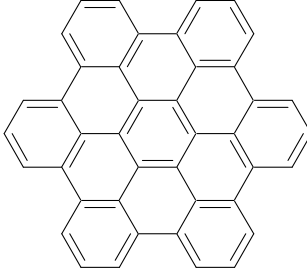
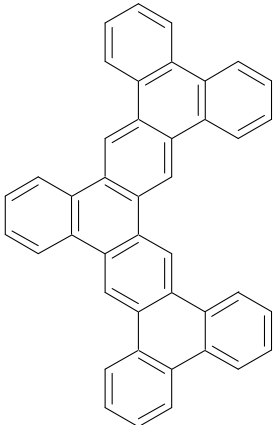
benzo[a]naphtho[2,1,8-lmn]perylene		n/a	C ₃₀ H ₁₆	376.45	C ₃₀ H ₁₆	557.4 372.6 559.0 374.1 601.8 499.7 556.9 469.8 482.0 413.9 525.8 467.9
benzo[a]naphtho[2,1,8-cde]perylene		n/a	C ₃₀ H ₁₆	376.45	C ₃₀ H ₁₆	558.0 383.4 559.6 385.0 595.3 502.7 545.2 467.5 472.4 412.9 517.8 467.3
tribenzo[a,ghi,o]perylene		n/a	C ₃₀ H ₁₆	376.45	C ₃₀ H ₁₆	559.9 383.5 561.5 385.0 602.1 513.9 562.2 488.5 474.8 418.7 522.8 475.1
dibenzo[c,m]picene		n/a	C ₃₀ H ₁₈	378.46	C ₃₀ H ₁₈	546.1 417.4 547.7 418.9 546.4 499.1 488.3 455.1 447.0 427.2 482.8 467.2
tetrabenz[a,c,h,j]anthracene		215-11-2	C ₃₀ H ₁₈	378.46	C ₃₀ H ₁₈	557.7 493.5 559.3 495.0 542.3 504.7 473.9 448.4 438.5 423.0 476.4 464.4
dibenzo(a,l)pentacene		227-09-8	C ₃₀ H ₁₈	378.46	C ₃₀ H ₁₈	558.3 383.7 560.0 385.2 585.7 493.1 547.9 469.9 496.3 436.3 526.6 476.7
benzo[a]hexacene		n/a	C ₃₀ H ₁₈	378.46	C ₃₀ H ₁₈	591.9 375.5 593.5 377.1 631.0 496.1 598.2 478.7 542.2 444.0 569.3 485.1

heptacene		258-38-8	C ₃₀ H ₁₈	378.46	C ₃₀ H ₁₈	629.3 367.3 630.9 368.9 680.6 499.0 652.6 487.5 592.2 451.5 615.9 493.4
ovalene		190-26-1	C ₃₂ H ₁₄	398.45	C ₃₂ H ₁₄	472.3 292.1 474.0 293.8 558.5 468.5 498.9 424.6 400.5 343.7 469.6 419.5
dinaphtho[2,1,8,7-defg:2',1',8',7'-qrst]pentacene		n/a	C ₃₂ H ₁₆	400.47	C ₃₂ H ₁₆	528.1 366.1 529.9 367.7 572.0 498.6 506.2 448.3 432.6 390.8 489.3 453.5
dibenzo(a,j)coronene		190-72-7	C ₃₂ H ₁₆	400.47	C ₃₂ H ₁₆	528.3 379.2 530.0 379.0 561.7 500.1 487.9 441.3 418.1 385.8 476.9 449.0
tetrapheno[10,11,12,1,2-defghij]pentaphene		n/a	C ₃₂ H ₁₆	400.47	C ₃₂ H ₁₆	530.2 355.8 531.9 357.4 584.5 498.6 525.0 454.9 446.8 395.1 501.7 458.0
dibenzo[a,d]coronene		n/a	C ₃₂ H ₁₆	400.47	C ₃₂ H ₁₆	543.7 386.3 545.5 387.9 583.7 517.7 522.3 472.4 442.0 406.1 499.9 469.2
benzo[e]phenanthro[2,3,4,5-pqrab]perylene		n/a	C ₃₂ H ₁₆	400.47	C ₃₂ H ₁₆	554.6 381.6 556.4 383.8 602.9 522.2 546.3 482.1 463.5 415.4 518.4 478.0

dibenzo[a,ghi]naphtho[2,1,8-cde]perylene		n/a	C ₃₂ H ₁₆ 400.47	C ₃₂ H ₁₆ 558.0 388.9 559.8 390.5 599.6 521.9 538.3 476.9 457.7 411.7 514.2 474.7
dibenzo[a,ghi]naphtho[2,1,8-lmn]perylene		n/a	C ₃₂ H ₁₆ 400.47	C ₃₂ H ₁₆ 565.0 370.3 566.7 372.0 623.0 519.6 572.0 485.5 484.8 417.2 537.5 479.8
dibenzo[a,cd]naphtho[8,1,2,3-fghi]perylene		n/a	C ₃₂ H ₁₆ 400.47	C ₃₂ H ₁₆ 565.9 390.7 567.6 392.4 609.9 525.5 549.3 480.9 468.0 415.7 523.4 479.1
dinaphtho[1,8-ab:8',1',2',3'-fghi]perylene		n/a	C ₃₂ H ₁₆ 400.47	C ₃₂ H ₁₆ 585.3 380.0 587.1 381.7 643.8 525.9 590.5 488.6 502.5 421.9 554.5 485.4
n/a		n/a	C ₃₂ H ₁₆ 400.47	C ₃₂ H ₁₆ 629.2 384.4 630.9 386.1 688.5 529.6 633.3 490.9 546.2 426.1 596.1 489.8
dibenzo(hi,uv)hexacene		192-54-1	C ₃₂ H ₁₈ 402.48	C ₃₂ H ₁₈ 577.2 424.9 578.9 426.6 591.7 528.9 528.1 480.7 472.9 440.8 517.1 491.3

anthra(1,2,3,4-rst)pentaphene	31541-07-8	C ₃₂ H ₁₈	402.48	C ₃₂ H ₁₈	638.4	451.8	640.1	453.4	661.5	570.3	620.4	548.0	544.9	488.5	583.1	537.7
n/a	n/a	C ₃₂ H ₁₈	402.48	C ₃₂ H ₁₈	662.2	433.9	664.0	435.5	703.4	564.1	664.0	539.9	577.8	477.5	618.2	531.3
benzo[p]naphtho[8,1,2-abc]coronene	n/a	C ₃₄ H ₁₆	424.49	C ₃₄ H ₁₆	568.4	383.7	570.3	385.5	628.3	541.1	563.2	493.7	468.1	415.4	533.1	487.6
n/a	n/a	C ₃₄ H ₁₆	424.49	C ₃₄ H ₁₆	584.5	385.7	586.4	387.4	647.2	545.4	582.8	498.6	487.1	421.3	550.1	493.5
benzo[uv]naphtho[2,1,8,7-fghi]hexacene	n/a	C ₃₄ H ₁₈	426.51	C ₃₄ H ₁₈	590.9	421.6	592.8	423.4	622.6	548.4	551.9	494.4	484.2	443.9	537.3	503.6
n/a	n/a	C ₃₄ H ₁₈	426.51	C ₃₄ H ₁₈	646.2	397.0	648.0	398.8	702.0	544.7	646.3	506.7	568.9	452.8	614.9	512.8

pyreno[1,10,9-abc]coronene		n/a	C ₃₆ H ₁₆	448.51	C ₃₆ H ₁₆	548.3 363.3 550.2 365.1 622.6 538.6 545.3 478.8 444.8 396.7 520.4 478.2
dibenzo[<i>ij,rst</i>]phenanthro[9,10,1,2-defg]pentaphene		n/a	C ₃₆ H ₁₈	450.53	C ₃₆ H ₁₈	613.9 449.4 615.9 451.2 638.7 575.6 546.0 499.2 474.9 442.3 539.8 511.9
benzo[<i>fg</i>]benzo[8,9]phenaleno[1,2,3,4,5- <i>rstuv</i>]pentaphene		n/a	C ₃₆ H ₁₈	450.53	C ₃₆ H ₁₈	743.5 450.4 745.4 452.2 808.3 613.7 750.0 572.7 640.5 489.2 697.3 562.3
n/a		n/a	C ₃₆ H ₂₀	452.54	C ₃₆ H ₂₀	657.6 484.1 659.5 486.0 664.2 594.8 583.0 530.9 524.5 489.4 574.6 545.5
tetrabenzo[<i>a,c,hi,qr</i>]pentacene		n/a	C ₃₆ H ₂₀	452.54	C ₃₆ H ₂₀	658.8 499.9 660.8 501.6 651.9 598.7 562.3 524.7 509.5 485.1 561.7 542.0
n/a		n/a	C ₃₆ H ₂₀	452.54	C ₃₆ H ₂₀	687.1 476.4 689.1 478.3 719.8 611.9 665.0 575.8 587.3 519.8 633.3 576.7
naphtho[7',8',1',2':5,10,4]anthra[1,9,8- <i>abcd</i>]coronene		41163-25-1	C ₃₈ H ₁₆	472.53	C ₃₈ H ₁₆	562.1 366.4 564.2 368.4 647.8 558.7 561.5 491.2 449.2 398.1 534.7 489.0

phenanthro[3,4,5,6-bcdef]ovalene		n/a	C ₄₀ H ₁₆	496.55	C ₄₀ H ₁₆	614.6 351.4 616.7 353.5 734.1 582.7 651.6 520.3 519.1 412.2 608.7 513.3
dinaphtho[2,1,8,7-hijk:2',1',8',7'-stuv]ovalene		n/a	C ₄₂ H ₁₆	520.58	C ₄₂ H ₁₆	614.0 356.7 616.2 358.8 743.7 605.1 652.3 535.0 507.8 415.6 608.3 525.9
hexabenzob[bc,ef,hi,kl,no,qr]coronene		190-24-9	C ₄₂ H ₁₈	522.59	C ₄₂ H ₁₈	680.8 469.7 683.4 471.9 742.5 652.5 622.0 552.8 515.7 464.7 607.8 562.9
n/a		n/a	C ₄₂ H ₂₄	528.64	C ₄₂ H ₂₄	794.9 675.3 797.2 677.5 769.7 710.4 662.8 621.6 610.8 584.6 665.5 644.4

^a UHF calculation converged on a structure having one or more cleaved bonds compared to RHF geometry.