Gas Phase Heat of Formation Values for Buckminsterfullerene (C_{60}), C70 Fullerene (C_{70}) Coronene, Corannulene, Sumanene and other Polycyclic Aromatic Hydrocarbons Calculated using Density Functional Theory (M06 2X) Coupled with a Versatile Inexpensive Group Equivalent Approach

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Supporting Information

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Table S1. Experimental $\Delta_f H^o_{g,298}$ Values and Literature References for Compounds Included in the Training and Test Sets.*

	Compound	Experimental $\Delta_f H^o_{g,298}$ (kJ/mol)	Reference
1	**methane**	-74.533 ± 0.057	1
2	ethane	-84 ± 0.4	2
3	**propane**	-104.63 ± 0.24	1
4	*n*-butane	-125.6 ± 0.67	3
5	*n*-pentane	-146.4 ± 0.67	4
6	*n*-hexane	-167.1	5
7	***n*-heptane**	-187.34 ± 0.74	1
8	***n*-octane**	-208.23 ± 0.79	1
9	*n*-nonane	-228.3	6
10	***n*-decane**	-249.7 ± 1.1	4
11	*n*-undecane	-270.3 ± 1.3	4
12	*n*-dodecane	-290.9 ± 1.4	4
13	*n*-tridecane	-311.5 ± 1.6	4
14	*n*-tetradecane	-332.1 ± 1.8	4
15	*n*-pentadecane	-354.8 ± 2.0	4
16	*n*-hexadecane	-374.9	7
17	*n*-heptadecane	-393.9 ± 2.4	4
18	*n*-octadecane	-414.6 ± 2.7	4
19	*n*-nonadecane	-435.1 ± 2.9	4
20	*n*-eicosane	-455.8 ± 3.1	4
21	cyclopropane	39.3	8
22	cyclobutane	28.37 ± 0.59	9
23	**cyclopentane**	-76.40 ± 0.79	10
24	**cyclohexane**	-122.07 ± 0.68	1
25	cycloheptane	-118.03 ± 0.8	9
26	cyclooctane	-124.39 ± 1.2	9
27	cyclononane	-132.76 ± 1.7	9
28	cyclodecane	-154.31 ± 1.7	9
29	cyclotetradecane	-274.47	11
30	**methylcyclopentane**	-106	5
31	**1,1-dimethylcyclopentane**	-138.3 ± 1.2	12
32	ethylcyclopentane	-127.1 ± 1.0	13
33	*n*-propylcyclopentane	-147.6	14
34	*n*-butylcyclopentane	-168.3 ± 1.5	13
35	*n*-pentylcyclopentane	-188.9 ± 1.5	13
36	*n*-hexylcyclopentane	-209.5 ± 1.6	13
37	*n*-heptylcyclopentane	-230.1 ± 1.8	13
38	*n*-octylcyclopentane	-250.7 ± 1.9	13
39	*n*-nonylcyclopentane	-271.3 ± 2.1	13

40	*n*-decylcyclopentane	-292.0 ± 2.3	13
41	*n*-undecylcyclopentane	-312.5 ± 2.5	13
42	*n*-dodecylcyclopentane	-333.2 ± 2.7	13
43	*n*-tridecylcyclopentane	-353.8 ± 2.9	13
44	*n*-tetradecylcyclopentane	-374.4 ± 3.1	13
45	*n*-pentadecylcyclopentane	-395.0 ± 3.3	13
46	*n*-hexadecylcyclopentane	-415.6 ± 3.6	13
47	**methycyclohexane**	-154.8 ± 1.0	13
48	**1,1-dimethylcyclohexane**	-180.874± 2.0	9
49	ethylcyclohexane	-171.8 ± 1.5	13
50	*n*-propylcyclohexane	-193.3 ± 1.3	13
51	*n*-butylcyclohexane	-213.2 ± 1.4	13
52	*n*-pentylcyclohexane	-233.8 ± 1.7	13
53	*n*-hexylcyclohexane	-254.4 ± 1.8	13
54	*n*-heptylcyclohexane	-275.0 ± 1.9	13
55	*n*-octylcyclohexane	-295.6 ± 2.1	13
56	*n*-nonylcyclohexane	-316.2 ± 2.3	13
57	*n*-decylcyclohexane	-336.9 ± 2.4	13
58	*n*-undecylcyclohexane	-357.4 ± 2.6	13
59	*n*-dodecylcyclohexane	-378.1 ± 2.8	13
60	*n*-tridecylcyclohexane	-398.7 ± 3.1	13
61	*n*-tetradecylcyclohexane	-419.3 ± 3.3	13
62	*n*-pentadecylcyclohexane	-439.9 ± 3.5	13
63	*n*-hexadecylcyclohexane	-460.5± 3.7	13
64	**2-methylpropane (isobutane)**	-135.27 ± 0.37	1
65	2-methylbutane	-154.18 ± 0.6	9
66	**2,2-dimethylpropane**	-167.9 ± 0.63	15
67	2-methylpentane	-174.3 ± 1.0	4
68	**3-methylpentane**	-171.6 ± 0.96	4
69	2-methylhexane	-195.0 ± 1.3	4
70	3-methylhexane	-192.3 ± 1.3	4
71	2,3-dimethylbutane	-177.8 ± 1.0	4
72	2,2-dimethylbutane	-185.6 ± 0.96	4
73	3-ethylpentane	-189.7 ± 1.2	4
74	2,2-dimethylpentane	-206.2 ± 1.3	4
75	2,3-dimethylpentane	-199.2 ± 1.3	4
76	2,4-dimethylpentane	-202.1 ± 0.96	4
77	3,3-dimethylpentane	-201.5 ± 0.92	4
78	2,2,3-trimethylbutane	-204.8 ± 1.1	4
79	2-methylheptane	-215.5 ± 1.3	4
80	3-methylheptane	-212.6 ± 1.1	4
81	4-methylheptane	-212.1 ± 1.2	4
82	3-ethylhexane	-210.9 ± 1.2	4
83	2,2-dimethylhexane	-224.7 ± 1.0	4
84	2,3-dimethylhexane	-213.9 ± 1.5	4

85	2,4-dimethylhexane	-219.4 ± 1.1	4
86	2,5-dimethylhexane	-222.6 ± 1.5	4
87	3,3-dimethylhexane	-220.1 ± 1.1	4
88	3,4-dimethylhexane	-213.0 ± 1.5	4
89	3-ethyl-2-methylpentane	-211.2 ± 1.3	4
90	3-ethyl-3-methylpentane	-215.0 ± 1.3	4
91	2,2,3-trimethylpentane	-220.1 ± 1.5	4
92	2,3,3-trimethylpentane	-216.4 ± 1.4	4
93	**2,2,4-trimethylpentane**	-223.7 ± 1.5	1
94	2,3,4-trimethylpentane	-217.4 ± 1.7	4
95	2,2,3,3-tetramethylbutane	-225.9 ± 1.9	4
96	bicyclo[4.1.0]heptane (norcarane)	2.0 ± 4.2	16
97	bicyclo[2.2.1]heptane (norbornane)	-52.0	17,18
98	tricyclo[4.2.0.0^{2,5}]octane, anti-	211.0 ± 3.0	19
99	tricyclo[4_2_0_0^{2,5}]octane,syn	235.0 ± 4.2	19
100	bicyclo[2.2.0]hexane	125.0	20
101	tricyclo[2.2.1.0^{2,6}]heptane (nortricyclene)	62.0 ± 2.3	21
102	**cubane**	597.1 ± 5.0	22,23
103	adamantane	-132.3	24
104	1-methyladamantane	-171.5 ± 2.9	25
105	2-methyladamantane	-156.5 ± 2.1	25
106	2,2-dimethyladamantane	-182.8 ± 2.9	25
107	1,3-dimethyladamantane	-206.6	26
108	1,3,5-trimethyladamantane	-243.5	26, 27
109	1,3,5,7- tetramethyladamantane	-281.0 ± 2.1	27
110	**toluene**	50.41 ± 0.37	1
111	p-xylene	17.9 ± 1.0	28
112	m-xylene	17.2 ± 0.75	28
113	o-xylene	19.0 ± 1.1	28
114	ethylbenzene	29.8 ± 0.84	28,29
115	1,3,5-trimethylbenzene	-15.94 ± 1.4	9
116	*n*-propylbenzene or 1-phenylpropane	7.82 ± 0.84	28, 29
117	isopropylbenzene	3.9 ± 1.1	28, 29
118	n-butylbenzene	-12.8	28, 30
119	t-butylbenzene	-22.7 ± 1.4	28
120	1-methyl-2-ethylbenzene	1.2 ± 1.2	28, 29
121	1-methyl-3-ethylbenzene	-1.9 ± 1.2	28,31
122	1-methyl-4-ethylbenzene	-3.3 ± 1.5	28,31
123	**phenol**	-91.8 ± 2.5	32
124	1,2-dihydroxybenzene (1,2-benzenediol)	-267.5 ±1.9	32
125	1,3-dihydroxybenzene (resorcinol)	-268 ±3.0	32
126	1,4-dihydroxybenzene (hydroquinone)	-260.3 ±1.0	32
127	1,2,3-benzenetriol (pyrogallol)	-447.2 ±1.0	32
128	1,2,4-benzenetriol	-439.6 ±1.1	32

129	1,3,5-benzenetriol	-444.7 ±3.0	32
130	2-methylphenol (ortho-cresol)	-128.3 ±0.9	32
131	3-methylphenol (meta-cresol)	-125.6 ±3.0	32
132	4-methylphenol (p-cresol)	-125.3 ±1.5	32
133	2.3-dimethylphenol	-157.3 ±1.1	32
134	2,4-dimethylphenol	-159.3 ±3.0	32
135	2,5-dimethylphenol (2,5-xylenol)	-161.7 ±0.5	32
136	2,6-dimethylphenol	-161.8 ±0.5	32
137	3,4-dimethylphenol	-156.6 ±0.6	32
138	3,5-dimethylphenol (3,5-xylenol)	-161.6 ±0.7	32
139	2,3,6-trimethylphenol	-192.9 ±1.4	32
140	2,4,6-trimethylphenol	-192.4 ±1.3	32
141	1-naphthol	-30.8 ± 1.	33
142	2-naphthol	-29.9 ± 1.7	33
143	1,2-naphthalenediol	-200.5 ± 1.8	33
144	1,3-naphthalenediol	-211.2 ± 1.9	33
145	1,4-naphthalenediol	-197.0 ± 1.8	33
146	ethene	52.53 + 0.14	1
147	**propene**	20.26 ± 0.29	1
148	**2-methylpropene (isobutene)**	-17.52 ± 0.51	1
149	1-butene	-0.01 ± 0.46	1
150	***trans*-2-butene**	-11.15 ± 0.49	1
151	***cis*-2-butene**	-7.3 ± 0.51	1
152	propadiene (allene)	190.06 + 0.32	1
153	1-pentene	-21.7 ± 2.7	34
154	*trans*-2-pentene	-31.4 ± 0.5	35
155	*cis*-2-pentene	-26.5 ± 0.5	35
156	**2-methyl-2-pentene**	-66.86 ± 1.51	9
157	**1,2-butadiene**	162.2 ± 0.59	36
158	1,3-butadiene	111.9 ± 0.96	37
159	1,2-pentadiene	140.6 ± 0.67	38
160	*trans*-1,3-pentadiene	75.77 ± 0.67	38
161	*cis*-1,3-pentadiene	82.72 ± 0.92	38
162	1,4-pentadiene	106.3 ± 1.3	38
163	2-methyl-1-butene	-34.8	39
164	3-methyl-1-butene	-25.5	39
165	2-methyl-2-butene	-41.5 ± 0.88	40
166	1-hexene	-41.5 ± 1.2	41
167	*trans*-2-hexene	-51.6 ± 0.8	42
168	*cis*-2-hexene	-47.0 ± 1.1	43
169	*trans*-3-hexene	-49.3 ± 1.0	43
170	*cis*-3-hexene	-45.9 ± 0.7	43
171	2-methyl-1-pentene	-59.37 ± 1.34	9
172	3-methyl-1-pentene	-49.497 ± 1.55	9
173	4-methyl-1-pentene	-51.254 ± 1.84	9

174	3-methyl-*cis*-2-pentene	-62.3 ± 1.51	9
175	3-methyl-*trans*-2-pentene	-63.137 ± 1.34	9
176	*cis*-4-methyl-2-pentene	-57.488 ± 1.21	9
177	1-octene	-80.1± 1.3	9
178	*trans*-4-methyl-2-pentene	-61.505 ± 1.46	9
179	1,5-hexadiene	84.14 ± 1.3	9
180	2-ethyl-1-butene	-56.024 ± 1.51	9
181	2,3-dimethyl-1-butene	-63.555 ± 2.1	9
182	3,3-dimethyl-1-butene	-60.71 ± 1.05	9
183	2,3-dimethyl-2-butene	-68.701 ± 1.05	9
184	2,3-dimethyl-1,3-butadiene	45.104 ± 1.26	9
185	cyclopropene	277	44
186	cyclobutene	157.0 ± 2.0	45
187	cycloheptene	-9.163 ± 1.0	9
188	*trans*-cyclooctene	20	20
189	1,3,5-cycloheptatriene	183.678 ± 1.51	9
190	**cyclopentene**	36.0	46
191	**cyclohexene**	-4.32 ± 0.98	47
192	1,3-cyclopentadiene	133.4	48
193	1,3-cyclohexadiene	104.58 ± 0.63	49
194	**1-methylcyclopentene**	-4.39	5
195	3-methylcyclopentene	9.67	46
196	**1,2-dimethylcyclopentene**	-41.4	46
197	**1-methylcyclohexene**	-43.263	9
198	norbornadiene	247.6 ± 3.1	50
199	**acetylene (ethyne)**	228.31 ± 0.14	1
200	**propyne**	185.67 ± 0.32	1
201	1-butyne	165.39± 0.85	1
202	2-butyne	145.77± 0.78	1
203	1-pentyne	144.3 ± 2.1	51
204	2-pentyne	128.9 ± 2.1	51
205	1-hexyne	122.3 ± 1.2	52
206	2-hexyne	107.7 ± 2.4	52
207	3-hexyne	105.4 ± 1.9	52
208	4-nonyne	42.0 ± 2.8	52
209	1-decyne	41.9 ± 3.4	52
210	2,4-hexadiyne	377.4	53
211	indane	60.9 ± 2.1	54
212	azulene	308	55
213	diphenylmethane	165± 2.2	54
214	bibenzyl	143 ± 2.0	56, 57,
215	benz[c]phenanthrene	291.2+ 4.6	58
216	triphenylmethane	280.3 ± 1.5	59
217	1-methylnaphthalene	116.9 ± 2.7	60
218	2-methylnaphthalene	116.1 ± 2.6	60

219	acenaphthene	156.8 ± 3.1	54
220	acenaphthylene	265.5 ± 5.2	54, 61
221	**anthracene**	227.1 ± 5.6	57, 62
222	benz[a]anthracene	278.7	54 &See text
223	**benzene**	83.2 ± 0.26	1
224	biphenyl	180.3 ± 3.3	54
225	biphenylene	420.4 ± 1.9	63
226	chrysene	263.5 ± 4.3	64
227	coronene	279.7 ± 7.1	65, 66 & see text
228	fluoranthene	289.8 ± 0.4 kJ/mol	67,68
229	fluorene	179.4 ± 3.0 kJ/mol	69
230	naphthacene	310.7 ± 4.2	70 & see text
231	**naphthalene**	150.6 ± 1.5	54
232	perylene	306 ± 0.8	9, 64, 71, 72 & see text
233	**phenanthrene**	202.2 ± 2.3	54
234	**pyrene**	224.0 + 2.2	73, 74
235	triphenylene	270.1 ± 4.4	54

*For a substantial number of compounds, two or more experimental $\Delta_f H^o_{g,298}$ values have been reported. Fortunately, $\Delta_f H^o_{g,298}$ values for several classes of compounds have been evaluated and recommended by others. For many PAHs, values listed are those recommended by Roux *et al.* [54] For phenol and substituted phenols, values listed are those recommended by Dorofeeva and Ryzhova[32]. For some compounds, experimental values listed are those mutually supportive of the theoretical values reported here. Compounds that are members of the training set are underlined and in bold.

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Table S2. Experimental $\Delta_f H^o_{s,298}$ and $\Delta_{sub} H^o_{g,298}$ used to calculate $\Delta_f H^o_{g,298}$ Values for Selected PAHs Included in the Training and Test Sets.

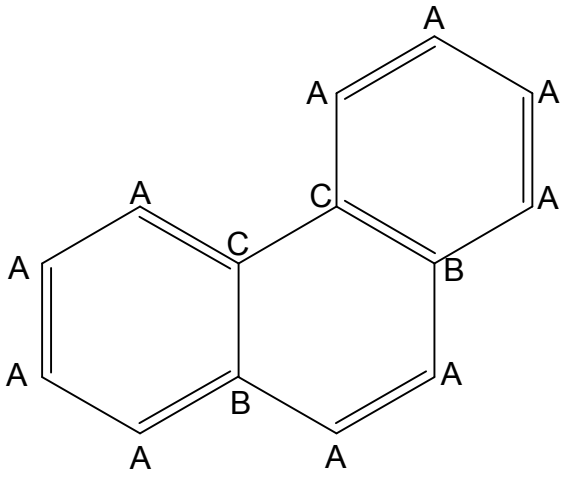
Compound	$\Delta_f H^o_{s,298}$	$\Delta_{sub} H^o_{298}$	$\Delta_f H^o_{g,298}$	**Reference***	$\Delta_f H^o_{g,298}$
	kJ/mol	kJ/mol	kJ/mol		kJ/mol
214 bibenzyl	51.5 ± 1.3	91.5 ± 0.7	143.0 ± 2.0	56, 57	n/a**
220 acenaphthylene	193.0 ± 4.0	72.5 ± 1.2	265.5 + 5.2	54, 61	(263.2 ± 3.7)
221 anthracene	125.5±5.6	101.6	227.1 ± 5.6	57, 62	(229.4 ± 2.9)
225 biphenylene	333.4 ± 1.1	87.0 ± 0.8	420.4 ± 1.9	63	(417.2 ± 1.9)
227 coronene	146.5 + 4.8	133.2 ± 2.3	279.7 +/- 7.1	64, 65	n/a**
228 fluoranthene	189.9 ± 0.4	100.0	289.8 ± 0.4	67,68	(291.4 ± 4.0)
234 pyrene	125.5 ± 1.2	98.5 ± 1.0	224.0 + 2.2	73, 74	(225.5 ± 2.5)

*See Table S1 for references

** n/a = not available

Data in parentheses are the $\Delta_f H^o_{g,298}$ values recommended by Roux *et al.*[53]. All $\Delta_f H^o_{g,298}$ values for PAHs used in this study were within the limits of uncertainty (2-4 kJ/mol) associated with recommended values where such values are available.

Table S3: Examples of Carbon Groups in PAHs and their Abbreviations/Designations Illustrated in Three Representative Compounds.



phenanthrene

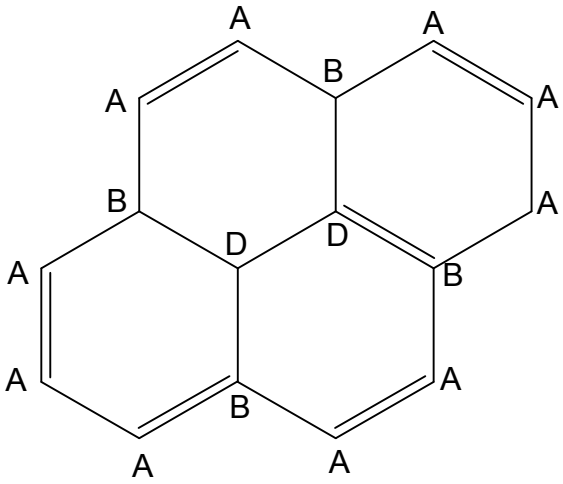
A = [C_B-H]

B = [C_{BF}-(C_B)$_2$ (C_{BF})]

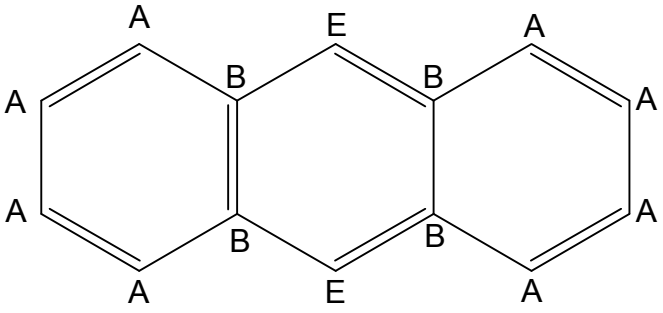
C= [C_{BF}-(C_B) (C_{BF})$_2$]

D = [C_{BF}-(C_{BF})$_3$]

E = [C_B-H-(C_{BF})$_2$]



pyrene



anthracene

Table S4. E_{Elec}, Correction Values (ZPE+ (H_T) +RT), and $H_{298.15}$ for Compounds Included in this Investigation.

	Compound	E_{Elec}	$ZPE+H_T+RT$	$ZPE+H_T+RT$	$H_{298.15}$
		hartrees	kcal/mol	hartrees	hartrees
1	methane	-40.499432	30.153	0.048052	-40.4513802
2	ethane	-79.801748	50.537	0.080536	-79.7212122
3	propane	-119.107324	69.555	0.110843	-118.9964811
4	*n*-butane	-158.412791	88.667	0.141300	-158.2714913
5	*n*-pentane	-197.718362	107.499	0.171310	-197.5470516
6	*n*-hexane	-237.02379	126.562	0.201689	-236.8221008
7	*n*-heptane	-276.329306	145.495	0.231861	-276.0974452
8	*n*-octane	-315.634768	164.517	0.262174	-315.3725937
9	*n*-nonane	-354.940295	183.489	0.292408	-354.6478869
10	*n*-decane	-394.245751	202.506	0.322714	-393.9230374
11	*n*-undecane	-433.551243	221.480	0.352951	-433.1982924
12	*n*-dodecane	-472.856714	240.503	0.383266	-472.4734484
13	*n*-tridecane	-512.162215	259.440	0.413444	-511.7487714
14	*n*-tetradecane	-551.467677	278.496	0.443811	-551.0238657
15	*n*-pentadecane	-590.773147	297.450	0.474016	-590.2991306
16	*n*-hexadecane	-630.078633	316.486	0.504352	-629.5742809
17	*n*-heptadecane	-669.384108	335.419	0.534524	-668.8495842
18	*n*-octadecane	-708.68958	354.449	0.564850	-708.1247300
19	*n*-nonadecane	-747.995068	373.387	0.595030	-747.4000384
20	*n*-eicosane	-787.300559	392.427	0.625372	-786.6751873
21	cyclopropane	-117.872824	54.629	0.087057	-117.7857672
22	cyclobutane	-157.176296	73.945	0.117839	-157.0584572
23	cyclopentane	-196.512618	93.678	0.149285	-196.3633327
24	cyclohexane	-235.828951	112.792	0.179745	-235.6492057
25	cycloheptane	-275.125225	132.101	0.210516	-274.9147088
26	cyclooctane	-314.425604	151.300	0.241112	-314.1844923

27	cyclononane	-353.727774	170.667	0.271975	-353.4557991
28	cyclodecane	-393.032684	189.451	0.301909	-392.7307749
29	cyclotetradecane	-550.268619	265.521	0.423134	-549.8454847
30	methylcyclopentane	-235.820693	112.269	0.178912	-235.6417811
31	1,1-dimethylcyclopentane	-275.129338	130.852	0.208526	-274.9208122
32	ethylcyclopentane	-275.126021	131.406	0.209409	-274.9166124
33	*n*-propylcyclopentane	-314.431474	150.435	0.239733	-314.1917408
34	*n*-butylcyclopentane	-353.737011	169.374	0.269914	-353.4670966
35	*n*-pentylcyclopentane	-393.042462	188.383	0.300207	-392.7422548
36	*n*-hexylcyclopentane	-432.3479	207.389	0.330495	-432.0174049
37	*n*-heptylcyclopentane	-471.653398	226.352	0.360715	-471.2926834
38	*n*-octylcyclopentane	-510.95882	245.422	0.391105	-510.5677155
39	*n*-nonylcyclopentane	-550.264298	264.373	0.421305	-549.8429932
40	*n*-decylcyclopentane	-589.569781	283.563	0.451886	-589.1178950
41	*n*-undecylcyclopentane	-628.875228	302.573	0.482180	-628.3930476
42	*n*-dodecylcyclopentane	-668.180732	321.495	0.512334	-667.6683975
43	*n*-tridecylcyclopentane	-707.486191	340.498	0.542618	-706.9435734
44	*n*-tetradecylcyclopentane	-746.791727	359.471	0.572853	-746.2188740
45	*n*-pentadecylcyclopentane	-786.09717	378.475	0.603138	-785.4940322
46	*n*-hexadecylcyclopentane	-825.402704	397.495	0.633448	-824.7692559
47	methycyclohexane	-275.137307	131.356	0.209329	-274.9279781
48	1,1-dimethylcyclohexane	-314.444326	150.040	0.239104	-314.2052222
49	ethylcyclohexane	-314.441817	150.569	0.239947	-314.2018702
50	*n*-propylcyclohexane	-353.747175	169.615	0.270298	-353.4768765
51	*n*-butylcyclohexane	-393.052854	188.657	0.300644	-392.7522102
52	*n*-pentylcyclohexane	-432.358302	207.627	0.330874	-432.0274276
53	*n*-hexylcyclohexane	-471.663682	226.629	0.361156	-471.3025260
54	*n*-heptylcyclohexane	-510.969156	245.632	0.391439	-510.5777168
55	*n*-octylcyclohexane	-550.274501	264.558	0.421600	-549.8529013

56	*n*-nonylcyclohexane	-589.579996	283.583	0.451918	-589.1280781
57	*n*-decylcyclohexane	-628.885395	302.566	0.482169	-628.4032258
58	*n*-undecylcyclohexane	-668.190853	321.584	0.512476	-667.6783767
59	*n*-dodecylcyclohexane	-707.496326	340.559	0.542715	-706.9536111
60	*n*-tridecylcyclohexane	-746.80179	359.580	0.573027	-746.2287633
61	*n*-tetradecylcyclohexane	-786.107499	378.671	0.603450	-785.5040489
62	*n*-pentadecylcyclohexane	-825.412773	397.854	0.634020	-824.7787528
63	*n*-hexadecylcyclohexane	-864.718314	416.945	0.664444	-864.0538704
64	2-methylpropane (isobutane)	-158.415073	88.269	0.140665	-158.2744075
65	2-methylbutane	-197.719783	107.252	0.170917	-197.5488662
66	2,2-dimethylpropane	-197.724334	106.955	0.170443	-197.5538905
67	2-methylpentane	-237.025155	126.267	0.201219	-236.8239359
68	3-methylpentane	-237.024225	126.443	0.201500	-236.8227254
69	2-methylhexane	-276.330634	145.224	0.231429	-276.0992050
70	3-methylhexane	-276.329565	145.407	0.231721	-276.0978444
71	2,3-dimethylbutane	-237.025407	125.986	0.200771	-236.8246357
72	2,2-dimethylbutane	-237.027863	125.847	0.200550	-236.8273132
73	3-ethylpentane	-276.328730	145.448	0.231786	-276.0969441
74	2,2-dimethylpentane	-276.333106	144.882	0.230884	-276.1022220
75	2,3-dimethylpentane	-276.330092	145.234	0.231445	-276.0986471
76	2,4-dimethylpentane	-276.332443	144.950	0.230992	-276.1014507
77	3,3-dimethylpentane	-276.332238	145.209	0.231405	-276.1008329
78	2,2,3-trimethylbutane	-276.33214	144.653	0.230519	-276.1016210
79	2-methylheptane	-315.636083	164.190	0.261653	-315.3744298
80	3-methylheptane	-315.635056	164.347	0.261903	-315.3731526
81	4-methylheptane	-315.634956	164.512	0.262166	-315.3727893
82	3-ethylhexane	-315.634142	164.482	0.262119	-315.3720235
83	2,2-dimethylhexane	-315.63863	163.782	0.261003	-315.3776270
84	2,3-dimethylhexane	-315.634507	164.178	0.261634	-315.3728729

85	2,4-dimethylhexane	-315.636937	164.055	0.261438	-315.3754989
86	2,5-dimethylhexane	-315.637204	164.184	0.261644	-315.3755604
87	3,3-dimethylhexane	-315.6374346	163.436	0.260452	-315.3769766
88	3,4-dimethylhexane	-315.634352	164.262	0.261768	-315.3725841
89	3-ethyl-2-methylpentane	-315.633481	164.474	0.262106	-315.3713752
90	3-ethyl-3-methylpentane	-315.63606	164.067	0.261457	-315.3746028
91	2,2,3-trimethylpentane	-315.63628	163.858	0.261124	-315.3751559
92	2,3,3-trimethylpentane	-315.635058	163.354	0.260321	-315.3747370
93	2,2,4-trimethylpentane	-315.637188	163.591	0.260699	-315.3764894
94	2,3,4-trimethylpentane	-315.635486	164.130	0.261558	-315.3739284
95	2,2,3,3-tetramethylbutane	-315.637584	163.330	0.260283	-315.3773013
96	bicyclo[4.1.0]heptane (norcarane)	-273.899678	116.749	0.186051	-273.7136268
97	bicyclo[2.2.1]heptane (norbornane)	-273.919445	117.143	0.186679	-273.7327659
98	tricyclo[4.2.0.0^{2,5}]octane, anti-	-311.934280	119.872	0.191028	-311.7432520
99	tricyclo[4.2.0.0^{2,5}]octane, syn-	-311.924167	119.872	0.191028	-311.7331390
100	bicyclo[2.2.0]hexane	-234.552653	96.878	0.154385	-234.3982682
101	tricyclo[2.2.1.0^{2,6}]heptane	-272.695197	101.608	0.161923	-272.5332745
102	cubane	-309.422982	88.974	0.141789	-309.2811930
103	adamantine	-390.664255	160.728	0.256136	-390.4081188
104	1-methyladamantane	-429.975139	178.355	0.284227	-429.6909125
105	2-methyladamantane	-429.970079	178.928	0.285140	-429.6849393
106	2,2-dimethyladamantane	-469.274598	197.682	0.315026	-468.9595719
107	1,3-dimethyladamantane	-469.285987	197.006	0.313949	-468.9720382
108	1,3,5-trimethyladamantane	-508.596687	215.211	0.342960	-508.2537267
109	1,3,5,7- tetramethyladamantane	-547.908691	234.444	0.373610	-547.5350810
110	toluene	-271.522208	86.015	0.137074	-271.3851345
111	*p*-xylene	-310.830792	104.603	0.166695	-310.6640966
112	*m*-xylene	-310.831081	104.600	0.166691	-310.6643904

113	*o*-xylene	-310.831824	104.650	0.166770	-310.6650537
114	ethylbenzene	-310.827698	105.068	0.167436	-310.6602616
115	1,3,5-trimethylbenzene	-350.139997	123.324	0.196529	-349.9434679
116	*n*-propylbenzene or 1-phenylpropane	-350.133572	124.181	0.197895	-349.9356791
117	isopropylbenzene	-350.134184	123.866	0.197393	-349.9367911
118	*n*-butylbenzene	-389.438967	143.128	0.228089	-389.2108782
119	t-butylbenzene	-389.440588	142.362	0.226868	-389.2137199
120	1-methyl-2-ethylbenzene	-350.136098	123.888	0.197428	-349.9386701
121	1-methyl-3-ethylbenzene	-350.136516	123.783	0.197261	-349.9392554
122	1-methyl-4-ethylbenzene	-350.136262	123.764	0.197230	-349.9390317
123	phenol	-307.441502	70.623	0.112545	-307.3289572
124	1,2-dihydroxybenzene (1,2-benzenediol)	-382.670489	74.087	0.118065	-382.5524239
125	1,3-dihydroxybenzene (resorcinol)	-382.670182	73.912	0.117786	-382.5523958
126	1,4-dihydroxybenzene (hydroquinone)	-382.666468	73.862	0.117706	-382.5487615
127	1,2,3-benzenetriol (pyrogallol)	-457.899749	77.323	0.123222	-457.7765271
128	1,2,4-benzenetriol	-457.896078	77.190	0.123010	-457.7730680
129	1,3,5-benzenetriol	-457.899261	77.251	0.123107	-457.7761538
130	2-methylphenol (ortho-cresol)	-346.751706	89.381	0.142438	-346.6092684
131	3-methylphenol (meta-cresol)	-346.75063	89.242	0.142216	-346.6084139
132	4-methylphenol (p-cresol)	-346.749545	89.253	0.142234	-346.6073114
133	2.3-dimethylphenol	-386.059586	108.053	0.172193	-385.8873927
134	2,4-dimethylphenol	-386.059807	108.051	0.172190	-385.8876169
135	2,5-dimethylphenol (2,5-xylenol)	-386.060456	108.034	0.172163	-385.8882930
136	2,6-dimethylphenol	-386.06131	108.131	0.172318	-385.8889924
137	3,4-dimethylphenol	-386.059443	107.892	0.171937	-385.8875063
138	3,5-dimethylphenol (3,5-xylenol)	-386.059663	107.952	0.172032	-385.8876307

139	2,3,6-trimethylphenol	-425.369228	126.825	0.202108	-425.1671197
140	2,4,6-trimethylphenol	-425.369296	126.874	0.202186	-425.1671096
141	1-naphthol	-461.069143	102.193	0.162855	-460.9062882
142	2-naphthol	-461.068750	102.096	0.162700	-460.9060498
143	1,2-naphthalenediol	-536.296851	105.594	0.168275	-536.1285764
144	1,3-naphthalenediol	-536.298098	105.577	0.168248	-536.1298505
145	1.4-naphtahlenediol	-536.294794	105.548	0.168201	-536.1265927
146	ethene	-78.568733	35.053	0.055860	-78.5128725
147	propene	-117.879056	54.102	0.086217	-117.7928390
148	2-methylpropene (isobutene)	-157.190293	72.812	0.116033	-157.0742598
149	1-butene	-157.18405	73.201	0.116653	-157.0673969
150	*trans*-2-butene	-157.188539	73.026	0.116374	-157.0721648
151	*cis*-2-butene	-157.186715	73.049	0.116411	-157.0703041
152	propadiene (allene)	-116.6365565	37.920	0.060429	-116.5761272
153	1-pentene	-196.489678	92.152	0.146853	-196.3428246
154	*trans*-2-pentene	-196.493553	92.136	0.146828	-196.3467251
155	*cis*-2-pentene	-196.491617	92.199	0.146928	-196.3446887
156	2-methyl-2-pentene	-235.801953	110.946	0.176804	-235.6251494
157	1,2-butadiene	-155.944783	57.529	0.091678	-155.8531048
158	1,3-butadiene	-155.961266	57.890	0.092254	-155.8690125
159	1,2-pentadiene	-195.250033	76.538	0.121971	-195.1280620
160	*trans*-1,3-pentadiene	-195.271502	76.807	0.122400	-195.1491024
161	*cis*-1,3-pentadiene	-195.269454	76.917	0.122575	-195.1468791
162	1,4-pentadiene	-195.260512	76.774	0.122347	-195.1381649
163	2-methyl-1-butene	-196.494587	92.026	0.146653	-196.3479344
164	3-methyl-1-butene	-196.491423	91.857	0.146383	-196.3450397
165	2-methyl-2-butene	-196.497061	91.855	0.146380	-196.3506809
166	1-hexene	-235.795131	111.192	0.177196	-235.6179354
167	*trans*-2-hexene	-235.799215	111.076	0.177011	-235.6222043

168	*cis*-2-hexene	-235.797242	111.186	0.177186	-235.6200560
169	*trans*-3-hexene	-235.798673	111.246	0.177282	-235.6213914
170	*cis*-3-hexene	-235.796463	111.309	0.177382	-235.6190810
171	2-methyl-1-pentene	-235.800152	110.999	0.176888	-235.6232640
172	3-methyl-1-pentene	-235.797234	110.862	0.176670	-235.6205643
173	4-methyl-1-pentene	-235.797588	110.833	0.176623	-235.6209645
174	3-methyl-*cis*-2-pentene	-235.801478	110.892	0.176718	-235.6247605
175	3-methyl-*trans*-2-pentene	-235.801420	110.972	0.176845	-235.6245750
176	*cis*-4-methyl-2-pentene	-235.798826	110.952	0.176813	-235.6220129
177	1-octene	-314.405179	149.236	0.237823	-314.1673565
178	*trans*-4-methyl-2-pentene	-235.800884	110.833	0.176623	-235.6242605
179	1,5-hexadiene	-234.566271	95.828	0.152712	-234.4135595
180	2-ethyl-1-butene	-235.800533	111.250	0.177288	-235.6223502
181	2,3-dimethyl-1-butene	-235.800942	110.862	0.176670	-235.6242723
182	3,3-dimethyl-1-butene	-235.799824	110.573	0.176209	-235.6236149
183	2,3-dimethyl-2-butene	-235.802592	110.677	0.176375	-235.6262171
184	2,3-dimethyl-1,3-butadiene	-234.581223	95.780	0.152635	-234.4285880
185	cyclopropane	-116.604750	38.589	0.061495	-116.5432546
186	cyclobutene	-155.943940	58.439	0.093128	-155.8508116
187	cycloheptene	-273.903031	116.653	0.185898	-273.7171328
188	*trans*-cyclooctene	-313.1891759	135.458	0.215866	-312.9733100
189	1,3,5-cycloheptatriene	-271.467492	86.005	0.137058	-271.3304344
190	cyclopentene	-195.289518	78.091	0.124446	-195.1650722
191	cyclohexene	-234.603414	97.472	0.155331	-234.4480826
192	1,3-cyclopentadiene	-194.070782	62.290	0.099265	-193.9715166
193	1,3-cyclohexadiene	-233.379614	82.015	0.130699	-233.2489149
194	1-methylcyclopentene	-234.60111	96.824	0.154299	-234.4468113
195	3-methylcyclopentene	-234.596948	96.820	0.154292	-234.4426556
196	1,2-dimethylcyclopentene	-273.911868	115.624	0.184258	-273.7276096

197	1-methylcyclohexene	-273.91443	116.180	0.185136	-273.7292940
198	norbornadiene	-271.442428	85.701	0.136573	-271.3058549
199	acetylene (ethyne)	-77.321604	19.506	0.031085	-77.2905192
200	propyne	-116.637330	38.607	0.061524	-116.5758059
201	1-butyne	-155.941979	57.808	0.092123	-155.8498562
202	2-butyne	-155.95124	58.089	0.092571	-155.8596654
203	1-pentyne	-195.248053	76.781	0.122358	-195.1256948
204	2-pentyne	-195.255957	77.196	0.123020	-195.1329374
205	1-hexyne	-234.553488	95.739	0.152570	-234.4009183
206	2-hexyne	-234.561955	96.287	0.153443	-234.4085120
207	3-hexyne	-234.560616	96.442	0.153690	-234.4069260
208	4-nonyne	-352.478177	153.490	0.244602	-352.2335753
209	1-decyne	-391.775263	171.809	0.273795	-391.5014682
210	2,4-hexadiyne	-232.103589	**66.199**	0.105495	**-231.9980943**
211	indane	-348.934269	109.785	0.174953	-348.7593156
212	azulene	-385.777431	97.881	0.155983	-385.6214478
213	diphenylmethane	-502.54762	140.701	0.224221	-502.3233989
214	bibenzyl	-541.854568	159.697	0.254493	-541.6000748
215	benz[c]phenanthrene	-693.089455	161.950	0.258084	-692.8313715
216	triphenylmethane	-733.572875	196.036	0.312403	-733.2604720
217	1-methylnaphthalene	-425.149338	117.542	0.187315	-424.9620231
218	2-methylnaphthalene	-425.149653	117.396	0.187082	-424.9625707
219	acenaphthene	-463.251851	122.048	0.194496	-463.0573553
220	acenaphthylene	-462.029780	106.949	0.170434	-461.8593461
221	anthracene	-539.460143	130.027	0.207211	-539.2529320
222	benz[a]anthracene	-693.093811	161.589	0.257508	-692.8363028
223	benzene	-232.213348	67.309	0.107264	-232.1060844
224	biphenyl	-463.244901	121.806	0.194110	-463.0507909
225	biphenylene	-461.972934	106.548	0.169795	-461.8031391

226	chrysene	-693.098269	161.715	0.257709	-692.8405600
227	coronene	-921.797274	187.178	0.298287	-921.4989871
228	fluoranthene	-615.675199	138.540	0.220777	-615.4544216
229	fluorene	-501.358814	125.807	0.200486	-501.1583280
230	naphthacene	-693.076947	161.324	0.257086	-692.8198611
231	naphthalene	-385.840207	98.689	0.157271	-385.6829362
232	perylene	-769.316	170.317	0.271417	-769.0445828
233	phenanthrene	-539.470828	130.233	0.207539	-539.2632887
234	pyrene	-615.698533	138.633	0.220926	-615.4776074
235	triphenylene	-693.099608	161.970	0.258115	-692.8414926
	corannulene	-768.067282	155.545	0.24788	-767.8194055
	sumanene	-807.345351	174.112	0.27746	-807.0678861
	buckminsterfullerene(C_{60})	-2286.050997	253.032	0.403232	-2285.6477652
	C70 fullerene (C_{70})	-2667.153959	295.955	0.471634	-2666.6823251

$H_{298} = E_{Elec} + ZPE + H_T + RT$

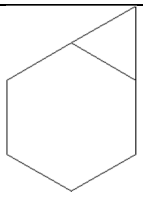
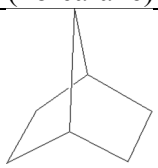
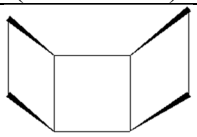
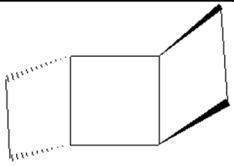
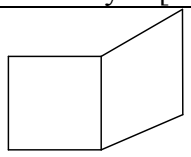
Table S5: Group Assignments and Number of Groups Assigned (Alkanes 1-95).

		CH_4	CH_3	CH_2	CH	>C<	CH_2 in a 5 member ring	CH in a 5 member ring	>C< in a 5 member ring	CH_2 in a 6 member	CH in a 6 member	>C< in a 6 member
1	methane	1										
2	ethane		2									
3	propane		2	1								
4	*n*-butane		2	2								
5	*n*-pentane		2	3								
6	*n*-hexane		2	4								
7	*n*-heptane		2	5								
8	*n*-octane		2	6								
9	*n*-nonane		2	7								
10	*n*-decane		2	8								
11	*n*-undecane		2	9								
12	*n*-dodecane		2	10								
13	*n*-tridecane		2	11								
14	*n*-tetradecane		2	12								
15	*n*-pentadecane		2	13								
16	*n*-hexadecane		2	14								
17	*n*-heptadecane		2	15								
18	*n*-octadecane		2	16								
19	*n*-nonadecane		2	17								
20	*n*-eicosane		2	18								
21	cyclopropane			3								
22	cyclobutane			4								
23	cyclopentane						5					
24	**cyclohexane**									6		
25	cycloheptane			7								
26	cyclooctane			8								
27	cyclononane			9								
28	cyclodecane			10								
29	cyclotetradecane			14								
30	methylcyclopentane		1				4	1				
31	1,1-dimethylcyclopentane		2				4		1			

32	ethylcyclopentane		1	1			4	1				
33	*n*-propylcyclopentane		1	2			4	1				
34	*n*-butylcyclopentane		1	3			4	1				
35	*n*-pentylcyclopentane		1	4			4	1				
36	*n*-hexylcyclopentane		1	5			4	1				
37	*n*-heptylcyclopentane		1	6			4	1				
38	*n*-octylcyclopentane		1	7			4	1				
39	*n*-nonylcyclopentane		1	8			4	1				
40	*n*-decylcyclopentane		1	9			4	1				
41	*n*-undecylcyclopentane		1	10			4	1				
42	*n*-dodecylcyclopentane		1	11			4	1				
43	*n*-tridecylcyclopentane		1	12			4	1				
44	*n*-tetradecylcyclopentane		1	13			4	1				
45	*n*-pentadecylcyclopentane		1	14			4	1				
46	*n*-hexadecylcyclopentane		1	15			4	1				
47	methycyclohexane		1							5	1	
48	1,1-dimethylcyclohexane		2							5		1
49	ethylcyclohexane		1	1						5	1	
50	*n*-propylcyclohexane		1	2						5	1	
51	*n*-butylcyclohexane		1	3						5	1	
52	*n*-pentylcyclohexane		1	4						5	1	
53	*n*-hexylcyclohexane		1	5						5	1	
54	*n*-heptylcyclohexane		1	6						5	1	
55	*n*-octylcyclohexane		1	7						5	1	
56	*n*-nonylcyclohexane		1	8						5	1	
57	*n*-decylcyclohexane		1	9						5	1	
58	*n*-undecylcyclohexane		1	10						5	1	
59	*n*-dodecylcyclohexane		1	11						5	1	
60	*n*-tridecylcyclohexane		1	12						5	1	
61	*n*-tetradecylcyclohexane		1	13						5	1	
62	*n*-pentadecylcyclohexane		1	14						5	1	
63	*n*-hexadecylcyclohexane		1	15						5	1	
64	2-methylpropane(isobutane)		3		1							
65	2-methylbutane		3	1	1							
66	2,2-dimethylpropane		4			1						
67	2-methylpentane		3	2	1							
68	3-methylpentane		3	2	1							
69	2-methylhexane		3	3	1							
70	3-methylhexane		3	3	1							
71	2,3-dimethylbutane		4		2							
72	2,2-dimethylbutane		4	1		1						
73	3-ethylpentane		3	3	1							
74	2,2-dimethylpentane		4	2		1						
75	R-2,3-dimethylpentane		4	1	2							
76	2,4-dimethylpentane		4	1	2							

77	3,3-dimethylpentane		4	2		1						
78	2,2,3-trimethylbutane		5		1	1						
79	2-methylheptane		3	4	1							
80	3-methylheptane		3	4	1							
81	4-methylheptane		3	4	1							
82	3-ethylhexane		3	4	1							
83	2,2-dimethylhexane		4	3		1						
84	2,3-dimethylhexane		4	2	2							
85	2,4-dimethylhexane		4	2	2							
86	2,5-dimethylhexane		4	2	2							
87	3,3-dimethylhexane		4	3		1						
88	3,4-dimethylhexane		4	2	2							
89	3-ethyl-2-methylpentane		4	2	2							
90	3-ethyl-3-methylpentane		4	3		1						
91	2,2,3-trimethylpentane		5	1	1	1						
92	2,3,3-trimethylpentane		5	1	1	1						
93	2,2,4-trimethylpentane		5	1	1	1						
94	2,3,4-trimethylpentane		5		3							
95	2,2,3,3-tetramethylbutane		6			2						

Table S5 Continued: Group Assignments and Number of Groups Assigned (Seven Polycyclic Alkanes 96-102).

		CH_3	CH_2	CH	CH_2 in a 6 member ring	CH in a 6 member ring	>C< in a 6 member ring	CH_2 in a 5 member ring	CH in a 5 member ring
96	 bicyclo[4.1.0]heptane (norcarane)		5	2					
97	 bicyclo[2.2.1]heptane (norbornane)							5	2
98	 *trans*-tricyclo[4.2.0.0^{2,5}]octane		4	4					
99	 *cis*- tricyclo[4.2.0.0^{2,5}]octane		4	4					
100	 bicyclo[2.2.0]hexane				4	2			

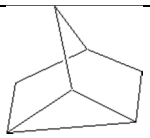
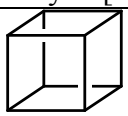
101	 tricyclo[2.2.1.$0^{2,6}$]heptane		3	4					
102	 cubane			8					

Table S5 Continued: Group Assignments and Number of Groups Assigned (The Adamantanes, Alkanes 103-109).

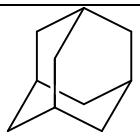
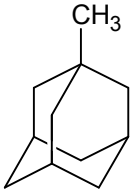
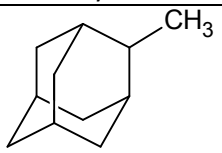
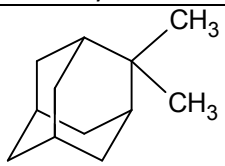
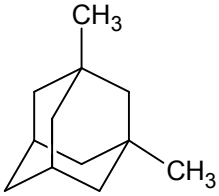
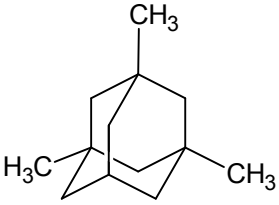
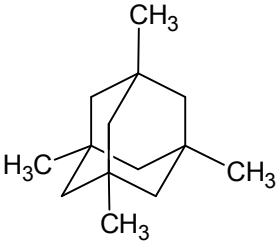
		CH_3	CH_2	CH	>C<
103	 adamantane		6	4	
104	 1-methyladamantane	1	6	3	1
`105	 2-methyladamantane	1	5	5	
106	 2,2-dimethyladamantane	2	5	4	1
107	 1,3-dimethyladamantane	2	6	2	2
108	 1,3,5-trimethyladamantane	3	6	1	3
109	 1,3,5,7-tetramethyladamantane	4	6		4

Table S5 Continued: Group Assignments and Number of Groups Assigned (Alkybenzenes 110-122).

		CH_3	CH_2	CH	>C<	C_B-(H)	C_B-(C)	ArC-CH_3	Phenyl-
110	toluene					5		1	
111	*p*-xylene					4		2	
112	*m*-xylene					4		2	
113	*o*-xylene					4		2	
114	ethylbenzene	1	1						1
115	1,3,5-trimethylbenzene					3		3	
116	*n*-propylbenzene	1	2						1
117	isopropylbenzene	2		1					1
118	*n-butylbenzene*	1	3						1
119	*t*-butylbenzene	3			1				1
120	1-methyl-2-ethylbenzene	2	1			4	2		
121	1-methyl-3-ethylbenzene	2	1			4	2		
122	1-methyl-4-ethylbenzene	2	1			4	2		

Table S5 Continued: Group Assignments and Number of Groups Assigned (Phenols and Naphthols 123-145).

		CH_3	CH_2	CH	>C<	C_B-(H)	C_B-(C)	ArC-OH	ArC- CH_3	$C_{BF}(C_B)_2(C_{BF})$
123	phenol					5		1		
124	1,2-dihydroxybenzene (1,2-benzenediol)					4		2		
125	1,3-dihydroxybenzene (resorcinol)					4		2		
126	1,4-dihydroxybenzene (hydroquinone)					4		2		
127	1,2,3-benzenetriol (pyrogallol)					3		3		
128	1,2,4-benzenetriol					3		3		
129	1,3,5-benzenetriol					3		3		
130	2-methylphenol (ortho-cresol)					4		1	1	
131	3-methylphenol (meta-cresol)					4		1	1	
132	4-methylphenol (p-cresol)					4		1	1	
133	2.3-dimethylphenol					3		1	2	
134	2,4-dimethylphenol					3		1	2	
135	2,5-dimethylphenol (2,5-xylenol)					3		1	2	
136	2,6-dimethylphenol					3		1	2	
137	3,4-dimethylphenol					3		1	2	
138	3,5-dimethylphenol (3,5-xylenol)					3		1	2	
139	2,3,6-trimethylphenol					2		1	3	
140	2,4,6-trimethylphenol					2		1	3	

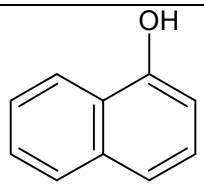
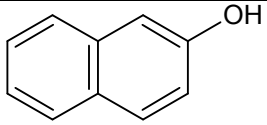
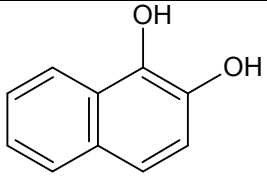
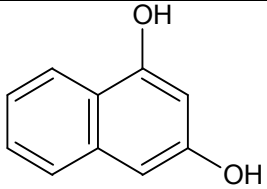
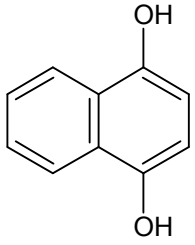
141	 1-naphthol					7	2	1		
142	 2-naphthol					7	2	1		
143	 1,2-naphthalenediol					6	2	2		
144	 1,3-naphthalenediol					6	2	2		
145	 1.4-naphtahlenediol					6	2	2		

Table S5 Continued: Group Assignments and Number of Groups Assigned (Alkenes 146-189).

		CH_3	CH_2	CH	>C<	$CH=CH_2$	*trans*-HC=CH	*cis*-HC=CH	$CH_2=C<$	>C=CH-	$HC=C=CH_2$
146	ethene					2	-1				
147	propene	1				1					
148	2-methylpropene (isobutene)	2							1		
149	1-butene	1	1			1					
150	*trans*-2-butene	2					1				
151	*cis*-2-butene	2						1			
152	propadiene (allene)					1	-1				1
153	1-pentene	1	2			1					
154	*trans*-2-pentene	2	1				1				
155	*cis*-2-pentene	2	1					1			
156	2-methyl-2-pentene	3	1							1	
157	1,2-butadiene	1									1
158	1,3-butadiene					2					
159	1,2-pentadiene	1	1								1
160	*trans*-1,3-pentadiene	1				1	1				
161	*cis*-1,3-pentadiene	1				1		1			
162	1,4-pentadiene		1			2					
163	2-methyl-1-butene	2	1						1		
164	3-methyl-1-butene	2		1		1					
165	2-methyl-2-butene	3								1	
166	1-hexene	1	3			1					

167	*trans*-2-hexene	2	2				1				
168	*cis*-2-hexene	2	2					1			
169	*trans*-3-hexene	2	2				1				
170	*cis*-3-hexene	2	2					1			
171	2-methyl-1-pentene	2	2						1		
172	3-methyl-1-pentene	2	1	1		1					
173	4-methyl-1-pentene	2	1	1		1					
174	3-methyl-*cis*-2-pentene	3	1	-2				1		1	
175	3-methyl-*trans*-2-pentene	3	1	-2			1			1	
176	*cis*-4-methyl-2-pentene	3		1				1			
177	1-octene	1	5			1					
178	*trans*-4-methyl-2-pentene	3		1			1				
179	1,5-hexadiene		2			2					
180	2-ethyl-1-butene	2	2						1		
181	2,3-dimethyl-1-butene	3		1					1		
182	3,3-dimethyl-1-butene	3			1	1					
183	2,3-dimethyl-2-butene	4				-2		1	2		
184	2,3-dimethyl-1,3-butadiene	2							2		
185	cyclopropene		1					1			
186	cyclobutene		2					1			
187	cycloheptene		5					1			
188	*trans*-cyclooctene		6					1			
189	1,3,5-cycloheptatriene		1					3			

Table S5 Continued: Group Assignments and Number of Groups Assigned (Cyclopentenes and Cyclohexenes 190-198).

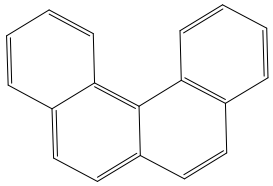
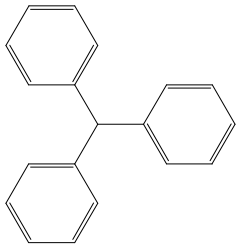
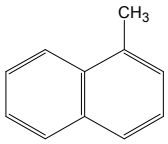
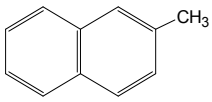
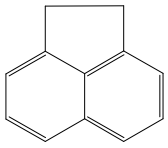
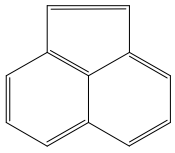
		CH_3	CH_2 in a 5 member ring	CH in a 5 member ring	>C< in a 5 member ring	HC=CH in a 5 member ring	HC=C< in a 5 member ring	>C=C< in a 5 member ring	CH_2 in a 6 member ring	CH in a 6 member ring	>C< in a 6 member ring	HC=CH in a 6 member ring	>C=CH i in a 6 member ring
190	cyclopentene		3			1							
191	cyclohexene								4			1	
192	1,3-cyclopentadiene		1			2							
193	1,3-cyclohexadiene								2			2	
194	1-methylcyclopentene	1	3				1						
195	3-methylcyclopentene	1	2	1		1							
196	1,2-dimethylcyclopentene	2	3					1					
197	1-methylcyclohexene	1							4				1
198	 norbornadiene		1							2		2	

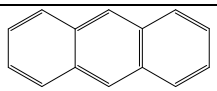
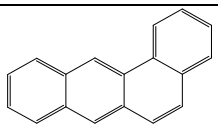
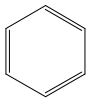
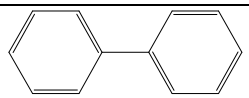
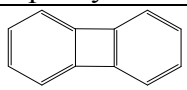
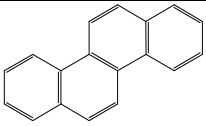
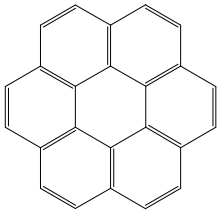
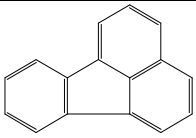
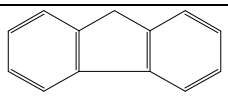
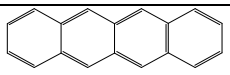
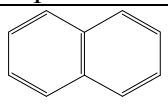
Table S5 Continued: Group Assignments and Number of Groups Assigned (Alkynes 199-210).

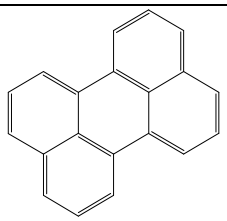
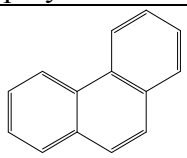
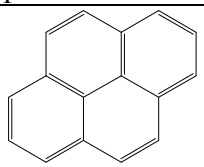
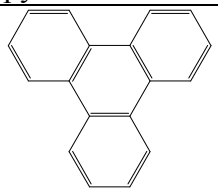
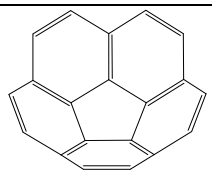
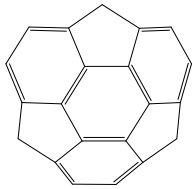
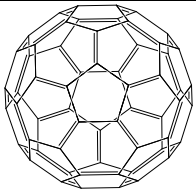
		CH_3	CH_2	CH	>C<	≡CH	≡C-
199	acetylene (ethyne)					2	
200	propyne	1	0			1	1
201	1-butyne	1	1			1	1
202	2-butyne	2					2
203	1-pentyne	1	2			1	1
204	2-pentyne	2	1				2
205	1-hexyne	1	3			1	1
206	2-hexyne	2	2				2
207	3-hexyne	2	2				2
208	4-nonyne	2	5				2
209	1-decyne	1	7			1	1
210	2,4-hexadiyne	2					4

Table S5 Continued: Group Assignments and Number of Groups Assigned (PAHs 211-235, plus corannulene, sumanene, C60 and C70).

		CH_3	CH_2	CH	>C<	Phenyl	C_B-(H)	C_B-(C)	ArC- CH_3	$C_{BF}(C_B)_2(C_{BF})$	C_{BF}-$(C_{BF})_3$	$C_{BF}(C_B)(C_{BF})_2$	C_B-H-$(C_{BF})_2$	HC=CH in a 5 member ring	HC=C-in a 5 member ring	CH_2in a 5 member ring	*cis*- HC=CH
211	indane						4	2								3	
212	azulene						5	1						1	1		
213	diphenylmethane		1				10	2									
214			2				10	2									

	bibenzyl																
215	 benzo[c]phenanthrene						12			3	1	2					
216	 triphenylmethane			1		3											
217	 1-methylnaphthalene						7	1	1	1							
218	 2-methylnaphthalene						7		1	2							
219	 acenaphthene		2				6	2		1	1						
220	 acenaphthylene						6	2		1	1						1

221	 anthracene						8			4			2				
222	 benz[a]anthracene						12			4		2					
223	 benzene						6										
224	 biphenyl						10	2									
225	 biphenylene						8	4									
226	 chrysene						12			2		4					
227	 coronene						12			6	6						
228	 fluoranthene						10	4		1	1						
229	 fluorene		1				8	2				2					
230	 naphthacene						8			6			4				
231	 napthalene						8			2							

232	 perylene						12			2	2	4					
233	 phenanthrene						10			2		2					
234	 pyrene						10			4	2						
235	 triphenylene						12	6									
	 corannulene						10			5	5						
	 sumanene		3				6	6			6						
	 buckminsterfullerene (C_{60})										60						

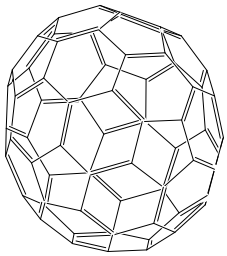
	 C70 fullerene (C_{70})										70						

Table S6: Data used to Calculate Composite $\Delta_f H^o_{g,298}$ Value for Pyrene.*

C_{60}	**Pyrene**	**Group Value**	**References**
$\Delta_f H^o_{g,298}$	**$\Delta_f H^o_{g,298}$**	**hartrees**	
kJ/mol	**kJ/mol**		
2508.0	224.0	-38.110050	Karton et al.[1]
2521.6	224.5	-38.110137	Karton et al.[1]
2535.2	224.9	-38.110223	Karton et al.[1]
2511.7	224.1	-38.110074	Wan and Karton [2]
2515.0	224.2	-38.110095	Wan and Karton [2]
2515.2	224.2	-38.110096	Wan and Karton [2]
2516	224.3	-38.110101	Dobek et al.[3]
2531	224.8	-38.110196	Dobek et al.[3]
2546	225.3	-38.110291	Dobek et al.[3]
2499.3	223.7	-38.109995	Chan et al.[4]
2520.0	224.4	-38.110126	Chan et al.[4]
2540.7	225.1	-38.110258	Chan et al.[4]
2529.6	224.7	-38.110187	Yu et al. [18]
2509.6	224.0	-38.110060	Yu et al. [18]
C_{70}	**Pyrene**	**Group Value**	**References**
$\Delta_f H^o_{g,298}$	**$\Delta_f H^o_{g,298}$**	**hartrees**	
kJ/mol	**kJ/mol**		
2665.7	223.6	-38.109966	Chan et al.[4]
2683.4	224.1	-38.110063	Chan et al.[4]
2701.1	224.6	-38.110159	Chan et al.[4]
2686.1	224.1	-38.110077	Sun et al.[21]
Composite Low	**223.9**	**-38.110033**	
Composite Mean	**224.4**	**-38.110129**	
Composite High	**224.9**	**-38.110224**	

Individual literature [1-4,18,21] $\Delta_f H^o_{g,298}$ values for C_{60} and C_{70} were used with training set values in place of pyrene. Linear regression analysis was then used to calculate group values for fused carbons bonded only to other fused carbons. These group values were then used to calculate a range of $\Delta_f H^o_{g,298}$ values for pyrene. Finally, the composite mean $\Delta_f H^o_{g,298}$ and standard deviation for pyrene was calculated along with the group value for the composite mean. Mean $\Delta_f H^o_{g,298}$ values as well as the upper and lower uncertainty values reported by Karton *et al.* [1], Dobek *et al.*[3] and Chan *et al.*[4] were used. Other $\Delta_f H^o_{g,298}$ values represent individual $\Delta_f H^o_{g,298}$ values for C_{60} and C_{70} reported by the various research groups [2, 18, 21].

Table S7. Comparison of Heat of Formation ($\Delta_f H^o_{g,298}$) Values Calculated using Density Functional Theory/Group Equivalents and other Approaches.

Compound	Reference/ Experimental	This study	Allison & Burgess [23]	Blanquart & Pitsch [22]	Sivar.amakr-ishman *et al.* [20]	Yu *et al.* [18]	Yu *et al.* [18]	Rayne [26]
				G3MP2B3	RCIR	Homo Iso	BCGA	G4MP2
	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol
1-methylnaphthalene	116.9	117.2	113.5		130.0			103.8
2-methylnaphthalene	116.1	116.3	108.7					102.9
acenaphthene	156.8	156.5	150.7		173.6			143.3
acenaphtylene	265.5	265.2	259.8		268.9	259.8	263.6	245.9
anthracene	227.1	227.1	222.6	230.11	225.1	234.7	233.9	210.8
benz[a]anthracene	278.7	279.7	277.1		286.1	279.1	275.3	254.7
benzene	83.2	83.2	75.2	82.99		82.8	80.3	
biphenyl	180.3	179.5	174.2		186.7			165.7
biphenylene	420.4	419.2	410.9		414.6			403.1
chrysene	263.5	261.9	271.1	259.86	278.8	259.0	262.8	
coronene	279.7	280.1	296.7	292.43	308.4	314.6	326.8	
fluoranthene	289.8	287.0	277.9		294.8	281.6	275.3	262.6
fluorene	179.4	182.9	179.6					172.2
naphthacene	310.7	311.7	310.5		319.4	324.7	319.2	
naphthalene	150.6	150.6	141.0	148.83	155.0	150.6	153.1	137.1
perylene	306.0	304.1	319.2	306.11	308.5	320.1	311.7	
phenanthrene	202.2	202.2	202.7	201.76	204.5	201.3	197.9	187.8
pyrene	224.0	224	221.3	226.09	237.5	235.1	250.2	203.4
triphenylene	270.1	269.7	275.1		281.8	274.9	268.6	
MAD		0.9 (1.2)*	6.3	3.0 (1.6)**	9.2 (7.9)**	8.1 (5.5)**	9.7 (6.6)**	16.5
RMS		1.3 (1.5)*	7.7	4.9 (2.1)**	11.5 (9.3)**	12.2 (7.7)**	16.0 (9.6)	17.3

*Values in parentheses represent analyses in which $\Delta_f H^o_{g,298}$ values of compounds in the training set have been omitted. **Values in parentheses represent analyses in which $\Delta_f H^o_{g,298}$ value of coronene has been omitted. *** Values in parentheses represent analyses in which $\Delta_f H^o_{g,298}$ value of biphenylene has been omitted.

Table S7 (Continued). Comparison of Heat of Formation ($\Delta_f H^o_{g,298}$) Values Calculated using Density Functional Theory/Group Equivalents and other Approaches.

Compound	Reference/ Experimental	Welsh [14]	Alberty and Reif [5,6]	Wang & Frenklach [12]	Wang & Frenklach [12]	Wang & Frenklach [12]	Wang & Frenklach [12]
				AM1	AM1 GC2	AM1 GC4a	AM1 GC4b
	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol
1-methylnaphthalene	116.9						
2-methylnaphthalene	116.1						
acenaphthene	156.8	154.0					
acenaphtylene	265.5	176.9					
anthracene	227.1	226.4	218.3	263.2	230.1	231.4	228.0
benz[a]anthracene	278.7	303.8	276.9	327.2	282.4	282.8	283.7
benzene	83.2		82.8	92.0	82.8	83.7	83.7
biphenyl	180.3	180.2					
biphenylene	420.4	191.9					
chrysene	263.5	275.6	267.7	319.2	274.5	274.1	280.3
coronene	279.7	352.8		402.5	331.0	286.6	296.2
fluoranthene	289.8	284.7					
fluorene	179.4	167.0					
naphthacene	310.7	297.0	286.1	363.6	318.8	319.7	315.1
naphthalene	150.6	158.4	150.6	169.9	149.0	149.8	148.1
perylene	306.0	330.0		373.6	319.7	304.6	315.5
phenanthrene	202.2	207.0	209.1	240.2	207.1	207.5	210.0
pyrene	224.0	225.8		281.6	239.7	225.5	227.2
triphenylene	270.1	276.1	258.5	315.9	271.1	270.3	281.6
MAD		31.7 (18.5)***	7.3	50.3	10.4	4.1	7.2
RMS		64.8 (31.7)***	10.5	57.6	17.3	5.3	9.0

Values in parentheses represent analyses in which $\Delta_f H^o_{g,298}$ value of coronene has been omitted. * Values in parentheses represent analyses in which $\Delta_f H^o_{g,298}$ value of biphenylene has been omitted.

Table S7 (Continued). Comparison of Heat of Formation ($\Delta_f H^o_{g,298}$) Values Calculated using Density Functional Theory/Group Equivalents and other Approaches

Compound	Reference/ Experimental	Herndon [13]	Herndon [13]	Herndon [13]	Schulman *et al.* [8]	Schulman *et al.* [8]	Schulman *et al.* [8]
		1	2	3	STO-3G	3-21 G	6-31 G*
	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol
1-methylnaphthalene	116.9						
2-methylnaphthalene	116.1						
acenaphthene	156.8	154.2	154.8	153.7			
acenaphtylene	265.5	265.9	266.0	264.9	278.7	274.9	264.4
anthracene	227.1	230.7	231.3	229.7	238.5	233.5	231.0
benz[a]anthracene	278.7	284.6	284.1	283.0	279.5	277.4	274.5
benzene	83.2	72.2	71.4	72.3	83.7	86.2	87.0
biphenyl	180.3	170.6	170.2	170.2			
biphenylene	420.4	412.1	411.6	411.5	449.8	446.0	419.2
chrysene	263.5	274.7	274.9	273.1	261.5	264.0	264.8
coronene	279.7				256.1	259.4	258.2
fluoranthene	289.8	285.9	285.8	284.3			
fluorene	179.4						
naphthacene	310.7				341.0	329.3	322.2
naphthalene	150.6	141.8	141.3	140.9	148.5	149.0	148.1
perylene	306.0	332.9	333.3	330.7	305.9	310.0	310.5
phenanthrene	202.2	203.5	203.4	202.4	199.6	200.8	201.7
Pyrene	224.0	230.5	231.0	228.9	219.7	215.9	214.2
triphenylene	270.1	276.2	275.4	274.6	255.6	261.5	265.3
MAD		7.6	7.7	7.1	10.4 (9.3)**	8.4 (7.4)**	5.4 (4.1)**
RMS		9.9	10.1	9.3	14.9 (13.9)**	11.5 (10.4)**	7.8 (5.2)**

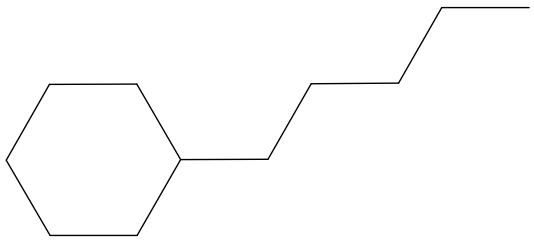
**Values in parentheses represent analyses in which $\Delta_f H^o_{g,298}$ value of coronene has been omitted.

Table S7 (Continued). Comparison of Heat of Formation ($\Delta_f H^o_{g,298}$) Values Calculated using Density Functional Theory/Group Equivalents and other Approaches.

Compound	Reference/ Experimental	Peck et al.[10]	Disch et al.[11]	Peck et al.[10] Disch et al.[11] (Composite)	Zauer[29]
	kJ/mol	kJ/mol	kJ/mol		*kJ/mol*
1-methylnaphthalene	116.9				
2-methylnaphthalene	116.1				
acenaphthene	156.8	146.0		146.0	146.8
acenaphtylene	265.5	264.0		264.0	286.2
anthracene	227.1	230.1		230.1	221.1
benz[a]anthracene	278.7				277.1
benzene	83.2	87.0	82.4	82.4	
biphenyl	180.3				165.1
biphenylene	420.4	419.7		419.7	430.9
chrysene	263.5	264.4		264.4	269.7
coronene	279.7	257.3	283.7	283.7	414.4
fluoranthene	289.8				312.4
fluorene	179.4				189.8
naphthacene	310.7	323.0		323.0	308.8
naphthalene	150.6	148.1		148.1	139.5
perylene	306.0	310.0	324.7	324.7	317.5
phenanthrene	202.2	201.3	205.4	205.4	201.1
pyrene	224.0	214.6	224.3	224.3	237.2
triphenylene	270.1	266.1	274.5	274.5	267.2
MAD		5.9	5.1	5.2	17.5 (9.7)**
RMS		8.4	8.0	8.1	35.5 (11.6)**

**Values in parentheses represent analyses in which $\Delta_f H^o_{g,298}$ value of coronene has been omitted.

Table S8: Selected Examples of Calculations used to Predict $\Delta_f H^o_{g,298}$ Values using the Density Functional Theory/Group Equivalent Approach.



pentylcyclohexane

(H_{298} = -432.027428)

Group present	Number of groups present	Group value (hartrees)
$-CH_3$	1	-39.844747
$-CH_2-$	4	-39.267306
$-CH_2-$ (in a cyclohexane ring)	5	-39.267119
–CH- (in a cyclohexane ring)	1	-38.688677

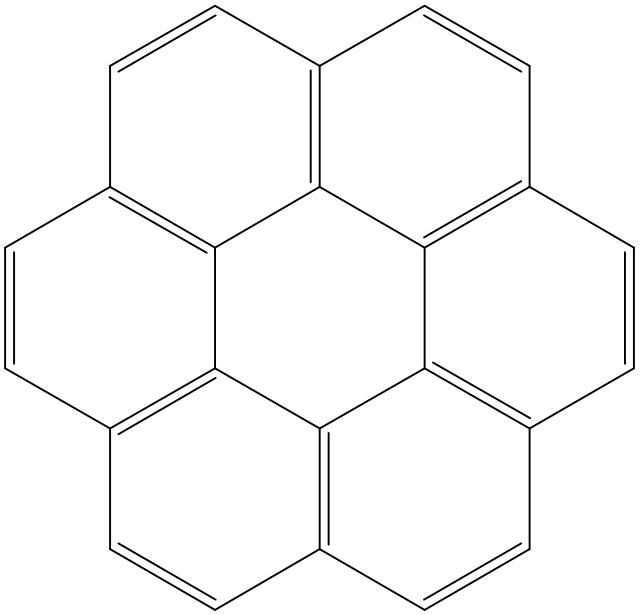
$$\Delta_f H^o_{298\ (g)} = H_{298} - \Sigma n_j \epsilon_j$$

$$\Delta_f H^o_{298\ (g)} = (-432.027428) - \big(\big((1)x(-39.844747)\big) + \big((4)x(-39.267306)\big) + \big((5)x(-39.267119)\big) + \big((1)x(-38.688677)\big)\big)$$

$$\Delta_f H^o_{298\ (g)} = ((-432.027428) - (-431.938243))$$

$\Delta_f H^o_{298\ (g)}$ =-0.089184 hartrees

$\Delta_f H^o_{298\ (g)}$ =-234.15 kJ/mol = -234.2 kJ/mol



coronene

(H_{298} = -921.4989871)

Group present	Number of groups present	Group value (hartrees)
C_B-H	12	-38.689629
C_{BF}-$(C_B)_2$(C_{BF})	6	-38.111633
C_{BF}-$(C_{BF})_3$	6	-38.110052

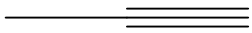
$\Delta_f H^o_{298\ (g)} = H_{298} - \Sigma n_j \epsilon_j$

$\Delta_f H^o_{298\ (g)} = (-921.4989871 - (((12)x(-38.689629)) + ((6)x(-38.111633)) + ((6)x(-38.110052)))$

$\Delta_f H^o_{298\ (g)} = ((-921.4989871) - (-921.605658))$

$\Delta_f H^o_{298\ (g)} = 0.106671$ hartrees

$\Delta_f H^o_{298\ (g)} = 280.06$ kJ/mol = 280.1 kJ/mol



propyne

(H_{298} = -116.5758059)

Group present	Number of groups present	Group value (hartrees)
$-CH_3$	1	-39.844747
≡C−	1	-38.113037
≡C−H	1	-38.688739

$\Delta_f H^o_{298\ (g)} = H_{298} - \Sigma n_j \epsilon_j$

$\Delta_f H^o_{298\ (g)} = (-116.5758059) - (\ (-39.844747) + (-38.113037) + (-38.688739)\ )$

$\Delta_f H^o_{298\ (g)} = (-116.5758059) - (-116.646523)$

$\Delta_f H^o_{298\ (g)} = 0.070717$ hartrees

$\Delta_f H^o_{298\ (g)} = 185.67$ kJ/mol = 185.7 kJ/mol