Supplementary Information

G4MP2 Energies for the 133,000 GDB9 Set of Molecules

Badri Narayanan,[1,2] Paul Redfern,[2] Rajeev S. Assary,[2] and Larry A. Curtiss[2]

[1]Department of Mechanical Engineering, University of Louisville, Louisville, Kentucky 40292

[2]Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439

Description of the G4MP2 database for GDB9 molecules

The atomic coordinates for equilibrium configurations of 133,296 molecules belonging to the GDB9 dataset, as well as their G4MP2-derived values of energy (at 0 K and 298 K), enthalpy, free energy, standard enthalpy of formation, and atomization energy are all provided as an ASE database (available at https://doi.org/10.18126/M23P9G).

The ASE database can be accessed using the ASE module within a Python script. Table S1 lists all the available quantities, and their associated ASE database keys; also an example Python script is provided (Code Snippet S1) showing how to extract G4MP2 data for a molecule whose InChI representation is known. Note, a user can obtain SMILES/InChI representation for any molecule from a variety of sources, including OpenBabel, PubChem, and others. Certain web-browser based packages, such as PubSketch (https://pubchem.ncbi.nlm.nih.gov/edit2/index.html), provide an online graphic-user-interface, wherein, a user can draw the molecule of interest and retrieve its InChI/SMILES representation.

Table S1. G4MP2 database for GDB9 molecules called `g4mp2-gdb9.gdb`. The database keys to access different G4MP2 values along with their units are provided. Note the atomic coordinates, and chemical formula of the molecules can also be accessed using the standard ASE Atoms class, and its associated methods (e.g., `get_positions()`, `get_chemical_symbols()`, `get_chemical_formula()`; see https://wiki.fysik.dtu.dk/ase/ase/atoms.html)

Quantity	Database key name	Units
Zero-point Energy	`g4mp2_ZPE`	Ha
Energy (0 K)	`g4mp2_E0K`	Ha
Energy (298 K)	`g4mp2_Energy`	Ha
Enthalpy (298 K)	`g4mp2_Enthalpy`	Ha
Free Energy (298 K)	`g4mp2_FreeE`	Ha
Standard enthalpy of formation	`g4mp2_Standard_Enthalpy_Formation`	kcal/mol
Atomization Energy	`g4mp2_AtomizationE`	kcal/mol
Isomeric SMILES	`smiles`	-
InChI	`InChI`	-

Code Snippet S1. Example Python script showing how to retrieve G4MP2 data from our database file (g4mp2-gdb9.db) for a GDB9 molecule using its InChI representation. Similarly, G4MP2 information can also be retrieved using SMILES representation, or for a collection of molecules using methods within ASE `Atoms` class.

```
import ase.db

# Connect to the ASE database
db = ase.db.connect('g4mp2-gdb9.db')

# Find a molecule using its InChI representation
mol = db.get(InChI='InChI=1S/C7H12O2/c1-2-4-6-5(3-8)7(4)9-6/h4-8H,2-3H2,1H3/t4-,5-
,6+,7-')

# Get G4MP2 properties

## Energy (0K), in Ha
E_0K = mol.g4mp2_E0K

## Energy (298 K), in Ha
Energy = mol.g4mp2_Energy

## Enthalpy (298 K), in Ha
Enthalpy = mol.g4mp2_Enthalpy

## Free Energy (298 K), in Ha
FreeE = mol.g4mp2_FreeE

## Standard enthalpy of formation, in kcal/mol
deltaH = mol.g4mp2_Standard_Enthalpy_Formation

## Atomization energy, in kcal/mol
deltaH = mol.g4mp2_AtomizationE

## SMILES
smiles = mol.Smiles
```

We can also use this retrieval technique to compute reaction energies. For example, Code Snippet S2 can be used to compute reaction energy of CH_3— O —CH_3 + H_2O → CH_3—OH + CH_3—OH

Code Snippet S2. Example Python script showing how to calculate reaction energy

```
import ase.db

# Connect to the ASE database
db = ase.db.connect('g4mp2-gdb9.db')

# InChI representations (from PubChem)
## Reactants R1 and R2
## R1: CH3-O-CH3
## R2: H2O

R1_inchi = 'InChI=1S/C2H6O/c1-3-2/h1-2H3'
R2_inchi = 'InChI=1S/H2O/h1H2'

## Product
## 2 * CH3-OH

P_inchi  = 'InChI=1S/CH4O/c1-2/h2H,1H3'


# Find reactants R1 and R2, and product P using their InChI representation

R1 = db.get(InChI = R1_inchi)
R2 = db.get(InChI = R2_inchi)

P  = db.get(InChI = P_inchi)


# Get G4MP2 energies

R1_E = R1.g4mp2_E0K
R2_E = R2.g4mp2_E0K
P_E  = P.g4mp2_E0K

# Calculate Reaction Energy in kcal/mol

Reaction_energy = (2*P_E – (R1_E + R2_E))* 627.509
```

Table S2 Comparison of G4MP2 and experimental (see text for reference) enthalpies of formation of the Pedley test set.

			ΔH_f^o(298 K) values (kcal/mol)		Difference (kcal/mol)
	Formula	Name	Expt	G4MP2	Expt -theory
1	CH4	Methane	-17.78	-17.65	-0.13
2	C2H2	Acetylene	54.54	54.25	0.29
3	C2H4	Ethylene	12.55	12.05	0.49
4	C2H6	Ethane	-20.03	-19.79	-0.24
5	C3H4	Propyne	44.19	44.07	0.12
6	C3H4	Allene	45.53	44.52	1.01
7	C3H4	Cyclopropene	66.23	67.51	-1.28
8	C3H6	Propene	4.78	4.47	0.31
9	C3H6	Cyclopropane	12.74	13.00	-0.26
10	C3H8	Propane	-25.02	-24.74	-0.28
11	C4H6	1-Butyne	39.48	39.67	-0.18
12	C4H6	2-Butyne	34.82	34.72	0.11
13	C4H6	1,2-Butadiene	38.79	38.15	0.64
14	C4H6	1,3-Butadiene	26.29	25.71	0.58
15	C4H6	Cyclobutene	37.45	38.26	-0.81
16	C4H6	Methylenecyclopropane	47.92	45.69	2.23
17	C4H6	1-Methylcyclopropene	58.22	57.20	1.02
18	C4H6	Bicyclo[1.1.0]butane	51.89	53.09	-1.20
19	C4H8	1-Butene	0.02	-0.20	0.22
20	C4H8	(Z)-2-Butene	-1.70	-1.53	-0.17
21	C4H8	(E)-2-Butene	-2.72	-2.76	0.04
22	C4H8	2-Methylpropene	-4.04	-4.30	0.26
23	C4H8	Cyclobutane	6.79	6.69	0.10
24	C4H10	Butane	-30.02	-29.83	-0.19
25	C4H10	2-Methylpropane	-32.07	-31.84	-0.23
26	C5H6	1,3-Cyclopentadiene	32.10	31.28	0.82
27	C5H8	1,2-Pentadiene	33.63	33.21	0.42
28	C5H8	(Z)-1,3-Pentadiene	19.46	19.31	0.15
29	C5H8	(E)-1,3-Pentadiene	18.19	18.01	0.18
30	C5H8	1,4-Pentadiene	25.24	24.87	0.37
31	C5H8	2,3-Pentadiene	31.81	31.66	0.16
32	C5H8	2-Methyl-1,3-butadiene	18.04	17.33	0.72
33	C5H8	Cyclopentene	8.10	8.33	-0.23

34	C5H8	Spiropentane	44.26	44.05	0.22
35	C5H8	Methylenecyclobutane	29.04	28.85	0.19
36	C5H10	1-Pentene	-5.09	-5.39	0.30
37	C5H10	(Z)-2-Pentene	-6.60	-6.24	-0.36
38	C5H10	(E)-2-Pentene	-7.62	-7.54	-0.09
39	C5H10	2-Methyl-1-butene	-8.44	-8.58	0.14
40	C5H10	3-Methyl-1-butene	-6.60	-7.14	0.54
41	C5H10	2-Methyl-2-butene	-9.99	-9.96	-0.03
42	C5H10	Cyclopentane	-18.26	-18.12	-0.14
43	C5H10	1,1-Dimethylcyclopropane	-1.96	-2.46	0.50
44	C5H12	Pentane	-35.11	-34.91	-0.20
45	C5H12	2-Methylbutane	-36.74	-35.56	-1.18
46	C5H12	2,2-Dimethylpropane	-40.18	-40.22	0.05
47	C6H6	Benzene	19.74	18.78	0.96
48	C6H8	1,3-Cyclohexadiene	25.38	24.86	0.52
49	C6H10	1,5-Hexadiene	20.10	19.32	0.78
50	C6H10	2,3-Dimethyl-1,3-butadiene	10.78	9.89	0.89
51	C6H10	1-Methylcyclopentene	-0.91	-0.91	0.00
52	C6H10	3-Methylcyclopentene	1.77	1.21	0.56
53	C6H10	4-Methylcyclopentene	3.49	1.26	2.23
54	C6H10	Cyclohexene	-1.20	-1.26	0.07
55	C6H10	Bicyclopropyl	30.93	32.00	-1.07
56	C6H10	Methylenecyclopentane	2.87	2.46	0.41
57	C6H10	Bicyclo[3.1.0]hexane	9.15	8.61	0.55
58	C6H12	1-Hexene	-10.40	-10.49	0.10
59	C6H12	(Z)-2-Hexene	-12.50	-11.50	-1.00
60	C6H12	(E)-2-Hexene	-12.88	-12.75	-0.14
61	C6H12	(Z)-3-Hexene	-11.38	-11.00	-0.38
62	C6H12	(E)-3-Hexene	-13.00	-12.36	-0.64
63	C6H12	2-Methyl-1-pentene	-14.20	-13.79	-0.41
64	C6H12	3-Methyl-1-pentene	-11.83	-12.44	0.61
65	C6H12	4-Methyl-1-pentene	-12.26	-12.63	0.37
66	C6H12	2-Methyl-2-pentene	-15.99	-14.78	-1.20
67	C6H12	(Z)-3-Methyl-2-pentene	-14.89	-14.38	-0.51
68	C6H12	(E)-3-Methyl-2-pentene	-15.08	-14.34	-0.74
69	C6H12	(Z)-4-Methyl-2-pentene	-13.74	-13.25	-0.50
70	C6H12	(E)-4-Methyl-2-pentene	-14.70	-14.54	-0.16
71	C6H12	2-Ethyl-1-butene	-13.38	-12.97	-0.41
72	C6H12	2,3-Dimethyl-1-butene	-14.96	-14.98	0.02

73	C6H12	3,3-Dimethyl-1-butene	-14.46	-14.91	0.45
74	C6H12	2,3-Dimethyl-2-butene	-16.30	-15.38	-0.92
75	C6H12	Methylcyclopentane	-25.38	-25.03	-0.36
76	C6H12	Cyclohexane	-29.49	-29.05	-0.44
77	C6H12	Ethylcyclobutane	-6.29	-6.57	0.28
78	C6H14	Hexane	-39.94	-40.01	0.07
79	C6H14	2-Methylpentane	-41.78	-41.51	-0.27
80	C6H14	3-Methylpentane	-41.13	-40.87	-0.26
81	C6H14	2,3-Dimethylbutane	-42.61	-42.14	-0.48
82	C6H14	2,2-Dimethylbutane	-44.48	-44.21	-0.27
83	C7H8	1,3,5-Cycloheptatriene	43.24	42.79	0.45
84	C7H8	Methylbenzene	12.05	10.89	1.15
85	C7H8	Quadricyclane	81.05	78.77	2.27
86	C7H10	1,3-Cycloheptadiene	22.54	22.03	0.51
87	C7H10	Tricyclo[4.1.0.02,4]heptane	35.66	36.45	-0.79
88	C7H12	1-Ethylcyclopentene	-4.71	-5.84	1.13
89	C7H12	Ethylidenecyclopentane	-4.33	-4.52	0.19
90	C7H12	1-Methylcyclohexene	-10.35	-10.21	-0.14
91	C7H12	Cycloheptene	-2.20	-1.65	-0.55
92	C7H12	Bicyclo[2.2.1]heptane	-13.12	-13.81	0.68
93	C7H12	1-Methyl-bicyclo[3.1.0]-hexane	0.36	-0.19	0.55
94	C7H14	1-Heptene	-14.89	-15.61	0.72
95	C7H14	5-Methyl-1-hexene	-15.70	-16.28	0.57
96	C7H14	(Z)-3-Methyl-3-hexene	-18.98	-19.31	0.33
97	C7H14	(E)-3-Methyl-3-hexene	-18.36	-19.19	0.84
98	C7H14	2,4-Dimethyl-1-pentene	-20.03	-21.30	1.27
99	C7H14	4,4-Dimethyl-1-pentene	-19.50	-20.52	1.02
100	C7H14	2,4-Dimethyl-2-pentene	-21.20	-21.85	0.65
101	C7H14	(Z)-4,4-Dimethyl-2-pentene	-17.35	-18.24	0.89
102	C7H14	(E)-4,4-Dimethyl-2-pentene	-21.22	-22.28	1.06
103	C7H14	3-Methyl-2-ethyl-1-butene	-19.00	-19.33	0.33
104	C7H14	2,3,3-Trimethyl-1-butene	-20.43	-21.77	1.33
105	C7H14	1,1-Dimethylcyclopentane	-33.03	-33.32	0.29
106	C7H14	cis-1,2-dimethylcyclopentane	-30.95	-31.28	0.33
107	C7H14	trans-1,2-dimethylcyclopentane	-32.65	-32.73	0.09
108	C7H14	cis-1,3-dimethylcyclopentane	-32.48	-32.34	-0.14
109	C7H14	trans-1,3-dimethylcyclopentane	-31.93	-32.07	0.14
110	C7H14	Ethylcyclopentane	-30.33	-30.63	0.30
111	C7H14	Methylcyclohexane	-36.97	-36.80	-0.17

112	C7H14	Cycloheptane	-28.23	-27.83	-0.39
113	C7H16	Heptane	-44.86	-45.13	0.27
114	C7H16	2-Methylhexane	-46.51	-45.81	-0.70
115	C7H16	3-Methylhexane	-45.72	-45.60	-0.13
116	C7H16	3-Ethylpentane	-45.32	-45.13	-0.18
117	C7H16	2,2-Dimethylpentane	-49.21	-49.32	0.11
118	C7H16	2,3-Dimethylpentane	-47.54	-46.69	-0.85
119	C7H16	2,4-Dimethylpentane	-48.21	-45.23	-2.98
120	C7H16	3,3-Dimethylpentane	-48.09	-48.52	0.43
121	C7H16	2,2,3-Trimethylbutane	-48.88	-49.23	0.35
122	C8H8	1,3,5,7-Cyclooctatetraene	70.72	69.52	1.20
123	C8H8	Ethenylbenzene	35.35	33.69	1.66
124	C8H10	Ethylbenzene	7.15	5.64	1.51
125	C8H10	1,2-Dimethylbenzene	4.57	2.81	1.75
126	C8H10	1,3-Dimethylbenzene	4.13	3.09	1.04
127	C8H10	1,4-Dimethylbenzene	4.30	3.21	1.09
128	C8H12	Bicyclo[2.2.2]oct-2-ene	4.90	4.30	0.60
129	C8H12	4-Ethenylcyclohexene	15.56	15.57	-0.01
130	C8H12	(Z,Z)-1,5-Cyclooctadiene	24.16	23.10	1.06
131	C8H14	(2-Propenyl)cyclopentane	-5.76	-5.98	0.22
132	C8H14	1-Ethylcyclohexene	-15.15	-14.67	-0.48
133	C8H14	Ethylidenecyclohexane	-14.70	-14.28	-0.42
134	C8H14	Ethenylcyclohexane	-11.69	-12.21	0.52
135	C8H14	Cyclooctene	-6.45	-6.14	-0.31
136	C8H14	Bicyclo[4.2.0]octane	-6.26	-5.98	-0.28
137	C8H14	Bicyclo[5.1.0]octane	-3.97	-2.55	-1.42
138	C8H14	cis-Bicyclo[3.3.0]octane	-22.20	-23.24	1.04
139	C8H14	trans-Bicyclo[3.3.0]octane	-15.92	-14.62	-1.30
140	C8H14	Bicyclo[2.2.2]octane	-23.66	-23.05	-0.61
141	C8H14	1-Methylbicyclo[4.1.0]-heptane	-4.97	-6.02	1.05
142	C8H16	1-Octene	-19.46	-20.72	1.27
143	C8H16	(Z)-2,2-Dimethyl-3-hexene	-21.34	-23.30	1.95
144	C8H16	(E)-2,2-Dimethyl-3-hexene	-25.74	-27.20	1.46
145	C8H16	2-Methyl-3-ethyl-1-pentene	-23.97	-26.16	2.18
146	C8H16	2,4,4-Trimethyl-1-pentene	-26.43	-27.88	1.44
147	C8H16	2,4,4-Trimethyl-2-pentene	-25.07	-26.66	1.59
148	C8H16	Propylcyclopentane	-35.30	-35.82	0.52
149	C8H16	Ethylcyclohexane	-41.04	-41.39	0.35
150	C8H16	1,1-Dimethylcyclohexane	-43.24	-44.18	0.94

151	C8H16	cis-1,2-Dimethylcyclohexane	-41.13	-41.91	0.77
152	C8H16	trans-1,2-Dimethylcyclohexane	-43.00	-43.63	0.63
153	C8H16	cis-1,3-Dimethylcyclohexane	-44.12	-44.58	0.46
154	C8H16	trans-1,3-Dimethylcyclohexane	-42.18	-42.74	0.56
155	C8H16	cis-1,4-Dimethylcyclohexane	-42.21	-42.76	0.55
156	C8H16	trans-1,4-Dimethyl-cyclohexane	-44.10	-44.54	0.45
157	C8H16	Cyclooctane	-29.73	-29.53	-0.21
158	C8H18	Octane	-49.86	-50.24	0.39
159	C8H18	2-Methylheptane	-51.48	-50.94	-0.54
160	C8H18	3-Methylheptane	-50.79	-51.15	0.36
161	C8H18	4-Methylheptane	-50.67	-51.11	0.44
162	C8H18	2,2-Dimethylhexane	-53.68	-54.53	0.85
163	C8H18	2,5-Dimethylhexane	-53.18	-52.42	-0.76
164	C9H8	Indene	39.05	36.31	2.75
165	C9H10	2,3-Dihydro-1H-indene	14.51	12.78	1.72
166	C9H10	Cyclopropylbenzene	35.97	35.71	0.26
167	C9H12	Propylbenzene	1.89	0.25	1.64
168	C9H12	(1-Methylethyl)benzene	0.96	-0.91	1.87
169	C9H12	1-Ethyl-2-methylbenzene	0.31	-1.82	2.13
170	C9H12	1-Ethyl-3-methylbenzene	-0.43	-2.19	1.76
171	C9H12	1-Ethyl-4-methylbenzene	-0.76	-2.04	1.28
172	C9H12	1,2,3-Trimethylbenzene	-2.27	-3.86	1.59
173	C9H12	1,2,4-Trimethylbenzene	-3.30	-4.88	1.58
174	C9H12	1,3,5-Trimethylbenzene	-3.80	-4.72	0.92
175	C9H12	(Z)-5-Ethylidene-bicyclo[2.2.1]hept-2-ene	34.82	33.16	1.66
176	CH2O	Formaldehyde	-25.96	-26.82	0.86
177	CH4O	Methanol	-48.16	-47.82	-0.34
178	C2H2O	Ketene	-11.35	-11.69	0.34
179	C2H4O	Acetaldehyde	-39.70	-39.61	-0.09
180	C2H4O	Oxirane	-12.57	-12.60	0.03
181	C2H6O	Ethanol	-56.21	-55.50	-0.72
182	C2H6O	Dimethyl ether	-44.00	-43.71	-0.29
183	C3H6O	2-Propen-1-ol	-29.76	-30.31	0.56
184	C3H6O	Propanal	-44.36	-44.75	0.39
185	C3H6O	Acetone	-51.94	-51.39	-0.54
186	C3H6O	Methyloxirane	-22.63	-22.33	-0.30
187	C3H6O	Oxetane	-19.24	-18.76	-0.48
188	C3H8O	1-Propanol	-60.97	-60.33	-0.64
189	C3H8O	2-Propanol	-65.20	-64.48	-0.72

190	C3H8O	Methoxyethane	-51.72	-51.79	0.07
191	C4H4O	Furan	-8.34	-8.49	0.15
192	C4H6O	trans-2-Butenal	-24.04	-24.86	0.81
193	C4H6O	Divinyl ether	-3.25	-3.04	-0.21
194	C4H8O	Butanal	-48.95	-49.58	0.63
195	C4H8O	2-Methylpropanal	-51.58	-50.96	-0.62
196	C4H8O	2-Butanone	-57.05	-56.61	-0.45
197	C4H8O	Ethoxyethene	-33.65	-31.61	-2.05
198	C4H8O	Tetrahydrofuran	-44.02	-42.96	-1.06
199	C4H10O	1-Butanol	-65.73	-65.27	-0.46
200	C4H10O	2-Methyl-1-propanol	-67.85	-67.62	-0.23
201	C4H10O	2-Butanol	-70.00	-69.86	-0.14
202	C4H10O	2-Methyl-2-propanol	-74.69	-74.43	-0.26
203	C4H10O	Diethyl ether	-60.25	-59.82	-0.44
204	C4H10O	1-Methoxypropane	-56.93	-56.52	-0.41
205	C4H10O	2-Methoxypropane	-60.23	-59.74	-0.48
206	C5H8O	Cyclopentanone	-45.91	-45.87	-0.04
207	C5H8O	Dihydro-2H-pyran	-29.90	-27.88	-2.01
208	C5H10O	3-Pentanone	-61.64	-61.79	0.15
209	C5H10O	2-Pentanone	-61.90	-61.48	-0.42
210	C5H10O	3-Methyl-2-butanone	-62.74	-62.41	-0.32
211	C5H10O	Tetrahydro-2H-pyran	-53.39	-52.65	-0.75
212	C5H10O	Pentanal	-54.61	-54.71	0.10
213	C5H10O	Propoxyethylene	-38.62	-36.38	-2.24
214	C5H10O	3,3-Dimethyloxetane	-35.42	-35.08	-0.34
215	C5H10O	Isopropyl vinyl ether	-41.54	-40.80	-0.74
216	C5H12O	1-Pentanol	-70.43	-70.40	-0.03
217	C5H12O	2-Pentanol	-74.74	-74.51	-0.23
218	C5H12O	3-Pentanol	-75.81	-74.43	-1.38
219	C5H12O	2-Methyl-1-butanol	-72.18	-71.53	-0.65
220	C5H12O	3-Methyl-1-butanol	-72.01	-70.66	-1.35
221	C5H12O	2-Methyl-2-butanol	-79.06	-78.88	-0.18
222	C5H12O	3-Methyl-2-butanol	-75.33	-75.85	0.52
223	C5H12O	2-Methoxy-2-methylpropane	-67.76	-67.76	0.00
224	C5H12O	1-Methoxybutane	-61.69	-61.49	-0.20
225	C5H12O	1-Ethoxypropane	-65.06	-64.58	-0.48
226	C6H6O	Phenol	-23.04	-22.73	-0.31
227	C6H6O	Vinylfuran	6.64	3.58	3.06
228	C6H10O	Cyclohexanone	-54.04	-54.39	0.35

229	C6H12O	2-Hexanone	-66.87	-66.63	-0.25
230	C6H12O	3,3-Dimethyl-2-butanone	-69.48	-69.74	0.26
231	C6H12O	3-Hexanone	-66.52	-66.69	0.18
232	C6H12O	2-Methyl-3-pentanone	-68.38	-67.82	-0.56
233	C6H12O	Cyclohexanol	-68.40	-69.34	0.94
234	C6H14O	Hexanol	-75.48	-75.52	0.04
235	C6H14O	Dipropyl ether	-70.00	-69.34	-0.66
236	C6H14O	Diisopropyl ether	-76.29	-76.11	-0.18
237	C7H6O	Benzaldehyde	-8.77	-10.12	1.35
238	C7H8O	Benzenemethanol	-24.00	-23.87	-0.13
239	C7H8O	2-Methylphenol	-30.74	-31.30	0.57
240	C7H8O	3-Methylphenol	-31.62	-30.67	-0.95
241	C7H8O	4-Methylphenol	-29.97	-30.12	0.15
242	C7H8O	Methoxybenzene	-16.23	-17.55	1.32
243	C7H10O	Bicyclo[2.2.1]heptan-2-one	-40.77	-40.54	-0.23
244	C7H10O	8-Oxatricyclo-[3.2.1.01,5]octane	6.43	8.00	-1.57
245	C7H14O	Heptanal	-63.05	-64.94	1.89
246	C7H14O	2,2-Dimethyl-3-pentanone	-74.98	-74.91	-0.06
247	C7H14O	2,4-Dimethyl-3-pentanone	-74.40	-74.07	-0.33
248	C7H16O	1-Heptanol	-80.40	-80.63	0.23
249	C8H8O	Acetophenone	-20.72	-21.02	0.30
250	C8H8O	Phenyl vinyl ether	5.43	4.75	0.67
251	C8H10O	2-Ethylphenol	-34.70	-36.31	1.61
252	C8H10O	3-Ethylphenol	-34.92	-35.93	1.02
253	C8H10O	4-Ethylphenol	-34.44	-35.41	0.97
254	C8H10O	2,3-Dimethylphenol	-37.57	-38.41	0.84
255	C8H10O	2,4-Dimethylphenol	-38.93	-38.61	-0.33
256	C8H10O	2,5-Dimethylphenol	-38.62	-38.76	0.14
257	C8H10O	2,6-Dimethylphenol	-38.67	-39.44	0.77
258	C8H10O	3,4-Dimethylphenol	-37.43	-38.33	0.90
259	C8H10O	3,5-Dimethylphenol	-38.60	-38.53	-0.07
260	C8H10O	Ethoxybenzene	-24.28	-25.76	1.48
261	C2H2O2	Ethanedial	-50.67	-51.59	0.93
262	C2H4O2	Acetic acid	-103.44	-102.29	-1.16
263	C2H4O2	Methyl formate	-84.97	-85.61	0.65
264	C2H6O2	1,2-Ethanediol	-92.61	-91.91	-0.70
265	C2H6O2	Dimethyl peroxide	-30.04	-29.07	-0.98
266	C3H4O2	2-Oxetanone	-67.61	-67.20	-0.41
267	C3H6O2	1,3-Dioxolane	-71.22	-70.79	-0.43

268	C3H6O2	Propanoic acid	-108.39	-107.38	-1.01
269	C3H6O2	Acetic acid methyl ester	-98.45	-97.46	-0.99
270	C3H8O2	1,2-propanediol	-100.69	-101.73	1.04
271	C3H8O2	Dimethoxymethane	-83.27	-83.47	0.20
272	C3H8O2	1,3-Propanediol	-93.71	-95.15	1.43
273	C4H4O2	4-Methylene-2-oxetanone	-45.46	-45.69	0.23
274	C4H4O2	Cyclobutane-1,3-dione	-44.53	-43.33	-1.20
275	C4H6O2	2,3-Butanedione	-78.18	-78.06	-0.12
276	C4H6O2	Acetic acid ethenyl ester	-75.26	-74.72	-0.55
277	C4H8O2	Acetic acid ethyl ester	-106.14	-105.26	-0.88
278	C4H8O2	1,4-Dioxane	-75.48	-75.00	-0.48
279	C4H8O2	2-Methyl-1,3-dioxolane	-84.13	-82.41	-1.72
280	C4H10O2	1,3-Butanediol	-103.54	-104.23	0.69
281	C4H10O2	1,1-Dimethoxyethane	-93.14	-91.69	-1.45
282	C4H10O2	Diethyl peroxide	-46.08	-44.64	-1.44
283	C4H10O2	1,4-Butanediol	-101.98	-100.86	-1.12
284	C5H6O2	2-Furanmethanol	-50.62	-51.29	0.67
285	C5H8O2	(E)-2-Butenoic acid methyl ester	-81.72	-80.98	-0.73
286	C5H10O2	Pentanoic acid	-117.57	-117.43	-0.14
287	C5H10O2	Propanoic acid ethyl ester	-110.80	-110.37	-0.43
288	C5H10O2	propan-2-yl acetate	-115.13	-114.23	-0.90
289	C5H10O2	4-Methyl-1,3-dioxane	-90.08	-90.64	0.56
290	C5H10O2	1,3-Dioxepane	-82.84	-84.82	1.98
291	C5H10O2	cis-2,4-Dimethyl-1,3-dioxolane	-91.44	-92.42	0.98
292	C5H10O2	trans-2,4-Dimethyl-1,3-dioxolane	-90.94	-91.16	0.22
293	C5H12O2	2,2-Dimethoxypropane	-102.68	-102.42	-0.26
294	C5H12O2	1,5-Pentanediol	-107.34	-105.72	-1.62
295	C5H12O2	Diethoxymethane	-99.14	-99.58	0.44
296	C6H4O2	2,5-cyclohexadiene-1,4-dione	-29.37	-28.20	-1.18
297	C6H6O2	1,4-Benzenediol	-63.41	-62.40	-1.01
298	C6H6O2	1,3-Benzenediol	-65.65	-64.40	-1.25
299	C6H10O2	(E)-2-Butenoic acid ethyl ester	-89.77	-88.81	-0.97
300	C6H12O2	Hexanoic acid	-122.35	-122.55	0.20
301	C6H12O2	Pentanoic acid methyl ester	-112.62	-112.62	0.00
302	C6H12O2	2,2-Dimethylpropanoic acid methyl ester	-118.14	-116.30	-1.84
303	C6H12O2	Acetic acid butyl ester	-116.06	-115.08	-0.98
304	C6H12O2	Tetrahydro-2-methoxy-2H-pyran	-95.51	-93.94	-1.57
305	C6H12O2	4,5-Dimethyl-1,3-dioxane	-97.78	-97.82	0.04
306	C6H14O2	1,2-Diethoxyethane	-97.56	-98.22	0.66

307	C6H14O2	1,1-Diethoxyethane	-108.39	-107.83	-0.56
308	C7H6O2	Benzoic acid	-70.29	-71.36	1.07
309	C7H6O2	2-Hydroxy-2,4,6-cycloheptatriene-1-one	-37.14	-37.38	0.24
310	C7H6O2	Formic acid phenyl ester	-51.58	-53.36	1.79
311	C7H6O2	3-(2-Furyl)-2-propenal	-25.31	-25.76	0.45
312	C7H12O2	4-Pentenoic acid ethyl ester	-92.16	-90.68	-1.48
313	C7H12O2	(Z)-3-Pentenoic acid ethyl ester	-92.64	-90.93	-1.71
314	C7H12O2	(E)-3-Pentenoic acid ethyl ester	-93.26	-92.25	-1.01
315	C7H12O2	(E)-2-Pentenoic acid ethyl ester	-94.24	-93.51	-0.73
316	C7H12O2	(E)-2-Butenoic acid propyl ester	-94.46	-93.64	-0.82
317	C7H12O2	(E)-2-Butenoic acid isopropyl ester	-98.26	-97.83	-0.43
318	C3H4O3	1,3-Dioxolan-2-one	-121.51	-121.27	-0.24
319	C3H6O3	1,3,5-Trioxane	-111.35	-111.22	-0.13
320	C3H8O3	1,2,3-Propanetriol	-139.27	-138.38	-0.89
321	C4H6O3	Acetic anhydride	-136.83	-136.74	-0.09
322	C4H10O3	Trimethoxymethane	-127.13	-126.62	-0.51
323	C5H4O3	3-Methyl-2,5-furandione	-106.88	-107.28	0.40
324	C5H10O3	Carbonic acid diethyl ester	-152.46	-151.58	-0.88
325	C5H10O3	1,3,6-Trioxacyclooctane	-111.64	-111.06	-0.58
326	C5H12O3	1,1,1-Trimethoxyethane	-136.88	-135.77	-1.11
327	C4H6O4	Butanedioic acid	-196.70	-195.01	-1.69
328	C4H8O4	1,3,5,7-Tetroxane	-148.23	-148.57	0.34
329	C4H10O4	2(R),3(S)-1,2,3,4-Butanetetrol	-185.28	-184.59	-0.69
330	C2N2	Cyanogen	73.30	73.52	-0.22
331	C4N2	2-Butynedinitrile	126.48	127.11	-0.63
332	CH5N	Methylamine	-5.50	-4.51	-0.99
333	C2H5N	Aziridine	30.23	30.54	-0.31
334	C2H7N	Ethylamine	-11.33	-11.17	-0.16
335	C2H7N	Dimethylamine	-4.45	-3.42	-1.03
336	C3H3N	2-Propenenitrile	43.16	44.31	-1.15
337	C3H5N	Propanenitrile	12.31	13.34	-1.03
338	C3H7N	Cyclopropylamine	18.40	20.55	-2.15
339	C3H9N	1-Propylamine	-16.78	-16.18	-0.60
340	C3H9N	2-Propylamine	-20.03	-19.44	-0.59
341	C3H9N	Trimethylamine	-5.66	-5.58	-0.09
342	C4H5N	1H-Pyrrole	25.88	25.49	0.40
343	C4H5N	Cyclopropanecarbonitrile	43.45	44.58	-1.12
344	C4H5N	3-Butenenitrile	37.72	39.53	-1.82
345	C4H5N	(E)-2-Butenenitrile	33.63	35.46	-1.83

346	C4H7N	Butanenitrile	8.03	8.07	-0.04
347	C4H7N	2-Methylpropanenitrile	5.57	6.87	-1.30
348	C4H9N	pyrrolidine	-0.81	-0.23	-0.59
349	C4H9N	Cyclobutylamine	9.85	11.23	-1.38
350	C4H11N	1-Butylamine	-21.99	-21.18	-0.81
351	C4H11N	2-Butylamine	-25.07	-24.75	-0.32
352	C4H11N	2-Methyl-2-propylamine	-28.90	-28.79	-0.11
353	C4H11N	Diethylamine	-17.33	-17.15	-0.18
354	C4H11N	2-Methylpropylamine	-23.59	-23.09	-0.50
355	C5H5N	Pyridine	33.56	32.67	0.88
356	C5H7N	1-Methyl-1H-pyrrole	24.64	24.00	0.64
357	C5H7N	(E)-2-Pentenenitrile	28.63	30.73	-2.10
358	C5H7N	(E)-3-Pentenenitrile	30.02	31.62	-1.60
359	C5H9N	2,2-Dimethylpropanenitrile	-0.60	-1.08	0.48
360	C5H9N	Pentanenitrile	2.51	2.96	-0.45
361	C5H11N	Piperidine	-11.28	-11.09	-0.20
362	C5H11N	Cyclopentylamine	-13.12	-12.14	-0.98
363	C6H7N	Aniline	20.82	20.18	0.64
364	C6H7N	2-Methylpyridine	23.71	22.55	1.16
365	C6H7N	3-Methylpyridine	25.43	24.50	0.93
366	C6H7N	4-Methylpyridine	24.88	24.00	0.88
367	C6H7N	Bicyclo[2.1.0]pentane-1-carbonitrile	65.03	66.37	-1.34
368	C6H7N	3-Methylenecyclobutane-carbonitrile	60.35	60.04	0.31
369	C6H7N	1-Cyclopentene-1-carbonitrile	37.40	37.86	-0.45
370	C6H9N	2,5-Dimethyl-1H-pyrrole	9.51	8.91	0.60
371	C6H13N	2-Methylpiperidine	-20.17	-20.32	0.15
372	C6H13N	Cyclohexylamine	-25.07	-24.60	-0.47
373	C6H15N	Triethylamine	-22.18	-22.72	0.54
374	C6H15N	Dipropylamine	-27.75	-26.97	-0.78
375	C6H15N	Diisopropylamine	-34.42	-32.18	-2.23
376	C7H5N	Benzonitrile	51.55	50.37	1.18
377	C7H9N	2,3-Dimethylpyridine	16.32	14.75	1.57
378	C7H9N	2,4-Dimethylpyridine	15.27	13.89	1.38
379	C7H9N	2,5-Dimethylpyridine	15.89	14.53	1.36
380	C7H9N	2,6-Dimethylpyridine	14.03	12.53	1.50
381	C7H9N	3,4-Dimethylpyridine	16.75	15.54	1.21
382	C7H9N	3,5-Dimethylpyridine	17.40	16.41	0.99
383	C7H9N	Benzylamine	20.98	19.85	1.13
384	C7H11N	Cyclohexanecarbonitrile	1.15	1.54	-0.39

385	C7H13N	1-Azabicyclo[2.2.2]octane	-1.00	-0.21	-0.80
386	C7H13N	Heptanenitrile	-7.41	-7.51	0.10
387	C8H7N	1H-Indole	37.40	37.38	0.02
388	CH6N2	Methylhydrazine	22.61	23.92	-1.31
389	C2H8N2	1,1-Dimethylhydrazine	20.05	20.45	-0.40
390	C4H2N2	(E)-Butenedinitrile	81.31	80.20	1.11
391	C4H4N2	Pyrimidine	46.82	44.35	2.47
392	C4H12N2	1,2-Butanediamine	-17.69	-15.24	-2.45
393	C6H8N2	Phenylhydrazine	48.49	50.37	-1.88
394	C4H12N4	1,1,4,4-Tetramethyl-2-tetrazene	64.70	67.01	-2.31
395	C2H5NO	Acetamide	-56.96	-55.12	-1.83
396	C3H3NO	Oxazole	-3.70	-3.80	0.09
397	C3H3NO	Isoxazole	18.79	19.28	-0.49
398	C3H7NO	propanamide	-61.88	-61.37	-0.50
399	C4H5NO	5-Methylisoxazole	8.15	8.40	-0.25
400	C4H5NO	3-Methylisoxazole	8.51	9.53	-1.02
401	C4H7NO	2-Methyl-2-oxazoline	-31.19	-29.61	-1.58
402	C4H9NO	Butanamide	-66.49	-66.30	-0.19
403	C5H5NO	2-Pyridinol	-19.05	-16.45	-2.60
404	C5H5NO	3-pyridinol	-10.44	-8.19	-2.25
405	C5H5NO	4-pyridinol	-9.75	-7.01	-2.75
406	C5H7NO	3,5-Dimethylisoxazole	-4.28	-1.32	-2.96
407	C5H9NO	2-Ethyl-2-oxazoline	-35.59	-34.09	-1.49
408	C5H11NO	Pentanamide	-69.36	-71.42	2.06
409	C6H7NO	2-Methyl-3-hydroxypyridine	-20.17	-18.38	-1.79
410	C6H7NO	2-Methyl-4-hydroxypyridine	-17.14	-17.10	-0.03
411	C6H7NO	2-Methyl-5-hydroxypyridine	-16.68	-17.82	1.14
412	C6H7NO	2-Methyl-6-hydroxypyridine	-28.73	-26.66	-2.06
413	C6H11NO	Hexahydro-2H-azepin-2-one	-58.84	-57.03	-1.81
414	C6H13NO	Hexanamide	-77.49	-75.30	-2.19
415	C6H13NO	N-Butylacetamide	-72.85	-72.22	-0.63
416	C7H7NO	1-Amino-2,4,6-cyclohepta-trien-1-one	9.44	7.16	2.28
417	CH3NO2	Methyl nitrite	-15.87	-15.40	-0.47
418	CH3NO2	Nitromethane	-17.76	-17.82	0.07
419	C2H5NO2	Nitroethane	-24.45	-24.35	-0.10
420	C2H5NO2	Glycine	-93.71	-93.42	-0.29
421	C3H7NO2	1-Nitropropane	-29.59	-29.11	-0.48
422	C3H7NO2	2-Nitropropane	-33.22	-33.11	-0.11
423	C4H9NO2	1-Nitrobutane	-34.39	-34.25	-0.14

424	C4H9NO2	2-Nitrobutane	-39.10	-38.87	-0.23
425	C4H9NO2	2-Methyl-2-nitropropane	-42.33	-41.73	-0.60
426	C5H11NO2	L-Valine	-108.77	-110.91	2.14
427	C6H5NO2	Nitrobenzene	16.13	13.87	2.26
428	C2H5NO3	Ethyl nitrate	-36.83	-36.36	-0.47
429	C3H7NO3	Propyl nitrate	-41.56	-41.19	-0.38
430	C3H7NO3	Isopropyl nitrate	-45.65	-45.15	-0.50
431	C4H3NO3	2-Nitrofuran	-6.88	-8.12	1.23
432	C4H6N2O	3-Amino-5-methylisoxazole	4.71	8.43	-3.72
433	C4H6N2O	Dimethylfurazan	25.65	26.88	-1.23
434	C5H8N2O	5-Amino-3,4-dimethyl-isoxazole	1.24	0.98	0.26
435	C5H10N2O	1-Nitrosopiperidine	3.97	7.32	-3.35
436	C6H4N2O	1,2,3-Benzoxadiazole	71.87	71.67	0.20
437	C2H6N2O2	N-Nitrodimethylamine	-1.15	-0.17	-0.98
438	C4H4N2O2	Uracil	-72.39	-70.09	-2.30
439	C4H6N2O2	Dimethylfurazan monoxide	24.45	25.72	-1.27
440	C5H10N2O2	1-Nitropiperidine	-10.64	-8.07	-2.56
441	C3H4N2O3	4,5-Dihydro-3-nitro-isoxazole	9.32	14.42	-5.10
442	C3H6N2O4	1,1-Dinitropropane	-24.07	-26.88	2.81
443	CF4	Carbon tetrafluoride	-223.14	-222.77	-0.37
444	C2FH3	Fluoroethylene	-33.17	-34.10	0.93
445	C3FH7	1-Fluoropropane	-68.33	-69.51	1.18
446	C6FH5	Fluorobenzene	-27.72	-27.75	0.03
447	C7FH7	1-Fluoro-4-methylbenzene	-35.25	-35.29	0.03
448	CF2H2	Difluoromethane	-108.08	-107.72	-0.36
449	C6F2H4	1,2-Difluorobenzene	-70.22	-69.82	-0.40
450	C6F2H4	1,3-Difluorobenzene	-73.90	-73.57	-0.34
451	C6F2H4	1,4-Difluorobenzene	-73.30	-72.76	-0.55
452	CF3H	Trifluoromethane	-166.20	-166.28	0.08
453	C2F3H3	1,1,1-Trifluoroethane	-177.96	-179.18	1.21
454	C2FH3O	Acetyl fluoride	-105.66	-104.70	-0.96
455	C3F4H4O	2,2,3,3-Tetrafluoro-1-propanol	-253.66	-253.75	0.10
456	C3F5H3O	2,2,3,3,3-Pentafluoro-1-propanol	-313.17	-310.62	-2.55
457	C2F3N	Trifluoroacetonitrile	-119.00	-118.90	-0.10
458	CF5N	Pentafluoromethylamine	-169.10	-167.99	-1.11
459	CF5N3	Pentafluoroguanidine	22.87	21.44	1.43

Table S3. Comparison of B3LYP/6-31+G(2df,p)//B3LYP/6-31G(2df,p) and experimental (see text for reference) enthalpies of formation of the Pedley test set.

			ΔH_f^o(298 K) values (kcal/mol)		Difference (kcal/mol)
	Formula	Name	Expt	B3LYP	Expt. -Theory
1	CH4	Methane	-17.78	-21.82	4.03
2	C2H2	Acetylene	54.54	57.38	-2.84
3	C2H4	Ethylene	12.55	10.73	1.82
4	C2H6	Ethane	-20.03	-25.50	5.47
5	C3H4	Propyne	44.19	44.01	0.18
6	C3H4	Allene	45.53	41.28	4.25
7	C3H4	Cyclopropene	66.23	65.94	0.29
8	C3H6	Propene	4.78	1.39	3.39
9	C3H6	Cyclopropane	12.74	9.88	2.86
10	C3H8	Propane	-25.02	-30.86	5.83
11	C4H6	1-Butyne	39.48	39.00	0.49
12	C4H6	2-Butyne	34.82	31.57	3.25
13	C4H6	1,2-Butadiene	38.79	33.49	5.30
14	C4H6	1,3-Butadiene	26.29	24.02	2.27
15	C4H6	Cyclobutene	37.45	37.05	0.40
16	C4H6	Methylenecyclopropane	47.92	41.98	5.94
17	C4H6	1-Methylcyclopropene	58.22	53.44	4.78
18	C4H6	Bicyclo[1.1.0]butane	51.89	52.53	-0.64
19	C4H8	1-Butene	0.02	-3.64	3.67
20	C4H8	(Z)-2-Butene	-1.70	-6.01	4.31
21	C4H8	(E)-2-Butene	-2.72	-7.48	4.75
22	C4H8	2-Methylpropene	-4.04	-7.97	3.94
23	C4H8	Cyclobutane	6.79	2.88	3.90
24	C4H10	Butane	-30.02	-36.22	6.20
25	C4H10	2-Methylpropane	-32.07	-37.07	5.00
26	C5H6	1,3-Cyclopentadiene	32.10	32.72	-0.62
27	C5H8	1,2-Pentadiene	33.63	28.26	5.37
28	C5H8	(Z)-1,3-Pentadiene	19.46	16.34	3.12
29	C5H8	(E)-1,3-Pentadiene	18.19	14.66	3.53
30	C5H8	1,4-Pentadiene	25.24	24.19	1.05
31	C5H8	2,3-Pentadiene	31.81	25.70	6.11
32	C5H8	2-Methyl-1,3-butadiene	18.04	15.62	2.42
33	C5H8	Cyclopentene	8.10	7.33	0.77
34	C5H8	Spiropentane	44.26	40.44	3.82

35	C5H8	Methylenecyclobutane	29.04	26.19	2.85
36	C5H10	1-Pentene	-5.09	-9.05	3.96
37	C5H10	(Z)-2-Pentene	-6.60	-10.93	4.33
38	C5H10	(E)-2-Pentene	-7.62	-12.51	4.89
39	C5H10	2-Methyl-1-butene	-8.44	-12.17	3.73
40	C5H10	3-Methyl-1-butene	-6.60	-9.73	3.13
41	C5H10	2-Methyl-2-butene	-9.99	-14.82	4.83
42	C5H10	Cyclopentane	-18.26	-21.30	3.04
43	C5H10	1,1-Dimethylcyclopropane	-1.96	-5.47	3.51
44	C5H12	Pentane	-35.11	-41.50	6.39
45	C5H12	2-Methylbutane	-36.74	-40.43	3.69
46	C5H12	2,2-Dimethylpropane	-40.18	-43.33	3.15
47	C6H6	Benzene	19.74	17.90	1.84
48	C6H8	1,3-Cyclohexadiene	25.38	25.83	-0.45
49	C6H10	1,5-Hexadiene	20.10	18.75	1.35
50	C6H10	2,3-Dimethyl-1,3-butadiene	10.78	8.57	2.21
51	C6H10	1-Methylcyclopentene	-0.91	-2.81	1.90
52	C6H10	3-Methylcyclopentene	1.77	0.88	0.89
53	C6H10	4-Methylcyclopentene	3.49	0.96	2.53
54	C6H10	Cyclohexene	-1.20	-2.09	0.89
55	C6H10	Bicyclopropyl	30.93	30.49	0.44
56	C6H10	Methylenecyclopentane	2.87	1.37	1.50
57	C6H10	Bicyclo[3.1.0]hexane	9.15	8.71	0.45
58	C6H12	1-Hexene	-10.40	-14.33	3.93
59	C6H12	(Z)-2-Hexene	-12.50	-16.34	3.84
60	C6H12	(E)-2-Hexene	-12.88	-17.91	5.03
61	C6H12	(Z)-3-Hexene	-11.38	-15.85	4.47
62	C6H12	(E)-3-Hexene	-13.00	-17.54	4.53
63	C6H12	2-Methyl-1-pentene	-14.20	-17.51	3.32
64	C6H12	3-Methyl-1-pentene	-11.83	-14.86	3.03
65	C6H12	4-Methyl-1-pentene	-12.26	-15.00	2.74
66	C6H12	2-Methyl-2-pentene	-15.99	-19.73	3.74
67	C6H12	(Z)-3-Methyl-2-pentene	-14.89	-18.86	3.97
68	C6H12	(E)-3-Methyl-2-pentene	-15.08	-18.98	3.89
69	C6H12	(Z)-4-Methyl-2-pentene	-13.74	-16.90	3.15
70	C6H12	(E)-4-Methyl-2-pentene	-14.70	-18.54	3.85
71	C6H12	2-Ethyl-1-butene	-13.38	-16.33	2.94
72	C6H12	2,3-Dimethyl-1-butene	-14.96	-17.24	2.28
73	C6H12	3,3-Dimethyl-1-butene	-14.46	-15.06	0.60

74	C6H12	2,3-Dimethyl-2-butene	-16.30	-19.94	3.64
75	C6H12	Methylcyclopentane	-25.38	-27.50	2.11
76	C6H12	Cyclohexane	-29.49	-31.61	2.12
77	C6H12	Ethylcyclobutane	-6.29	-10.05	3.77
78	C6H14	Hexane	-39.94	-46.77	6.83
79	C6H14	2-Methylpentane	-41.78	-46.67	4.89
80	C6H14	3-Methylpentane	-41.13	-45.69	4.56
81	C6H14	2,3-Dimethylbutane	-42.61	-45.53	2.92
82	C6H14	2,2-Dimethylbutane	-44.48	-46.65	2.17
83	C7H8	1,3,5-Cycloheptatriene	43.24	44.85	-1.61
84	C7H8	Methylbenzene	12.05	9.51	2.53
85	C7H8	Quadricyclane	81.05	84.76	-3.71
86	C7H10	1,3-Cycloheptadiene	22.54	21.84	0.70
87	C7H10	Tricyclo[4.1.0.02,4]heptane	35.66	39.52	-3.86
88	C7H12	1-Ethylcyclopentene	-4.71	-7.51	2.80
89	C7H12	Ethylidenecyclopentane	-4.33	-6.48	2.15
90	C7H12	1-Methylcyclohexene	-10.35	-11.47	1.12
91	C7H12	Cycloheptene	-2.20	-1.63	-0.57
92	C7H12	Bicyclo[2.2.1]heptane	-13.12	-10.56	-2.56
93	C7H12	1-Methyl-bicyclo[3.1.0]-hexane	0.36	0.29	0.07
94	C7H14	1-Heptene	-14.89	-19.61	4.72
95	C7H14	5-Methyl-1-hexene	-15.70	-18.48	2.78
96	C7H14	(Z)-3-Methyl-3-hexene	-18.98	-23.81	4.83
97	C7H14	(E)-3-Methyl-3-hexene	-18.36	-23.86	5.50
98	C7H14	2,4-Dimethyl-1-pentene	-20.03	-23.46	3.44
99	C7H14	4,4-Dimethyl-1-pentene	-19.50	-20.19	0.69
100	C7H14	2,4-Dimethyl-2-pentene	-21.20	-25.64	4.44
101	C7H14	(Z)-4,4-Dimethyl-2-pentene	-17.35	-18.81	1.46
102	C7H14	(E)-4,4-Dimethyl-2-pentene	-21.22	-23.69	2.47
103	C7H14	3-Methyl-2-ethyl-1-butene	-19.00	-21.27	2.27
104	C7H14	2,3,3-Trimethyl-1-butene	-20.43	-21.11	0.68
105	C7H14	1,1-Dimethylcyclopentane	-33.03	-32.98	-0.05
106	C7H14	cis-1,2-dimethylcyclopentane	-30.95	-31.77	0.82
107	C7H14	trans-1,2-dimethylcyclopentane	-32.65	-34.03	1.38
108	C7H14	cis-1,3-dimethylcyclopentane	-32.48	-34.07	1.59
109	C7H14	trans-1,3-dimethylcyclopentane	-31.93	-33.78	1.85
110	C7H14	Ethylcyclopentane	-30.33	-32.82	2.49
111	C7H14	Methylcyclohexane	-36.97	-38.27	1.30
112	C7H14	Cycloheptane	-28.23	-30.09	1.86

113	C7H16	Heptane	-44.86	-52.05	7.19
114	C7H16	2-Methylhexane	-46.51	-50.90	4.39
115	C7H16	3-Methylhexane	-45.72	-49.96	4.24
116	C7H16	3-Ethylpentane	-45.32	-48.95	3.64
117	C7H16	2,2-Dimethylpentane	-49.21	-51.74	2.53
118	C7H16	2,3-Dimethylpentane	-47.54	-49.55	2.01
119	C7H16	2,4-Dimethylpentane	-48.21	-51.82	3.61
120	C7H16	3,3-Dimethylpentane	-48.09	-49.92	1.83
121	C7H16	2,2,3-Trimethylbutane	-48.88	-49.62	0.74
122	C8H8	1,3,5,7-Cyclooctatetraene	70.72	73.72	-3.00
123	C8H8	Ethenylbenzene	35.35	33.96	1.39
124	C8H10	Ethylbenzene	7.15	4.49	2.65
125	C8H10	1,2-Dimethylbenzene	4.57	1.61	2.95
126	C8H10	1,3-Dimethylbenzene	4.13	1.23	2.91
127	C8H10	1,4-Dimethylbenzene	4.30	1.29	3.01
128	C8H12	Bicyclo[2.2.2]oct-2-ene	4.90	10.32	-5.42
129	C8H12	4-Ethenylcyclohexene	15.56	18.49	-2.93
130	C8H12	(Z,Z)-1,5-Cyclooctadiene	24.16	25.36	-1.20
131	C8H14	(2-Propenyl)cyclopentane	-5.76	-5.41	-0.35
132	C8H14	1-Ethylcyclohexene	-15.15	-15.66	0.51
133	C8H14	Ethylidenecyclohexane	-14.70	-15.36	0.66
134	C8H14	Ethenylcyclohexane	-11.69	-10.98	-0.71
135	C8H14	Cyclooctene	-6.45	-5.29	-1.16
136	C8H14	Bicyclo[4.2.0]octane	-6.26	-4.42	-1.84
137	C8H14	Bicyclo[5.1.0]octane	-3.97	-1.92	-2.04
138	C8H14	cis-Bicyclo[3.3.0]octane	-22.20	-20.83	-1.37
139	C8H14	trans-Bicyclo[3.3.0]octane	-15.92	-12.92	-3.00
140	C8H14	Bicyclo[2.2.2]octane	-23.66	-19.79	-3.87
141	C8H14	1-Methylbicyclo[4.1.0]-heptane	-4.97	-5.03	0.06
142	C8H16	1-Octene	-19.46	-24.88	5.42
143	C8H16	(Z)-2,2-Dimethyl-3-hexene	-21.34	-23.76	2.41
144	C8H16	(E)-2,2-Dimethyl-3-hexene	-25.74	-28.72	2.98
145	C8H16	2-Methyl-3-ethyl-1-pentene	-23.97	-27.31	3.34
146	C8H16	2,4,4-Trimethyl-1-pentene	-26.43	-27.19	0.75
147	C8H16	2,4,4-Trimethyl-2-pentene	-25.07	-27.23	2.16
148	C8H16	Propylcyclopentane	-35.30	-38.08	2.78
149	C8H16	Ethylcyclohexane	-41.04	-42.55	1.52
150	C8H16	1,1-Dimethylcyclohexane	-43.24	-42.56	-0.67
151	C8H16	cis-1,2-Dimethylcyclohexane	-41.13	-41.27	0.14

152	C8H16	trans-1,2-Dimethylcyclohexane	-43.00	-43.46	0.46
153	C8H16	cis-1,3-Dimethylcyclohexane	-44.12	-44.85	0.73
154	C8H16	trans-1,3-Dimethylcyclohexane	-42.18	-42.50	0.31
155	C8H16	cis-1,4-Dimethylcyclohexane	-42.21	-42.59	0.38
156	C8H16	trans-1,4-Dimethyl-cyclohexane	-44.10	-44.89	0.79
157	C8H16	Cyclooctane	-29.73	-30.89	1.16
158	C8H18	Octane	-49.86	-57.32	7.46
159	C8H18	2-Methylheptane	-51.48	-56.17	4.69
160	C8H18	3-Methylheptane	-50.79	-56.16	5.37
161	C8H18	4-Methylheptane	-50.67	-56.06	5.39
162	C8H18	2,2-Dimethylhexane	-53.68	-57.02	3.34
163	C8H18	2,5-Dimethylhexane	-53.18	-55.97	2.80
164	C9H8	Indene	39.05	39.04	0.01
165	C9H10	2,3-Dihydro-1H-indene	14.51	13.93	0.58
166	C9H10	Cyclopropylbenzene	35.97	36.81	-0.84
167	C9H12	Propylbenzene	1.89	-1.00	2.89
168	C9H12	(1-Methylethyl)benzene	0.96	-0.67	1.62
169	C9H12	1-Ethyl-2-methylbenzene	0.31	-2.40	2.71
170	C9H12	1-Ethyl-3-methylbenzene	-0.43	-3.79	3.36
171	C9H12	1-Ethyl-4-methylbenzene	-0.76	-3.75	2.99
172	C9H12	1,2,3-Trimethylbenzene	-2.27	-4.73	2.45
173	C9H12	1,2,4-Trimethylbenzene	-3.30	-6.60	3.30
174	C9H12	1,3,5-Trimethylbenzene	-3.80	-7.03	3.23
175	C9H12	(Z)-5-Ethylidene-bicyclo[2.2.1]hept-2-ene	34.82	40.44	-5.62
176	CH2O	Formaldehyde	-25.96	-27.69	1.73
177	CH4O	Methanol	-48.16	-48.73	0.57
178	C2H2O	Ketene	-11.35	-15.88	4.52
179	C2H4O	Acetaldehyde	-39.70	-42.90	3.20
180	C2H4O	Oxirane	-12.57	-15.12	2.55
181	C2H6O	Ethanol	-56.21	-57.68	1.46
182	C2H6O	Dimethyl ether	-44.00	-49.67	5.67
183	C3H6O	2-Propen-1-ol	-29.76	-30.15	0.40
184	C3H6O	Propanal	-44.36	-49.02	4.66
185	C3H6O	Acetone	-51.94	-55.76	3.83
186	C3H6O	Methyloxirane	-22.63	-25.81	3.17
187	C3H6O	Oxetane	-19.24	-22.54	3.30
188	C3H8O	1-Propanol	-60.97	-62.99	2.02
189	C3H8O	2-Propanol	-65.20	-66.66	1.46
190	C3H8O	Methoxyethane	-51.72	-58.34	6.62

191	C4H4O	Furan	-8.34	-9.88	1.54
192	C4H6O	trans-2-Butenal	-24.04	-28.78	4.74
193	C4H6O	Divinyl ether	-3.25	-7.43	4.18
194	C4H8O	Butanal	-48.95	-54.23	5.28
195	C4H8O	2-Methylpropanal	-51.58	-54.65	3.07
196	C4H8O	2-Butanone	-57.05	-61.65	4.60
197	C4H8O	Ethoxyethene	-33.65	-37.15	3.50
198	C4H8O	Tetrahydrofuran	-44.02	-46.68	2.66
199	C4H10O	1-Butanol	-65.73	-68.16	2.43
200	C4H10O	2-Methyl-1-propanol	-67.85	-69.14	1.29
201	C4H10O	2-Butanol	-70.00	-72.01	2.01
202	C4H10O	2-Methyl-2-propanol	-74.69	-74.89	0.20
203	C4H10O	Diethyl ether	-60.25	-66.94	6.69
204	C4H10O	1-Methoxypropane	-56.93	-63.51	6.58
205	C4H10O	2-Methoxypropane	-60.23	-65.68	5.45
206	C5H8O	Cyclopentanone	-45.91	-48.28	2.36
207	C5H8O	Dihydro-2H-pyran	-29.90	-30.48	0.58
208	C5H10O	3-Pentanone	-61.64	-67.36	5.72
209	C5H10O	2-Pentanone	-61.90	-66.86	4.95
210	C5H10O	3-Methyl-2-butanone	-62.74	-66.36	3.62
211	C5H10O	Tetrahydro-2H-pyran	-53.39	-56.07	2.67
212	C5H10O	Pentanal	-54.61	-59.54	4.93
213	C5H10O	Propoxyethylene	-38.62	-42.35	3.72
214	C5H10O	3,3-Dimethyloxetane	-35.42	-37.54	2.12
215	C5H10O	Isopropyl vinyl ether	-41.54	-45.77	4.23
216	C5H12O	1-Pentanol	-70.43	-73.48	3.04
217	C5H12O	2-Pentanol	-74.74	-77.42	2.68
218	C5H12O	3-Pentanol	-75.81	-77.56	1.75
219	C5H12O	2-Methyl-1-butanol	-72.18	-73.52	1.34
220	C5H12O	3-Methyl-1-butanol	-72.01	-72.13	0.12
221	C5H12O	2-Methyl-2-butanol	-79.06	-79.27	0.21
222	C5H12O	3-Methyl-2-butanol	-75.33	-76.85	1.52
223	C5H12O	2-Methoxy-2-methylpropane	-67.76	-71.72	3.96
224	C5H12O	1-Methoxybutane	-61.69	-68.69	7.01
225	C5H12O	1-Ethoxypropane	-65.06	-72.12	7.07
226	C6H6O	Phenol	-23.04	-22.95	-0.09
227	C6H6O	Vinylfuran	6.64	1.67	4.98
228	C6H10O	Cyclohexanone	-54.04	-55.82	1.78
229	C6H12O	2-Hexanone	-66.87	-72.15	5.27

230	C6H12O	3,3-Dimethyl-2-butanone	-69.48	-71.19	1.71
231	C6H12O	3-Hexanone	-66.52	-72.55	6.03
232	C6H12O	2-Methyl-3-pentanone	-68.38	-72.22	3.84
233	C6H12O	Cyclohexanol	-68.40	-67.76	-0.64
234	C6H14O	Hexanol	-75.48	-78.75	3.27
235	C6H14O	Dipropyl ether	-70.00	-77.30	7.30
236	C6H14O	Diisopropyl ether	-76.29	-81.63	5.34
237	C7H6O	Benzaldehyde	-8.77	-11.45	2.68
238	C7H8O	Benzenemethanol	-24.00	-22.47	-1.53
239	C7H8O	2-Methylphenol	-30.74	-31.57	0.83
240	C7H8O	3-Methylphenol	-31.62	-31.33	-0.29
241	C7H8O	4-Methylphenol	-29.97	-30.84	0.87
242	C7H8O	Methoxybenzene	-16.23	-21.04	4.81
243	C7H10O	Bicyclo[2.2.1]heptan-2-one	-40.77	-36.73	-4.04
244	C7H10O	8-Oxatricyclo-[3.2.1.01,5]octane	6.43	10.06	-3.63
245	C7H14O	Heptanal	-63.05	-70.11	7.06
246	C7H14O	2,2-Dimethyl-3-pentanone	-74.98	-76.72	1.74
247	C7H14O	2,4-Dimethyl-3-pentanone	-74.40	-77.03	2.63
248	C7H16O	1-Heptanol	-80.40	-84.02	3.62
249	C8H8O	Acetophenone	-20.72	-22.43	1.70
250	C8H8O	Phenyl vinyl ether	5.43	2.44	2.98
251	C8H10O	2-Ethylphenol	-34.70	-36.31	1.61
252	C8H10O	3-Ethylphenol	-34.92	-36.33	1.42
253	C8H10O	4-Ethylphenol	-34.44	-35.91	1.47
254	C8H10O	2,3-Dimethylphenol	-37.57	-38.49	0.92
255	C8H10O	2,4-Dimethylphenol	-38.93	-39.43	0.50
256	C8H10O	2,5-Dimethylphenol	-38.62	-39.40	0.77
257	C8H10O	2,6-Dimethylphenol	-38.67	-39.58	0.90
258	C8H10O	3,4-Dimethylphenol	-37.43	-38.81	1.39
259	C8H10O	3,5-Dimethylphenol	-38.60	-39.64	1.04
260	C8H10O	Ethoxybenzene	-24.28	-29.75	5.47
261	C2H2O2	Ethanedial	-50.67	-52.65	1.98
262	C2H4O2	Acetic acid	-103.44	-104.29	0.85
263	C2H4O2	Methyl formate	-84.97	-89.93	4.97
264	C2H6O2	1,2-Ethanediol	-92.61	-91.56	-1.06
265	C2H6O2	Dimethyl peroxide	-30.04	-37.23	7.18
266	C3H4O2	2-Oxetanone	-67.61	-70.64	3.02
267	C3H6O2	1,3-Dioxolane	-71.22	-74.65	3.43
268	C3H6O2	Propanoic acid	-108.39	-110.16	1.77

269	C3H6O2	Acetic acid methyl ester	-98.45	-102.98	4.53
270	C3H8O2	1,2-propanediol	-100.69	-100.83	0.13
271	C3H8O2	Dimethoxymethane	-83.27	-90.43	7.16
272	C3H8O2	1,3-Propanediol	-93.71	-94.06	0.34
273	C4H4O2	4-Methylene-2-oxetanone	-45.46	-49.17	3.71
274	C4H4O2	Cyclobutane-1,3-dione	-44.53	-46.68	2.16
275	C4H6O2	2,3-Butanedione	-78.18	-82.33	4.15
276	C4H6O2	Acetic acid ethenyl ester	-75.26	-79.82	4.56
277	C4H8O2	Acetic acid ethyl ester	-106.14	-111.51	5.37
278	C4H8O2	1,4-Dioxane	-75.48	-79.00	3.52
279	C4H8O2	2-Methyl-1,3-dioxolane	-84.13	-86.36	2.23
280	C4H10O2	1,3-Butanediol	-103.54	-103.06	-0.48
281	C4H10O2	1,1-Dimethoxyethane	-93.14	-98.64	5.50
282	C4H10O2	Diethyl peroxide	-46.08	-54.11	8.03
283	C4H10O2	1,4-Butanediol	-101.98	-99.86	-2.12
284	C5H6O2	2-Furanmethanol	-50.62	-50.30	-0.33
285	C5H8O2	(E)-2-Butenoic acid methyl ester	-81.72	-87.42	5.70
286	C5H10O2	Pentanoic acid	-117.57	-120.72	3.16
287	C5H10O2	Propanoic acid ethyl ester	-110.80	-117.30	6.49
288	C5H10O2	propan-2-yl acetate	-115.13	-120.04	4.91
289	C5H10O2	4-Methyl-1,3-dioxane	-90.08	-93.68	3.60
290	C5H10O2	1,3-Dioxepane	-82.84	-88.61	5.77
291	C5H10O2	cis-2,4-Dimethyl-1,3-dioxolane	-91.44	-96.18	4.74
292	C5H10O2	trans-2,4-Dimethyl-1,3-dioxolane	-90.94	-94.94	3.99
293	C5H12O2	2,2-Dimethoxypropane	-102.68	-107.09	4.41
294	C5H12O2	1,5-Pentanediol	-107.34	-105.32	-2.02
295	C5H12O2	Diethoxymethane	-99.14	-107.61	8.47
296	C6H4O2	2,5-cyclohexadiene-1,4-dione	-29.37	-28.21	-1.16
297	C6H6O2	1,4-Benzenediol	-63.41	-61.87	-1.54
298	C6H6O2	1,3-Benzenediol	-65.65	-64.03	-1.63
299	C6H10O2	(E)-2-Butenoic acid ethyl ester	-89.77	-95.94	6.17
300	C6H12O2	Hexanoic acid	-122.35	-126.01	3.66
301	C6H12O2	Pentanoic acid methyl ester	-112.62	-119.31	6.69
302	C6H12O2	2,2-Dimethylpropanoic acid methyl ester	-118.14	-119.87	1.73
303	C6H12O2	Acetic acid butyl ester	-116.06	-121.92	5.86
304	C6H12O2	Tetrahydro-2-methoxy-2H-pyran	-95.51	-97.65	2.15
305	C6H12O2	4,5-Dimethyl-1,3-dioxane	-97.78	-99.65	1.87
306	C6H14O2	1,2-Diethoxyethane	-97.56	-106.88	9.32
307	C6H14O2	1,1-Diethoxyethane	-108.39	-115.75	7.36

308	C7H6O2	Benzoic acid	-70.29	-71.35	1.06
309	C7H6O2	2-Hydroxy-2,4,6-cycloheptatriene-1-one	-37.14	-42.96	5.82
310	C7H6O2	Formic acid phenyl ester	-51.58	-55.93	4.36
311	C7H6O2	3-(2-Furyl)-2-propenal	-25.31	-29.44	4.12
312	C7H12O2	4-Pentenoic acid ethyl ester	-92.16	-95.25	3.09
313	C7H12O2	(Z)-3-Pentenoic acid ethyl ester	-92.64	-96.83	4.19
314	C7H12O2	(E)-3-Pentenoic acid ethyl ester	-93.26	-98.21	4.95
315	C7H12O2	(E)-2-Pentenoic acid ethyl ester	-94.24	-100.86	6.62
316	C7H12O2	(E)-2-Butenoic acid propyl ester	-94.46	-101.14	6.68
317	C7H12O2	(E)-2-Butenoic acid isopropyl ester	-98.26	-104.47	6.22
318	C3H4O3	1,3-Dioxolan-2-one	-121.51	-126.25	4.74
319	C3H6O3	1,3,5-Trioxane	-111.35	-114.56	3.20
320	C3H8O3	1,2,3-Propanetriol	-139.27	-136.97	-2.30
321	C4H6O3	Acetic anhydride	-136.83	-142.71	5.88
322	C4H10O3	Trimethoxymethane	-127.13	-134.32	7.19
323	C5H4O3	3-Methyl-2,5-furandione	-106.88	-110.78	3.89
324	C5H10O3	Carbonic acid diethyl ester	-152.46	-160.07	7.61
325	C5H10O3	1,3,6-Trioxacyclooctane	-111.64	-116.17	4.53
326	C5H12O3	1,1,1-Trimethoxyethane	-136.88	-141.97	5.09
327	C4H6O4	Butanedioic acid	-196.70	-195.01	-1.70
328	C4H8O4	1,3,5,7-Tetroxane	-148.23	-154.32	6.09
329	C4H10O4	2(R),3(S)-1,2,3,4-Butanetetrol	-185.28	-179.74	-5.54
330	C2N2	Cyanogen	73.30	71.58	1.73
331	C4N2	2-Butynedinitrile	126.48	122.17	4.32
332	CH5N	Methylamine	-5.50	-9.58	4.08
333	C2H5N	Aziridine	30.23	26.00	4.24
334	C2H7N	Ethylamine	-11.33	-17.20	5.87
335	C2H7N	Dimethylamine	-4.45	-11.26	6.81
336	C3H3N	2-Propenenitrile	43.16	42.86	0.30
337	C3H5N	Propanenitrile	12.31	10.31	2.00
338	C3H7N	Cyclopropylamine	18.40	16.83	1.58
339	C3H9N	1-Propylamine	-16.78	-22.54	5.77
340	C3H9N	2-Propylamine	-20.03	-24.65	4.63
341	C3H9N	Trimethylamine	-5.66	-14.55	8.88
342	C4H5N	1H-Pyrrole	25.88	23.35	2.53
343	C4H5N	Cyclopropanecarbonitrile	43.45	42.90	0.55
344	C4H5N	3-Butenenitrile	37.72	39.04	-1.33
345	C4H5N	(E)-2-Butenenitrile	33.63	32.09	1.54
346	C4H7N	Butanenitrile	8.03	4.67	3.36

347	C4H7N	2-Methylpropanenitrile	5.57	4.29	1.28
348	C4H9N	pyrrolidine	-0.81	-5.00	4.19
349	C4H9N	Cyclobutylamine	9.85	7.96	1.89
350	C4H11N	1-Butylamine	-21.99	-27.27	5.28
351	C4H11N	2-Butylamine	-25.07	-29.34	4.26
352	C4H11N	2-Methyl-2-propylamine	-28.90	-31.87	2.97
353	C4H11N	Diethylamine	-17.33	-25.50	8.17
354	C4H11N	2-Methylpropylamine	-23.59	-28.41	4.82
355	C5H5N	Pyridine	33.56	27.94	5.61
356	C5H7N	1-Methyl-1H-pyrrole	24.64	20.00	4.65
357	C5H7N	(E)-2-Pentenenitrile	28.63	27.07	1.56
358	C5H7N	(E)-3-Pentenenitrile	30.02	29.59	0.43
359	C5H9N	2,2-Dimethylpropanenitrile	-0.60	-1.97	1.37
360	C5H9N	Pentanenitrile	2.51	-0.65	3.16
361	C5H11N	Piperidine	-11.28	-15.38	4.10
362	C5H11N	Cyclopentylamine	-13.12	-14.71	1.59
363	C6H7N	Aniline	20.82	17.22	3.60
364	C6H7N	2-Methylpyridine	23.71	17.23	6.48
365	C6H7N	3-Methylpyridine	25.43	19.21	6.22
366	C6H7N	4-Methylpyridine	24.88	18.76	6.12
367	C6H7N	Bicyclo[2.1.0]pentane-1-carbonitrile	65.03	66.60	-1.57
368	C6H7N	3-Methylenecyclobutane-carbonitrile	60.35	59.97	0.38
369	C6H7N	1-Cyclopentene-1-carbonitrile	37.40	37.02	0.38
370	C6H9N	2,5-Dimethyl-1H-pyrrole	9.51	4.33	5.18
371	C6H13N	2-Methylpiperidine	-20.17	-23.57	3.40
372	C6H13N	Cyclohexylamine	-25.07	-25.71	0.64
373	C6H15N	Triethylamine	-22.18	-30.74	8.56
374	C6H15N	Dipropylamine	-27.75	-35.86	8.12
375	C6H15N	Diisopropylamine	-34.42	-37.99	3.57
376	C7H5N	Benzonitrile	51.55	49.86	1.69
377	C7H9N	2,3-Dimethylpyridine	16.32	9.53	6.80
378	C7H9N	2,4-Dimethylpyridine	15.27	8.09	7.18
379	C7H9N	2,5-Dimethylpyridine	15.89	8.62	7.27
380	C7H9N	2,6-Dimethylpyridine	14.03	6.63	7.40
381	C7H9N	3,4-Dimethylpyridine	16.75	10.36	6.39
382	C7H9N	3,5-Dimethylpyridine	17.40	10.58	6.82
383	C7H9N	Benzylamine	20.98	18.49	2.50
384	C7H11N	Cyclohexanecarbonitrile	1.15	3.11	-1.97
385	C7H13N	1-Azabicyclo[2.2.2]octane	-1.00	-0.33	-0.67

386	C7H13N	Heptanenitrile	-7.41	-11.21	3.80
387	C8H7N	1H-Indole	37.40	36.22	1.19
388	CH6N2	Methylhydrazine	22.61	16.02	6.59
389	C2H8N2	1,1-Dimethylhydrazine	20.05	10.93	9.12
390	C4H2N2	(E)-Butenedinitrile	81.31	78.48	2.83
391	C4H4N2	Pyrimidine	46.82	36.44	10.39
392	C4H12N2	1,2-Butanediamine	-17.69	-19.21	1.52
393	C6H8N2	Phenylhydrazine	48.49	44.37	4.12
394	C4H12N4	1,1,4,4-Tetramethyl-2-tetrazene	64.70	46.68	18.02
395	C2H5NO	Acetamide	-56.96	-60.51	3.56
396	C3H3NO	Oxazole	-3.70	-7.82	4.11
397	C3H3NO	Isoxazole	18.79	14.23	4.56
398	C3H7NO	propanamide	-61.88	-67.52	5.64
399	C4H5NO	5-Methylisoxazole	8.15	2.04	6.11
400	C4H5NO	3-Methylisoxazole	8.51	3.45	5.06
401	C4H7NO	2-Methyl-2-oxazoline	-31.19	-36.09	4.90
402	C4H9NO	Butanamide	-66.49	-72.77	6.28
403	C5H5NO	2-Pyridinol	-19.05	-21.72	2.67
404	C5H5NO	3-pyridinol	-10.44	-12.51	2.06
405	C5H5NO	4-pyridinol	-9.75	-11.77	2.02
406	C5H7NO	3,5-Dimethylisoxazole	-4.28	-8.66	4.38
407	C5H9NO	2-Ethyl-2-oxazoline	-35.59	-40.97	5.38
408	C5H11NO	Pentanamide	-69.36	-78.05	8.69
409	C6H7NO	2-Methyl-3-hydroxypyridine	-20.17	-22.69	2.52
410	C6H7NO	2-Methyl-4-hydroxypyridine	-17.14	-22.23	5.10
411	C6H7NO	2-Methyl-5-hydroxypyridine	-16.68	-22.72	6.03
412	C6H7NO	2-Methyl-6-hydroxypyridine	-28.73	-32.56	3.83
413	C6H11NO	Hexahydro-2H-azepin-2-one	-58.84	-61.68	2.84
414	C6H13NO	Hexanamide	-77.49	-82.13	4.64
415	C6H13NO	N-Butylacetamide	-72.85	-80.62	7.77
416	C7H7NO	1-Amino-2,4,6-cyclohepta-trien-1-one	9.44	-0.66	10.10
417	CH3NO2	Methyl nitrite	-15.87	-22.63	6.76
418	CH3NO2	Nitromethane	-17.76	-25.60	7.84
419	C2H5NO2	Nitroethane	-24.45	-33.33	8.88
420	C2H5NO2	Glycine	-93.71	-96.55	2.84
421	C3H7NO2	1-Nitropropane	-29.59	-38.31	8.72
422	C3H7NO2	2-Nitropropane	-33.22	-41.25	8.03
423	C4H9NO2	1-Nitrobutane	-34.39	-43.62	9.22
424	C4H9NO2	2-Nitrobutane	-39.10	-46.70	7.60

425	C4H9NO2	2-Methyl-2-nitropropane	-42.33	-48.46	6.13
426	C5H11NO2	L-Valine	-108.77	-112.31	3.54
427	C6H5NO2	Nitrobenzene	16.13	6.99	9.14
428	C2H5NO3	Ethyl nitrate	-36.83	-49.50	12.67
429	C3H7NO3	Propyl nitrate	-41.56	-54.69	13.13
430	C3H7NO3	Isopropyl nitrate	-45.65	-57.96	12.31
431	C4H3NO3	2-Nitrofuran	-6.88	-16.74	9.86
432	C4H6N2O	3-Amino-5-methylisoxazole	4.71	0.33	4.38
433	C4H6N2O	Dimethylfurazan	25.65	16.26	9.39
434	C5H8N2O	5-Amino-3,4-dimethyl-isoxazole	1.24	-8.49	9.73
435	C5H10N2O	1-Nitrosopiperidine	3.97	-2.60	6.57
436	C6H4N2O	1,2,3-Benzoxadiazole	71.87	63.96	7.91
437	C2H6N2O2	N-Nitrodimethylamine	-1.15	-16.10	14.96
438	C4H4N2O2	Uracil	-72.39	-79.42	7.02
439	C4H6N2O2	Dimethylfurazan monoxide	24.45	11.38	13.07
440	C5H10N2O2	1-Nitropiperidine	-10.64	-20.61	9.98
441	C3H4N2O3	4,5-Dihydro-3-nitro-isoxazole	9.32	1.98	7.35
442	C3H6N2O4	1,1-Dinitropropane	-24.07	-38.78	14.71
443	CF4	Carbon tetrafluoride	-223.14	-236.58	13.44
444	C2FH3	Fluoroethylene	-33.17	-38.69	5.52
445	C3FH7	1-Fluoropropane	-68.33	-76.20	7.87
446	C6FH5	Fluorobenzene	-27.72	-32.70	4.98
447	C7FH7	1-Fluoro-4-methylbenzene	-35.25	-40.78	5.52
448	CF2H2	Difluoromethane	-108.08	-113.36	5.28
449	C6F2H4	1,2-Difluorobenzene	-70.22	-79.03	8.81
450	C6F2H4	1,3-Difluorobenzene	-73.90	-82.76	8.86
451	C6F2H4	1,4-Difluorobenzene	-73.30	-82.00	8.70
452	CF3H	Trifluoromethane	-166.20	-175.44	9.23
453	C2F3H3	1,1,1-Trifluoroethane	-177.96	-190.51	12.54
454	C2FH3O	Acetyl fluoride	-105.66	-110.64	4.98
455	C3F4H4O	2,2,3,3-Tetrafluoro-1-propanol	-253.66	-265.42	11.77
456	C3F5H3O	2,2,3,3,3-Pentafluoro-1-propanol	-313.17	-326.81	13.64
457	C2F3N	Trifluoroacetonitrile	-119.00	-129.78	10.78
458	CF5N	Pentafluoromethylamine	-169.10	-190.72	21.62
459	CF5N3	Pentafluoroguanidine	22.87	-11.94	34.82

Table S4. Comparison of M06-2X/6-311+G(3df,2p)//B3LYP/6-31G(2df,p) and experimental (see text for reference) enthalpies of formation of the Pedley test set.

			ΔH_f^o(298 K) values (kcal/mol)		Difference (kcal/mol)
	Formula	Name	Expt.	M06-2X	Expt. - Theory
1	CH4	Methane	-17.78	-15.74	-2.05
2	C2H2	Acetylene	54.54	55.66	-1.12
3	C2H4	Ethylene	12.55	14.50	-1.95
4	C2H6	Ethane	-20.03	-17.91	-2.11
5	C3H4	Propyne	44.19	44.62	-0.43
6	C3H4	Allene	45.53	44.83	0.71
7	C3H4	Cyclopropene	66.23	64.78	1.45
8	C3H6	Propene	4.78	6.75	-1.97
9	C3H6	Cyclopropane	12.74	10.94	1.80
10	C3H8	Propane	-25.02	-22.61	-2.41
11	C4H6	1-Butyne	39.48	40.66	-1.17
12	C4H6	2-Butyne	34.82	34.53	0.29
13	C4H6	1,2-Butadiene	38.79	38.67	0.12
14	C4H6	1,3-Butadiene	26.29	28.74	-2.45
15	C4H6	Cyclobutene	37.45	39.68	-2.23
16	C4H6	Methylenecyclopropane	47.92	43.53	4.39
17	C4H6	1-Methylcyclopropene	58.22	54.47	3.75
18	C4H6	Bicyclo[1.1.0]butane	51.89	47.80	4.09
19	C4H8	1-Butene	0.02	2.50	-2.48
20	C4H8	(Z)-2-Butene	-1.70	0.76	-2.45
21	C4H8	(E)-2-Butene	-2.72	-0.46	-2.26
22	C4H8	2-Methylpropene	-4.04	-1.78	-2.26
23	C4H8	Cyclobutane	6.79	7.95	-1.16
24	C4H10	Butane	-30.02	-27.28	-2.73
25	C4H10	2-Methylpropane	-32.07	-29.11	-2.97
26	C5H6	1,3-Cyclopentadiene	32.10	33.83	-1.73
27	C5H8	1,2-Pentadiene	33.63	34.22	-0.59
28	C5H8	(Z)-1,3-Pentadiene	19.46	22.37	-2.92
29	C5H8	(E)-1,3-Pentadiene	18.19	21.00	-2.81
30	C5H8	1,4-Pentadiene	25.24	28.27	-3.03
31	C5H8	2,3-Pentadiene	31.81	32.48	-0.67
32	C5H8	2-Methyl-1,3-butadiene	18.04	20.49	-2.45
33	C5H8	Cyclopentene	8.10	10.86	-2.76
34	C5H8	Spiropentane	44.26	38.56	5.70

35	C5H8	Methylenecyclobutane	29.04	30.59	-1.55
36	C5H10	1-Pentene	-5.09	-2.23	-2.86
37	C5H10	(Z)-2-Pentene	-6.60	-3.40	-3.19
38	C5H10	(E)-2-Pentene	-7.62	-4.73	-2.89
39	C5H10	2-Methyl-1-butene	-8.44	-5.55	-2.88
40	C5H10	3-Methyl-1-butene	-6.60	-3.67	-2.93
41	C5H10	2-Methyl-2-butene	-9.99	-7.25	-2.74
42	C5H10	Cyclopentane	-18.26	-15.77	-2.49
43	C5H10	1,1-Dimethylcyclopropane	-1.96	-3.07	1.11
44	C5H12	Pentane	-35.11	-31.89	-3.22
45	C5H12	2-Methylbutane	-36.74	-32.42	-4.31
46	C5H12	2,2-Dimethylpropane	-40.18	-36.57	-3.61
47	C6H6	Benzene	19.74	19.47	0.27
48	C6H8	1,3-Cyclohexadiene	25.38	27.77	-2.39
49	C6H10	1,5-Hexadiene	20.10	23.18	-3.08
50	C6H10	2,3-Dimethyl-1,3-butadiene	10.78	13.38	-2.60
51	C6H10	1-Methylcyclopentene	-0.91	2.07	-2.98
52	C6H10	3-Methylcyclopentene	1.77	4.65	-2.88
53	C6H10	4-Methylcyclopentene	3.49	4.70	-1.21
54	C6H10	Cyclohexene	-1.20	1.23	-2.42
55	C6H10	Bicyclopropyl	30.93	27.48	3.45
56	C6H10	Methylenecyclopentane	2.87	5.35	-2.48
57	C6H10	Bicyclo[3.1.0]hexane	9.15	7.90	1.25
58	C6H12	1-Hexene	-10.40	-6.85	-3.55
59	C6H12	(Z)-2-Hexene	-12.50	-8.16	-4.34
60	C6H12	(E)-2-Hexene	-12.88	-9.48	-3.41
61	C6H12	(Z)-3-Hexene	-11.38	-7.57	-3.81
62	C6H12	(E)-3-Hexene	-13.00	-9.02	-3.99
63	C6H12	2-Methyl-1-pentene	-14.20	-10.24	-3.96
64	C6H12	3-Methyl-1-pentene	-11.83	-8.47	-3.36
65	C6H12	4-Methyl-1-pentene	-12.26	-8.78	-3.48
66	C6H12	2-Methyl-2-pentene	-15.99	-11.44	-4.55
67	C6H12	(Z)-3-Methyl-2-pentene	-14.89	-11.05	-3.84
68	C6H12	(E)-3-Methyl-2-pentene	-15.08	-11.04	-4.04
69	C6H12	(Z)-4-Methyl-2-pentene	-13.74	-9.51	-4.23
70	C6H12	(E)-4-Methyl-2-pentene	-14.70	-10.89	-3.81
71	C6H12	2-Ethyl-1-butene	-13.38	-9.31	-4.07
72	C6H12	2,3-Dimethyl-1-butene	-14.96	-11.12	-3.84
73	C6H12	3,3-Dimethyl-1-butene	-14.46	-10.69	-3.77

74	C6H12	2,3-Dimethyl-2-butene	-16.30	-12.06	-4.24
75	C6H12	Methylcyclopentane	-25.38	-21.79	-3.60
76	C6H12	Cyclohexane	-29.49	-26.44	-3.05
77	C6H12	Ethylcyclobutane	-6.29	-4.02	-2.26
78	C6H14	Hexane	-39.94	-36.51	-3.43
79	C6H14	2-Methylpentane	-41.78	-37.73	-4.05
80	C6H14	3-Methylpentane	-41.13	-37.09	-4.04
81	C6H14	2,3-Dimethylbutane	-42.61	-38.14	-4.47
82	C6H14	2,2-Dimethylbutane	-44.48	-39.98	-4.50
83	C7H8	1,3,5-Cycloheptatriene	43.24	45.87	-2.63
84	C7H8	Methylbenzene	12.05	12.25	-0.20
85	C7H8	Quadricyclane	81.05	75.44	5.61
86	C7H10	1,3-Cycloheptadiene	22.54	25.05	-2.52
87	C7H10	Tricyclo[4.1.0.02,4]heptane	35.66	32.92	2.74
88	C7H12	1-Ethylcyclopentene	-4.71	-2.51	-2.20
89	C7H12	Ethylidenecyclopentane	-4.33	-1.40	-2.92
90	C7H12	1-Methylcyclohexene	-10.35	-7.18	-3.17
91	C7H12	Cycloheptene	-2.20	1.17	-3.37
92	C7H12	Bicyclo[2.2.1]heptane	-13.12	-9.41	-3.71
93	C7H12	1-Methyl-bicyclo[3.1.0]-hexane	0.36	0.30	0.05
94	C7H14	1-Heptene	-14.89	-11.47	-3.42
95	C7H14	5-Methyl-1-hexene	-15.70	-11.91	-3.79
96	C7H14	(Z)-3-Methyl-3-hexene	-18.98	-15.31	-3.67
97	C7H14	(E)-3-Methyl-3-hexene	-18.36	-15.20	-3.16
98	C7H14	2,4-Dimethyl-1-pentene	-20.03	-17.00	-3.02
99	C7H14	4,4-Dimethyl-1-pentene	-19.50	-15.61	-3.89
100	C7H14	2,4-Dimethyl-2-pentene	-21.20	-17.52	-3.68
101	C7H14	(Z)-4,4-Dimethyl-2-pentene	-17.35	-13.42	-3.93
102	C7H14	(E)-4,4-Dimethyl-2-pentene	-21.22	-17.75	-3.47
103	C7H14	3-Methyl-2-ethyl-1-butene	-19.00	-15.11	-3.89
104	C7H14	2,3,3-Trimethyl-1-butene	-20.43	-16.96	-3.48
105	C7H14	1,1-Dimethylcyclopentane	-33.03	-28.90	-4.13
106	C7H14	cis-1,2-dimethylcyclopentane	-30.95	-27.20	-3.75
107	C7H14	trans-1,2-dimethylcyclopentane	-32.65	-28.53	-4.12
108	C7H14	cis-1,3-dimethylcyclopentane	-32.48	-28.11	-4.37
109	C7H14	trans-1,3-dimethylcyclopentane	-31.93	-27.76	-4.17
110	C7H14	Ethylcyclopentane	-30.33	-26.81	-3.52
111	C7H14	Methylcyclohexane	-36.97	-33.24	-3.73
112	C7H14	Cycloheptane	-28.23	-24.96	-3.27

113	C7H16	Heptane	-44.86	-41.13	-3.74
114	C7H16	2-Methylhexane	-46.51	-41.56	-4.95
115	C7H16	3-Methylhexane	-45.72	-41.32	-4.40
116	C7H16	3-Ethylpentane	-45.32	-40.92	-4.40
117	C7H16	2,2-Dimethylpentane	-49.21	-44.44	-4.77
118	C7H16	2,3-Dimethylpentane	-47.54	-42.05	-5.49
119	C7H16	2,4-Dimethylpentane	-48.21	-40.76	-7.44
120	C7H16	3,3-Dimethylpentane	-48.09	-43.74	-4.34
121	C7H16	2,2,3-Trimethylbutane	-48.88	-44.07	-4.81
122	C8H8	1,3,5,7-Cyclooctatetraene	70.72	73.29	-2.57
123	C8H8	Ethenylbenzene	35.35	35.82	-0.47
124	C8H10	Ethylbenzene	7.15	7.70	-0.55
125	C8H10	1,2-Dimethylbenzene	4.57	4.64	-0.07
126	C8H10	1,3-Dimethylbenzene	4.13	5.10	-0.97
127	C8H10	1,4-Dimethylbenzene	4.30	5.25	-0.95
128	C8H12	Bicyclo[2.2.2]oct-2-ene	4.90	9.18	-4.28
129	C8H12	4-Ethenylcyclohexene	15.56	19.82	-4.26
130	C8H12	(Z,Z)-1,5-Cyclooctadiene	24.16	26.68	-2.51
131	C8H14	(2-Propenyl)cyclopentane	-5.76	-1.49	-4.27
132	C8H14	1-Ethylcyclohexene	-15.15	-10.92	-4.23
133	C8H14	Ethylidenecyclohexane	-14.70	-10.56	-4.14
134	C8H14	Ethenylcyclohexane	-11.69	-7.84	-3.85
135	C8H14	Cyclooctene	-6.45	-2.83	-3.62
136	C8H14	Bicyclo[4.2.0]octane	-6.26	-2.62	-3.64
137	C8H14	Bicyclo[5.1.0]octane	-3.97	-2.68	-1.29
138	C8H14	cis-Bicyclo[3.3.0]octane	-22.20	-18.80	-3.40
139	C8H14	trans-Bicyclo[3.3.0]octane	-15.92	-18.80	2.88
140	C8H14	Bicyclo[2.2.2]octane	-23.66	-18.52	-5.14
141	C8H14	1-Methylbicyclo[4.1.0]-heptane	-4.97	-5.37	0.40
142	C8H16	1-Octene	-19.46	-16.08	-3.38
143	C8H16	(Z)-2,2-Dimethyl-3-hexene	-21.34	-17.83	-3.51
144	C8H16	(E)-2,2-Dimethyl-3-hexene	-25.74	-22.04	-3.70
145	C8H16	2-Methyl-3-ethyl-1-pentene	-23.97	-21.19	-2.79
146	C8H16	2,4,4-Trimethyl-1-pentene	-26.43	-22.64	-3.80
147	C8H16	2,4,4-Trimethyl-2-pentene	-25.07	-21.20	-3.87
148	C8H16	Propylcyclopentane	-35.30	-31.43	-3.88
149	C8H16	Ethylcyclohexane	-41.04	-37.17	-3.87
150	C8H16	1,1-Dimethylcyclohexane	-43.24	-39.33	-3.91
151	C8H16	cis-1,2-Dimethylcyclohexane	-41.13	-37.40	-3.74

152	C8H16	trans-1,2-Dimethylcyclohexane	-43.00	-39.07	-3.93
153	C8H16	cis-1,3-Dimethylcyclohexane	-44.12	-40.00	-4.12
154	C8H16	trans-1,3-Dimethylcyclohexane	-42.18	-38.14	-4.04
155	C8H16	cis-1,4-Dimethylcyclohexane	-42.21	-40.00	-2.20
156	C8H16	trans-1,4-Dimethyl-cyclohexane	-44.10	-40.00	-4.09
157	C8H16	Cyclooctane	-29.73	-26.30	-3.44
158	C8H18	Octane	-49.86	-45.74	-4.12
159	C8H18	2-Methylheptane	-51.48	-46.17	-5.31
160	C8H18	3-Methylheptane	-50.79	-46.26	-4.53
161	C8H18	4-Methylheptane	-50.67	-46.16	-4.51
162	C8H18	2,2-Dimethylhexane	-53.68	-49.08	-4.60
163	C8H18	2,5-Dimethylhexane	-53.18	-47.30	-5.88
164	C9H8	Indene	39.05	38.64	0.41
165	C9H10	2,3-Dihydro-1H-indene	14.51	15.08	-0.57
166	C9H10	Cyclopropylbenzene	35.97	34.03	1.94
167	C9H12	Propylbenzene	1.89	2.83	-0.95
168	C9H12	(1-Methylethyl)benzene	0.96	2.13	-1.18
169	C9H12	1-Ethyl-2-methylbenzene	0.31	0.88	-0.57
170	C9H12	1-Ethyl-3-methylbenzene	-0.43	0.57	-1.00
171	C9H12	1-Ethyl-4-methylbenzene	-0.76	0.71	-1.47
172	C9H12	1,2,3-Trimethylbenzene	-2.27	-1.93	-0.34
173	C9H12	1,2,4-Trimethylbenzene	-3.30	-2.36	-0.94
174	C9H12	1,3,5-Trimethylbenzene	-3.80	-2.59	-1.21
175	C9H12	(Z)-5-Ethylidene-bicyclo[2.2.1]hept-2-ene	34.82	39.40	-4.58
176	CH2O	Formaldehyde	-25.96	-26.10	0.15
177	CH4O	Methanol	-48.16	-48.18	0.02
178	C2H2O	Ketene	-11.35	-14.49	3.13
179	C2H4O	Acetaldehyde	-39.70	-39.58	-0.12
180	C2H4O	Oxirane	-12.57	-16.19	3.62
181	C2H6O	Ethanol	-56.21	-55.77	-0.44
182	C2H6O	Dimethyl ether	-44.00	-45.81	1.81
183	C3H6O	2-Propen-1-ol	-29.76	-30.12	0.36
184	C3H6O	Propanal	-44.36	-44.76	0.41
185	C3H6O	Acetone	-51.94	-51.72	-0.21
186	C3H6O	Methyloxirane	-22.63	-25.55	2.91
187	C3H6O	Oxetane	-19.24	-20.50	1.26
188	C3H8O	1-Propanol	-60.97	-60.36	-0.61
189	C3H8O	2-Propanol	-65.20	-64.40	-0.80
190	C3H8O	Methoxyethane	-51.72	-53.41	1.69

191	C4H4O	Furan	-8.34	-11.62	3.28
192	C4H6O	trans-2-Butenal	-24.04	-24.53	0.49
193	C4H6O	Divinyl ether	-3.25	-5.23	1.98
194	C4H8O	Butanal	-48.95	-49.20	0.25
195	C4H8O	2-Methylpropanal	-51.58	-50.42	-1.16
196	C4H8O	2-Butanone	-57.05	-56.78	-0.27
197	C4H8O	Ethoxyethene	-33.65	-33.17	-0.48
198	C4H8O	Tetrahydrofuran	-44.02	-44.69	0.66
199	C4H10O	1-Butanol	-65.73	-64.85	-0.87
200	C4H10O	2-Methyl-1-propanol	-67.85	-66.99	-0.86
201	C4H10O	2-Butanol	-70.00	-69.23	-0.78
202	C4H10O	2-Methyl-2-propanol	-74.69	-73.45	-1.24
203	C4H10O	Diethyl ether	-60.25	-60.91	0.66
204	C4H10O	1-Methoxypropane	-56.93	-57.86	0.93
205	C4H10O	2-Methoxypropane	-60.23	-60.80	0.57
206	C5H8O	Cyclopentanone	-45.91	-46.23	0.32
207	C5H8O	Dihydro-2H-pyran	-29.90	-30.05	0.15
208	C5H10O	3-Pentanone	-61.64	-61.76	0.12
209	C5H10O	2-Pentanone	-61.90	-61.22	-0.68
210	C5H10O	3-Methyl-2-butanone	-62.74	-61.80	-0.94
211	C5H10O	Tetrahydro-2H-pyran	-53.39	-54.30	0.90
212	C5H10O	Pentanal	-54.61	-53.85	-0.76
213	C5H10O	Propoxyethylene	-38.62	-37.65	-0.98
214	C5H10O	3,3-Dimethyloxetane	-35.42	-35.19	-0.23
215	C5H10O	Isopropyl vinyl ether	-41.54	-41.73	0.19
216	C5H12O	1-Pentanol	-70.43	-69.51	-0.92
217	C5H12O	2-Pentanol	-74.74	-73.59	-1.14
218	C5H12O	3-Pentanol	-75.81	-73.66	-2.16
219	C5H12O	2-Methyl-1-butanol	-72.18	-70.53	-1.64
220	C5H12O	3-Methyl-1-butanol	-72.01	-69.61	-2.40
221	C5H12O	2-Methyl-2-butanol	-79.06	-77.48	-1.58
222	C5H12O	3-Methyl-2-butanol	-75.33	-74.55	-0.78
223	C5H12O	2-Methoxy-2-methylpropane	-67.76	-68.07	0.31
224	C5H12O	1-Methoxybutane	-61.69	-62.36	0.67
225	C5H12O	1-Ethoxypropane	-65.06	-65.37	0.31
226	C6H6O	Phenol	-23.04	-25.03	1.99
227	C6H6O	Vinylfuran	6.64	1.40	5.24
228	C6H10O	Cyclohexanone	-54.04	-54.21	0.17
229	C6H12O	2-Hexanone	-66.87	-65.86	-1.01

230	C6H12O	3,3-Dimethyl-2-butanone	-69.48	-68.32	-1.16
231	C6H12O	3-Hexanone	-66.52	-66.20	-0.31
232	C6H12O	2-Methyl-3-pentanone	-68.38	-66.86	-1.52
233	C6H12O	Cyclohexanol	-68.40	-68.61	0.21
234	C6H14O	Hexanol	-75.48	-74.14	-1.34
235	C6H14O	Dipropyl ether	-70.00	-69.81	-0.19
236	C6H14O	Diisopropyl ether	-76.29	-75.71	-0.58
237	C7H6O	Benzaldehyde	-8.77	-10.75	1.98
238	C7H8O	Benzenemethanol	-24.00	-24.81	0.82
239	C7H8O	2-Methylphenol	-30.74	-32.93	2.19
240	C7H8O	3-Methylphenol	-31.62	-32.36	0.74
241	C7H8O	4-Methylphenol	-29.97	-31.69	1.72
242	C7H8O	Methoxybenzene	-16.23	-20.99	4.76
243	C7H10O	Bicyclo[2.2.1]heptan-2-one	-40.77	-38.72	-2.05
244	C7H10O	8-Oxatricyclo-[3.2.1.01,5]octane	6.43	6.31	0.12
245	C7H14O	Heptanal	-63.05	-63.10	0.05
246	C7H14O	2,2-Dimethyl-3-pentanone	-74.98	-73.11	-1.87
247	C7H14O	2,4-Dimethyl-3-pentanone	-74.40	-72.15	-2.25
248	C7H16O	1-Heptanol	-80.40	-78.75	-1.65
249	C8H8O	Acetophenone	-20.72	-21.67	0.95
250	C8H8O	Phenyl vinyl ether	5.43	1.82	3.60
251	C8H10O	2-Ethylphenol	-34.70	-37.16	2.46
252	C8H10O	3-Ethylphenol	-34.92	-36.90	1.98
253	C8H10O	4-Ethylphenol	-34.44	-36.27	1.83
254	C8H10O	2,3-Dimethylphenol	-37.57	-39.55	1.98
255	C8H10O	2,4-Dimethylphenol	-38.93	-39.54	0.60
256	C8H10O	2,5-Dimethylphenol	-38.62	-39.87	1.25
257	C8H10O	2,6-Dimethylphenol	-38.67	-40.48	1.81
258	C8H10O	3,4-Dimethylphenol	-37.43	-39.45	2.02
259	C8H10O	3,5-Dimethylphenol	-38.60	-39.60	1.00
260	C8H10O	Ethoxybenzene	-24.28	-28.54	4.26
261	C2H2O2	Ethanedial	-50.67	-52.39	1.72
262	C2H4O2	Acetic acid	-103.44	-105.10	1.66
263	C2H4O2	Methyl formate	-84.97	-89.41	4.44
264	C2H6O2	1,2-Ethanediol	-92.61	-94.65	2.04
265	C2H6O2	Dimethyl peroxide	-30.04	-31.06	1.02
266	C3H4O2	2-Oxetanone	-67.61	-70.49	2.88
267	C3H6O2	1,3-Dioxolane	-71.22	-76.32	5.09
268	C3H6O2	Propanoic acid	-108.39	-110.15	1.76

269	C3H6O2	Acetic acid methyl ester	-98.45	-101.62	3.18
270	C3H8O2	1,2-propanediol	-100.69	-103.96	3.26
271	C3H8O2	Dimethoxymethane	-83.27	-89.03	5.76
272	C3H8O2	1,3-Propanediol	-93.71	-97.20	3.48
273	C4H4O2	4-Methylene-2-oxetanone	-45.46	-49.22	3.76
274	C4H4O2	Cyclobutane-1,3-dione	-44.53	-46.36	1.84
275	C4H6O2	2,3-Butanedione	-78.18	-74.45	-3.73
276	C4H6O2	Acetic acid ethenyl ester	-75.26	-78.87	3.60
277	C4H8O2	Acetic acid ethyl ester	-106.14	-108.92	2.78
278	C4H8O2	1,4-Dioxane	-75.48	-80.70	5.22
279	C4H8O2	2-Methyl-1,3-dioxolane	-84.13	-87.18	3.05
280	C4H10O2	1,3-Butanediol	-103.54	-105.78	2.24
281	C4H10O2	1,1-Dimethoxyethane	-93.14	-96.64	3.50
282	C4H10O2	Diethyl peroxide	-46.08	-45.84	-0.24
283	C4H10O2	1,4-Butanediol	-101.98	-102.44	0.45
284	C5H6O2	2-Furanmethanol	-50.62	-55.67	5.05
285	C5H8O2	(E)-2-Butenoic acid methyl ester	-81.72	-84.72	3.00
286	C5H10O2	Pentanoic acid	-117.57	-119.31	1.75
287	C5H10O2	Propanoic acid ethyl ester	-110.80	-113.87	3.07
288	C5H10O2	propan-2-yl acetate	-115.13	-117.17	2.04
289	C5H10O2	4-Methyl-1,3-dioxane	-90.08	-95.35	5.26
290	C5H10O2	1,3-Dioxepane	-82.84	-90.50	7.66
291	C5H10O2	cis-2,4-Dimethyl-1,3-dioxolane	-91.44	-96.37	4.93
292	C5H10O2	trans-2,4-Dimethyl-1,3-dioxolane	-90.94	-95.28	4.34
293	C5H12O2	2,2-Dimethoxypropane	-102.68	-106.78	4.10
294	C5H12O2	1,5-Pentanediol	-107.34	-106.95	-0.39
295	C5H12O2	Diethoxymethane	-99.14	-103.94	4.80
296	C6H4O2	2,5-cyclohexadiene-1,4-dione	-29.37	-28.70	-0.68
297	C6H6O2	1,4-Benzenediol	-63.41	-67.50	4.09
298	C6H6O2	1,3-Benzenediol	-65.65	-69.84	4.18
299	C6H10O2	(E)-2-Butenoic acid ethyl ester	-89.77	-92.00	2.23
300	C6H12O2	Hexanoic acid	-122.35	-123.94	1.60
301	C6H12O2	Pentanoic acid methyl ester	-112.62	-115.71	3.10
302	C6H12O2	2,2-Dimethylpropanoic acid methyl ester	-118.14	-118.57	0.43
303	C6H12O2	Acetic acid butyl ester	-116.06	-117.91	1.85
304	C6H12O2	Tetrahydro-2-methoxy-2H-pyran	-95.51	-98.66	3.16
305	C6H12O2	4,5-Dimethyl-1,3-dioxane	-97.78	-101.84	4.06
306	C6H14O2	1,2-Diethoxyethane	-97.56	-102.32	4.76
307	C6H14O2	1,1-Diethoxyethane	-108.39	-111.44	3.06

308	C7H6O2	Benzoic acid	-70.29	-74.79	4.50
309	C7H6O2	2-Hydroxy-2,4,6-cycloheptatriene-1-one	-37.14	-29.36	-7.78
310	C7H6O2	Formic acid phenyl ester	-51.58	-58.77	7.19
311	C7H6O2	3-(2-Furyl)-2-propenal	-25.31	-29.89	4.58
312	C7H12O2	4-Pentenoic acid ethyl ester	-92.16	-93.07	0.91
313	C7H12O2	(Z)-3-Pentenoic acid ethyl ester	-92.64	-94.90	2.26
314	C7H12O2	(E)-3-Pentenoic acid ethyl ester	-93.26	-94.90	1.64
315	C7H12O2	(E)-2-Pentenoic acid ethyl ester	-94.24	-96.15	1.91
316	C7H12O2	(E)-2-Butenoic acid propyl ester	-94.46	-96.46	2.00
317	C7H12O2	(E)-2-Butenoic acid isopropyl ester	-98.26	-100.23	1.97
318	C3H4O3	1,3-Dioxolan-2-one	-121.51	-129.22	7.71
319	C3H6O3	1,3,5-Trioxane	-111.35	-120.75	9.39
320	C3H8O3	1,2,3-Propanetriol	-139.27	-143.54	4.27
321	C4H6O3	Acetic anhydride	-136.83	-142.72	5.89
322	C4H10O3	Trimethoxymethane	-127.13	-135.66	8.53
323	C5H4O3	3-Methyl-2,5-furandione	-106.88	-112.41	5.53
324	C5H10O3	Carbonic acid diethyl ester	-152.46	-159.04	6.58
325	C5H10O3	1,3,6-Trioxacyclooctane	-111.64	-120.99	9.35
326	C5H12O3	1,1,1-Trimethoxyethane	-136.88	-144.23	7.35
327	C4H6O4	Butanedioic acid	-196.70	-202.26	5.56
328	C4H8O4	1,3,5,7-Tetroxane	-148.23	-159.23	10.99
329	C4H10O4	2(R),3(S)-1,2,3,4-Butanetetrol	-185.28	-187.13	1.85
330	C2N2	Cyanogen	73.30	74.84	-1.54
331	C4N2	2-Butynedinitrile	126.48	127.15	-0.67
332	CH5N	Methylamine	-5.50	-3.77	-1.73
333	C2H5N	Aziridine	30.23	27.70	2.54
334	C2H7N	Ethylamine	-11.33	-10.22	-1.11
335	C2H7N	Dimethylamine	-4.45	-3.51	-0.93
336	C3H3N	2-Propenenitrile	43.16	45.79	-2.62
337	C3H5N	Propanenitrile	12.31	14.14	-1.83
338	C3H7N	Cyclopropylamine	18.40	17.86	0.55
339	C3H9N	1-Propylamine	-16.78	-14.89	-1.89
340	C3H9N	2-Propylamine	-20.03	-17.84	-2.19
341	C3H9N	Trimethylamine	-5.66	-6.11	0.44
342	C4H5N	1H-Pyrrole	25.88	23.44	2.44
343	C4H5N	Cyclopropanecarbonitrile	43.45	41.59	1.86
344	C4H5N	3-Butenenitrile	37.72	41.07	-3.36
345	C4H5N	(E)-2-Butenenitrile	33.63	36.60	-2.97
346	C4H7N	Butanenitrile	8.03	9.22	-1.19

347	C4H7N	2-Methylpropanenitrile	5.57	8.34	-2.77
348	C4H9N	pyrrolidine	-0.81	0.24	-1.06
349	C4H9N	Cyclobutylamine	9.85	12.06	-2.21
350	C4H11N	1-Butylamine	-21.99	-19.32	-2.67
351	C4H11N	2-Butylamine	-25.07	-22.65	-2.42
352	C4H11N	2-Methyl-2-propylamine	-28.90	-26.16	-2.73
353	C4H11N	Diethylamine	-17.33	-16.23	-1.10
354	C4H11N	2-Methylpropylamine	-23.59	-21.27	-2.32
355	C5H5N	Pyridine	33.56	31.65	1.91
356	C5H7N	1-Methyl-1H-pyrrole	24.64	21.92	2.72
357	C5H7N	(E)-2-Pentenenitrile	28.63	32.35	-3.72
358	C5H7N	(E)-3-Pentenenitrile	30.02	33.17	-3.15
359	C5H9N	2,2-Dimethylpropanenitrile	-0.60	1.35	-1.95
360	C5H9N	Pentanenitrile	2.51	4.56	-2.05
361	C5H11N	Piperidine	-11.28	-10.48	-0.80
362	C5H11N	Cyclopentylamine	-13.12	-10.20	-2.92
363	C6H7N	Aniline	20.82	19.18	1.63
364	C6H7N	2-Methylpyridine	23.71	22.02	1.69
365	C6H7N	3-Methylpyridine	25.43	24.11	1.32
366	C6H7N	4-Methylpyridine	24.88	23.52	1.36
367	C6H7N	Bicyclo[2.1.0]pentane-1-carbonitrile	65.03	64.08	0.96
368	C6H7N	3-Methylenecyclobutane-carbonitrile	60.35	61.25	-0.91
369	C6H7N	1-Cyclopentene-1-carbonitrile	37.40	39.80	-2.39
370	C6H9N	2,5-Dimethyl-1H-pyrrole	9.51	7.74	1.77
371	C6H13N	2-Methylpiperidine	-20.17	-18.70	-1.47
372	C6H13N	Cyclohexylamine	-25.07	-22.24	-2.83
373	C6H15N	Triethylamine	-22.18	-20.94	-1.24
374	C6H15N	Dipropylamine	-27.75	-25.25	-2.50
375	C6H15N	Diisopropylamine	-34.42	-29.49	-4.93
376	C7H5N	Benzonitrile	51.55	50.69	0.86
377	C7H9N	2,3-Dimethylpyridine	16.32	14.71	1.61
378	C7H9N	2,4-Dimethylpyridine	15.27	13.92	1.35
379	C7H9N	2,5-Dimethylpyridine	15.89	14.67	1.23
380	C7H9N	2,6-Dimethylpyridine	14.03	12.52	1.51
381	C7H9N	3,4-Dimethylpyridine	16.75	15.52	1.23
382	C7H9N	3,5-Dimethylpyridine	17.40	16.66	0.74
383	C7H9N	Benzylamine	20.98	20.57	0.41
384	C7H11N	Cyclohexanecarbonitrile	1.15	3.64	-2.50
385	C7H13N	1-Azabicyclo[2.2.2]octane	-1.00	1.60	-2.61

386	C7H13N	Heptanenitrile	-7.41	-4.95	-2.46
387	C8H7N	1H-Indole	37.40	35.60	1.80
388	CH6N2	Methylhydrazine	22.61	23.21	-0.60
389	C2H8N2	1,1-Dimethylhydrazine	20.05	19.32	0.74
390	C4H2N2	(E)-Butenedinitrile	81.31	81.16	0.15
391	C4H4N2	Pyrimidine	46.82	41.57	5.25
392	C4H12N2	1,2-Butanediamine	-17.69	-14.03	-3.66
393	C6H8N2	Phenylhydrazine	48.49	47.87	0.63
394	C4H12N4	1,1,4,4-Tetramethyl-2-tetrazene	64.70	64.16	0.53
395	C2H5NO	Acetamide	-56.96	-57.46	0.50
396	C3H3NO	Oxazole	-3.70	-8.01	4.31
397	C3H3NO	Isoxazole	18.79	17.45	1.34
398	C3H7NO	propanamide	-61.88	-63.64	1.76
399	C4H5NO	5-Methylisoxazole	8.15	6.71	1.44
400	C4H5NO	3-Methylisoxazole	8.51	8.02	0.49
401	C4H7NO	2-Methyl-2-oxazoline	-31.19	-32.48	1.29
402	C4H9NO	Butanamide	-66.49	-68.14	1.65
403	C5H5NO	2-Pyridinol	-19.05	-20.18	1.14
404	C5H5NO	3-pyridinol	-10.44	-12.18	1.74
405	C5H5NO	4-pyridinol	-9.75	-10.93	1.18
406	C5H7NO	3,5-Dimethylisoxazole	-4.28	-2.66	-1.62
407	C5H9NO	2-Ethyl-2-oxazoline	-35.59	-36.45	0.87
408	C5H11NO	Pentanamide	-69.36	-72.76	3.40
409	C6H7NO	2-Methyl-3-hydroxypyridine	-20.17	-21.91	1.74
410	C6H7NO	2-Methyl-4-hydroxypyridine	-17.14	-20.60	3.47
411	C6H7NO	2-Methyl-5-hydroxypyridine	-16.68	-21.22	4.54
412	C6H7NO	2-Methyl-6-hydroxypyridine	-28.73	-30.11	1.38
413	C6H11NO	Hexahydro-2H-azepin-2-one	-58.84	-59.57	0.73
414	C6H13NO	Hexanamide	-77.49	-76.03	-1.45
415	C6H13NO	N-Butylacetamide	-72.85	-73.65	0.80
416	C7H7NO	1-Amino-2,4,6-cyclohepta-trien-1-one	9.44	4.52	4.92
417	CH3NO2	Methyl nitrite	-15.87	-14.68	-1.19
418	CH3NO2	Nitromethane	-17.76	-17.17	-0.58
419	C2H5NO2	Nitroethane	-24.45	-23.84	-0.61
420	C2H5NO2	Glycine	-93.71	-97.52	3.80
421	C3H7NO2	1-Nitropropane	-29.59	-28.02	-1.56
422	C3H7NO2	2-Nitropropane	-33.22	-31.75	-1.47
423	C4H9NO2	1-Nitrobutane	-34.39	-32.68	-1.72
424	C4H9NO2	2-Nitrobutane	-39.10	-37.07	-2.03

425	C4H9NO2	2-Methyl-2-nitropropane	-42.33	-39.87	-2.45
426	C5H11NO2	L-Valine	-108.77	-113.17	4.40
427	C6H5NO2	Nitrobenzene	16.13	13.60	2.53
428	C2H5NO3	Ethyl nitrate	-36.83	-38.16	1.33
429	C3H7NO3	Propyl nitrate	-41.56	-42.64	1.07
430	C3H7NO3	Isopropyl nitrate	-45.65	-46.44	0.79
431	C4H3NO3	2-Nitrofuran	-6.88	-11.83	4.95
432	C4H6N2O	3-Amino-5-methylisoxazole	4.71	5.29	-0.58
433	C4H6N2O	Dimethylfurazan	25.65	27.01	-1.37
434	C5H8N2O	5-Amino-3,4-dimethyl-isoxazole	1.24	-2.25	3.49
435	C5H10N2O	1-Nitrosopiperidine	3.97	6.89	-2.93
436	C6H4N2O	1,2,3-Benzoxadiazole	71.87	49.00	22.87
437	C2H6N2O2	N-Nitrodimethylamine	-1.15	-3.50	2.35
438	C4H4N2O2	Uracil	-72.39	-78.84	6.44
439	C4H6N2O2	Dimethylfurazan monoxide	24.45	26.16	-1.71
440	C5H10N2O2	1-Nitropiperidine	-10.64	-10.37	-0.27
441	C3H4N2O3	4,5-Dihydro-3-nitro-isoxazole	9.32	12.57	-3.25
442	C3H6N2O4	1,1-Dinitropropane	-24.07	-25.24	1.17
443	CF4	Carbon tetrafluoride	-223.14	-231.37	8.23
444	C2FH3	Fluoroethylene	-33.17	-35.08	1.91
445	C3FH7	1-Fluoropropane	-68.33	-70.16	1.83
446	C6FH5	Fluorobenzene	-27.72	-30.72	3.00
447	C7FH7	1-Fluoro-4-methylbenzene	-35.25	-37.61	2.35
448	CF2H2	Difluoromethane	-108.08	-110.84	2.77
449	C6F2H4	1,2-Difluorobenzene	-70.22	-76.40	6.18
450	C6F2H4	1,3-Difluorobenzene	-73.90	-80.25	6.35
451	C6F2H4	1,4-Difluorobenzene	-73.30	-79.44	6.13
452	CF3H	Trifluoromethane	-166.20	-171.98	5.77
453	C2F3H3	1,1,1-Trifluoroethane	-177.96	-185.56	7.60
454	C2FH3O	Acetyl fluoride	-105.66	-107.54	1.87
455	C3F4H4O	2,2,3,3-Tetrafluoro-1-propanol	-253.66	-265.51	11.85
456	C3F5H3O	2,2,3,3,3-Pentafluoro-1-propanol	-313.17	-323.25	10.08
457	C2F3N	Trifluoroacetonitrile	-119.00	-124.97	5.96
458	CF5N	Pentafluoromethylamine	-169.10	-178.71	9.61
459	CF5N3	Pentafluoroguanidine	22.87	11.26	11.61

Table S5. Comparison of ωB97X-D/6-311+G(3df,2p)//B3LYP/6-31G(2df,p) and experimental (see text for reference) enthalpies of formation of the Pedley test set.

			ΔH_f^o(298 K) values (kcal/mol)		Difference (kcal/mol)
	Formula	Name	Expt.	wB97-XD	Expt. - Theory
1	CH4	Methane	-17.78	-16.54	-1.24
2	C2H2	Acetylene	54.54	58.47	-3.93
3	C2H4	Ethylene	12.55	14.37	-1.82
4	C2H6	Ethane	-20.03	-19.26	-0.77
5	C3H4	Propyne	44.19	46.96	-2.77
6	C3H4	Allene	45.53	45.90	-0.37
7	C3H4	Cyclopropene	66.23	68.35	-2.12
8	C3H6	Propene	4.78	6.21	-1.43
9	C3H6	Cyclopropane	12.74	12.46	0.28
10	C3H8	Propane	-25.02	-24.36	-0.66
11	C4H6	1-Butyne	39.48	42.61	-3.12
12	C4H6	2-Butyne	34.82	36.47	-1.65
13	C4H6	1,2-Butadiene	38.79	39.33	-0.54
14	C4H6	1,3-Butadiene	26.29	29.08	-2.79
15	C4H6	Cyclobutene	37.45	38.59	-1.14
16	C4H6	Methylenecyclopropane	47.92	45.45	2.47
17	C4H6	1-Methylcyclopropene	58.22	57.39	0.83
18	C4H6	Bicyclo[1.1.0]butane	51.89	52.95	-1.07
19	C4H8	1-Butene	0.02	1.56	-1.53
20	C4H8	(Z)-2-Butene	-1.70	-0.31	-1.39
21	C4H8	(E)-2-Butene	-2.72	-1.41	-1.32
22	C4H8	2-Methylpropene	-4.04	-2.50	-1.54
23	C4H8	Cyclobutane	6.79	5.50	1.29
24	C4H10	Butane	-30.02	-29.49	-0.53
25	C4H10	2-Methylpropane	-32.07	-31.02	-1.05
26	C5H6	1,3-Cyclopentadiene	32.10	33.66	-1.56
27	C5H8	1,2-Pentadiene	33.63	34.45	-0.82
28	C5H8	(Z)-1,3-Pentadiene	19.46	22.22	-2.76
29	C5H8	(E)-1,3-Pentadiene	18.19	20.89	-2.70
30	C5H8	1,4-Pentadiene	25.24	28.06	-2.82
31	C5H8	2,3-Pentadiene	31.81	32.68	-0.87
32	C5H8	2-Methyl-1,3-butadiene	18.04	20.87	-2.83
33	C5H8	Cyclopentene	8.10	9.41	-1.31

34	C5H8	Spiropentane	44.26	41.80	2.46
35	C5H8	Methylenecyclobutane	29.04	28.47	0.56
36	C5H10	1-Pentene	-5.09	-3.65	-1.44
37	C5H10	(Z)-2-Pentene	-6.60	-4.96	-1.64
38	C5H10	(E)-2-Pentene	-7.62	-6.15	-1.48
39	C5H10	2-Methyl-1-butene	-8.44	-6.76	-1.67
40	C5H10	3-Methyl-1-butene	-6.60	-4.82	-1.77
41	C5H10	2-Methyl-2-butene	-9.99	-8.47	-1.52
42	C5H10	Cyclopentane	-18.26	-18.48	0.22
43	C5H10	1,1-Dimethylcyclopropane	-1.96	-2.34	0.38
44	C5H12	Pentane	-35.11	-34.60	-0.51
45	C5H12	2-Methylbutane	-36.74	-34.95	-1.79
46	C5H12	2,2-Dimethylpropane	-40.18	-38.35	-1.82
47	C6H6	Benzene	19.74	20.12	-0.37
48	C6H8	1,3-Cyclohexadiene	25.38	27.39	-2.01
49	C6H10	1,5-Hexadiene	20.10	22.52	-2.42
50	C6H10	2,3-Dimethyl-1,3-butadiene	10.78	13.90	-3.12
51	C6H10	1-Methylcyclopentene	-0.91	0.05	-0.96
52	C6H10	3-Methylcyclopentene	1.77	2.75	-0.99
53	C6H10	4-Methylcyclopentene	3.49	2.75	0.74
54	C6H10	Cyclohexene	-1.20	-0.26	-0.94
55	C6H10	Bicyclopropyl	30.93	30.51	0.41
56	C6H10	Methylenecyclopentane	2.87	3.36	-0.49
57	C6H10	Bicyclo[3.1.0]hexane	9.15	8.15	1.00
58	C6H12	1-Hexene	-10.40	-8.76	-1.63
59	C6H12	(Z)-2-Hexene	-12.50	-10.21	-2.29
60	C6H12	(E)-2-Hexene	-12.88	-11.37	-1.51
61	C6H12	(Z)-3-Hexene	-11.38	-9.64	-1.74
62	C6H12	(E)-3-Hexene	-13.00	-10.92	-2.08
63	C6H12	2-Methyl-1-pentene	-14.20	-11.98	-2.22
64	C6H12	3-Methyl-1-pentene	-11.83	-10.11	-1.72
65	C6H12	4-Methyl-1-pentene	-12.26	-10.40	-1.86
66	C6H12	2-Methyl-2-pentene	-15.99	-13.20	-2.79
67	C6H12	(Z)-3-Methyl-2-pentene	-14.89	-12.84	-2.05
68	C6H12	(E)-3-Methyl-2-pentene	-15.08	-12.79	-2.29
69	C6H12	(Z)-4-Methyl-2-pentene	-13.74	-11.35	-2.39
70	C6H12	(E)-4-Methyl-2-pentene	-14.70	-12.56	-2.14
71	C6H12	2-Ethyl-1-butene	-13.38	-11.12	-2.27
72	C6H12	2,3-Dimethyl-1-butene	-14.96	-12.59	-2.37

73	C6H12	3,3-Dimethyl-1-butene	-14.46	-11.46	-3.00
74	C6H12	2,3-Dimethyl-2-butene	-16.30	-13.46	-2.84
75	C6H12	Methylcyclopentane	-25.38	-24.99	-0.39
76	C6H12	Cyclohexane	-29.49	-29.27	-0.23
77	C6H12	Ethylcyclobutane	-6.29	-7.57	1.29
78	C6H14	Hexane	-39.94	-39.72	-0.22
79	C6H14	2-Methylpentane	-41.78	-40.71	-1.07
80	C6H14	3-Methylpentane	-41.13	-40.08	-1.05
81	C6H14	2,3-Dimethylbutane	-42.61	-40.93	-1.69
82	C6H14	2,2-Dimethylbutane	-44.48	-42.33	-2.15
83	C7H8	1,3,5-Cycloheptatriene	43.24	46.52	-3.28
84	C7H8	Methylbenzene	12.05	12.46	-0.41
85	C7H8	Quadricyclane	81.05	78.05	3.00
86	C7H10	1,3-Cycloheptadiene	22.54	23.92	-1.38
87	C7H10	Tricyclo[4.1.0.02,4]heptane	35.66	35.89	-0.23
88	C7H12	1-Ethylcyclopentene	-4.71	-4.89	0.18
89	C7H12	Ethylidenecyclopentane	-4.33	-3.84	-0.48
90	C7H12	1-Methylcyclohexene	-10.35	-9.02	-1.33
91	C7H12	Cycloheptene	-2.20	-0.72	-1.47
92	C7H12	Bicyclo[2.2.1]heptane	-13.12	-12.51	-0.61
93	C7H12	1-Methyl-bicyclo[3.1.0]-hexane	0.36	-0.10	0.46
94	C7H14	1-Heptene	-14.89	-13.89	-1.00
95	C7H14	5-Methyl-1-hexene	-15.70	-14.23	-1.48
96	C7H14	(Z)-3-Methyl-3-hexene	-18.98	-17.66	-1.32
97	C7H14	(E)-3-Methyl-3-hexene	-18.36	-17.53	-0.82
98	C7H14	2,4-Dimethyl-1-pentene	-20.03	-18.99	-1.04
99	C7H14	4,4-Dimethyl-1-pentene	-19.50	-17.13	-2.37
100	C7H14	2,4-Dimethyl-2-pentene	-21.20	-19.62	-1.58
101	C7H14	(Z)-4,4-Dimethyl-2-pentene	-17.35	-15.20	-2.16
102	C7H14	(E)-4,4-Dimethyl-2-pentene	-21.22	-19.09	-2.13
103	C7H14	3-Methyl-2-ethyl-1-butene	-19.00	-16.91	-2.09
104	C7H14	2,3,3-Trimethyl-1-butene	-20.43	-17.90	-2.54
105	C7H14	1,1-Dimethylcyclopentane	-33.03	-32.10	-0.93
106	C7H14	cis-1,2-dimethylcyclopentane	-30.95	-30.73	-0.22
107	C7H14	trans-1,2-dimethylcyclopentane	-32.65	-32.26	-0.39
108	C7H14	cis-1,3-dimethylcyclopentane	-32.48	-31.87	-0.61
109	C7H14	trans-1,3-dimethylcyclopentane	-31.93	-31.54	-0.39
110	C7H14	Ethylcyclopentane	-30.33	-30.60	0.27
111	C7H14	Methylcyclohexane	-36.97	-36.43	-0.54

112	C7H14	Cycloheptane	-28.23	-28.50	0.27
113	C7H16	Heptane	-44.86	-44.85	-0.01
114	C7H16	2-Methylhexane	-46.51	-45.18	-1.33
115	C7H16	3-Methylhexane	-45.72	-44.99	-0.74
116	C7H16	3-Ethylpentane	-45.32	-44.55	-0.76
117	C7H16	2,2-Dimethylpentane	-49.21	-47.39	-1.82
118	C7H16	2,3-Dimethylpentane	-47.54	-45.47	-2.07
119	C7H16	2,4-Dimethylpentane	-48.21	-44.29	-3.92
120	C7H16	3,3-Dimethylpentane	-48.09	-46.65	-1.44
121	C7H16	2,2,3-Trimethylbutane	-48.88	-46.63	-2.24
122	C8H8	1,3,5,7-Cyclooctatetraene	70.72	74.36	-3.64
123	C8H8	Ethenylbenzene	35.35	36.99	-1.64
124	C8H10	Ethylbenzene	7.15	7.40	-0.25
125	C8H10	1,2-Dimethylbenzene	4.57	4.59	-0.03
126	C8H10	1,3-Dimethylbenzene	4.13	4.85	-0.72
127	C8H10	1,4-Dimethylbenzene	4.30	5.01	-0.70
128	C8H12	Bicyclo[2.2.2]oct-2-ene	4.90	7.55	-2.65
129	C8H12	4-Ethenylcyclohexene	15.56	18.71	-3.15
130	C8H12	(Z,Z)-1,5-Cyclooctadiene	24.16	25.32	-1.16
131	C8H14	(2-Propenyl)cyclopentane	-5.76	-4.49	-1.27
132	C8H14	1-Ethylcyclohexene	-15.15	-13.41	-1.75
133	C8H14	Ethylidenecyclohexane	-14.70	-13.04	-1.66
134	C8H14	Ethenylcyclohexane	-11.69	-10.30	-1.39
135	C8H14	Cyclooctene	-6.45	-5.39	-1.06
136	C8H14	Bicyclo[4.2.0]octane	-6.26	-6.92	0.66
137	C8H14	Bicyclo[5.1.0]octane	-3.97	-3.62	-0.35
138	C8H14	cis-Bicyclo[3.3.0]octane	-22.20	-23.13	0.92
139	C8H14	trans-Bicyclo[3.3.0]octane	-15.92	-23.13	7.21
140	C8H14	Bicyclo[2.2.2]octane	-23.66	-22.09	-1.57
141	C8H14	1-Methylbicyclo[4.1.0]-heptane	-4.97	-6.13	1.15
142	C8H16	1-Octene	-19.46	-19.01	-0.44
143	C8H16	(Z)-2,2-Dimethyl-3-hexene	-21.34	-20.16	-1.19
144	C8H16	(E)-2,2-Dimethyl-3-hexene	-25.74	-23.93	-1.81
145	C8H16	2-Methyl-3-ethyl-1-pentene	-23.97	-23.70	-0.27
146	C8H16	2,4,4-Trimethyl-1-pentene	-26.43	-24.53	-1.91
147	C8H16	2,4,4-Trimethyl-2-pentene	-25.07	-23.21	-1.86
148	C8H16	Propylcyclopentane	-35.30	-35.77	0.47
149	C8H16	Ethylcyclohexane	-41.04	-41.01	-0.03
150	C8H16	1,1-Dimethylcyclohexane	-43.24	-42.63	-0.60

151	C8H16	cis-1,2-Dimethylcyclohexane	-41.13	-41.10	-0.04
152	C8H16	trans-1,2-Dimethylcyclohexane	-43.00	-42.61	-0.38
153	C8H16	cis-1,3-Dimethylcyclohexane	-44.12	-43.60	-0.52
154	C8H16	trans-1,3-Dimethylcyclohexane	-42.18	-41.91	-0.27
155	C8H16	cis-1,4-Dimethylcyclohexane	-42.21	-43.59	1.38
156	C8H16	trans-1,4-Dimethyl-cyclohexane	-44.10	-43.59	-0.51
157	C8H16	Cyclooctane	-29.73	-30.60	0.86
158	C8H18	Octane	-49.86	-49.97	0.12
159	C8H18	2-Methylheptane	-51.48	-50.32	-1.16
160	C8H18	3-Methylheptane	-50.79	-50.34	-0.45
161	C8H18	4-Methylheptane	-50.67	-50.28	-0.39
162	C8H18	2,2-Dimethylhexane	-53.68	-52.58	-1.10
163	C8H18	2,5-Dimethylhexane	-53.18	-51.28	-1.90
164	C9H8	Indene	39.05	38.96	0.09
165	C9H10	2,3-Dihydro-1H-indene	14.51	13.97	0.54
166	C9H10	Cyclopropylbenzene	35.97	36.65	-0.68
167	C9H12	Propylbenzene	1.89	2.00	-0.11
168	C9H12	(1-Methylethyl)benzene	0.96	1.50	-0.54
169	C9H12	1-Ethyl-2-methylbenzene	0.31	0.21	0.10
170	C9H12	1-Ethyl-3-methylbenzene	-0.43	-0.22	-0.21
171	C9H12	1-Ethyl-4-methylbenzene	-0.76	-0.06	-0.70
172	C9H12	1,2,3-Trimethylbenzene	-2.27	-2.21	-0.06
173	C9H12	1,2,4-Trimethylbenzene	-3.30	-2.88	-0.42
174	C9H12	1,3,5-Trimethylbenzene	-3.80	-3.33	-0.47
175	C9H12	(Z)-5-Ethylidene-bicyclo[2.2.1]hept-2-ene	34.82	38.06	-3.23
176	CH2O	Formaldehyde	-25.96	-26.31	0.36
177	CH4O	Methanol	-48.16	-47.67	-0.49
178	C2H2O	Ketene	-11.35	-14.24	2.89
179	C2H4O	Acetaldehyde	-39.70	-40.45	0.75
180	C2H4O	Oxirane	-12.57	-13.95	1.38
181	C2H6O	Ethanol	-56.21	-55.63	-0.59
182	C2H6O	Dimethyl ether	-44.00	-44.32	0.32
183	C3H6O	2-Propen-1-ol	-29.76	-29.20	-0.55
184	C3H6O	Propanal	-44.36	-45.79	1.43
185	C3H6O	Acetone	-51.94	-52.96	1.03
186	C3H6O	Methyloxirane	-22.63	-23.83	1.19
187	C3H6O	Oxetane	-19.24	-20.86	1.62
188	C3H8O	1-Propanol	-60.97	-60.60	-0.37
189	C3H8O	2-Propanol	-65.20	-64.40	-0.80

190	C3H8O	Methoxyethane	-51.72	-52.35	0.63
191	C4H4O	Furan	-8.34	-9.33	0.99
192	C4H6O	trans-2-Butenal	-24.04	-25.33	1.28
193	C4H6O	Divinyl ether	-3.25	-2.97	-0.28
194	C4H8O	Butanal	-48.95	-50.70	1.75
195	C4H8O	2-Methylpropanal	-51.58	-51.58	0.00
196	C4H8O	2-Butanone	-57.05	-58.18	1.13
197	C4H8O	Ethoxyethene	-33.65	-31.87	-1.78
198	C4H8O	Tetrahydrofuran	-44.02	-44.42	0.40
199	C4H10O	1-Butanol	-65.73	-65.58	-0.14
200	C4H10O	2-Methyl-1-propanol	-67.85	-67.12	-0.73
201	C4H10O	2-Butanol	-70.00	-69.44	-0.57
202	C4H10O	2-Methyl-2-propanol	-74.69	-73.30	-1.39
203	C4H10O	Diethyl ether	-60.25	-60.35	0.09
204	C4H10O	1-Methoxypropane	-56.93	-57.22	0.29
205	C4H10O	2-Methoxypropane	-60.23	-60.04	-0.19
206	C5H8O	Cyclopentanone	-45.91	-48.76	2.85
207	C5H8O	Dihydro-2H-pyran	-29.90	-28.75	-1.15
208	C5H10O	3-Pentanone	-61.64	-63.36	1.72
209	C5H10O	2-Pentanone	-61.90	-63.12	1.22
210	C5H10O	3-Methyl-2-butanone	-62.74	-63.42	0.68
211	C5H10O	Tetrahydro-2H-pyran	-53.39	-53.87	0.48
212	C5H10O	Pentanal	-54.61	-55.85	1.24
213	C5H10O	Propoxyethylene	-38.62	-36.77	-1.85
214	C5H10O	3,3-Dimethyloxetane	-35.42	-36.22	0.80
215	C5H10O	Isopropyl vinyl ether	-41.54	-40.71	-0.83
216	C5H12O	1-Pentanol	-70.43	-70.75	0.31
217	C5H12O	2-Pentanol	-74.74	-74.44	-0.29
218	C5H12O	3-Pentanol	-75.81	-74.31	-1.50
219	C5H12O	2-Methyl-1-butanol	-72.18	-71.37	-0.81
220	C5H12O	3-Methyl-1-butanol	-72.01	-70.71	-1.30
221	C5H12O	2-Methyl-2-butanol	-79.06	-77.62	-1.44
222	C5H12O	3-Methyl-2-butanol	-75.33	-74.83	-0.51
223	C5H12O	2-Methoxy-2-methylpropane	-67.76	-67.18	-0.58
224	C5H12O	1-Methoxybutane	-61.69	-62.21	0.53
225	C5H12O	1-Ethoxypropane	-65.06	-65.22	0.16
226	C6H6O	Phenol	-23.04	-23.11	0.07
227	C6H6O	Vinylfuran	6.64	4.12	2.53
228	C6H10O	Cyclohexanone	-54.04	-56.61	2.57

229	C6H12O	2-Hexanone	-66.87	-68.27	1.39
230	C6H12O	3,3-Dimethyl-2-butanone	-69.48	-69.65	0.17
231	C6H12O	3-Hexanone	-66.52	-68.30	1.79
232	C6H12O	2-Methyl-3-pentanone	-68.38	-68.76	0.38
233	C6H12O	Cyclohexanol	-68.40	-69.68	1.28
234	C6H14O	Hexanol	-75.48	-75.88	0.40
235	C6H14O	Dipropyl ether	-70.00	-70.10	0.10
236	C6H14O	Diisopropyl ether	-76.29	-75.91	-0.38
237	C7H6O	Benzaldehyde	-8.77	-10.05	1.28
238	C7H8O	Benzenemethanol	-24.00	-22.93	-1.06
239	C7H8O	2-Methylphenol	-30.74	-31.10	0.36
240	C7H8O	3-Methylphenol	-31.62	-30.89	-0.73
241	C7H8O	4-Methylphenol	-29.97	-30.21	0.24
242	C7H8O	Methoxybenzene	-16.23	-18.13	1.90
243	C7H10O	Bicyclo[2.2.1]heptan-2-one	-40.77	-41.56	0.79
244	C7H10O	8-Oxatricyclo-[3.2.1.01,5]octane	6.43	6.09	0.34
245	C7H14O	Heptanal	-63.05	-66.13	3.08
246	C7H14O	2,2-Dimethyl-3-pentanone	-74.98	-74.73	-0.25
247	C7H14O	2,4-Dimethyl-3-pentanone	-74.40	-74.35	-0.05
248	C7H16O	1-Heptanol	-80.40	-81.00	0.60
249	C8H8O	Acetophenone	-20.72	-21.18	0.46
250	C8H8O	Phenyl vinyl ether	5.43	4.70	0.72
251	C8H10O	2-Ethylphenol	-34.70	-35.76	1.06
252	C8H10O	3-Ethylphenol	-34.92	-35.95	1.03
253	C8H10O	4-Ethylphenol	-34.44	-35.32	0.88
254	C8H10O	2,3-Dimethylphenol	-37.57	-38.02	0.45
255	C8H10O	2,4-Dimethylphenol	-38.93	-38.17	-0.77
256	C8H10O	2,5-Dimethylphenol	-38.62	-38.57	-0.05
257	C8H10O	2,6-Dimethylphenol	-38.67	-38.81	0.14
258	C8H10O	3,4-Dimethylphenol	-37.43	-38.24	0.82
259	C8H10O	3,5-Dimethylphenol	-38.60	-38.58	-0.02
260	C8H10O	Ethoxybenzene	-24.28	-26.20	1.92
261	C2H2O2	Ethanedial	-50.67	-52.55	1.88
262	C2H4O2	Acetic acid	-103.44	-104.96	1.52
263	C2H4O2	Methyl formate	-84.97	-87.95	2.99
264	C2H6O2	1,2-Ethanediol	-92.61	-92.63	0.02
265	C2H6O2	Dimethyl peroxide	-30.04	-29.21	-0.83
266	C3H4O2	2-Oxetanone	-67.61	-71.50	3.89
267	C3H6O2	1,3-Dioxolane	-71.22	-73.01	1.79

268	C3H6O2	Propanoic acid	-108.39	-110.15	1.76
269	C3H6O2	Acetic acid methyl ester	-98.45	-100.34	1.89
270	C3H8O2	1,2-propanediol	-100.69	-102.04	1.34
271	C3H8O2	Dimethoxymethane	-83.27	-85.07	1.80
272	C3H8O2	1,3-Propanediol	-93.71	-95.91	2.20
273	C4H4O2	4-Methylene-2-oxetanone	-45.46	-49.68	4.22
274	C4H4O2	Cyclobutane-1,3-dione	-44.53	-49.31	4.79
275	C4H6O2	2,3-Butanedione	-78.18	-75.39	-2.78
276	C4H6O2	Acetic acid ethenyl ester	-75.26	-77.07	1.81
277	C4H8O2	Acetic acid ethyl ester	-106.14	-108.15	2.01
278	C4H8O2	1,4-Dioxane	-75.48	-77.09	1.61
279	C4H8O2	2-Methyl-1,3-dioxolane	-84.13	-84.28	0.15
280	C4H10O2	1,3-Butanediol	-103.54	-104.67	1.13
281	C4H10O2	1,1-Dimethoxyethane	-93.14	-93.07	-0.08
282	C4H10O2	Diethyl peroxide	-46.08	-44.66	-1.42
283	C4H10O2	1,4-Butanediol	-101.98	-101.61	-0.37
284	C5H6O2	2-Furanmethanol	-50.62	-52.58	1.96
285	C5H8O2	(E)-2-Butenoic acid methyl ester	-81.72	-83.31	1.59
286	C5H10O2	Pentanoic acid	-117.57	-120.30	2.73
287	C5H10O2	Propanoic acid ethyl ester	-110.80	-113.27	2.47
288	C5H10O2	propan-2-yl acetate	-115.13	-116.73	1.60
289	C5H10O2	4-Methyl-1,3-dioxane	-90.08	-92.13	2.05
290	C5H10O2	1,3-Dioxepane	-82.84	-86.86	4.02
291	C5H10O2	cis-2,4-Dimethyl-1,3-dioxolane	-91.44	-93.94	2.50
292	C5H10O2	trans-2,4-Dimethyl-1,3-dioxolane	-90.94	-92.74	1.80
293	C5H12O2	2,2-Dimethoxypropane	-102.68	-102.72	0.05
294	C5H12O2	1,5-Pentanediol	-107.34	-106.71	-0.63
295	C5H12O2	Diethoxymethane	-99.14	-101.06	1.92
296	C6H4O2	2,5-cyclohexadiene-1,4-dione	-29.37	-28.60	-0.78
297	C6H6O2	1,4-Benzenediol	-63.41	-64.35	0.94
298	C6H6O2	1,3-Benzenediol	-65.65	-66.70	1.05
299	C6H10O2	(E)-2-Butenoic acid ethyl ester	-89.77	-91.10	1.33
300	C6H12O2	Hexanoic acid	-122.35	-125.44	3.09
301	C6H12O2	Pentanoic acid methyl ester	-112.62	-115.59	2.97
302	C6H12O2	2,2-Dimethylpropanoic acid methyl ester	-118.14	-117.23	-0.91
303	C6H12O2	Acetic acid butyl ester	-116.06	-118.08	2.02
304	C6H12O2	Tetrahydro-2-methoxy-2H-pyran	-95.51	-95.66	0.15
305	C6H12O2	4,5-Dimethyl-1,3-dioxane	-97.78	-98.96	1.18
306	C6H14O2	1,2-Diethoxyethane	-97.56	-99.76	2.20

307	C6H14O2	1,1-Diethoxyethane	-108.39	-109.04	0.65
308	C7H6O2	Benzoic acid	-70.29	-72.83	2.54
309	C7H6O2	2-Hydroxy-2,4,6-cycloheptatriene-1-one	-37.14	-28.12	-9.02
310	C7H6O2	Formic acid phenyl ester	-51.58	-56.31	4.73
311	C7H6O2	3-(2-Furyl)-2-propenal	-25.31	-27.52	2.21
312	C7H12O2	4-Pentenoic acid ethyl ester	-92.16	-92.21	0.05
313	C7H12O2	(Z)-3-Pentenoic acid ethyl ester	-92.64	-94.17	1.53
314	C7H12O2	(E)-3-Pentenoic acid ethyl ester	-93.26	-94.17	0.91
315	C7H12O2	(E)-2-Pentenoic acid ethyl ester	-94.24	-95.73	1.49
316	C7H12O2	(E)-2-Butenoic acid propyl ester	-94.46	-95.99	1.54
317	C7H12O2	(E)-2-Butenoic acid isopropyl ester	-98.26	-99.66	1.40
318	C3H4O3	1,3-Dioxolan-2-one	-121.51	-126.91	5.40
319	C3H6O3	1,3,5-Trioxane	-111.35	-113.93	2.58
320	C3H8O3	1,2,3-Propanetriol	-139.27	-139.63	0.36
321	C4H6O3	Acetic anhydride	-136.83	-141.58	4.75
322	C4H10O3	Trimethoxymethane	-127.13	-128.81	1.68
323	C5H4O3	3-Methyl-2,5-furandione	-106.88	-112.00	5.12
324	C5H10O3	Carbonic acid diethyl ester	-152.46	-156.04	3.58
325	C5H10O3	1,3,6-Trioxacyclooctane	-111.64	-114.46	2.82
326	C5H12O3	1,1,1-Trimethoxyethane	-136.88	-137.22	0.34
327	C4H6O4	Butanedioic acid	-196.70	-201.11	4.41
328	C4H8O4	1,3,5,7-Tetroxane	-148.23	-149.40	1.17
329	C4H10O4	2(R),3(S)-1,2,3,4-Butanetetrol	-185.28	-181.71	-3.56
330	C2N2	Cyanogen	73.30	77.32	-4.02
331	C4N2	2-Butynedinitrile	126.48	132.21	-5.72
332	CH5N	Methylamine	-5.50	-5.57	0.07
333	C2H5N	Aziridine	30.23	28.52	1.72
334	C2H7N	Ethylamine	-11.33	-12.42	1.09
335	C2H7N	Dimethylamine	-4.45	-5.00	0.55
336	C3H3N	2-Propenenitrile	43.16	47.25	-4.09
337	C3H5N	Propanenitrile	12.31	14.71	-2.40
338	C3H7N	Cyclopropylamine	18.40	18.20	0.20
339	C3H9N	1-Propylamine	-16.78	-17.52	0.74
340	C3H9N	2-Propylamine	-20.03	-20.14	0.12
341	C3H9N	Trimethylamine	-5.66	-6.87	1.21
342	C4H5N	1H-Pyrrole	25.88	23.62	2.26
343	C4H5N	Cyclopropanecarbonitrile	43.45	44.76	-1.31
344	C4H5N	3-Butenenitrile	37.72	42.41	-4.69
345	C4H5N	(E)-2-Butenenitrile	33.63	37.55	-3.92

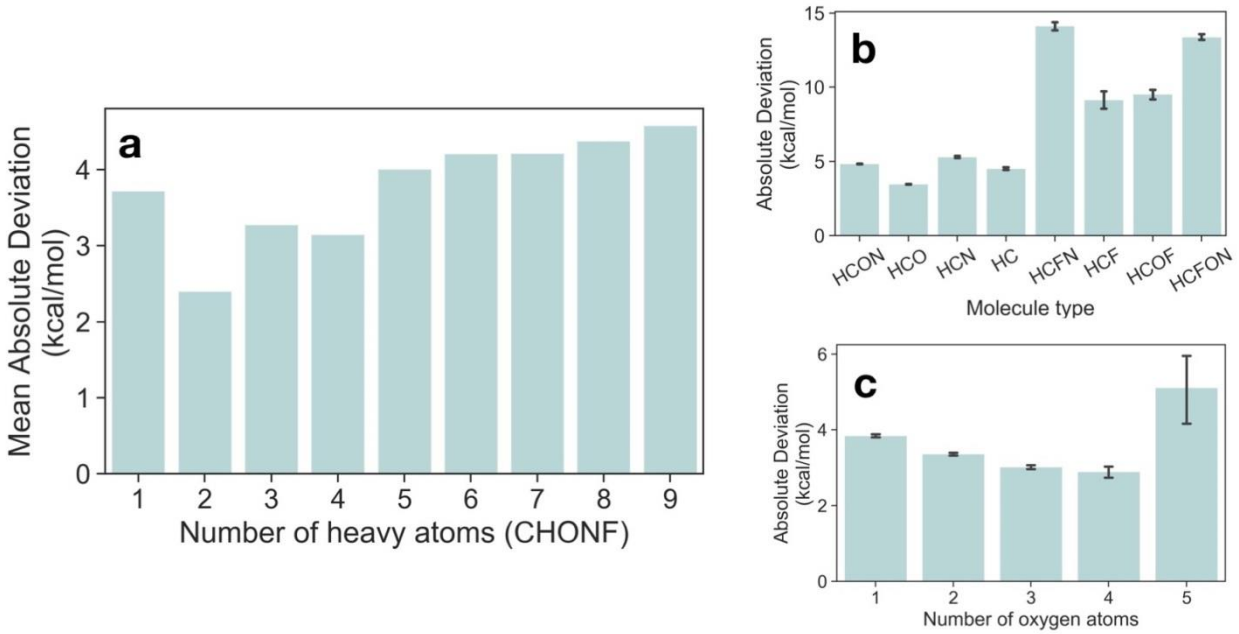
346	C4H7N	Butanenitrile	8.03	9.35	-1.32
347	C4H7N	2-Methylpropanenitrile	5.57	8.70	-3.13
348	C4H9N	pyrrolidine	-0.81	-2.26	1.44
349	C4H9N	Cyclobutylamine	9.85	8.74	1.11
350	C4H11N	1-Butylamine	-21.99	-22.35	0.37
351	C4H11N	2-Butylamine	-25.07	-25.24	0.17
352	C4H11N	2-Methyl-2-propylamine	-28.90	-28.31	-0.59
353	C4H11N	Diethylamine	-17.33	-18.57	1.25
354	C4H11N	2-Methylpropylamine	-23.59	-24.09	0.50
355	C5H5N	Pyridine	33.56	31.74	1.82
356	C5H7N	1-Methyl-1H-pyrrole	24.64	22.29	2.35
357	C5H7N	(E)-2-Pentenenitrile	28.63	32.85	-4.22
358	C5H7N	(E)-3-Pentenenitrile	30.02	34.00	-3.98
359	C5H9N	2,2-Dimethylpropanenitrile	-0.60	1.80	-2.40
360	C5H9N	Pentanenitrile	2.51	4.20	-1.69
361	C5H11N	Piperidine	-11.28	-12.92	1.64
362	C5H11N	Cyclopentylamine	-13.12	-13.79	0.67
363	C6H7N	Aniline	20.82	18.87	1.95
364	C6H7N	2-Methylpyridine	23.71	21.60	2.11
365	C6H7N	3-Methylpyridine	25.43	23.77	1.66
366	C6H7N	4-Methylpyridine	24.88	23.10	1.78
367	C6H7N	Bicyclo[2.1.0]pentane-1-carbonitrile	65.03	65.92	-0.88
368	C6H7N	3-Methylenecyclobutane-carbonitrile	60.35	60.86	-0.51
369	C6H7N	1-Cyclopentene-1-carbonitrile	37.40	39.69	-2.29
370	C6H9N	2,5-Dimethyl-1H-pyrrole	9.51	6.70	2.81
371	C6H13N	2-Methylpiperidine	-20.17	-21.48	1.31
372	C6H13N	Cyclohexylamine	-25.07	-25.66	0.59
373	C6H15N	Triethylamine	-22.18	-23.52	1.34
374	C6H15N	Dipropylamine	-27.75	-28.54	0.79
375	C6H15N	Diisopropylamine	-34.42	-32.61	-1.81
376	C7H5N	Benzonitrile	51.55	52.94	-1.38
377	C7H9N	2,3-Dimethylpyridine	16.32	14.01	2.31
378	C7H9N	2,4-Dimethylpyridine	15.27	12.99	2.28
379	C7H9N	2,5-Dimethylpyridine	15.89	13.81	2.09
380	C7H9N	2,6-Dimethylpyridine	14.03	11.57	2.46
381	C7H9N	3,4-Dimethylpyridine	16.75	14.83	1.93
382	C7H9N	3,5-Dimethylpyridine	17.40	15.85	1.55
383	C7H9N	Benzylamine	20.98	20.05	0.93
384	C7H11N	Cyclohexanecarbonitrile	1.15	2.91	-1.76

385	C7H13N	1-Azabicyclo[2.2.2]octane	-1.00	-0.75	-0.25
386	C7H13N	Heptanenitrile	-7.41	-6.29	-1.12
387	C8H7N	1H-Indole	37.40	36.27	1.13
388	CH6N2	Methylhydrazine	22.61	20.70	1.91
389	C2H8N2	1,1-Dimethylhydrazine	20.05	17.51	2.54
390	C4H2N2	(E)-Butenedinitrile	81.31	84.10	-2.79
391	C4H4N2	Pyrimidine	46.82	41.12	5.70
392	C4H12N2	1,2-Butanediamine	-17.69	-17.34	-0.34
393	C6H8N2	Phenylhydrazine	48.49	46.77	1.73
394	C4H12N4	1,1,4,4-Tetramethyl-2-tetrazene	64.70	60.62	4.08
395	C2H5NO	Acetamide	-56.96	-59.81	2.85
396	C3H3NO	Oxazole	-3.70	-6.25	2.54
397	C3H3NO	Isoxazole	18.79	17.29	1.49
398	C3H7NO	propanamide	-61.88	-66.09	4.21
399	C4H5NO	5-Methylisoxazole	8.15	5.98	2.17
400	C4H5NO	3-Methylisoxazole	8.51	7.21	1.29
401	C4H7NO	2-Methyl-2-oxazoline	-31.19	-32.58	1.39
402	C4H9NO	Butanamide	-66.49	-71.08	4.59
403	C5H5NO	2-Pyridinol	-19.05	-21.12	2.07
404	C5H5NO	3-pyridinol	-10.44	-10.86	0.41
405	C5H5NO	4-pyridinol	-9.75	-11.65	1.90
406	C5H7NO	3,5-Dimethylisoxazole	-4.28	-4.05	-0.23
407	C5H9NO	2-Ethyl-2-oxazoline	-35.59	-36.94	1.35
408	C5H11NO	Pentanamide	-69.36	-76.21	6.85
409	C6H7NO	2-Methyl-3-hydroxypyridine	-20.17	-20.83	0.66
410	C6H7NO	2-Methyl-4-hydroxypyridine	-17.14	-21.75	4.61
411	C6H7NO	2-Methyl-5-hydroxypyridine	-16.68	-20.41	3.73
412	C6H7NO	2-Methyl-6-hydroxypyridine	-28.73	-31.46	2.73
413	C6H11NO	Hexahydro-2H-azepin-2-one	-58.84	-63.02	4.18
414	C6H13NO	Hexanamide	-77.49	-80.05	2.57
415	C6H13NO	N-Butylacetamide	-72.85	-77.16	4.31
416	C7H7NO	1-Amino-2,4,6-cyclohepta-trien-1-one	9.44	3.42	6.02
417	CH3NO2	Methyl nitrite	-15.87	-17.48	1.61
418	CH3NO2	Nitromethane	-17.76	-22.18	4.42
419	C2H5NO2	Nitroethane	-24.45	-28.92	4.47
420	C2H5NO2	Glycine	-93.71	-98.01	4.29
421	C3H7NO2	1-Nitropropane	-29.59	-33.66	4.07
422	C3H7NO2	2-Nitropropane	-33.22	-36.93	3.71
423	C4H9NO2	1-Nitrobutane	-34.39	-38.81	4.42

424	C4H9NO2	2-Nitrobutane	-39.10	-42.54	3.43
425	C4H9NO2	2-Methyl-2-nitropropane	-42.33	-44.50	2.17
426	C5H11NO2	L-Valine	-108.77	-113.98	5.21
427	C6H5NO2	Nitrobenzene	16.13	10.38	5.75
428	C2H5NO3	Ethyl nitrate	-36.83	-43.11	6.28
429	C3H7NO3	Propyl nitrate	-41.56	-48.01	6.45
430	C3H7NO3	Isopropyl nitrate	-45.65	-51.58	5.93
431	C4H3NO3	2-Nitrofuran	-6.88	-14.38	7.49
432	C4H6N2O	3-Amino-5-methylisoxazole	4.71	2.99	1.72
433	C4H6N2O	Dimethylfurazan	25.65	23.20	2.45
434	C5H8N2O	5-Amino-3,4-dimethyl-isoxazole	1.24	-4.81	6.06
435	C5H10N2O	1-Nitrosopiperidine	3.97	1.57	2.40
436	C6H4N2O	1,2,3-Benzoxadiazole	71.87	47.70	24.17
437	C2H6N2O2	N-Nitrodimethylamine	-1.15	-8.96	7.81
438	C4H4N2O2	Uracil	-72.39	-81.13	8.74
439	C4H6N2O2	Dimethylfurazan monoxide	24.45	19.38	5.07
440	C5H10N2O2	1-Nitropiperidine	-10.64	-17.14	6.51
441	C3H4N2O3	4,5-Dihydro-3-nitro-isoxazole	9.32	7.02	2.30
442	C3H6N2O4	1,1-Dinitropropane	-24.07	-34.54	10.48
443	CF4	Carbon tetrafluoride	-223.14	-227.05	3.92
444	C2FH3	Fluoroethylene	-33.17	-34.53	1.35
445	C3FH7	1-Fluoropropane	-68.33	-70.65	2.32
446	C6FH5	Fluorobenzene	-27.72	-29.33	1.61
447	C7FH7	1-Fluoro-4-methylbenzene	-35.25	-36.68	1.43
448	CF2H2	Difluoromethane	-108.08	-109.47	1.39
449	C6F2H4	1,2-Difluorobenzene	-70.22	-74.27	4.05
450	C6F2H4	1,3-Difluorobenzene	-73.90	-78.18	4.28
451	C6F2H4	1,4-Difluorobenzene	-73.30	-77.36	4.06
452	CF3H	Trifluoromethane	-166.20	-169.26	3.06
453	C2F3H3	1,1,1-Trifluoroethane	-177.96	-182.89	4.92
454	C2FH3O	Acetyl fluoride	-105.66	-107.85	2.19
455	C3F4H4O	2,2,3,3-Tetrafluoro-1-propanol	-253.66	-259.52	5.86
456	C3F5H3O	2,2,3,3,3-Pentafluoro-1-propanol	-313.17	-315.51	2.35
457	C2F3N	Trifluoroacetonitrile	-119.00	-120.90	1.89
458	CF5N	Pentafluoromethylamine	-169.10	-175.59	6.49
459	CF5N3	Pentafluoroguanidine	22.87	9.51	13.37

Table S6 Twelve molecules deleted due to other experimental data differing by more than 1 kcal/mol

Formula	**Name**	**Other experimental data**
C8H8	Cubane	F. Agapito, et al J. Phys. Chem. A 2015, 119, 2998−3007
C8H12	trans-1,2-Diethenylcyclobutane	https://webbook.nist.gov/chemistry/
C2H6O2	Ethyl hydroperoxide	https://webbook.nist.gov/chemistry/; J. Simmie et al, J. Phys. Chem. A 2008, 112, 5010
C3H2O3	1,3-Dioxol-2-one	C. Sousa et al J. Phys. Chem. A 2017, 121, 9474
C4H6O3	4-Methyl-1,3-dioxolan-2-one	https://webbook.nist.gov/chemistry/
C5H4O3	Furancarboxylic acid	M. Roux, et al J. Phys. Chem. A 2003, 107, 11460
C4H6O4	Dimethyl Oxalate	Chickos, J.S., et al. Struct Chem (1996) 7: 391.
C6H7N	2-Cyclopentene-1-carbonitrile	https://webbook.nist.gov/chemistry/
C6H9N	Cyclopentanecarbonitrile	https://webbook.nist.gov/chemistry/
CH4N2O	Urea	https://webbook.nist.gov/chemistry/; O. Dorofeeva et al, J. Chem. Thermodynamics 41 (2009) 433
C4H8N2O2	2,3-Butanedione dioxime	"The Chemistry of Hydroxylamines, Oximes and Hydroxamic Acids," Part 1 Edited by Zvi Rappoport and Joel F. Liebman, Wiley West Sussex England 2009,
C4FH9N2O2	N-Fluoro-n-butylnitramine	https://webbook.nist.gov/chemistry/



Supplemental Fig. S1 Mean absolute deviations between B3LYP/6-31G(2df,p) and G4MP2 enthalpies of formation for the GDB-9 database of 130 K molecules as a function of (a) molecule size, (b) molecule type, also including the standard deviation of the absolute differences, and (c) number of oxygens (for CHO group only). In panels (b) and (c), the standard deviation of the absolute differences is shown as errors bars.