Table I. Deviations of Calculated Heats of Formation From Experiment.[a]

		c-SVWNV(30)		BLYP		B3LYP	
Name	expt.	3-21G*	3-21+G*	3-21G*	3-21+G*	3-21G*	3-21+G*
LiH	33.3	-15.4	-12.7	0.1	0.1	0.0	0.0
BeH	81.7	2.2	5.1	6.0	6.1	6.5	6.6
CH	142.5	-14.3	-10.9	-3.2	-2.6	-4.6	-4.0
CH2(3B1)	93.7	-6.3	-2.5	-3.9	-4.0	-3.0	-3.2
CH2(1A1)	102.8	-25.5	-20.3	-9.4	-8.4	-10.7	-9.7
CH3	35.0	-15.1	-10.5	-2.9	-3.6	-1.9	-2.6
CH4	-17.9	-17.5	-12.9	-2.3	-4.2	-0.9	-2.8
NH	85.2	-17.8	-12.7	-3.5	-1.4	-6.4	-4.2
NH2	45.1	-31.1	-22.4	-9.9	-5.7	-13.8	-9.6
NH3	-11.0	-39.5	-23.9	-18.1	-9.6	-20.6	-12.4
OH	9.4	-17.2	-8.3	-11.9	-6.1	-14.6	-9.0
OH2	-57.8	-32.4	-16.5	-27.9	-17.1	-31.5	-21.0
FH	-65.1	-21.2	-5.0	-22.7	-10.4	-25.2	-13.5
SiH2(1A1)	65.2	-16.5	-11.7	1.0	1.7	1.8	2.0
SiH2(3B1)	86.2	-5.4	-1.0	1.3	1.6	2.9	2.7
SiH3	47.9	-16.6	-11.0	1.4	1.6	4.0	3.7
SiH4	8.2	-26.8	-20.2	-0.4	-0.4	3.5	3.1
PH2	33.1	-15.1	-11.1	3.5	3.4	3.4	3.2
PH3	1.3	-22.3	-17.3	0.3	0.0	0.8	0.5
SH2	-4.9	-12.4	-8.5	-5.1	-5.3	-5.1	-5.4
ClH	-22.1	-3.8	-3.7	-5.7	-4.9	-5.9	-5.6
Li2	51.6	-12.4	-9.7	-3.1	-3.2	-3.0	-3.1
LiF	-80.1	-4.1	0.3	-1.3	1.0	-8.2	-2.2
C2H2	54.2	-4.0	-3.2	-7.5	-10.8	-12.5	-15.0
C2H4	12.5	-10.7	-8.2	-6.3	-10.8	-8.1	-11.8
C2H6	-20.1	-16.9	-12.8	-5.6	-11.3	-3.7	-8.9
CN	104.9	-5.7	-8.5	-3.7	-8.3	-20.2	-23.2
HCN	31.5	-11.3	-11.8	-5.5	-8.9	-16.9	-19.2
CO	-26.4	-5.0	-14.0	-15.3	-25.4	-27.6	-35.9
HCO	10.0	1.7	-4.0	-7.5	-15.6	-20.1	-26.3
H2CO	-26.0	-4.8	-7.8	-9.6	-16.2	-20.2	-25.0
H3COH	-48.0	-19.0	-12.7	-17.3	-17.7	-22.3	-21.7
N2	0.0	-36.1	-36.6	-22.2	-24.7	-39.1	-40.2
H2NNH2	22.8	-46.3	-32.3	-22.0	-17.8	-30.4	-25.6
O2	0.0	18.9	6.6	2.4	-10.6	-18.7	-29.0
HOOH	-32.5	-6.6	-2.9	-12.3	-13.5	-26.4	-27.1
F2	0.0	39.9	24.7	23.7	7.0	8.9	-6.6
CO2	-94.1	15.6	-2.1	-14.0	-32.3	-37.3	-51.7
Na2	34.0	2.7	-2.0	10.4	10.9	8.6	9.1
Si2	139.9	4.0	6.9	2.1	2.2	-3.2	-4.3
P2	34.3	-7.0	-5.9	3.4	2.2	-3.7	-4.5
S2	30.7	12.9	12.9	2.6	0.4	-3.2	-5.0
Cl2	0.0	12.2	7.6	-5.1	-5.2	-9.2	-9.8
NaCl	-43.6	-6.5	-4.3	-5.5	-2.7	-4.6	-2.2

SiO	-24.6	3.9	2.5	-0.1	-3.1	-11.4	-12.6
SC	66.9	0.1	1.7	-6.0	-7.0	-14.3	-14.7
SO	1.2	11.8	10.4	-0.7	-3.9	-13.0	-14.7
FCl	-13.2	19.6	15.9	3.3	0.6	-5.6	-7.6
Si2H6	19.1	-34.5	-24.3	-2.3	-2.5	4.9	3.9
CH3Cl	-19.6	-2.0	-2.2	-5.4	-8.2	-6.0	-8.7
H3CSH	-5.5	-10.9	-7.5	-6.5	-10.4	-6.3	-9.8
HOCl	-17.8	2.9	2.4	-8.6	-9.4	-18.0	-18.3
SO2	-71.0	7.2	2.0	-20.4	-27.5	-44.6	-48.6
BF3	-271.4	52.1	12.1	7.9	-34.7	-7.7	-43.1
BCl3	-96.3	28.6	21.1	-18.8	-20.2	-20.8	-22.3
AlF3	-289.0	41.1	19.1	16.0	-9.1	3.3	-14.7
AlCl3	-139.7	20.4	12.2	-11.9	-14.5	-8.9	-12.0
CF4	-223.0	77.3	25.7	6.4	-47.3	-17.9	-64.5
CCl4	-22.9	43.4	30.5	-23.2	-28.0	-31.9	-37.0
COS	-33.1	24.2	11.6	-1.5	-15.7	-18.9	-30.5
CS2	28.0	26.2	23.1	4.0	-1.9	-7.0	-11.8
COF2	-149.1	45.1	10.8	-5.0	-40.8	-30.1	-60.2
SiF4	-386.0	56.6	15.9	11.2	-33.6	-3.5	-40.6
SiCl4	-158.4	29.1	18.1	-24.1	-27.2	-21.8	-25.7
N2O	19.6	-8.7	-19.9	-15.4	-27.7	-48.9	-57.3
ClNO	12.4	12.9	0.3	-2.5	-14.0	-32.1	-41.2
NF3	-31.6	59.9	36.9	26.1	0.4	-11.1	-32.3
PF3	-229.1	37.8	17.4	5.2	-17.8	-11.4	-29.7
O3	34.1	34.1	15.9	7.1	-12.3	-38.8	-54.2
F2O	5.9	63.6	41.1	35.7	11.5	6.8	-14.6
ClF3	-38.0	57.5	55.9	11.8	9.8	-20.3	-20.2
C2F4	-157.4	97.5	46.5	16.4	-37.2	-15.2	-59.3
C2Cl4	-3.0	58.7	43.6	-23.1	-30.4	-33.6	-40.2
CF3CN	-118.4	66.0	24.0	4.2	-40.6	-28.2	-65.6
CH3CCH (propyne)	44.2	-1.4	-1.2	-9.9	-17.2	-14.5	-20.3
CH2=C=CH2 (allene)	45.5	2.5	2.3	-6.3	-13.9	-12.0	-18.1
C3H4 (cyclopropene)	66.2	-5.9	-7.1	-18.9	-27.5	-24.1	-31.2
CH3CH=CH2 (propylene)	4.8	-9.1	-6.5	-10.1	-17.9	-11.4	-17.9
C3H6 (cyclopropane)	12.7	-10.9	-9.6	-17.2	-26.3	-17.0	-25.0
C3H8 (propane)	-25.0	-15.9	-11.9	-9.9	-19.2	-7.2	-15.5
CH2CHCHCH2 (butadiene)	26.3	-1.2	-0.2	-13.7	-23.5	-18.7	-26.4
C4H6 (2-butyne)	34.8	1.1	0.2	-12.4	-23.9	-16.4	-26.0
C4H6 (methylene cyclopropane)	47.9	2.2	1.3	-16.4	-28.3	-20.1	-30.0
C4H6 (bicyclobutane)	51.9	-5.6	-7.4	-30.0	-42.8	-33.1	-44.0
C4H6 (cyclobutene)	37.4	1.3	-0.2	-18.9	-31.4	-22.5	-32.9
C4H8 (cyclobutane)	6.8	-2.4	-2.0	-15.0	-28.5	-14.1	-25.8
C4H8 (isobutene)	-4.0	-8.1	-5.7	-15.2	-26.6	-15.8	-25.3
C4H10 (trans butane)	-30.0	-15.0	-11.3	-14.2	-27.2	-10.9	-22.3
C4H10 (isobutane)	-32.1	-14.6	-10.3	-15.1	-27.7	-11.6	-22.5
C5H8 (spiropentane)	44.3	-1.9	-2.1	-31.1	-45.7	-32.4	-44.7
C6H6 (benzene)	19.7	25.6	19.5	-22.2	-39.9	-29.3	-43.3

CH2F2	-107.7	19.0	10.7	-4.3	-16.8	-16.1	-25.2
CHF3	-166.6	45.7	19.2	-0.8	-30.7	-19.1	-43.8
CH2Cl2	-22.8	12.6	8.3	-11.0	-14.2	-14.0	-17.3
CHCl3	-24.7	27.4	19.1	-17.2	-21.0	-23.0	-27.0
CH3NH2 (methylamine)	-5.5	-32.7	-22.8	-15.2	-14.7	-18.3	-17.0
CH3CN (methyl cyanide)	18.0	-7.7	-8.9	-6.8	-14.2	-17.5	-23.3
CH3NO2 (nitromethane)	-17.8	0.7	-3.1	-19.4	-29.5	-51.5	-57.1
CH3ONO (methyl nitrate)	-15.9	11.8	-2.0	-5.5	-24.6	-39.4	-54.0
CH3SiH3 (methyl silane)	-7.0	-28.4	-21.0	-5.7	-8.3	-0.5	-3.3
HCOOH (formic acid)	-90.5	4.5	-3.4	-18.9	-30.8	-36.8	-45.4
HCOOCH3 (methyl formate)	-85.0	12.8	1.0	-13.1	-31.8	-32.1	-46.1
CH3CONH2 (acetamide)	-57.0	-7.1	-7.2	-19.7	-29.5	-33.6	-40.4
C2H4NH (aziridine)	30.2	-25.0	-22.0	-22.8	-29.0	-30.3	-34.9
NCCN (cyanogen)	73.3	7.2	-3.4	-0.2	-13.2	-25.7	-35.9
(CH3)2-NH (dimethylamine)	-4.4	-26.5	-20.9	-14.3	-20.8	-17.6	-22.6
CH3CH2NH2 (trans ethylamine)	-11.3	-29.6	-20.5	-17.3	-21.2	-19.9	-22.5
CH2CO (ketene)	-11.4	14.8	4.6	-4.7	-18.9	-19.2	-30.7
C2H4O (oxirane)	-12.6	-5.5	-6.6	-18.3	-26.3	-28.4	-34.3
CH3CHO (acetaldehyde)	-39.7	-2.4	-5.1	-12.8	-22.6	-22.8	-30.4
HCOCOH (glyoxal)	-50.7	12.9	0.6	-17.0	-33.6	-39.5	-51.9
CH3CH2OH (ethanol)	-56.2	-17.6	-11.2	-21.0	-25.1	-25.4	-27.9
CH3OCH3 (dimethylether)	-44.0	-8.8	-9.4	-11.1	-21.1	-17.1	-24.8
C2H4S (thiirane)	19.6	0.4	0.4	-11.9	-19.8	-14.4	-21.2
(CH3)2-SO (dimethyl sulfoxide)	-36.2	-9.8	-2.3	-24.1	-28.0	-33.8	-34.9
C2H5SH (ethanethiol)	-11.1	-10.3	-6.5	-11.1	-18.2	-10.2	-16.4
CH3SCH3 (dimethyl sulfide)	-8.9	-8.9	-5.4	-8.6	-16.0	-8.1	-14.6
CH2=CHF (vinyl flouride)	-33.2	15.0	8.2	-1.5	-13.8	-10.7	-20.0
C2H5Cl (ethyl chloride)	-26.8	-0.8	-1.1	-9.5	-15.8	-9.5	-15.3
CH2=CHCl (vinyl chloride)	8.9	10.5	8.4	-5.9	-11.2	-9.8	-14.4
CH2=CHCN (acrylonitrile)	43.2	-1.2	-4.5	-11.0	-21.0	-25.4	-33.1
CH3COCH3 (acetone)	-51.9	-0.3	-2.6	-16.4	-29.5	-25.5	-35.8
CH3COOH (acetic acid)	-103.4	5.6	-1.6	-23.0	-37.8	-39.6	-50.7
CH3COF (acetyl fluoride)	-105.7	23.4	8.9	-9.1	-29.3	-26.3	-42.6
CH3COCl (acetyl chloride)	-58.0	17.8	7.7	-13.7	-27.4	-27.7	-38.7
CH3CH2CH2Cl (propyl chloride)	-31.5	0.4	0.1	-13.4	-23.3	-12.6	-21.5
(CH3)2-CHOH (isopropanol)	-65.2	-14.5	-8.9	-24.3	-32.7	-28.0	-34.3
C2H5OCH3 (methyl ethyl ether)	-51.7	-7.3	-7.6	-14.6	-28.0	-19.9	-30.6
(CH3)3-N (trimethylamine)	-5.7	-20.5	-17.5	-14.9	-27.1	-18.0	-28.1
C4H4O (furan)	-8.3	28.3	15.2	-18.1	-38.7	-32.5	-48.9
C4H4S (thiophene)	27.5	22.6	19.2	-20.5	-32.8	-27.6	-37.3
C4H5N (pyrrole)	25.9	12.0	7.6	-20.7	-34.8	-31.2	-41.9
C5H5N (pyridine)	33.6	19.0	11.5	-21.6	-39.1	-35.7	-49.1
H2	0.0	-16.1	-13.5	0.6	0.6	0.7	0.7
CCH	135.1	2.7	1.8	-5.5	-9.2	-13.4	-16.3
C2H3 (2A')	71.6	-3.4	-1.2	-3.9	-7.5	-7.0	-9.9
CH3CO (2A')	-2.4	3.6	-0.9	-10.1	-20.8	-22.1	-30.6
H2COH (2A)	-4.1	-10.5	-7.7	-13.8	-16.6	-20.5	-21.8

CH3CH2O (2A")	-3.7	-5.7	-3.0	-9.1	-15.5	-14.1	-19.0
CH3S (2A')	29.8	-2.3	0.1	-0.8	-4.4	-1.2	-4.5
C2H5 (2A')	28.9	-13.0	-8.9	-5.5	-10.0	-4.4	-8.4
(CH3)2-CH (2A')	21.5	-10.6	-6.5	-8.6	-16.5	-7.2	-14.0
(CH3)3-C (t-butyl radical)	12.3	-9.4	-5.4	-13.5	-25.2	-11.6	-21.6
NO2	7.9	10.0	-2.8	-9.2	-23.1	-45.1	-54.8
NO	21.6	-12.6	-17.5	-13.1	-19.3	-31.8	-35.9
ClO	24.2	13.5	11.6	0.4	-0.6	-10.1	-11.2
SH	34.2	-6.5	-3.8	-1.2	-1.3	-1.5	-1.6
CH3O	4.1	-5.6	-2.4	-5.0	-7.4	-10.6	-11.9
CH3-CH=C=CH2 (methyl allene)	38.8	3.0	2.9	-10.4	-21.4	-15.6	-24.6
C5H8 (isoprene)	18.0	-0.1	0.7	-19.6	-32.9	-23.6	-34.3
C5H10 (cyclopentane)	-18.3	1.0	0.8	-19.4	-36.9	-16.5	-31.6
C5H12 (n-pentane)	-35.1	-14.4	-10.9	-18.8	-35.6	-14.8	-29.4
C5H12 (neopentane)	-40.2	-13.5	-8.8	-21.5	-37.2	-16.6	-30.2
C6H8 (1,3 cyclohexadiene)	25.4	16.3	13.2	-24.7	-42.8	-29.1	-43.7
C6H8 (1,4 cyclohexadiene)	25.0	15.1	10.8	-25.9	-44.9	-30.0	-45.5
C6H12 (cyclohexane)	-29.5	3.6	2.7	-24.8	-46.3	-20.7	-39.2
C6H14 (n-hexane)	-39.9	-13.4	-10.1	-22.9	-43.5	-18.2	-36.1
C6H14 (3-methyl pentane)	-41.1	-12.4	-9.0	-24.7	-44.9	-19.6	-37.1
C6H5CH3 (toluene)	12.0	26.5	20.9	-27.2	-47.8	-33.7	-50.0
C7H16 (n-heptane)	-44.9	-12.6	-9.7	-27.4	-51.7	-22.0	-43.1
C8H8 (cyclooctatetraene)	70.7	31.8	26.4	-34.5	-55.7	-45.5	-61.8
C8H18 (n-octane)	-49.9	-11.8	-9.1	-31.7	-59.8	-25.7	-50.0
C10H8 (naphthalene)	35.9	61.5	47.4	-39.3	-69.7	-52.5	-76.2
C10H8 (azulene)	69.1	61.0	47.8	-38.8	-68.4	-55.8	-78.5
CH3COOCH3 (methyl acetate)	-98.4	13.7	2.3	-18.2	-39.5	-35.9	-52.6
(CH3)3-COH (t-butanol)	-74.7	-11.8	-6.5	-28.7	-41.1	-31.4	-41.0
C6H5NH2 (aniline)	20.8	20.7	16.1	-29.3	-47.6	-41.0	-54.8
C6H5OH (phenol)	-23.0	33.1	22.7	-32.2	-54.4	-46.3	-63.3
C4H6O (divinyl ether)	-3.3	13.3	5.1	-15.3	-34.1	-28.6	-43.3
C4H8O (tetrahydrofuran)	-44.0	8.4	4.1	-20.1	-38.0	-25.8	-40.3
C5H8O (cyclopentanone)	-45.9	19.6	11.9	-23.1	-45.5	-32.0	-50.2
C6H4O2 benzoquinone	-29.4	50.9	31.0	-30.6	-59.9	-59.8	-82.4
C4H4N2 pyrimidine	46.8	12.0	2.2	-21.4	-39.7	-42.3	-56.3
C2H6O2S dimethyl sulphone	-89.2	-5.3	-7.0	-39.0	-52.1	-53.9	-63.3
C6H5Cl (chlorobenzene)	12.4	42.9	32.8	-26.1	-44.2	-35.2	-49.6
N=-C-CH2-CH2-C=-N (1,2-dicyano ethane)	50.1	2.3	-5.0	-15.5	-32.3	-37.7	-50.7
C4H4N2 (pyrazine)	46.9	8.5	-1.1	-24.6	-42.8	-45.9	-59.8
CH3-C(=O)-C=-CH (acetyl acetylene)	15.6	14.5	6.2	-19.7	-36.2	-36.3	-49.2
CH3-CH=CH-CHO (crotonaldehyde)	-24.0	9.3	4.8	-18.0	-33.4	-31.1	-43.0
CH3-C(=O)-O-C(=O)-CH3 (acetic anhydride)	-136.8	35.7	12.9	-23.5	-57.7	-52.2	-79.4
C4H6S (2,5-dihydrothiophene)	20.8	14.8	12.4	-18.5	-32.8	-22.0	-33.8
(CH3)2-CH-CN (isobutale nitrile)	5.6	-8.1	-9.0	-17.1	-31.1	-26.2	-37.6
CH3-CO-CH2-CH3 (methly ethyl ketone)	-57.1	2.2	-2.1	-19.5	-38.0	-27.8	-42.9
(CH3)2-CH-CHO (isobutanal)	-51.6	-0.6	-3.9	-22.1	-39.2	-30.5	-44.2
C4H8O2 (1,4-dioxane)	-75.5	20.4	9.9	-23.7	-47.8	-37.5	-56.3

C4H8S (tetrahydrothiophene)	-8.2	7.8	7.4	-19.1	-34.4	-18.4	-31.6
(CH3)3-C-Cl (t-butyl chloride)	-43.5	3.5	3.8	-19.0	-31.9	-17.1	-28.5
CH3-CH2-CH2-CH2-Cl (n-butyl chloride)	-37.0	0.5	0.0	-18.4	-32.0	-16.9	-28.9
C4H8NH (tetrahydropyrrole)	-0.8	-9.8	-7.8	-23.8	-38.0	-26.9	-38.4
CH3-CH2-CH(CH3)-NO2 (nitro-s-butane)	-39.1	9.5	1.9	-29.8	-52.7	-59.7	-76.2
CH3-CH2-O-CH2-CH3 (Diethyl ether)	-60.3	-6.8	-6.9	-19.1	-36.0	-23.8	-37.3
CH3-CH(OCH3)2 (acetaldehyde dimethyl acetal)	-93.1	7.9	-0.6	-21.0	-45.6	-33.1	-52.6
(CH3)3C-SH (t-butanethiol)	-26.2	-5.8	-1.1	-21.0	-34.4	-18.2	-29.7
CH3-CH2-S-S-CH2-CH3 (Diethyl disulfide)	-17.9	-1.3	2.4	-21.9	-37.1	-22.4	-35.3
(CH3)3C-NH2 (t-butylamine)	-28.9	-26.7	-17.7	-28.2	-39.2	-28.7	-37.4
Si(CH3)4 (Tetramethylsilane)	-55.7	-33.3	-23.0	-23.0	-33.7	-14.0	-23.7
C5H6S (2-methyl thiophene)	20.0	23.8	20.4	-24.7	-40.5	-31.2	-43.8
C5H7N (N-methyl pyrrole)	24.6	13.8	8.6	-23.4	-41.6	-33.7	-47.9
C5H10O (Tetrahydropyran)	-53.4	12.3	6.4	-24.1	-47.1	-28.9	-47.7
CH3-CH2-CO-CH2-CH3 (Diethyl ketone)	-61.6	5.7	-0.4	-22.1	-45.2	-29.5	-48.8
C5H10O2 (Isopropyl acetate)	-115.1	17.3	5.4	-25.9	-55.2	-41.6	-65.0
C5H10S (Tetrahydrothiopyran)	-15.2	10.3	9.8	-24.2	-43.1	-22.4	-38.5
cyc-C5H10NH (piperidine)	-11.3	-5.8	-5.6	-27.7	-47.2	-29.8	-45.8
(CH3)3C-O-CH3 (t-butyl methyl ether)	-67.8	-2.0	-2.9	-23.8	-44.9	-27.1	-44.2
C6H4F2 (1,3-DiFluorobenzene)	-73.9	81.6	50.5	-8.6	-48.5	-30.0	-61.9
C6H4F2 (1,4-DiFluorobenzene)	-73.3	81.6	50.9	-8.5	-48.0	-29.8	-61.4
C6H5F (Fluorobenzene)	-27.7	53.3	35.2	-15.6	-43.9	-29.9	-52.4
(CH3)2CH-O-CH(CH3)2 (Di-isopropyl ether)	-76.3	-1.4	-2.6	-27.1	-52.3	-30.1	-50.7
SF6	-291.7	120.8	46.1	14.2	-62.9	-16.9	-87.3
P4	14.1	-7.6	-7.1	-13.7	-17.5	-22.2	-25.2
SO3	-94.6	14.8	-1.1	-30.2	-48.2	-61.9	-75.3
SCl2	-4.2	18.2	13.8	-9.1	-10.1	-16.1	-17.1
POCl3	-133.8	26.7	13.5	-24.1	-31.9	-36.1	-42.1
PCl5	-86.1	42.5	30.4	-29.2	-30.9	-36.2	-38.3
Cl2O2S	-84.8	26.9	11.7	-34.9	-47.9	-61.7	-70.9
PCl3	-69.0	20.3	13.7	-13.4	-14.1	-19.7	-20.8
Cl2S2	-4.0	31.6	27.9	-6.0	-7.4	-18.5	-19.9
SiCl2	-40.3	14.0	10.3	-7.1	-7.5	-9.4	-10.6
CF3Cl	-169.5	67.2	30.3	-1.5	-38.2	-23.3	-53.8
C2F6	-321.3	125.1	51.5	8.4	-69.3	-30.7	-96.1
CF3	-111.3	58.8	24.6	8.0	-28.1	-13.3	-43.6
C6H5 (phenyl radical)	81.2	33.3	26.3	-19.0	-36.3	-27.9	-41.6
PF5	-38.1	423.1	368.3	353.6	293.5	332.2	280.5

[a] Deviations in kcal/mol. Deviation=Experiment-Theory.