Pergamon

Tetrahedron Vol. 50, No. 3, pp. 627-638, 1994

0040-4020/94 $6.00+0.00

0040-4020(93)E0065-N

Addendum to SAM1 Results Previously Published

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Key words: SAM1; semiempirical; AM1; PM3; NDDO

Abstract: Corrected data and additional molecules are presented for the new SAM1 semiempirical method recently published by M.J.S Dewar, J.Y. Yu, and C. Jie.

INTRODUCTION

Recently Dewar *et. al.*[1] published results of a new method entitled SAM1 in this journal. In that paper they presented extensive tables of ΔH_f data representing the performance of their new SAM1 method *vs.* AM1 and PM3. This table was prepared using an older version of a program that is not generally available to the scientific community. SAM1 will be distributed for general use through the **AMPAC 4.5**[2] program. Our work with AMPAC 4.5's implementation of SAM1 and the more advanced and reliable algorithms it contains revealed significant discrepancies (about 15% of the entries) in the older program's performance. We therefore intend this re-publication of those tables to correct any inconsistencies existing in the literature. Additionally, we have added several molecules of interest and deleted species where the experimental data was especially questionable. We have also performed more extensive statistical analyses by element. The tables here are numbered to correspond to the tables in the original paper. It should be noted that the overall errors listed for the sets of compounds in the original paper have changed only very slightly. The discussion of results in that paper is still accurate and appropriate in the context of this new data.

TABLE 1. CALCULATED HEATS OF FORMATION[1] OF NEUTRAL CLOSED SHELL MOLECULES

	ΔH_f		Error[2] calculated by:		
Molecule	Expt'l	SAM1	SAM1	AM1	PM3
Hydrogen	0.0	0.2	0.2	-5.2	-13.4
Methane	-17.8	-16.2	1.6	9.0	4.7
Ethane	-20.0	-21.1	-1.1	2.6	1.9
Propane	-25.0	-25.8	-0.8	0.7	1.4
n-Butane	-30.0	-30.6	-0.6	-1.1	0.9
n-Pentane	-35.1	-35.3	-0.2	-2.8	0.7
n-Hexane	-39.9	-40.1	-0.2	-4.9	0.0
n-Heptane	-44.9	-44.8	0.1	-6.8	-0.4
n-Octane	-49.8	-49.6	0.2	-8.7	-0.9
n-Nonane	-54.5	-54.2	0.3	-10.9	-1.7
n-Decane	-59.6	-59.1	0.5	-12.6	-2.0

Molecule (Table 1 cont'd)	ΔH_f Expt'l	ΔH_f SAM1	Error[2] calculated by: SAM1	AM1	PM3
n-Undecane	-64.7	-63.8	0.9	-14.4	-2.3
n-Dodecane	-69.2	-68.5	0.7	-16.7	-3.2
iso-Butane	-32.1	-30.3	1.8	2.7	2.5
2-Methylbutane	-36.7	-34.1	2.6	1.3	2.3
neo-Pentane	-40.2	-34.6	5.6	7.4	4.4
Cyclopropane	12.7	17.0	4.3	5.1	3.5
Cyclobutane	6.8	0.7	-6.1	-7.8	-10.6
Cyclopentane	-18.3	-26.0	-7.7	-10.5	-5.2
Methylcyclopentane	-25.4	-31.0	-5.6	-8.7	-4.5
Cyclohexane (chair)	-29.5	-30.5	-1.0	-9.0	-1.5
trans-Bicyclopropyl	30.9	42.4	11.5	8.7	5.1
Spiropentane	44.3	49.9	5.6	6.2	-1.2
Bicyclobutane	51.9	75.3	23.4	26.2	17.3
Bicyclo[2.1.0]pentane	37.8	45.6	7.8	8.3	0.0
Bicyclo[2.2.1]heptane	-13.1	-12.0	1.1	-1.3	-0.5
Bicyclo[2.2.2]octane	-23.7	-27.6	-3.9	-12.3	-4.1
Adamantane	-32.2	-30.1	2.1	-11.0	-2.4
Cubane	148.7	134.6	-14.1	2.5	-34.9
Ethene	12.5	15.9	3.4	3.9	4.1
Propene	4.8	5.2	0.4	1.8	1.6
1-Butene	0.0	1.0	1.0	0.5	1.8
cis-2-Butene	-1.7	-3.7	-2.0	-0.4	-0.8
trans-2-Butene	-2.7	-5.3	-2.6	-0.6	-1.1
iso-Butene	-4.0	-4.5	-0.5	2.8	0.7
1-Pentene	-5.1	-4.6	0.5	-1.6	1.1
cis-2-Pentene	-6.6	-9.2	-2.6	-2.1	-2.0
trans-2-Pentene	-7.6	-10.1	-2.5	-2.1	-1.1
1-Dodecene	-39.5	-37.9	1.6	-15.1	-2.4
Propadiene (Allene)	45.5	43.2	-2.3	0.6	1.6
1,2-Butadiene	38.8	33.2	-5.6	-1.6	-0.8
trans-1,3-Butadiene	26.3	31.2	4.9	3.6	4.7
2,3-Dimethyl-1,3-butadiene	10.8	13.0	2.2	6.5	4.3
E-1,3-Pentadiene	18.2	20.1	1.9	1.6	2.5
Z-1,3-Pentadiene	19.5	21.7	2.2	1.1	1.8
1,4-Pentadiene	25.2	26.6	1.4	-0.4	1.4
1,5-Hexadiene	20.1	22.9	2.8	-1.6	1.9
Methylenecyclopropane	47.9	46.3	-1.6	-0.2	-3.4
Methylenecyclobutene	29.1	24.1	-5.0	-4.0	-9.4
Cyclopropene	66.2	72.4	6.2	8.6	2.0
1-Methylcyclopropene	58.2	59.4	1.2	6.5	-0.8
1,2-Dimethylcyclopropene	46.4	46.9	0.5	8.2	0.3
Cyclobutene	37.5	45.1	7.6	8.3	0.2
1,2-Dimethylcyclobutene	19.8	20.2	0.4	7.2	-3.6
Cyclopentene	8.1	3.3	-4.8	-5.1	-5.1
Cyclohexene (half-chair)	-1.2	-5.4	-4.2	-8.8	-3.7
1,3-Cyclopentadiene	32.1	35.8	3.7	5.0	-0.3
1,3-Cyclohexadiene	25.4	20.2	-5.2	-7.7	-5.0
Fulvene	53.5	60.0	6.5	9.2	2.7
1,3,5-Cycloheptatriene	43.2	44.4	1.2	-2.1	3.2
Norbornadiene	58.8	62.1	3.3	8.9	0.0
Benzene	19.7	19.6	-0.1	2.3	3.8
Toluene	12.0	9.7	-2.3	2.4	2.1
Ethylbenzene	7.1	5.1	-2.0	1.6	2.4
Styrene	35.3	36.4	1.1	3.4	3.9
Naphthalene	35.9	33.9	-2.0	4.7	4.8
1-Methylnaphthalene	27.0	25.3	-1.7	6.9	5.6
2-Methylnaphthalene	25.5	24.0	-1.5	7.5	5.7

Molecule (Table 1 cont'd)	ΔH_f Expt'l	ΔH_f SAM1	Error[2] SAM1	Error[2] AM1	Error[2] PM3
Azulene	69.1	79.0	9.9	16.0	12.2
Diphenylmethane	33.2	40.9	7.7	21.2	15.8
Anthracene	55.2	52.2	-3.0	7.7	6.5
Phenanthrene	49.5	45.2	-4.3	7.9	5.5
Biphenyl	43.4	40.6	-2.8	4.2	4.7
Acetylene	54.6	54.8	0.2	0.2	-3.9
Propyne	44.2	40.0	-4.2	-0.8	-4.0
1-Butyne	39.5	34.9	-4.6	-2.0	-3.8
2-Butyne	34.8	25.7	-9.1	-2.8	-5.0
Butadiyne	113.0	112.4	-0.6	-6.9	-10.5
1-Buten-3-yne (vinylacetylene)	72.8	68.5	-4.3	-4.9	-6.4
Nitrogen	0.0	12.7	12.7	11.2	17.6
Ammonia	-11.0	-5.7	5.3	3.7	7.9
Hydrazine	22.8	12.1	-10.7	-9.1	-2.1
Methylamine	-5.5	-5.5	0.0	-1.9	0.3
Ethylamine	-11.3	-10.9	0.4	-3.8	-1.2
n-Propylamine	-16.8	-15.4	1.4	-5.3	-1.1
iso-Propylamine	-20.0	-15.4	4.6	0.9	1.3
tert-Butylamine	-28.9	-19.6	9.3	7.6	3.7
Cyclopropylamine	18.4	25.4	7.0	0.8	1.1
Aniline	20.8	19.6	-1.2	-0.3	0.5
N,N-Diethylamine	-4.4	-5.3	-0.9	-1.2	-3.5
Trimethylamine	-5.7	-4.4	1.3	4.0	-5.2
Pyrrolidine	-0.8	-6.8	-6.0	-9.6	-11.2
Acetaldehyde Imine	30.2	40.1	9.9	2.9	1.4
1,2-Ethanediamine	-4.2	-0.9	3.3	-8.6	-1.4
Methylhydrazine	22.6	12.7	-9.9	-5.3	-4.7
Phenylhydrazine	48.5	39.6	-8.9	-1.8	-0.9
1,2-Dimethylhydrazine	22.0	16.8	-5.2	-0.4	-6.4
Hydrogen Cyanide	32.3	33.8	1.5	-1.3	0.7
Acetonitrile (Methylcyanide)	15.4	18.0	2.6	3.9	7.9
Propane Nitrile (Ethylcyanide)	12.3	12.4	0.1	0.7	6.3
Cyclobuytylcyanide	34.2	32.3	-1.9	-3.7	-1.8
Benzonitrile (Phenylcyanide)	51.6	50.9	-0.7	1.8	6.9
Acrylonitrile (Cyanoethene)	43.2	47.6	4.4	1.8	7.0
Cyanogen	73.3	77.8	4.5	-5.4	4.2
Malononitrile (1,3-Dicyanopropanane	63.5	56.6	-6.9	-9.2	0.9
Maleonitrile (1,2-Dicyanoethene)	81.3	80.9	-0.4	-5.3	4.7
Dicyanoacetylene	126.5	136.4	9.9	-6.7	1.6
Cyanoamine	32.0	33.7	1.7	-2.3	4.2
Hydrogen isocyanate	-24.3	-15.9	8.4	9.1	9.0
Methyl Isocyanide	39.1	23.0	-16.1	11.3	15.6
cis-Diimine	50.9	38.4	-12.5	-18.5	-8.0
Diazomethane	55.0	58.4	3.4	7.6	6.0
trans-Azopropane	12.3	7.5	-4.8	1.1	-1.8
trans-Azoisopropane	8.6	7.2	-1.4	6.2	-2.8
cis-Azoisopropane	20.0	7.3	-12.7	-10.3	-13.2
Pyrrole	25.9	36.0	10.1	14.0	1.2
1-H-Tetrazole	79.9	89.9	10.0	29.7	6.3
Pyridine	33.6	32.1	-1.5	-1.6	-3.2
1,2-Diazabenzene (Pyridazine)	66.5	48.7	-17.8	-11.2	-10.5
1,3-Diazabenzene (Pyrimidine)	46.8	46.3	-0.5	-2.9	-8.8
1,4-Diazabenzene (Pyrazine)	46.9	46.4	-0.5	-2.7	-7.6
trans-Diisopropyl-diazene	8.6	7.2	-1.4	6.2	-2.8
Phenazine	82.2	80.8	-1.4	10.8	3.3
Benzocinnoline	94.8	72.0	-22.8	-4.6	-10.1
Oxygen (singlet)	22.0	15.6	-6.4	-21.3	-3.6

Molecule (Table 1 cont'd)	ΔH_f Expt'l	ΔH_f SAM1	Error[2] calculated by: SAM1	AM1	PM3
Ozone	34.1	42.9	8.8	3.7	17.0
Carbon Dioxide	-94.1	-86.0	8.1	14.2	9.0
Carbon Monoxide	-26.4	-33.0	-6.6	20.7	6.7
Water	-57.8	-57.0	0.8	-1.4	4.4
Hydrogen Peroxide	-32.5	-44.9	-12.4	-2.8	-8.3
Methanol	-48.1	-51.8	-3.7	-8.5	-3.8
Ethanol	-56.2	-57.5	-1.3	-6.4	-0.7
Propanol	-61.0	-64.2	-3.2	-9.6	-2.6
iso-Propanol	-65.2	-64.0	1.2	-2.8	1.2
tert-Butanol	-74.7	-70.1	4.6	3.1	3.4
Phenol	-23.0	-22.7	0.3	0.8	1.3
Ethylene glycol	-92.6	-97.8	-5.2	-18.7	-6.5
1,3-Propane diol	-93.7	-101.1	-7.4	-22.3	-8.7
o-Hydroxyphenol (Catechol)	-65.0	-64.2	0.8	-1.3	0.0
m-Hydroxyphenol (Resorcinol)	-65.7	-65.7	0.0	-1.1	-1.6
p-Hydroxyphenol (Hydroquinone)	-63.4	-63.6	-0.2	-2.3	-2.7
Dimethylether	-44.0	-45.9	-1.9	-9.2	-4.3
Diethylether	-60.3	-57.4	2.9	-4.7	0.7
Ethyleneoxide (oxirane)	-12.6	-8.1	4.5	3.6	4.4
Oxetane	-19.2	-15.2	4.0	-6.3	-7.5
Tetrahydrofuran	-44.0	-51.5	-7.5	-14.4	-7.3
Furan	-8.3	3.7	12.0	11.3	4.3
Dimethoxymethane	-83.3	-86.4	-3.1	-20.0	-6.9
1,3-Dioxolane	-71.2	-82.3	-11.1	-22.5	-11.1
Divinylether	-3.3	5.1	8.4	7.2	3.5
Ethylvinylether	-33.7	-27.6	6.1	0.3	3.7
Anisole	-16.2	-13.7	2.5	2.0	2.8
1,3,5-Trioxane	-113.3	-120.2	-6.9	-29.7	-9.1
Dimethylperoxide	-30.0	-32.1	-2.1	3.0	-4.1
Diethylperoxide	-46.1	-43.2	2.9	7.8	6.2
Formaldehyde	-26.0	-28.5	-2.5	-5.5	-8.1
Acetaldehyde	-39.7	-41.7	-2.0	-1.8	-4.5
Propionaldehyde	-44.4	-47.6	-3.2	-3.1	-4.8
Butanal	-48.9	-51.9	-3.0	-5.7	-5.2
2-Butenal	-24.0	-26.0	-2.0	-3.0	-4.9
Benzaldehyde	-8.8	-11.0	-2.2	-0.1	-1.8
trans-Glyoxal	-50.7	-57.8	-7.1	-8.0	-13.6
Ketene	-11.4	-10.3	1.1	5.7	2.2
Acetone	-51.9	-53.3	-1.4	2.8	-1.4
Methylethyl ketone	-57.1	-58.6	-1.5	1.9	-0.3
2,3-Butanedione	-78.2	-85.2	-7.0	4.1	-5.8
2,4-Pentanedione	-91.0	-91.4	-0.4	5.4	-0.6
p-Benzoquinone	-29.4	-29.5	-0.1	4.4	-2.1
Formic Acid	-90.5	-90.5	0.0	-6.9	-3.9
Acetic Acid	-103.4	-102.1	1.3	0.4	1.4
Propionic Acid	-108.4	-108.4	0.0	-0.7	2.0
Benzoic Acid	-70.3	-70.2	0.1	2.4	4.1
Oxalic Acid	-173.0	-171.1	1.9	0.6	-1.0
Salicylic Acid	-118.3	-117.8	0.5	3.9	4.1
Methyl Formate	-85.0	-84.3	0.7	-6.1	-2.1
Methyl Acetate	-98.4	-95.6	2.8	2.0	4.4
Acetic Anhydride	-136.8	-138.7	-1.9	5.1	1.8
Maleic Anhydride	-95.2	-81.9	13.3	20.3	11.8
2-Hydroxypyridine	-19.0	-11.9	7.1	7.2	0.9
3-Hydroxypyridine	-10.4	-10.9	-0.5	-1.2	-3.8
4-Hydroxypyridine	-9.8	-11.3	-1.5	-2.9	-5.4
Glycine	-93.7	-96.1	-2.4	-7.8	-2.3

Molecule (Table 1 cont'd)	ΔH_f Expt'l	ΔH_f SAM1	Error[2] calculated by: SAM1	AM1	PM3
Alanine	-111.4	-102.3	9.1	6.4	10.3
Formamide	-44.5	-39.8	4.7	-0.2	2.7
Acetamide	-57.0	-51.0	6.0	6.3	6.2
Propionamide	-61.9	-56.7	5.2	4.8	6.2
n-Butyramide	-66.5	-60.8	5.7	3.6	6.0
Dimethylformamide	-45.8	-38.7	7.1	8.9	1.3
Hydroxyamine	-10.0	-17.1	-7.1	-12.5	-3.3
Hyponitrous Acid	23.8	14.4	-9.4	-21.6	-10.0
Dinitrogen Oxide	19.6	15.6	-4.0	8.9	5.8
Dinitrogen Trioxide	19.8	20.0	0.2	2.0	3.9
Dinitrogen Tetroxide	2.2	6.3	4.1	22.7	9.1
Dinitrogen Pentoxide	2.7	-8.5	-11.2	3.1	-17.0
Nitrous Acid	-18.3	-27.4	-9.1	-21.1	3.4
Nitric Acid	-32.1	-39.8	-7.7	-5.2	-5.7
Methyl Nitrite	-15.9	-19.8	-3.9	-15.9	6.8
Methyl Nitrate	-29.2	-34.9	-5.7	-2.2	-3.3
Ethyl Nitrate	-36.8	-42.1	-5.3	-1.3	-1.2
Nitromethane	-17.7	-15.9	1.8	7.8	1.8
Nitroethane	-24.5	-22.9	1.6	7.7	3.1
1,1,1-Trinitroethane	-12.4	-19.7	-7.3	33.5	1.0
1-Nitropropane	-29.6	-28.4	1.2	6.0	2.8
2-Nitropropane	-33.2	-29.4	3.8	11.7	6.1
1-Nitrobutane	-34.4	-32.5	1.9	4.0	2.8
2-Nitrobutane	-39.1	-33.9	5.2	10.9	7.2
Dinitromethane	-14.1	-13.0	1.1	17.3	2.4
Trinitromethane	0.0	-10.5	-10.5	25.0	-4.7
1,1-Dinitropropane	-24.1	-26.8	-2.7	14.9	2.2
1,1,1-Trinitropropane	-18.4	-22.8	-4.4	34.0	8.4
N-Nitrodimethylamine	-1.1	-0.9	0.2	22.8	2.4
o-Nitroaniline	15.2	10.2	-5.0	5.5	-2.4
m-Nitroaniline	14.0	14.4	0.4	10.0	-1.5
p-Nitroaniline	14.1	11.8	-2.3	5.4	-3.4
Nitrobenzene	16.1	14.1	-2.0	9.2	-1.6
o-Dinitrobenzene	21.0	15.3	-5.7	17.6	-5.8
m-Dinitrobenzene	12.9	9.4	-3.5	20.2	-3.7
p-Dinitrobenzene	14.0	9.0	-5.0	19.3	-3.9
1,3,5-Trinitrobenzene	14.9	5.5	-9.4	30.0	-8.0
p-Nitrotoluene	7.4	3.4	-4.0	9.9	-2.7
2,4-Dinitrotoluene	7.9	0.3	-7.6	18.3	-5.9
2,4,6-Trinitrotoluene (TNT)	10.4	-0.9	-11.3	30.8	-7.0
Fluorine	0.0	2.1	2.1	-22.5	-21.7
Hydrogen Fluoride	-65.3	-72.7	-7.4	-9.0	2.6
Methyl Fluoride	-56.0	-61.0	-5.0	-5.0	2.2
Difluoromethane	-108.1	-112.9	-4.8	-8.0	4.3
Trifluoromethane	-166.2	-169.8	-3.6	-6.3	4.2
Tetrafluoromethane	-223.1	-225.5	-2.4	-2.6	-2.0
Ethyl Fluoride	-63.0	-64.3	-1.3	-3.3	2.8
1,1-Difluoroethane	-118.8	-115.0	3.8	0.2	6.9
1,1,1-Trifluoroethane	-178.0	-171.4	6.6	5.4	5.7
Perfluoroethane	-321.3	-315.7	5.6	8.1	3.5
1-Fluoropropane	-68.3	-69.8	-1.5	-5.0	-2.7
2-Fluoropropane	-70.1	-67.2	2.9	0.3	3.3
Perfluorocyclobutane	-368.7	-375.9	-7.2	1.5	-10.5
Vinyl Fluoride	-33.2	-31.2	2.0	-0.8	4.6
1,1-Difluoroethene	-80.1	-80.4	-0.3	-4.2	0.5
Trifluoroethene	-117.3	-124.3	-7.0	-13.3	-4.2
Perfluoroethene	-157.5	-166.2	-8.7	-17.6	-10.7

Molecule (Table 1 cont'd)	ΔH_f Expt'l	ΔH_f SAM1	Error[2] calculated by: SAM1	AM1	PM3
Fluorobenzene	-27.7	-24.2	3.5	4.4	7.5
o-Difluorobenzene	-70.2	-66.6	3.6	3.8	7.1
m-Difluorobenzene	-73.9	-66.9	7.0	6.0	10.6
p-Difluorobenzene	-73.3	-67.1	6.2	5.3	10.0
Pentafluorobenzene	-192.8	-188.1	4.7	0.8	4.2
Perfluorobenzene	-228.3	-226.2	2.1	-2.9	-1.0
Hypofluorous Acid	-23.5	-17.3	6.2	0.9	-5.7
Difluorine Oxide	5.9	15.3	9.4	4.6	-10.7
Trifluoromethylhypofluorite	-182.8	-173.1	9.7	5.1	-4.5
2,2,2-Trifluoroethanol	-212.3	-213.0	-0.7	-5.2	1.0
2,2,3,3,3-Pentafluoropropanol	-313.2	-309.4	3.8	3.8	5.4
Pentafluorophenol	-228.7	-227.6	1.1	-4.0	-2.6
Perfluoroacetone	-334.0	-341.1	-7.1	2.4	-6.0
Perfluoroacetic Acid	-246.5	-244.5	2.0	3.8	2.5
p-Fluorobenzoic Acid	-118.2	-114.2	4.0	5.2	8.7
Carbonyl Fluoride	-152.9	-142.1	10.8	6.6	11.3
Formyl Flouride	-90.0	-87.9	2.1	-2.9	1.2
Acetyl Fluoride	-105.8	-97.9	7.9	7.0	7.1
Fluorocyanide	8.6	0.6	-8.0	-13.0	-2.1
Difluoroamine	-16.0	-19.9	-3.9	-7.9	4.6
Nitrogen Trifluoride	-29.8	-40.4	-10.6	-10.2	5.4
Tetrafluorohydrazine	-2.0	-8.2	-6.2	13.0	3.1
cis-Difluorodiimine	16.4	14.8	-1.6	4.4	11.6
trans-Difluorodiimine	19.4	24.0	4.6	11.9	9.8
Trifluoroacetonitrile	-119.0	-113.3	5.7	-0.5	4.0
Nitrosyl fluoride	-15.7	-15.2	0.5	-10.8	12.4
Nitryl Fluoride	-26.0	-22.5	3.5	4.7	0.4
Chlorine	0.0	2.8	2.8	-14.2	-11.6
Hydrogen Chloride	-22.1	-23.9	-1.8	-2.5	1.6
Methylchloride	-19.6	-21.4	-1.8	0.7	4.9
Dichloromethane	-22.8	-25.6	-2.8	-3.0	5.7
Chloroform	-24.8	-28.2	-3.4	-4.2	3.9
Carbon Tetrachloride	-22.9	-28.6	-5.7	-5.2	-3.1
Ethyl Chloride	-26.8	-28.3	-1.5	0.6	4.7
1,1-Dichloroethane	-30.5	-33.8	-3.3	-0.6	4.0
1,2-Dichloroethane	-30.3	-33.3	-3.0	-3.5	5.6
1,1,1-Trichloroethane	-34.6	-37.3	-2.7	2.7	2.7
1,1,2-Trichloroethane	-36.1	-36.6	-0.5	-1.1	8.4
Perchloroethane	-34.3	-36.9	-2.6	-1.5	-2.2
n-Propylchloride	-31.5	-33.5	-2.0	-1.5	4.1
iso-Propylchloride	-34.6	-34.9	-0.3	3.3	4.8
1,2-Dichloropropane	-38.9	-39.6	-0.7	0.7	7.3
1,3-Dichloropropane	-38.0	-39.3	-1.3	-2.7	7.6
iso-Butylchloride	-38.1	-36.9	1.2	1.1	5.5
tert-Butylchloride	-43.5	-41.1	2.4	9.0	5.7
1-Chloropentane	-41.8	-42.5	-0.7	-4.4	3.7
Cyclohexylchloride	-39.1	-40.8	-1.7	-6.6	2.1
Vinyl Chloride	8.9	5.4	-3.5	-3.0	0.8
1,1-Dichloroethene	0.6	-0.8	-1.4	-0.6	2.5
cis-1,2-Dichloroethene	1.2	-2.9	-4.1	-4.5	2.8
trans-1,2-Dichloroethene	1.1	-2.7	-3.8	-4.5	2.5
Trichloroethylene	-1.9	-7.6	-5.7	-6.5	-0.4
Perchloroethene	-2.6	-10.8	-8.2	-9.8	-5.5
2-Chloropropene	-5.0	-5.3	-0.3	3.4	3.9
Chlorobenzene	12.4	10.1	-2.3	2.4	4.3
o-Dichlorobenzene	7.2	3.7	-3.5	2.0	3.9
m-Dichlorobenzene	6.1	2.2	-3.9	2.1	4.1

Molecule (Table 1 cont'd)	ΔH_f Expt'l	ΔH_f SAM1	Error[2] calculated by: SAM1	AM1	PM3
p-Dichlorobenzene	5.4	1.9	-3.5	2.6	4.7
Perchlorobenzene	-8.5	-11.0	-2.5	0.7	-0.6
Benzylchloride	4.5	3.6	-0.9	3.7	7.6
p-Chlorotoluene	4.5	0.0	-4.5	2.6	2.8
p-Chloroethylbenzene	-0.9	-4.7	-3.8	2.2	3.5
Chloroacetylene	51.1	49.7	-1.4	-3.3	-4.5
Hypochlorous Acid	-17.8	-18.2	-0.4	-4.0	-16.5
Dichlorine Oxide	21.0	19.9	-1.1	-1.5	-37.2
m-Chlorophenol	-36.6	-32.0	4.6	7.4	8.2
p-Chlorophenol	-34.8	-31.8	3.0	5.5	6.4
Pentachlorophenol	-53.8	-46.9	6.9	9.1	5.5
Chloroacetic Acid	-104.0	-103.8	0.2	-2.8	2.5
o-Chlorobenzoic Acid	-77.7	-75.0	2.7	7.6	7.5
m-Chlorobenzoic Acid	-81.7	-78.5	3.2	7.4	9.4
p-Chlorobenzoic Acid	-81.5	-79.2	2.3	6.9	8.9
Carbonyl Dichloride (Phosgene)	-52.4	-50.1	2.3	5.1	3.3
Acetyl Chloride	-58.0	-58.5	-0.5	7.3	4.9
TrichloroAcetyl Chloride	-57.3	-58.7	-1.4	4.0	0.6
Oxalyl Chloride	-80.3	-78.6	1.7	11.8	3.7
Benzoyl Chloride	-24.7	-25.9	-1.2	9.0	6.4
Cyanogen Chloride	32.9	29.0	-3.9	-8.2	-1.3
p-Chloronitrobenzene	9.1	5.5	-3.6	10.1	-0.7
Chlorine Fluoride	-12.0	-6.9	5.1	1.5	-9.7
Chlorofluoromethane	-62.0	-65.1	-3.1	-3.3	4.4
Chlorodifluoromethane	-115.1	-114.2	0.9	0.9	5.4
Dichlorofluoromethane	-67.0	-66.4	0.6	1.8	5.0
Dichlorodifluoromethane	-114.1	-109.0	5.1	7.1	-1.9
Trichlorofluoromethane	-64.1	-63.8	0.3	3.2	-3.2
1,2-Dichloro-1,1,2,2-tetrafluoroethane	-219.0	-205.0	14.0	20.0	6.7
Chloropentafluorobenzene	-194.1	-188.6	5.5	1.4	1.9
Chlorotrifluoroethene	-132.7	-121.1	11.6	3.9	7.4
Fluorine Hypochlorite	12.9	22.1	9.2	8.5	-20.0
Nitrosyl Chloride	12.4	13.6	1.2	-7.7	-7.9
Nitryl Chloride	2.9	4.3	1.4	11.7	-15.9
Bromine	7.4	-2.8	-10.2	-12.7	-2.5
Hydrogen Bromide	8.7	-6.6	2.1	-1.8	14.0
Methyl Bromide	-8.5	-11.2	-2.7	2.3	6.5
Dibromomethane	0.0	-2.7	-2.7	-1.0	7.9
Tribromomethane	5.7	8.9	3.2	0.7	11.9
Carbon Tetrabromide	20.1	23.5	3.4	-4.2	12.8
Ethylbromide	-14.8	-18.3	-3.5	1.7	3.4
1,2-Dibromoethane	-9.0	-15.0	-6.0	1.1	5.6
n-Propylbromide	-20.8	-23.5	-2.7	0.9	4.1
iso-Propylbromide	-23.8	-24.9	-1.1	5.9	3.0
1,2-Dibromopropane	-17.1	-19.1	-2.0	4.8	5.5
n-Butylbromide	-25.6	-28.4	-2.8	-1.2	3.5
sec-Butylbromide	-28.8	-29.0	-0.2	4.7	3.0
tert-Butylbromide	-31.6	-31.0	0.6	11.0	1.3
n-Pentylbromide	-30.8	-33.3	-2.5	-2.8	3.3
Bromoethene (Vinyl bromide)	18.9	16.8	-2.1	-0.9	4.9
3-Bromo-propene (Allylbromide)	10.8	8.4	-2.4	0.2	2.6
trans-1-Bromopropene	10.5	5.4	-5.1	-2.6	3.1
cis-1-Bromopropene	9.8	6.3	-3.5	-1.4	4.9
Bromoacetylene	59.2	61.2	2.0	-4.8	10.6
Bromobenzene	25.2	21.1	-4.1	1.6	5.8
Hypobromous Acid	-19.0	-21.3	-2.3	-5.7	-14.9
Bromoacetone	-43.3	-46.9	-3.6	2.5	0.9

Molecule (Table 1 cont'd)	ΔH_f Expt'l	ΔH_f SAM1	Error[2] calculated by: SAM1	AM1	PM3
p-Bromobenzoic Acid	-69.4	-68.1	1.3	7.1	11.5
Carbonyl Bromide	-27.1	-26.5	0.6	9.3	1.8
Acetyl Bromide	-45.5	-46.7	-1.2	11.2	2.0
Benzoylbromide	-11.7	-14.0	-2.3	12.5	3.2
Cyanogen Bromide	44.5	39.9	-4.6	-12.0	9.1
Nitrosyl bromide	19.6	19.7	0.1	1.7	-13.0
Bromine Fluoride	-14.0	-6.2	7.8	6.8	-7.2
Bromodifluoromethane	-101.6	-100.1	1.5	4.8	2.2
Bromotrifluoromethane	-154.9	-148.6	6.3	10.4	-2.9
Dibromodifluoromethane	-91.0	-80.8	10.2	16.9	-3.1
1-Bromo-2-fluoroethane	-60.0	-59.9	0.1	-0.7	8.8
1,2-Dibromo-1,1,2,2-tetrafluoroethane	-188.6	-178.0	10.6	23.4	-5.7
Pentafluorobromobenzene	-170.2	-176.4	-6.2	-9.5	-5.8
Bromine Chloride	3.5	-6.9	-10.4	-14.1	-6.7
Bromotrichloromethane	-10.0	-15.6	-5.6	-4.7	-4.1
1-Bromo-1-chloroethane	-20.0	-22.4	-2.4	2.5	4.1
1-Bromo-2-chloroethane	-21.0	-22.4	-1.4	0.8	7.9
1,2-Dibromo-1,2-dichloroethane	-8.8	-13.6	-4.8	-4.8	-2.4
Iodine	14.9	17.4	2.5	4.9	5.8
Hydrogen Iodide	6.3	15.1	8.8	1.6	22.5
Methyl Iodide	3.5	6.7	3.2	2.2	5.9
Diiodomethane	28.0	28.6	0.6	-6.5	5.5
Triiodomethane	50.4	50.3	-0.1	-12.6	10.2
Carbon Tetraiodide	62.4	74.9	12.5	-8.2	40.3
Ethyliodide	-1.8	-2.3	-0.5	0.3	7.3
1-Propyliodide	-7.2	-7.6	-0.4	0.6	4.3
1,2-Diiodoethane	16.0	13.8	-2.2	-0.3	7.3
1,2-Diiodopropane	8.5	6.1	-2.4	2.6	10.1
n-Butyliodide	-12.0	-12.5	-0.5	-2.7	3.7
tert-Butyliodide	-17.2	-17.6	-0.4	-2.7	3.7
Iodoethene (Vinyl iodide)	31.0	34.0	3.0	-1.2	4.2
3-Iodopropene (Allyl Iodide)	21.9	23.4	1.5	0.5	5.2
cis-Diiodoethene	49.6	54.7	5.1	-6.1	13.2
trans-Diiodoethene	49.6	51.0	1.4	-5.5	5.7
cis-1-Iodopropene	20.7	22.9	2.2	-0.2	8.5
trans-1-Iodopropene	22.3	23.6	1.3	-2.6	3.1
Cyclohexyl Iodide	-12.0	-16.6	-4.6	-8.0	0.3
Iodobenzene	39.4	36.4	-3.0	-1.3	5.3
o-Diiodobenzene	60.2	52.1	-8.1	-6.2	13.6
o-Iodotoluene	31.7	26.9	-4.8	0.1	7.2
m-Iodotoluene	31.9	26.3	-5.6	-1.4	3.5
p-Iodotoluene	29.1	26.4	-2.7	1.3	6.3
1-Iodonaphthalene	55.9	50.9	-5.0	2.6	10.1
2-Iodonaphthalene	56.2	50.4	-5.8	0.6	5.7
Cyanogen Iodide	53.7	56.6	2.9	-9.5	11.4
Iodoacetone	-31.2	-30.0	1.2	2.3	4.9
p-Iodobenzoic Acid	-54.5	-53.1	1.4	3.6	10.1
Benzyl Iodide	25.0	28.2	3.2	5.9	13.3
Acetyl Iodide	-30.2	-33.8	-3.6	9.5	0.3
Benzoyl Iodide	2.5	-2.5	-5.0	11.7	5.5
Nitrosyl Iodide	26.8	24.7	-2.1	5.4	-8.6
Iodine Fluoride	-22.7	-13.0	9.7	13.8	14.9
2,2,2-Trifluoroethyl Iodide	-154.1	-146.0	8.1	4.6	15.2
Iodine Chloride	4.3	-0.1	-4.4	-8.9	6.5
Iodine Bromide	9.8	9.0	-0.8	-3.8	5.9

1. In kcal/mol. 2. Error = $E_{calc.} - E_{expt'l}$

TABLE 2. ERROR ANALYSIS FOR CALCULATED HEATS OF FORMATION OF NEUTRAL CLOSED SHELL MOLECULES

Elements	Number of Examples[1]	Type of Error[2]	Procedure SAM1	AM1	PM3
C, H	79	MU	3.35	5.91	3.99
		MS	0.25	0.45	-0.11
		SD	4.96	4.98	4.91
		RMS	4.94	7.70	6.31
O	138	MU	3.93	8.51	5.33
		MS	-0.34	3.12	-0.19
		SD	3.22	10.92	7.04
		RMS	5.08	11.32	7.01
N	103	MU	5.11	9.03	5.22
		MS	-1.43	3.38	0.35
		SD	4.23	11.43	6.55
		RMS	6.62	11.86	6.53
C, H, O, N	222	MU	4.24	7.46	4.50
		MS	-0.54	1.27	-0.20
		SD	5.82	7.04	4.12
		RMS	5.83	10.24	6.09
F	63	MU	5.15	6.46	6.10
		MS	2.09	1.11	1.53
		SD	3.34	8.36	7.42
		RMS	6.12	8.36	7.52
Cl	70	MU	3.16	4.82	5.68
		MS	-0.64	0.73	1.24
		SD	2.68	6.14	7.65
		RMS	4.13	6.14	7.70
Br	42	MU	3.55	5.56	5.80
		MS	-1.18	1.34	2.54
		SD	4.44	7.55	6.45
		RMS	4.54	7.58	6.87
I	37	MU	3.53	4.37	8.52
		MS	0.18	4.37	8.05
		SD	2.92	5.80	7.53
		RMS	4.56	5.74	10.95
F, Cl, Br, I	186	MU	3.66	5.15	6.30
		MS	-0.13	0.43	3.03
		SDS	4.64	4.36	5.29
		RMS	4.62	6.17	8.21
C, H, O, N, F, Cl, Br, I	408	MU	3.97	6.40	5.32
		MS	-0.35	0.89	1.27
		SDS	5.31	6.07	4.77
		RMS	5.31	8.82	7.14

1. The total of the number examples is greater than the total number of species due to overlap in the categories.
2. MU=mean unsigned error; MS=mean signed error, SD=standard deviation, RMS=root mean square error.

TABLE 3. CALCULATED HEATS OF FORMATION[1] OF IONS AND RADICALS

	ΔH_f		Error[2] calculated by:		
Species	Expt'l	SAM1	SAM1	AM1	PM3
C2	200.2	177.8	-22.4	22.4	31.7
C3	196.0	180.6	-15.4	16.4	10.7
C4	232.0	245.1	13.1	38.7	33.9
CH	142.4	144.6	2.2	2.6	4.4
Carbene (singlet)	99.8	108.8	9.0	11.1	13.4
Carbene (triplet)	92.3	86.9	-5.4	-11.5	-16.7
Methyl radical	34.8	30.6	-4.2	-3.5	-5.0
Ethyl radical	25.7	17.4	-8.3	-7.6	-8.4
n-Propyl radical	16.8	12.8	-4.0	-12.5	-12.0
iso-Propyl radical	22.3	4.7	-17.6	-15.6	-16.9
sec-Butyl radical	17.0	-0.1	-17.1	-17.0	-16.9
tert-Butyl radical	11.0	-7.0	-18.0	-13.9	-17.1
Vinyl radical	63.4	64.7	1.3	1.3	-0.1
Allyl radical	40.0	40.6	0.6	-1.4	-0.4
Azidyl radical	99.0	110.0	11.0	8.4	7.0
Cyanide radical	104.0	110.4	6.4	10.4	24.0
Cyanomethyl radical	59.0	63.3	4.3	-1.7	3.0
Aminomethyl radical	38.0	39.5	1.5	-22.3	-17.2
O2 (triplet)	0.0	-13.2	-13.2	-27.1	-4.2
Hydroxyl radical	9.3	1.7	-7.6	-8.4	-6.3
Nitrogen Oxide	21.6	15.8	-5.8	-20.6	-7.1
Cyanate radical	38.1	49.2	11.1	0.8	-5.7
2,2,2-Trifluoroethyl radical	-124.0	-126.5	-2.5	-7.4	-7.2
Difluoroamidyl radical	10.1	-11.0	-21.1	-16.5	1.8
Carbonylchloride radical	-21.0	-31.0	-10.0	-0.4	-1.1
Bromoxy radical	30.1	32.0	1.9	5.5	-9.3
Iodoxy radical	41.8	38.2	-3.6	-4.8	-10.9
Hydrogen cation	365.7	362.0	-3.7	-50.8	-12.1
Trihydrogen cation	264.5	236.3	-28.2	-40.6	-49.3
Hydronium cation	138.9	139.9	1.0	4.6	20.2
Methyl cation	262.9	262.6	-0.3	-10.5	-6.3
Ethyl cation	215.6	212.2	-3.4	1.5	7.3
iso-Propyl cation	190.9	178.8	-12.1	1.0	6.4
1-Methylcyclopentyl cation	167.0	149.5	-17.5	0.5	7.5
Cyclohexyl cation	175.0	167.0	-8.0	-0.7	11.1
Vinyl cation	268.9	257.7	-11.2	-7.4	-5.0
Allyl cation	226.0	226.0	0.0	0.2	6.7
Benzyl cation	215.0	211.8	-3.2	7.1	12.4
Tropylium cation	203.0	196.4	-6.6	7.4	18.0
Ammonium cation	155.0	142.1	-12.9	-4.4	-1.6
Methylamino cation	178.0	171.9	-6.1	-1.7	7.3
Cyanide cation	430.9	432.3	1.4	-10.9	13.0
Oxonium cation	168.0	155.2	-12.8	-6.7	-1.7
Hydrogen carbonyl cation	197.3	192.4	-4.9	-9.8	-20.4
Nitrosyl cation	235.3	236.4	1.1	-7.2	2.9
Nitronium cation	231.3	188.8	-42.5	-10.2	-22.9
Methylene Fluoride cation	199.0	182.1	-16.9	-18.6	1.3
Trifluoromethyl cation	96.7	82.6	-14.1	-14.6	2.9
Fluoroethyl cation	157.0	149.9	-7.1	0.6	16.5
Methyl anion	33.2	43.5	10.3	24.5	18.3
Ethyl anion	35.1	26.8	-8.3	-0.4	-3.3
iso-Propyl anion	28.2	12.3	-15.9	11.4	13.4
Diphenylmethyl anion	31.3	33.3	2.0	4.8	-3.6
tert-Butyl anion	16.0	-0.8	-16.8	-12.9	-16.0

Species (Table 3 cont'd)	ΔH_f		Error[2] calculated by:		
	Expt'l	SAM1	SAM1	AM1	PM3
Cyclopropyl anion	57.5	64.0	6.5	8.7	3.4
Vinyl anion	52.9	45.8	-7.1	14.9	8.8
Allyl anion	29.9	27.9	-2.0	-2.3	-4.7
Cyclopentadienyl anion	19.6	25.2	5.6	5.6	-3.7
Cycloheptatrienyl anion	53.3	52.0	-1.3	-13.7	-10.2
Monoacetylide anion	65.5	58.0	-7.5	23.6	10.9
Oxygen anion	24.3	29.4	5.1	22.5	12.6
Hydroxide anion	-32.7	-19.9	12.8	18.6	15.2
Methoxide anion	-33.2	-36.4	-3.2	-5.3	-4.7
Methoxymethyl anion	-2.6	-8.9	-6.3	-6.0	-5.2
Vinyl oxide anion	-39.4	-33.1	6.3	33.2	-0.5
Phenyloxide anion	-39.4	-35.9	3.5	-1.6	-4.7
Ethynyloxide anion	-12.2	-6.6	5.6	7.3	-0.7
Formate anion	-110.9	-101.1	9.8	1.5	0.0
Dimethylketo anion	-48.5	-41.4	7.1	4.9	-0.2
Methylamide anion	29.4	39.5	10.1	4.7	-2.1
Pyrrole anion	18.9	32.3	13.4	9.2	-7.4
Cyanide anion	17.7	25.5	7.8	26.3	10.0
Ethylcyanide anion	21.5	23.3	1.8	-3.5	-4.4
iso-Propylcyanide anion	15.3	8.9	-6.4	-7.4	-9.1
Cyclopropylcyanide anion	53.8	47.7	-6.1	2.4	-0.2
Benzylcyanide anion	29.4	34.4	5.0	14.1	14.5
Propional anion	-45.2	-43.5	1.7	-4.7	-7.1
Nitrate anion	-73.4	-77.2	-3.8	-15.4	-19.9
Nitromethyl anion	-27.2	-22.9	4.3	-2.0	-16.1
Flouride anion	-61.0	-32.4	28.6	64.4	29.8
2,2-Difluoroethoxide anion	-147.7	-157.9	-10.2	-17.0	-7.9
Triflouroacetate anion	-289.2	-299.9	-10.7	1.9	-1.2
Difluoroamide anion	-22.2	-13.9	8.3	-3.0	-8.8
m-Fluoroamide phenyl anion	-31.5	-21.1	10.4	-0.7	-4.4
Chloride anion	-55.7	-41.8	13.9	19.6	4.5
3-Chloropropionate anion	-139.8	-132.0	7.8	2.1	5.0
4-Chloro-n-butyrate anion	-140.0	-133.5	6.5	-2.0	2.5
3-Chloro-n-butyrate anion	-147.2	-137.3	9.9	4.8	5.3
m-Chloroamide phenyl anion	6.2	10.2	4.0	-0.6	-4.5
Bromide anion	-52.4	-30.1	22.3	30.6	-5.2
Iodide anion	-47.0	-16.5	30.5	43.2	-19.2

1. In kcal/mol. 2. Error = $E_{calc.} - E_{expt'l}$

TABLE 4. ERROR ANALYSIS FOR CALCULATED HEATS OF FORMATION OF IONS AND RADICALS

Elements	Number of Examples	Type of Error[1]	Procedure SAM1	AM1	PM3
Radicals	27	MU	8.84	11.47	10.83
		MS	-4.21	-2.76	-1.21
		SD	10.22	14.64	14.06
		RMS	5.93	7.97	7.55
Anions	42	MU	8.73	11.98	7.84
		MS	3.70	7.29	-0.50
		SD	10.28	16.28	10.26
		RMS	7.34	12.00	6.89
Cations	22	MU	9.77	9.86	11.89
		MS	-9.45	-7.78	0.65
		SD	10.43	14.12	15.88
		RMS	6.84	7.79	7.64
All	91	MU	9.01	11.32	9.61
		MS	-1.83	0.66	-0.43
		SD	11.57	16.45	12.82
		RMS	11.65	16.37	12.76

1. MU=mean unsigned error; MS=mean signed error, SD=standard deviation, RMS=root mean square error.

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(*Received in USA* 10 *August* 1993; *accepted* 22 *August* 1993)