Table 4: Thermodynamic Database for Combustion and Air-Pollution Use.

DEDICATED TO THE MEMORY OF WILLIAM (BILL) C. GARDINER (1933-2000), PROFESSOR OF CHEMISTRY AT THE UNIVERSITY OF TEXAS, AUSTIN. INITIATOR AND FIRST PUBLISHER OF THIS DATABASE. MAY HE REST IN PEACE.

The Database was last updated on December 2000
Discard Previous Versions

IT IS STRICTLY FORBIDDEN TO INCLUDE THIS DATABASE AS IS OR PARTS OF IT IN ANY COMMERCIAL DATABASE, SOFTWARE, FIRMWARE OR HARDWARE AND ANY OTHER TYPE OF COMMERCIAL USE WITHOUT WRITTEN PERMISSION FROM THE AUTHOR.

ORIGIN OF CALCULATIONS: A-Species calculated by M.B. Colket B-Ihsan Barin database C-CHEMKIN database D-Delaware University J-JANAF tables.
L-NASA Glen (Lewis) Research Center
P- Thermodynamic Research Center (Formerly American Petroleum Institute)
R-Russian Tables (TSIV) T- Technion-Israel Inst. Technology

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AIR calculated from ingredients %N2=78.084 %O2=20.9476 %Ar=0.9365 %CO2=0.0319
This format is not capable of automatic formula calculation for this species!!!
See New NASA Polynomials  REF=McBride & Gordon NASA RP-1271 1992     Sructure
for automatic formula calculation should be:
N   1.56O   0.42AR  0.01C   0.00     Max Lst Sq Error Cp @ 2500 K 0.19%
AIR               L 9/95                  0.G   200.000  6000.000  B  28.96518 1
 3.08792717E+00 1.24597184E-03-4.23718945E-07 6.74774789E-11-3.97076972E-15    2
-9.95262755E+02 5.95960930E+00 3.56839620E+00-6.78729429E-04 1.55371476E-06    3
-3.29937060E-12-4.66395387E-13-1.06234659E+03 3.71582965E+00-1.50965000E+01    4

AL(cr) REF ELEMEN CODA89AL 1.   0.   0.   0.S   200.000   933.610  B  26.98154 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00 1.01040191E+00 1.20769743E-02-2.62083556E-05    3
 2.64282413E-08-9.01916513E-12-6.54454196E+02-5.00471254E+00 0.00000000E+00    4

AL(L) REF ELEMENT CODA89AL 1.   0.   0.   0.L   933.610  6000.000  B  26.98154 1
 3.81862551E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-9.49651808E+01-1.75229704E+01 3.81862551E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-9.49651808E+01-1.75229704E+01 0.00000000E+00    4

Al  HF298=329.7+/-4.2 KJ   REF=JANAF
AL                J 6/83AL 1.   0.   0.   0.G   200.000  6000.000  B  26.98154 1
 2.53385701E+00-4.65859492E-05 2.82798048E-08-8.54362013E-12 1.02207983E-15    2
 3.89045662E+04 5.37984179E+00 3.11112433E+00-3.59382310E-03 8.14749313E-06    3
-8.08808966E-09 2.93132463E-12 3.88283390E+04 2.84045730E+00 3.96535695E+04    4

AlH   SIGMA=1  STATWT=1  Be=6.3907  WE=1682.56  WEXE=29.09  ALPHAE=0.1858
HF298=259.4+/-20 KJ  REF=JANAF
ALH               J 6/63AL 1.H  1.   0.   0.G   300.000  5000.000  B  27.98948 1
 3.33668980E+00 1.28778640E-03-4.98699410E-07 9.22946330E-11-6.34516940E-15    2
 3.00917610E+04 3.09548828E+00 3.65768570E+00-1.97446980E-03 6.86633980E-06    3
-6.20414040E-09 1.86631030E-12 3.01464580E+04 2.08851108E+00 3.11985222E+04    4
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In Table 4, the units of the enthalpy of formation HF298 and HF0 are abreviated to kJ and kcal instead of kJ/mol and kcal/mol.

Table 4 (continued)

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AlO  T0=0    STSTWT=2  Be=0.64136  WE=979.23  WEXE=6.97   ALFAE=0.0058
T0=5282.     STATWT=4  Be=0.5365   WE=728.5   WEXE=4.15   ALFAE=0.0050
T0=20635.2   STATWT=2  Be=0.60408  WE=870.05  WEXE=3.52   ALFAE=0.00447
T0=33055.    STATWT=4  Be=0.60     WE=856.    WEXE=6.     ALFAE=0.004
T0=30200.    STATWT=4  Be=0.565    WE=820.    WEXE=5.0    ALFAE=0.004
T0=31600.    STATWT=8  Be=0.565    WE=820.    WEXE=5.0    ALFAE=0.004
T0=33000.    STATWT=4  Be=0.565    WE=820.    WEXE=5.0    ALFAE=0.004
T0=34700.    STATWT=4  Be=0.565    WE=820.    WEXE=5.0    ALFAE=0.004
T0=34900.    STATWT=2  Be=0.565    WE=820.    WEXE=5.0    ALFAE=0.004
TO=40187.    STATWT=2  Be=0.5652   WE=817.5   WEXE=4.8    ALFAE=0.0046
HF298=66.9+/-8 kJ  REF=JANAF
ALO                J12/79AL 1.O  1.   0.   0.G   300.000  5000.000  A  42.98094 1
 3.31390640E+00 1.04524210E-03 2.74855330E-07-1.79286060E-10 1.99878130E-14    2
 7.09433360E+03 7.20963426E+00 2.81161030E+00 3.95842610E-03-3.36953040E-06    3
 6.73304970E-10 4.00894550E-13 7.06550370E+03 9.20895756E+00 8.05147516E+03    4

AlOH  SIGMA=1  STATWT=1  B0=0.538347 cm-1   NU=1600,1000(2),900    HF298=-179.9
+/- 13 kJ   REF=JANAF
ALOH               J12/67AL 1.O  1.H  1.   0.G   300.000  5000.000  C  43.98888 1
 3.68606740E+00 3.36368220E-03-1.24662440E-06 2.13822050E-10-1.38983190E-14    2
-2.30461050E+04 3.69015562E+00 2.61322110E+00 2.77168940E-03 7.41578300E-06    3
-1.13546020E-08 4.55695590E-12-2.25867970E+04 1.00753303E+01-2.16392416E+04    4

AlO2  ALUMINUM OXIDE  SIGMA=2 B0=0.184455cm-1  T0(STATWT)=0(4),15000(4),20000(2)
NU=930,700,200(2)  HF298=-86.19+/-32 KJ   REF=JANAF
ALO2               J12/79AL 1.O  2.   0.   0.G   300.000  5000.000  C  58.98034 1
 6.60646410E+00 1.08022520E-03-5.22293440E-07 1.13242200E-10-8.52909680E-15    2
-1.25324320E+04-8.01717584E+00 3.25451480E+00 1.42758440E-02-2.11032480E-05    3
 1.50562590E-08-4.21426140E-12-1.18125820E+04 8.30255496E+00-1.03664132E+04    4

AlO2H  ALUMINUM HYDROXIDE OXIDE  SIGMA=1  STATWT=1  IA=0.1301  IB=16.9121
IC=17.0422   NU=3400,1200,1100,700,500,400  HF298=-460+/-63 KJ  REF=JANAF
ALO2H              J12/68AL 1.O  2.H  1.   0.G   300.000  5000.000  B  59.98828 1
 6.42643460E+00 3.22303620E-03-1.21393480E-06 2.10745000E-10-1.38280000E-14    2
-5.76261540E+04-7.45759253E+00 2.48004560E+00 1.61492640E-02-1.60335240E-05    3
 6.44661660E-09-4.09947690E-13-5.66827590E+04 1.23070710E+01-5.53546581E+04    4

Al2O  ALUMINUM OXIDE  SIGMA=2  T0(STATWT)=0(1),23286(1),34331(3),36233(1)
B0=0.104378 cm-1  NU=994,471,160(2)  HF298=-145.2+/-17 KJ   REF=JANAF
AL2O               J12/79AL 2.O  1.   0.   0.G   300.000  5000.000  B  69.96248 1
 6.77206270E+00 8.25500920E-04-3.62910010E-07 6.95313000E-11-4.73452110E-15    2
-1.96431970E+04-8.77233125E+00 4.07326560E+00 1.13076130E-02-1.65651620E-05    3
 1.17842840E-08-3.30055030E-12-1.90542300E+04 4.40834835E+00-1.74618202E+04    4

Al2O2   SIGMA=4  STATWT=1  IA=8.6080  IB=14.5167  IC=23.1247  NU=650,600,496,
400,350,200  HF298=-394.6+/- 32 KJ   REF=JANAF
AL2O2              J12/79AL 2.O  2.   0.   0.G   300.000  5000.000  C  85.96188 1
 9.15909760E+00 9.68539270E-04-4.32585130E-07 8.51788400E-11-6.16153700E-15    2
-5.04280590E+04-1.91564680E+01 2.75964110E+00 2.99975990E-02-5.21904970E-05    3
 4.22826860E-08-1.30753600E-11-4.92260320E+04 1.11007720E+01-4.74536598E+04    4

AL2O3  HF298=-1675.7 kJ  REF=JANAF
AL2O3(S)           J12/79AL 2.O  3.   0.   0.S   300.000  2327.000  C 101.96128 1
 1.18336660E+01 3.77088780E-03-1.78631910E-07-5.60088070E-10 1.40768250E-13    2
-2.05711310E+05-6.35998350E+01-4.91383090E+00 7.93984430E-02-1.32379180E-04    3
 1.04467500E-07-3.15663300E-11-2.02626220E+05 1.54780730E+01-2.01540284E+05    4
AL2O3(L)           J12/79AL 2.O  3.   0.   0.L  2327.000  6000.000  C 101.96128 1
 2.31482410E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-2.11405200E+05-1.38602050E+02 2.31482410E+01 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-2.11405200E+05-1.38602050E+02 0.00000000E+00    4
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Ar  HF298=0.  REF=C.E. Moore "Atomic Energy Levels" NSRDS-NBS 35 (1971) p.211
AR REF ELEMENT    L 6/88AR 1     0     0     0G   200.000  6000.000  A  39.94800 1
 0.25000000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-0.74537500E+03 0.43796749E+01 0.25000000E+01 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-0.74537500E+03 0.43796749E+01 0.00000000E+00    4

Ar+  HF298=1526.8 KJ  REF=C.E. Moore "Atomic Energy Levels" NSRDS-NBS 35 (1971)
Ar+               L10/92AR 1.E -1.    0.    0.G   298.150  6000.000  A  39.94745 1
 2.86999547E+00-1.42547242E-04 9.36688776E-09 2.92580859E-12-3.58247941E-16    2
 1.82702617E+05 3.53229975E+00 2.59316097E+00-1.32892944E-03 5.26503944E-06    3
-5.97956691E-09 2.18967862E-12 1.82878368E+05 5.44980570E+00 1.83628186E+05    4

B  HF298=560+/-12 kJ   REF=JANAF
B                 J 6/83B  1.    0.    0.    0.G   200.000  6000.000  B  10.81100 1
 2.49860273E+00 1.40267322E-06 1.09458278E-09-1.20006414E-12 2.43121994E-16    2
 6.66075914E+04 4.21887979E+00 2.51054099E+00-6.23801328E-05 1.42178099E-07    3
-1.41697796E-10 5.15018749E-14 6.66053894E+04 4.16367209E+00 6.73521350E+04    4

B(S) REF ELEMENT  J 3/79B  1.    0.    0.    0.S   300.000  2350.000  B  10.81000 1
 0.12508638E 01 0.34056258E-02-0.24349586E-05 0.87414463E-09-0.10498288E-12    2
-0.60694437E 03-0.75854277E 01-0.17810789E 01 0.16367573E-01-0.23992225E-04    3
 0.17285547E-07-0.48891231E-11-0.16242365E 02 0.69007440E 01 0.0       E 00    4

B(L) REF ELEMENT  J 3/79B  1.    0.    0.    0.L  2350.000  5000.000  B  10.81000 1
 0.38245440E 01     0.00000000     0.00000000     0.00000000     0.00000000    2
 0.34140016E 04-0.20732328E 02 0.38245440E 01     0.00000000     0.00000000    3
     0.00000000     0.00000000 0.34140016E 04-0.20732328E 02     0.00000000    4

BCl  SIGMA=1  STATWT=1  BE=0.6914   WE=843.65   WEXE=5.167    ALFAE=0.00657
HF298=141.4 kJ  REF=JANAF
BCL               J12/64B  1.CL 1.    0.    0.G   300.000  5000.000  B  46.26370 1
 4.10205710E+00 4.86591930E-04-1.88643260E-07 3.58333420E-11-2.50990690E-15    2
 1.56879580E+04 1.95525119E+00 2.83644630E+00 4.43688120E-03-4.38875220E-06    3
 1.51610780E-09 3.26461950E-14 1.60013610E+04 8.34533209E+00 1.70084902E+04    4

BClF  SIGMA=1   STATWT=2  IA=0.7794  IB=14.8586  IC=15.638  NU=1220,929,360
HF298=-314+/-29 kJ  REF=JANAF
BCLF              J12/64B  1.CL 1.F  1.    0.G   300.000  5000.000  C  65.26210 1
 5.70767570E+00 1.41002030E-03-6.01141370E-07 1.13670440E-10-7.93680630E-15    2
-3.96933270E+04-1.53503845E+00 3.31202340E+00 7.41987630E-03-4.34859490E-06    3
-1.13740570E-09 1.37638900E-12-3.90175480E+04 1.09483562E+01-3.77402953E+04    4

BCl2  SIGMA=2  T0(STATWT)=0(2),11000(2),28003(1),28153(1),29455(1),29542(1)
IA=1.4577  IB=24.2203  IC=25.678  NU=725,700,250  HF298=-79.5+/-12.6 kJ
REF=JANAF
BCL2              J 6/72B  1.CL 2.    0.    0.G   300.000  5000.000  C  81.71640 1
 6.44598380E+00 5.79279480E-04-2.60497050E-07 6.35963580E-11-5.39822150E-15    2
-1.16613040E+04-4.46086977E+00 3.29747860E+00 1.20825760E-02-1.61237550E-05    3
 9.62658560E-09-2.05991990E-12-1.09565370E+04 1.10425333E+01-9.56076191E+03    4

BCl3  SIGMA=6 STATWT=1  IA=IB=27.0443  IC=54.0887  NU=986.3(2),471.0,470.6,243.0
HF298=-403.0+/-2.1 kJ  REF=JANAF
BCL3              J12/64B  1.CL 3.    0.    0.G   300.000  5000.000  B 117.16910 1
 8.59853800E+00 1.55319230E-03-6.70006020E-07 1.27891120E-10-9.00000590E-15    2
-5.13570710E+04-1.51584297E+01 3.73952650E+00 1.81058130E-02-2.13404610E-05    3
 1.08283350E-08-1.73259670E-12-5.02146090E+04 9.05312747E+00-4.84628831E+04    4
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Table 4 (continued)

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BF    SIGMA=1   STATWT=1   BE=1.5286   WE=1410.3   WEXE=11.98   ALFAE=0.0168
HF298=-115.9+/-13.8 kJ   REF=JANAF
BF                J12/64B  1.F  1.   0.   0.G   300.000  5000.000  B  29.80940 1
 3.57718880E+00 1.01929080E-03-4.12515640E-07 7.71964380E-11-5.34987410E-15    2
-1.51272640E+04 3.26612227E+00 3.46136090E+00-9.56854680E-04 6.01357440E-06    3
-6.49780570E-09 2.23553490E-12-1.49698200E+04 4.46077947E+00-1.39390003E+04    4

BF2   SIGMA=2  T0(STATWT)=0(2),16000(2)  IA=0.7385  IB=7.3289  IC=8.0674
NU=1213,1080,500   HF298=-589.9+/-13 kJ  REF=JANAF
BF2               J 6/72B  1.F  2.   0.   0.G   300.000  5000.000  C  48.80781 1
 5.44474570E+00 1.75332110E-03-7.84444740E-07 1.57198590E-10-1.13110710E-14    2
-7.28603670E+04-2.27331909E+00 3.03093030E+00 7.24110210E-03-2.82509190E-06    3
-2.89204130E-09 2.00461020E-12-7.21511020E+04 1.04457036E+01-7.09553140E+04    4

BF3  SIGMA=6  STATWT=1 IA=IB=8.0838  IC=16.1676  NU=1463.3(2),888,696.7,480.7(2)
HF298=-1135.6+/-1.7 kJ   REF=JANAF
BF3               J 6/69B  1.F  3.0  0.   0.G   300.000  5000.000  B  67.80621 1
 7.02419850E+00 3.22215590E-03-1.37051540E-06 2.59196710E-10-1.81223100E-14    2
-1.39180720E+05-1.11843009E+01 2.44682440E+00 1.52763120E-02-1.07846170E-05    3
 6.89075020E-10 1.48931870E-12-1.37901350E+05 1.25678211E+01-1.36586061E+05    4

BH  BORANE    STATWT=1   BE=12.036   WE=2368   WEXE=49   ALFAE=0.413
HF298=442.7+/-8.4 kJ  REF=JANAF
BH                J12/64B  1.H  1.   0.   0.G   300.000  5000.000  C  11.81894 1
 2.89190790E+00 1.58329460E-03-5.82617290E-07 1.02420680E-10-6.76695690E-15    2
 5.23287140E+04 3.79624329E+00 3.68622060E+00-1.30554350E-03 2.67421050E-06    3
-9.10737380E-10-1.55911360E-13 5.21763300E+04-5.52454012E-02 5.32391023E+04    4

BHF2  DIFLUOROBORANE  SIGMA=2  STATWT=1  IA=1.0402  IB=7.9974  IC=9.0376
NU=2640,1411,1174,1158,928,544  HF298=-733.9+/-3.3 kJ   REF=JANAF
BHF2              J12/65B  1.H  1.F  2.   0.G   300.000  5000.000  B  49.81575 1
 5.31845270E+00 4.74444660E-03-1.93378580E-06 3.55083820E-10-2.42936670E-14    2
-9.03750120E+04-3.04314020E+00 2.40536020E+00 9.27558440E-03 1.33864610E-06    3
-8.68078950E-09 4.12110150E-12-8.93884090E+04 1.28880442E+01-8.82623625E+04    4

BH2   SIGMA=2  STATWT=2  B0=5.807235  NU=2650,2430,840  HF298=201+/-63 kJ
REF=JANAF
BH2               J12/64B  1.H  2.   0.   0.G   300.000  5000.000  C  12.82688 1
 3.36252850E+00 3.90128540E-03-1.50975510E-06 2.66728050E-10-1.77130530E-14    2
 2.29190280E+04 1.25928259E+00 2.39582820E+00 7.47762600E-03-7.20195140E-06    3
 4.58263980E-09-1.25106800E-12 2.31626500E+04 6.07647039E+00 2.41541598E+04    4

BH3   SIGMA=6  STATWT=1  IA=IB=0.3378  IC=0.6757  NU=2976(2),2394,1765(2),802
HF298=106.7+/-10 kJ  REF=JANAF
BH3               J12/64B  1.H  3.   0.   0.G   300.000  5000.000  C  13.83482 1
 2.06217260E+00 7.26558950E-03-2.75103370E-06 4.78037090E-10-3.13342850E-14    2
 1.19237530E+04 8.84945083E+00 3.94870330E+00-5.21705430E-04 7.64811640E-06    3
-4.61486940E-09 5.63186160E-13 1.16188090E+04-4.55174579E-02 1.28316429E+04    4

BO   SIGMA=1  T0(STATWT)=0(2),23836(2),23959(2),39957(2),43175(2) BE=1.800
WE=1895.66  WEXE=11.90  ALFAE=0.01676   HF298=0+/-8 kJ   REF=JANAF
BO                J 6/68B  1.O  1.   0.   0.G   300.000  5000.000  B  26.81040 1
 3.15649560E+00 1.38165890E-03-5.50496300E-07 9.91166780E-11-6.41645460E-15    2
-1.03034220E+03 6.03748954E+00 3.72972500E+00-2.08783240E-03 5.73628490E-06    3
-4.38948280E-09 1.09166320E-12-1.06188590E+03 3.62554104E+00-1.45402311E-01    4
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BOCl   (OBCl)  SIGMA=1   STATWT=1    B0=0.165056   NU=1850,690,400(2)
HF298=-316.3+/-29 kJ   REF=JANAF
BOCL              J12/65B  1.O  1.CL 1.   0.G   300.000  5000.000  C  62.26310 1
 5.71355660E+00 1.86646890E-03-7.74878980E-07 1.43985720E-10-9.93177450E-15    2
-3.99773530E+04-4.88040355E+00 3.27053210E+00 1.02277500E-02-1.20701630E-05    3
 7.20255620E-09-1.69147380E-12-3.93782080E+04 7.34930225E+00-3.80417115E+04    4

BOF   (OBF)   SIGMA=1   STATWT=1    B0=0.309392   NU=1900,1050,500(2)
HF298=-602+/-13 kJ   REF=JANAF
BOF               J12/65B  1.O  1.F  1.   0.G   200.000  6000.000  C  45.80880 1
 5.39296603E+00 2.07444500E-03-7.93600586E-07 1.33476571E-10-8.21779331E-15    2
-7.43113852E+04-4.76500545E+00 2.23703738E+00 1.33495496E-02-1.81530614E-05    3
 1.36093676E-08-4.24382397E-12-7.35283735E+04 1.10069410E+01-7.24035451E+04    4

BOF2   OBF2   SIGMA=2   T0(STATWT)=0(2),17171(2),22390(2)  IA=7.4051  IB=8.4655
IC=15.8706  NU=1377,1100,856,850,500,491  HF298=-837+/-15 kJ  REF=JANAF
BOF2              J12/66B  1.O  1.F  2.   0.G   300.000  5000.000  C  64.80721 1
 7.30772330E+00 2.99036200E-03-1.30596170E-06 2.53082420E-10-1.76873330E-14    2
-1.03345760E+05-1.11924159E+01 1.74459770E+00 1.86932770E-02-1.52461640E-05    3
 2.65594700E-09 1.37986060E-12-1.01867580E+05 1.73531391E+01-1.00645369E+05    4

BO2   SIGMA=2   T0(STATWT)=0(2),149(2),18291.6(4),24508(2)   B0=0.33036
NU=1321.7,1056,454   HF298=-285+/-8 kJ  REF=JANAF
BO2               J 6/68B  1.O  2.   0.   0.G   300.000  5000.000  B  42.80980 1
 5.81984340E+00 1.86265740E-03-8.13027970E-07 1.57358210E-10-1.09442380E-14    2
-3.62551170E+04-6.56090797E+00 3.12120480E+00 8.46808830E-03-4.59722780E-06    3
-1.64200210E-09 1.66582330E-12-3.54833070E+04 7.54789163E+00-3.42194143E+04    4

B2    SIGMA=2  T0=0(3)  BE=1.236121  WE=1061.61  WEXE=9.536  ALFAE=0.01442411
   T0=1271(5)     BE=1.305    WE=1215.81   WEXE=9.995    ALFAE=0.0113
   T0=14829(3)    BE=1.275    WE=1114.83   WEXE=16.318   ALFAE=0.0175
   T0=30573.4(3)  BE1.183086  WE=946.59    WEXE=2.652    ALFAE0.1133323
HF298=829.7+/-33.5 kJ   REF=JANAF
B2                J 3/79B  2.   0.   0.   0.G   200.000  6000.000  B  21.62200 1
 5.23869155E+00-5.23607507E-04 1.69704978E-07-2.06549042E-11 9.41435925E-16    2
 9.79873828E+04-6.00742217E+00 3.79099744E+00-5.87536359E-03 3.00514162E-05    3
-3.91439173E-08 1.60419428E-11 9.87229998E+04 3.43463203E+00 9.97878648E+04    4

B2O   SIGMA=2  STATWT=1  IA=0.1624  IB=5.3179  IC=5.4803  NU=1800,1250,600
HF298=96+/-105 kJ   REF=JANAF
B2O               J 6/66B  2.O  1.   0.   0.G   300.000  5000.000  C  37.62140 1
 4.73005380E+00 2.39414860E-03-1.00083240E-06 1.86975100E-10-1.29536720E-14    2
 9.88533540E+03-6.35851289E-01 3.52947300E+00 3.19938260E-03 3.03292570E-06    3
-5.74912550E-09 2.28473490E-12 1.03632010E+04 6.23963143E+00 1.15742290E+04    4

B2O2  (BO)2   SIGMA=2   STATWT=1   B0=0.112313    NU=2065,1910,570,565,285
HF298=-456.1+/-8.4 kJ   REF=JANAF
B2O2              J12/64B  2.O  2.   0.   0.G   300.000  5000.000  B  53.62080 1
 6.99385740E+00 3.59403930E-03-1.47536110E-06 2.72251240E-10-1.86959960E-14    2
-5.72961780E+04-1.21677771E+01 3.68070780E+00 1.53611320E-02-1.86060970E-05    3
 1.21714510E-08-3.24110180E-12-5.64866470E+04 4.35612734E+00-5.48483506E+04    4

B2O3(L)   HF298=-1253.4 kJ   REF=JANAF
B2O3(L)           J 6/71B  2.O  3.0  0.0  0.L   300.000  3000.000  B  69.61820 1
 0.15600114E 02     0.00000000     0.00000000     0.00000000     0.00000000    2
-0.15684455E 06-0.83126444E 02 0.31433274E 02-0.21578039E 00 0.64057986E-03    3
-0.70572420E-06 0.26509150E-09-0.15490139E 06-0.12803880E 03-0.15074514E+06    4
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B2O3   SIGMA=2  STATWT=1  IA=2.9763  IB=31.0977  IC=34.0740  NU=2073(2),1240,
730,521,480,460,457,172  HF298=-836.0+/-4.2 kJ   REF=JANAF
B2O3              J 6/71B  2.O  3.   0.   0.G   300.000  5000.000  B  69.62020 1
 8.39941060E+00 4.74363380E-03-1.95523040E-06 3.61877490E-10-2.49072320E-14    2
-1.03571580E+05-1.58100009E+01 3.66088370E+00 2.02620760E-02-2.19473380E-05    3
 1.22530040E-08-2.70384020E-12-1.02365240E+05 8.10622068E+00-1.00544127E+05    4

B3O3Cl3  (BOCl)3 TRICHLOROBOROXIN  SIGMA=6  STATWT=1  IA=IB=97.7637  IC=195.5274
NU=1300(2),1037,980(2),920(2),807,690,600,400(3),390(2),333,150(2),140,120(2)
HF298=-1632+/-8 kJ   REF=JANAF
B3O3CL3           J 3/65B  3.O  3.CL 3.   0.G   300.000  5000.000  C 186.78930 1
 1.92825640E+01 6.31725810E-03-2.72429260E-06 5.20479100E-10-3.66777900E-14    2
-2.03208830E+05-6.78851521E+01 4.04449830E+00 5.42605970E-02-5.57507610E-05    3
 2.22231280E-08-1.41812950E-12-1.99416320E+05 9.05672255E+00-1.96248045E+05    4

B3O3F3  (BOF)3   TRIFLUOROBOROXIN  SIGMA=6  STATWT=1  IA=IB=45.8345  IC=91.6691
NU=1450(2),1381(2),1280,1233,966(2),790,714,630(2),570,440,420(2),220(2),185(2),
170   HF298=-2365.2+/-4.2 kJ   REF=JANAF
B3O3F3            J 3/65B  3.O  3.F  3.   0.G   300.000  5000.000  C 137.42641 1
 1.68586160E+01 8.86857540E-03-3.78810580E-06 7.18704010E-10-5.03769170E-14    2
-2.90931040E+05-5.98587523E+01 3.07988610E+00 4.56365920E-02-3.30988260E-05    3
 2.55388390E-09 4.43587610E-12-2.87122130E+05 1.14753917E+01-2.84460743E+05    4

B3O3H3   SIGMA=6  STATWT=1   IA=IB=13.971  IC=27.9421   NU=2620(2),2530,1560,
1404(2),1335(2),1115(2),940(2),920,903,735,550,400(2),300,230(2)
HF298=-1218+/-42 kJ   REF=JANAF
B3O3H3            J 3/65B  3.O  3.H  3.   0.G   200.000  6000.000  C  83.45502 1
 1.21201212E+01 1.22811209E-02-4.60922487E-06 7.65824542E-10-4.67623793E-14    2
-1.51648629E+05-3.98918007E+01 2.76989078E+00 2.53425900E-02 1.22486701E-05    3
-3.73057611E-08 1.74556897E-11-1.48431026E+05 1.15218019E+01-1.46436050E+05    4

H3B3O6   (HBO2)3   SIGMA=3   STATWT=1   IA=43.6915  IB=45.5585  IC=89.2499
NU=3500(3),1300(2),1100,1150,1000(4),950,900(2),750(2),600(3),550,500(2),450(2),
350(3),250,200(2)   HF298=-2272+/-13 kJ  REF=JANAF
H3B3O6            J12/64H  3.B  3.O  6.   0.G   300.000  5000.000  C 131.45322 1
 2.01535790E+01 1.30162860E-02-5.06696190E-06 9.03082530E-10-6.05324100E-14    2
-2.81040920E+05-7.96763324E+01-2.27051160E+00 8.70248940E-02-9.15877140E-05    3
 3.94453920E-08-3.66660350E-12-2.75695230E+05 3.25296526E+01-2.73237150E+05    4

BR   HF298=111.86+/-0.06  REF=JANAF
BR                J 6/82BR  1    0    0    0G   200.000  6000.000  A  79.90400 1
 0.20866945E+01 0.71459733E-03-0.27080691E-06 0.41519029E-10-0.23016335E-14    2
 0.12857696E+05 0.90837335E+01 0.24820782E+01 0.18570465E-03-0.64313029E-06    3
 0.84642045E-09-0.30137068E-12 0.12709455E+05 0.68740409E+01 0.13453589E+05    4

BrO  T0=0 STATWT=2  Be=0.4299  De=0.594E-6 ALPHAE=0.003639  WE=727.05 WEXE=4.932
T0=968  STATWT=2  Be=0.4299  De=0.594E-6 ALPHAE=0.003639  WE=727.05 WEXE=4.932
T0=27871  STATWT=2  Be=0.314  De=0.474E-6 ALPHAE=0.0034  WE=511.3 WEXE=4.83
T0=29321   STATWT=2  Be=0.314  De=0.474E-6 ALPHAE=0.0034  WE=511.3 WEXE=4.8
HF298=125.8+/-2.4 kJ  REF=M.W.Chase JPCRD 25 (1996), 1069      Max Lst Sq Error
Cp @ 400 K 0.45 %.
BRO               T02/97BR 1.O  1.   0.   0.G   200.000  6000.000  A  95.90340 1
 5.07219100E+00-4.35812081E-04 1.75747890E-07-2.82506168E-11 1.92290510E-15    2
 1.35030084E+04-1.08904614E+00 2.55466821E+00 6.43468019E-03-2.95159758E-06    3
-4.90190824E-09 3.64995652E-12 1.41165412E+04 1.17071098E+01 1.51301760E+04    4
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BrO2  Br-O-O  SIGMA=1  STATWT=2  IA=1.2011  IB=21.5417  IC=22.7428  NU=1487,250,
160  HF298=108.0+/-40. kJ REF=M.W.Chase JPCRD 25 (1996), 1069   Max Lst Sq Error
Cp @ 1300 K 0.21 %.
BrO2  Br-O-O      T02/97BR 1.O  2.   0.   0.G   200.000  6000.000  B 111.90280 1
 6.00363127E+00 9.92540840E-04-3.82278926E-07 6.45667378E-11-3.98629626E-15    2
 1.10621232E+04 3.62860950E-02 5.09638120E+00 3.60676575E-03-4.28370757E-06    3
 3.72707925E-09-1.47204500E-12 1.13407206E+04 4.78601414E+00 1.29893403E+04    4

BrO2  O-Br-O   SIGMA=2  STATWT=2  IA=3.0275  IB=10.2087  IC=13.2361  NU=800,300,
852  HF298=152.0+/-25. kJ REF=M.W.Chase JPCRD 25 (1996), 1069   Max Lst Sq Error
Cp @ 400 K 0.18 %.
BrO2  O-Br-O      T02/97BR 1.O  2.   0.   0.G   200.000  6000.000  B 111.90280 1
 6.24396373E+00 7.82813558E-04-3.08534350E-07 5.28853891E-11-3.29803612E-15    2
 1.62066239E+04-3.61634966E+00 3.07292385E+00 1.13245422E-02-1.28765411E-05    3
 5.90293758E-09-6.56032315E-13 1.69641688E+04 1.22438586E+01 1.82812938E+04    4

BrO3   SIGMA=3  STATWT=2  IA=IB=12.2156  IC=14.7352  NU=442,800,320.(2),828.(2)
HF298=221.0+/-50. kJ REF=M.W.Chase JPCRD 25 (1996), 1069    Max Lst Sq Error
Cp @ 1200 K 0.21 %.
BrO3              T02/97BR 1.O  3.   0.   0.G   200.000  6000.000  C 127.90220 1
 8.69236256E+00 1.35841486E-03-5.36468670E-07 9.20768329E-11-5.74736730E-15    2
 2.36159592E+04-1.64447310E+01 1.49818242E+00 3.04080397E-02-4.72006811E-05    3
 3.49686979E-08-1.00736007E-11 2.51344798E+04 1.84248093E+01 2.65800390E+04    4

BR2 REF ELEMENT   J 6/82BR  2    0    0    0G   200.000  6000.000  A 159.80800 1
 0.49231991E+01-0.85447779E-03 0.59229129E-06-0.12767491E-09 0.84730953E-14    2
-0.15175171E+04 0.15060691E+01 0.33427017E+01 0.63460452E-02-0.13621151E-04    3
 0.13151888E-07-0.46776728E-11-0.11821285E+04 0.90749722E+01 0.00000000E+00    4

Br2O  BrBr-O  SIGMA=1  STATWT=3  IA=4.7079  IB=51.8084  IC=56.5163   NU=804,150,
236  HF298=168.0+/-20. kJ REF=M.W.Chase JPCRD 25 (1996), 1069   Max Lst Sq Error
Cp @ 1200 K 0.13 %
Br2O   BrBr-O     T02/97BR 2.O  1.   0.   0.G   200.000  6000.000  B 175.80740 1
 6.61241475E+00 4.02586598E-04-1.58975806E-07 2.72841078E-11-1.70297367E-15    2
 1.81249753E+04-3.99723764E-01 4.44451500E+00 9.35658684E-03-1.49756620E-05    3
 1.14829127E-08-3.42674585E-12 1.85758718E+04 1.00676579E+01 2.02056405E+04    4

Br2O Br-O-Br  SIGMA=2  STATWT=1  IA=2.5488  IB=62.1189  IC=64.6677  NU=526.1,180,
623.4  HF298=107.6+/-3.5 kJ REF=M.W.Chase JPCRD 25 (1996), 1069 Max Lst Sq Error
Cp @ 1200 K 0.094%
Br2O   Br-O-Br    T02/97BR 2.O  1.   0.   0.G   200.000  6000.000  B 175.80740 1
 6.60036780E+00 4.19198661E-04-1.66518672E-07 2.86896506E-11-1.79550923E-15    2
 1.08520131E+04-2.99978832E+00 3.04140956E+00 1.75424857E-02-3.28632899E-05    3
 2.86038685E-08-9.44453191E-12 1.14930042E+04 1.36453473E+01 1.29412317E+04    4

C(GR) REF ELEMENT P 4/83C  1    0    0    0C   200.000  5000.000  B  12.01100 1
 0.14556924E+01 0.17170638E-02-0.69758410E-06 0.13528316E-09-0.96764905E-14    2
-0.69512804E+03-0.85256842E+01-0.31087207E+00 0.44035369E-02 0.19039412E-05    3
-0.63854697E-08 0.29896425E-11-0.10865079E+03 0.11138295E+01 0.00000000E+00    4

C  HF298=716.68 KJ REF=C.E. Moore "Selected Tables of Atomic Spectra"  NSRDS-NBS
Sec 3 (1970) p A6 I.
C                 L 7/88C  1    0    0    0G   200.000  6000.000  A  12.01100 1
 0.26055830E+01-0.19593434E-03 0.10673722E-06-0.16423940E-10 0.81870580E-15    2
 0.85411742E+05 0.41923868E+01 0.25542395E+01-0.32153772E-03 0.73379223E-06    3
-0.73223487E-09 0.26652144E-12 0.85442681E+05 0.45313085E+01 0.86195097E+05    4
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C+  HF298=1809.4 KJ    REF=C.E. Moore "Selected Tables of Atomic Spectra"
NSRDS-NBS Sec 3 (1970) p A6 I.
C+                L 7/88C  1E  -1    0     0G   298.150  6000.000  A  12.01045 1
 0.25085352E+01-0.10859950E-04 0.53707035E-08-0.11827082E-11 0.97126910E-16    2
 0.21687829E+06 0.43173958E+01 0.26152397E+01-0.55378388E-03 0.10634864E-05    3
-0.92375636E-09 0.30077457E-12 0.21686085E+06 0.38265288E+01 0.21762369E+06    4

CBrClF2  HALON 1211 FC-12B1  STATWT=1  SIGMA=1  IAIBIC=6.3E-113  NU=1102,872,
648,440,337,220,1150,425,290   HF298=-435+/-15 KJ   REF=TSIV 1979   Max Lst sq
Error Cp @ 1200 K 0.28%
CBRClF2           RUS 79C   1F   2CL  1BR  1G   200.000  6000.000  B 165.36451 1
 0.10796522E+02 0.22669030E-02-0.89010449E-06 0.15221044E-09-0.94769732E-14    2
-0.56074618E+05-0.24866158E+02 0.21055312E+01 0.35677153E-01-0.52831950E-04    3
 0.38479959E-07-0.11114638E-10-0.54135708E+05 0.17730129E+02-0.52318176E+05    4

CBrF3 Freon 1301  STATWT=1 SIGMA=3  IAIBIC=2.36E-113  NU=1084,761.4,351,1209(2),
548(2),302.7(2)  HF298=-648.8 KJ  REF=TSIV   Max Lst Sq Error Cp @ 1300 K 0.33%.
CBRF3 Freon 1301  RUS 79C   1F   3BR  1    0G   200.000  6000.000  B 148.91021 1
 0.10243611E+02 0.28215023E-02-0.11045573E-05 0.18851925E-09-0.11722236E-13    2
-0.81715359E+05-0.24553036E+02 0.19219428E+01 0.31086171E-01-0.38589387E-04    3
 0.23185006E-07-0.54663797E-11-0.79689272E+05 0.17106925E+02-0.78032259E+05    4

CBr2F2  Halon 1202   FC-12B2     SIGMA=2  IAIBIC=1693.E-115    NU=1090,623,340,
165,282,1153,367,831,330  HF298=-380+/-15 KJ   REF=TSIV 1979  Max Lst Sq Error
Cp @ 1200 K .26%
CBR2F2            RUS 79C   1F   2BR  2    0G   200.000  6000.000  B 209.81581 1
 0.10938166E+02 0.21205324E-02-0.83247738E-06 0.14233906E-09-0.88616291E-14    2
-0.49463655E+05-0.24751195E+02 0.28677215E+01 0.33279106E-01-0.49637736E-04    3
 0.36511709E-07-0.10661103E-10-0.47665972E+05 0.14781450E+02-0.45703234E+05    4

CCl  CHLOROMETHYLIDENE  T0(STATWT)=0(2),134.92(2),20000(4),36004(4)  Be=0.0066
WE=876.4  WEXE 6.15  ALPHAE=0.0066  HF298=502.1+/-20 KJ  REF=JANAF
CCL               J12/69C  1CL   10   00   0G   300.000  5000.000  B  47.4637  1
 0.40984727E 01 0.50077845E-03-0.20012833E-06 0.38680992E-10-0.25441113E-14    2
 0.59076599E 05 0.33501736E 01 0.31953557E 01 0.28076318E-02-0.16043845E-05    3
-0.57744065E-09 0.61409732E-12 0.59325077E 05 0.80351732E 01 0.60387056E+05    4

CClF  RADICAL  SIGMA=1  STATWT=1 IAIBIC=210E 117  NU=1145,445,742  T0=13000
SIGMA=1  STATWT=3  REF=TSIV  HF298=25.876 KJ Max Lst Sq Error Cp @ 6000 K 0.48%.
CCLF              T 7/95C   1CL  1F   1    0G   200.000  6000.000  B  66.46210 1
 0.54307520E+01 0.50150344E-03-0.22180016E-06 0.64210243E-10-0.56789849E-14    2
 0.13122940E+04-0.42533125E+00 0.35204286E+01 0.56648447E-02-0.48259157E-05    3
 0.11531380E-08 0.25649091E-12 0.18509860E+04 0.94809134E+01 0.31121497E+04    4

COClF  CARBONIC CHLORIDE FLUORIDE   SIGMA=1   STATWT=1   IA=7.480   IB=16.008
IC=23.31  NU=1868,1095,776,667,501,415  HF298=-426.8+/-33 KJ  REF=JANAF
COCLF             J 6/61C  1.O  1.CL 1.F  1.G   300.000  5000.000  B  82.46150 1
 7.08810810E+00 3.18164790E-03-1.37633160E-06 2.65440050E-10-1.89289690E-14    2
-5.38837810E+04-8.68499361E+00 1.70666610E+00 2.27225650E-02-3.01156390E-05    3
 2.04835660E-08-5.65722280E-12-5.26199020E+04 1.79876256E+01-5.13293738E+04    4

CClF2 RADICAL  STATWT=2  IAIBIC=3700.E-117    NU=1148,1208,761,599,400,350
REF=TSIV 1979 HF298=-275 KJ  Max Lst Sq Error Cp @ 1300 K 0.3%
CCLF2             RUS 79C   1F   2CL  1    0G   200.000  6000.000  B  85.46051 1
 0.80282121E+01 0.20189090E-02-0.79048024E-06 0.13492662E-09-0.83903043E-14    2
-0.35924267E+05-0.12621010E+02 0.22332425E+01 0.20740417E-01-0.23401456E-04    3
 0.11899516E-07-0.20885418E-11-0.34478176E+05 0.16591709E+02-0.33074709E+05    4
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CClF3  CHLOROTRIFLUOROMETHANE  SIGMA=3  IA=14.6768  IB=IC=25.3677  NU=1217(2),
1106,782,560(2),474,350(2)  HF298=-707.93+/-3.3 KJ  REF=JANAF
CCLF3   FC-13      J 6/69C   1F   3CL  1    0G   200.000  6000.000  B 104.45891 1
 0.10091094E+02 0.29780933E-02-0.11659765E-05 0.19901491E-09-0.12375419E-13    2
-0.88819890E+05-0.25287649E+02 0.11848463E+01 0.33290012E-01-0.41344756E-04    3
 0.24726788E-07-0.57670412E-11-0.86657686E+05 0.19274742E+02-0.85143923E+05    4

ClCN  CYANOGEN CHLORIDE  SIGMA=1   B0=0.19817  D0=5.503E-8  NU=2215.5,714.52,
378.3  x11=-4  x22=-0.65  x33=-7  x12=-6.8  x23=-7.236  x13=-2.8  g22=0.95
ALPHA1=8.25E-4  ALPHA2=-5.46E-4  ALPHA3=1.06E-3  HF298=137.95 kJ  REF=JANAF
CLCN               J 6/66CL 1.C  1.N  1.   0.G   300.000  5000.000  A  61.47044 1
 5.49200210E+00 2.09872480E-03-7.74159140E-07 1.38238820E-10-9.23348640E-15    2
 1.47491610E+04-3.73046245E+00 3.33908540E+00 1.03974680E-02-1.37046500E-05    3
 9.50619620E-09-2.59252600E-12 1.52375390E+04 6.83103255E+00 1.65917045E+04    4

COCl  CARBONYL CHLORIDE  SIGMA=1  STATWT=2  IA=0.7159  IB=13.0005  IC=13.7165
NU=1880,570,281  HF298=-62.8+/-42 KJ REF=JANAF
COCL               J12/65C  1.O  1.CL 1.   0.G   300.000  5000.000  B  63.46310 1
 5.42912360E+00 1.61215350E-03-6.60062800E-07 1.21271140E-10-8.28586010E-15    2
-9.33050070E+03 3.82874056E-01 4.28637920E+00 5.08689800E-03-5.07294110E-06    3
 2.96479830E-09-7.70934530E-13-9.01252120E+03 6.25118670E+00-7.54776465E+03    4

CCl2   DICHLOROMETHYLENE  SIGMA=2  T0(STATWT)=0(1),4000(3),17500(1)  IA=2.1829
IB=21.4029  IC=23.5858  NU=748,721,350   HF298=238.5+/-21 KJ  REF=JANAF
CCL2               J12/68C  1CL  20   00    0G   300.000  5000.000  B  82.9164  1
 0.37184999E 01 0.53449745E-02-0.23431284E-05 0.41806177E-09-0.26765295E-13    2
 0.27554793E 05 0.96459795E 01 0.28588505E 01 0.13957938E-01-0.20038898E-04    3
 0.13500726E-07-0.31669715E-11 0.27363926E 05 0.12243313E 02 0.28684152E+05    4

CCl2F RADICAL   STATWT=2  IAIBIC=12000.E-117  NU=747,919,1143,300,400,350
REF= TSIV 1979  HF298=-105 KJ Max Lst Sq Error Cp @ 1300 0.24%
CCL2F              RUS 79C   1F   1CL  2    0G   200.000  6000.000  C 101.91480 1
 0.84345756E+01 0.16113470E-02-0.63289029E-06 0.10824563E-09-0.67404226E-14    2
-0.15533481E+05-0.13322229E+02 0.24855872E+01 0.23260491E-01-0.31755314E-04    3
 0.20955723E-07-0.54319496E-11-0.14161751E+05 0.16091138E+02-0.12628525E+05    4

CCl2F2 DICLORODIFLUOROMETHANE FREON-12 SIGMA=3 IA=21.216  IB= 31.929  IC=38.148
NU=1099,261.5,667,457,5,322,918,436,1162,446  REF=Tsuboi,Ishii,& Itoh 22 Int.
Symp. Shock-Waves 1999 London  HF298=-117.9 kcal. REF=TRC-75 Max Lst Sq Error
Cp @ 1200 K 0.29%.
CCL2F2 FREON-12   T 9/99C  1.F  2.CL 2.   0.G   200.000  6000.000  B 120.91321 1
 1.06559336E+01 2.41165412E-03-9.46969699E-07 1.61937898E-10-1.00827794E-14    2
-6.30799044E+04-2.63102587E+01 1.41679928E+00 3.77483497E-02-5.54644732E-05    3
 4.00119306E-08-1.14401332E-11-6.10131047E+04 1.90076580E+01-5.93292449E+04    4

CCL2O PHOSGEN   HF298=-52.46 Kcal  REF=Gurvich 91
COCL2              RUS 91C  1.O  1.CL 2.   0.G   200.000  6000.000  B  98.91580 1
 7.86018378E+00 2.13271500E-03-8.22077158E-07 1.38951133E-10-8.58406653E-15    2
-2.91056423E+04-1.19011907E+01 1.70787910E+00 2.89369464E-02-4.93289116E-05    3
 4.16910139E-08-1.37057391E-11-2.78350932E+04 1.76202114E+01-2.63996315E+04    4

CCl3  TRICHLOROMETHYL RADICAL  SIGMA=6  STATWT=2  IA=IB=26.7361  IC=53.4723
NU=898(2),460,450,240  HF298=79.5=/-8 KJ  REF=JANAF
CCL3               J 6/70C  1.CL 3.   0.   0.G   300.000  5000.000  B 118.36910 1
 8.78154730E+00 1.35161300E-03-5.82494530E-07 1.10986970E-10-7.79372640E-15    2
 6.63441510E+03-1.53161324E+01 3.71533570E+00 1.94437960E-02-2.46278410E-05    3
 1.37864640E-08-2.66389340E-12 7.78200200E+03 9.71604259E+00 9.56234693E+03    4
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CCl3F TRICHLOROFLUOROMETHANE  FC-11  TRC DATA EXTRAPOLATED TO 5000 K USING
WILHOIT'S POLYNOMIALS. HF298=-68.1 Kcal.
CCL3F   FC-11      P12/75C  1.CL 3.F  1.   0.G   298.150  5000.000  C 137.36840 1
 0.11246530E 02 0.17837698E-02-0.69260443E-06 0.11740724E-09-0.72640292E-14    2
-0.38108309E 05-0.28275976E 02 0.48287687E 01 0.18981740E-01-0.10360662E-04    3
-0.78472127E-08 0.68452752E-11-0.36446184E 05 0.46341471E 01-0.34269462E 05    4

CCl4  CARBONTETRACHLORIDE  SIGMA=12 IAIBIC=118000.E-117  NU=797(3),460,315(3),
220(2)  HF298=-95.6 kJ    REF=Gurvich 1991.
CCL4               L12/81C  1.CL 4.   0.   0.G   298.150  5000.000  B 153.82300 1
 1.17390960E+01 1.28375530E-03-4.96502590E-07 8.35250200E-11-5.11072240E-15    2
-1.54190900E+04-3.07909700E+01 5.79662990E+00 1.79774390E-02-1.09565460E-05    3
-6.66818070E-09 6.45548980E-12-1.39409650E+04-5.70110920E-01-1.15237980E+04    4

CD  METHYLIDENE-D RAD  SIGMA=1.  T0=0(2)=18(2)   WE=2101  WEXE=34.7  BE=7.808
ALFAE=.212   T0=23182(4) WE=2144.5  WEXE=48.7  BE=8.032  ALFAE=.26   T0=25993(2)
WE=1808  WEXE=201.5  BE=7.171  ALFAE=.528   T0=31828(2)  WE=2073.4  WEXE=5.7
BE=7.880  ALFAE=0.282  RHO=1.0E-5  REF=BURCAT (1980) MAX LST SQ ERROR CP @ 5000K
0.52 % HF298=593.3 KJ
CD                 T 2/80C  1D   1    0     0G   300.000  5000.000  B  14.0251  1
 0.26841459E+01 0.18855776E-02-0.48628311E-06 0.38441708E-10 0.64605384E-15    2
 0.70531750E+05 0.70322804E+01 0.35427971E+01-0.47720969E-03 0.10656331E-05    3
 0.73458772E-09-0.74328873E-12 0.70311938E+05 0.26416878E+01 0.71355979E+05    4

CDH3  METHANE-D  STATWT=1.  SIGMA=3.  A0=C0=5.25  B0=3.878  NU=2945,2200,1300,
3017(2),1471(2),1155(2)  REF=BURCAT (1980) MAX LST SQ ERROR CP @ 1300K 0.94% .
HF298=-78.45 KJ
CDH3               T05/79C  1D   1H   3     0G   300.000  5000.000  B  17.0489  1
 0.29389458E+01 0.84684640E-02-0.28219238E-05 0.41319725E-09-0.21738508E-13    2
-0.10964586E+05 0.42781033E+01 0.26380539E+01 0.41823313E-02 0.72133871E-05    3
-0.58564389E-08 0.79961938E-12-0.10462590E+05 0.75096125E+01-0.94354328E+04    4

CDO  FORMYL-D RAD  STATWT=2.  SIGMA=1  A0=14.69  B0=1.281375  C0=1.171465
NU=1937,847,1800  X12=-13.1,X22=-2.44,X23=-3.87,Y222=.0096  ALFA1=.006   ALFA2=
.002    ALFA3=.02  T0=9162  B0=1.1011   REF=BROWN & RAMSAY  MAX LST SQ ERROR CP
@ 1300 K 0.49%  HF0=9.63 KCAL REF=CHO, TSIV.
CDO                T 5/92D   1C   1O   1     0G   200.000  6000.000  B  30.02450 1
 0.41069843E+01 0.28191796E-02-0.10558996E-05 0.17632198E-09-0.10799344E-13    2
 0.33780018E+04 0.30182660E+01 0.39575311E+01-0.10167964E-02 0.10248940E-04    3
-0.10651298E-07 0.34974109E-11 0.36824264E+04 0.49663632E+01 0.48883217E+04    4

CD2  METHYLENE-D2 RAD  SIGMA=2.  T0=0(3)=30300(1)  IA=.0744  IB=.60878  IC=.6831
NU=2115,767,2345   T0=2600(1)  IA=.24223  IB=.50049  IC=.74272  NU=2209,926,2273
T0=9700(1)  IA=.06458  IB=.6511  IC=.71567  NU=2093,545,2338  REF=Burcat 1980
HF298=382.59 KJ   MAX LST SQ ERROR CP @ 1300K 0.72% .
CD2                T05/80C  1D   2    0     0G   300.000  5000.000  B  16.0392  1
 0.36602430E+01 0.33572798E-02-0.12381643E-05 0.20197106E-09-0.12083819E-13    2
 0.44684898E+05 0.25685925E+01 0.38409843E+01 0.12651016E-02 0.18910869E-05    3
-0.77415541E-09-0.25377709E-12 0.44799531E+05 0.22334236E+01 0.46014570E+05    4

CD2O  METHANAL-D2 (FORMALDEHIDE-D2)  STATWT=1.   SIGMA=2  IA=.59244  IB=2.5995
IC=3.2048  NU=2056,1700,1106,2160,990,938  REF=CHAO,WILHOIT & HALL MAX LST SQ
ERROR CP @ 1300 K 0.8 % .HF298=-27.46 KCAL.
CD2O               T 8/81C  1D   2O   1     0G   300.000  5000.000  B  32.0386  1
 0.46622076E+01 0.50203055E-02-0.18413848E-05 0.29739944E-09-0.17558905E-13    2
-0.15805738E+05-0.17688099E+01 0.25921259E+01 0.59901401E-02 0.39293818E-05    3
-0.62653172E-08 0.18746567E-11-0.14881922E+05 0.10390113E+02-0.13818716E+05    4
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CD3 METHYL-D3-RAD  STATWT=1.  SIGMA=6.   IA=IB=.596  IC=1.191  T0=0(2),46200(2)
NU=2153,463,2381(2),1026(2)  REF=BURCAT(1980)  MAX LST SQ ERROR CP @ 1300K 0.71%
HF298=138.69 KJ
CD3                 T11/79C  1D   3    0     0G   300.000  5000.000  B  18.0533  1
 0.44567032E+01 0.49626939E-02-0.17476059E-05 0.27139846E-09-0.15351469E-13    2
 0.14782500E+05-0.23810688E+01 0.34687710E+01 0.49496330E-02 0.19827057E-05    3
-0.36768906E-08 0.12036257E-11 0.15276805E+05 0.36025786E+01 0.16680117E+05    4

CD3NO2 Nitro-Methane D3 STATWT=1 SYMNO=3 IA = 6.96802 IB = 10.1365 IC = 15.945
IRED=0.88227 V(2)=0.16 kcal/mole ROSYM=2  NU = 435,542,631,885,942,1038,1046,
1075,1404,1548,898,2147,2283,2317   HF(298)= -14.768 kcal/mole  REF = A. Burcat
TAE Report 824a May 1999  Max Lst Sq Error Cp @ 1300 K 0.61%
CD3NO2              T01/00C  1.D  3.N  1.O  2.G   200.000  6000.000  B  64.05885 1
 8.82522748E+00 9.35166732E-03-3.53835387E-06 5.90989862E-10-3.62227246E-14    2
-1.13067808E+04-2.08804860E+01 2.37203218E+00 1.42408389E-02 2.16286890E-05    3
-4.09339693E-08 1.78857173E-11-8.89033378E+03 1.55850830E+01-7.43151250E+03    4

CD4   METHANE-D4  STATWT=1.  SIGMA=12.  A0=B0=C0=2.634  NU=2109,1092(2),2259(3),
996(3)  REF=BURCAT (1980) MAX LST SQ ERROR CP @ 1300K 0.94% . HF298=-89.01 KJ
CD4    RRHO         T05/79C  1D   4    0     0G   300.000  5000.000  B  20.0674  1
 0.47153826E+01 0.75838268E-02-0.27129208E-05 0.42667048E-09-0.24420637E-13    2
-0.12937410E+05-0.61998917E+01 0.19176292E+01 0.91806799E-02 0.47843714E-05    3
-0.88772119E-08 0.29830964E-11-0.11712711E+05 0.10130220E+02-0.10705742E+05    4

CD4  METHANE-D4 ANHARMONIC. DATA AS FOR RRHO.  X11=-13.6,X12=-1.54,X13=-40.6,
X14=-2.2,X22=-.2,X23=-4.8,X24=-10.9,X33=-9.6,X34=-12.7,X44=-6.4  ALFA1=.07
ALFA2=-.06  ALFA3=.03  ALFA4=.05  REF=TSIV(CH4)  MAX LST SQ ERROR CP @ 1300K .9%
CD4 * ANHARMONIC  T06/81C  1D   4    0     0G   300.000  5000.000  A  20.0674  1
 0.44482183E+01 0.81195608E-02-0.27020378E-05 0.43419712E-09-0.24605867E-13    2
-0.12860102E+05-0.47861973E+01 0.19425707E+01 0.89269280E-02 0.54267666E-05    3
-0.89088488E-08 0.28879408E-11-0.11714484E+05 0.10036650E+02-0.10705742E+05    4

CF  FLUOROMETHYLIDENE   SIGMA=1   Be=1.4172 cm-1  WE=1308.1    WEXE=11.10
ALPHAE=0.0184        T0(STATWT)=0(2),77.11(2),25000(4),42705(2),49452(2)
HF298=255.2+/-8 KJ  REF=JANAF
CF                  J 6/70C  1.F  1.   0.   0.G   300.000  5000.000  B  31.00940 1
 3.68696790E+00 9.11434910E-04-3.64638550E-07 6.74828540E-11-4.52695960E-15    2
 2.94781250E+04 4.17450994E+00 3.46551430E+00-6.87798050E-04 5.67847660E-06    3
-6.45829820E-09 2.29882480E-12 2.96555980E+04 5.88135474E+00 3.06967621E+04    4

FCN  CYANOGEN FLUORIDE  STATWT=1  SIGMA=1  B0=0.353106 cm-1  NU=2290,1077,420(2)
HF298=35.98+/-16.7 kJ  REF=JANAF
FCN                 J 6/69F  1.C  1.N  1.   0.G   300.000  5000.000  C  45.01614 1
 5.08985570E+00 2.41706840E-03-9.76827660E-07 1.78134420E-10-1.21185670E-14    2
 2.57807810E+03-2.87278107E+00 3.25169410E+00 8.30731440E-03-8.36663580E-06    3
 4.41256440E-09-9.08824230E-13 3.05511980E+03 6.44214763E+00 4.32821878E+03    4

COF  CARBONYLFLUORIDE  SIGMA=1  STATWT=2  IA=0.3399  IB=7.8768  IC=8.2167
NU=1855,1018,626  HF298=-171.5+/-63 KJ  REF=JANAF
COF                 J12/65C  1.O  1.F  1.   0.G   300.000  5000.000  B  47.00880 1
 4.89082140E+00 2.21797030E-03-9.25507250E-07 1.72701200E-10-1.19553430E-14    2
-2.23579840E+04 9.92783959E-01 3.20197270E+00 5.58377700E-03-1.49054810E-06    3
-2.31260690E-09 1.36143530E-12-2.18170430E+04 1.00607391E+01-2.06312897E+04    4

CF2  DIFLUOROMETHYLENE  SIGMA=2  IAIBIC=48.8015E-117  NU=1222,1110,665
T0=16000 STATWT=3  T0=37226  STATWT=1  HF298=-182.00+/- 6.3 KJ  REF=JANAF
CF2                 J 6/70C  1.F  2.   0.   0.G   300.000  5000.000  B  50.00781 1
 5.22671420E+00 2.08376800E-03-9.90372780E-07 2.12648480E-10-1.58311140E-14    2
-2.37558470E+04-1.91090412E+00 2.76888210E+00 7.23729620E-03-1.60281520E-06    3
-4.55123790E-09 2.66480110E-12-2.30157860E+04 1.11376959E+01-2.18904653E+04    4
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CF2O  HF298=-152.96 Kcal  REF= Gurvich 1991
COF2                RUS 91C  1.O  1.F  2.   0.G   200.000  6000.000  B  66.00721 1
 6.81631730E+00 3.16473282E-03-1.21776269E-06 2.05582261E-10-1.26893125E-14    2
-7.95482716E+04-9.52864566E+00 2.12979489E+00 1.41019723E-02-5.94381359E-06    3
-5.30544790E-09 3.97367469E-12-7.81745339E+04 1.51109093E+01-7.69738686E+04    4

CF3  TRIFLUOROMETHYL   SIGMA=3  STATWT=2  IAIBIC=961.0547E-117  NU=1259(2),1090,
701,500(2)  HF298=-470.28+/-4.2 KJ  REF=JANAF
CF3                 J 6/69C  1.F  3.   0.   0.G   300.000  5000.000  C  69.00621 1
 7.20126220E+00 3.06639350E-03-1.31441810E-06 2.49969250E-10-1.75509280E-14    2
-5.92386310E+04-1.09457100E+01 2.06501680E+00 1.64241580E-02-1.08381460E-05    3
-8.53179970E-10 2.38780700E-12-5.78119760E+04 1.57046930E+01-5.65626016E+04    4

CF3I  TRIFLUOROIODOMETHANE  SIGMA=3  IA=14.7097  IB=IC=54.7578  NU=1185(2),1074,
742,539(2),284,260(2)  HF298=-589.11+/-3.3 KJ  REF=JANAF
CF3I                J 6/69C   1F   3I   1    0G   200.000  6000.000  B 195.91068 1
 0.10375057E+02 0.26880979E-02-0.10525827E-05 0.17967408E-09-0.11173263E-13    2
-0.74551179E+05-0.24024941E+02 0.25628907E+01 0.28507572E-01-0.33699705E-04    3
 0.18730304E-07-0.39219886E-11-0.72621870E+05 0.15237838E+02-0.70853243E+05    4

CF3O2  CF3OO* RADICAL SIGMA=1  STATWT=2  IA=14.4736  IB=24.9063  IC=25.19106
IR(OO)=2.0124  ROT BARRIER V(3)=1217.14 cm-1 ROSYM=3  NU=1341,1288,1251,1124,
878.6,686.6,593.2,570.8,442,420,278.8  HF298=-149.95 kcal  REF=Melius database
F42D private communication (HF298=-173.5 kcal REF=Bozzelli's Therm)  Max Lst Sq
Error Cp @ 1300 K 0.33%.
CF3OO  RADICAL    T10/97C  1.F  3.O  2.   0.G   200.000  6000.000  B 101.00501 1
 1.22037091E+01 3.39739140E-03-1.33527750E-06 2.28468036E-10-1.42307780E-14    2
-7.99109047E+04-3.41946453E+01 1.55041706E+00 3.73972544E-02-4.08839888E-05    3
 1.89635072E-08-2.54712965E-12-7.72518205E+04 1.95583929E+01-7.54523069E+04    4

CF4 TETRAFLUOROMETHANE  FC-14  SIGMA=12 IA=IB=IC=14.255  NU=422(2),610(3),896,
1315(3)  HF298=-223. kcal. REF=Zachariah, Westmoreland, Burgess, Tsang& Melius
JPC 100,(1996),8737-8747 Max Lst Sq Error Cp @ 1300 K 0.41%
CF4    FC-14      T 9/99C  1.F  4.   0.   0.G   200.000  6000.000  B  88.00461 1
 9.44099184E+00 3.62071082E-03-1.41228609E-06 2.40482377E-10-1.49298254E-14    2
-1.15774828E+05-2.47051920E+01 1.10989749E+00 2.86535601E-02-2.84860924E-05    3
 1.18222921E-08-1.22468827E-12-1.13589057E+05 1.77898592E+01-1.12213468E+05    4

CH  METHYLIDENE RADICAL CALCULATED FROM TSIV TABLES. HF298=597.36 KJ
CH                  RUS 79C  1H   1    0     0G   200.000  6000.000  A  13.01894 1
 0.25209062E+01 0.17653726E-02-0.46147581E-06 0.59288567E-10-0.33473209E-14    2
 0.71134082E+05 0.74053223E+01 0.34898166E+01 0.32383554E-03-0.16889906E-05    3
 0.31621733E-08-0.14060907E-11 0.70799939E+05 0.20840111E+01 0.71845485E+05    4

CHBrF2  (HBFC-22B1)   STATWT=1  SIGMA=1  IAIBIC=8.79E 114    NU=3031,1280,1136,
717,577,240,1344,1108,323  HF298=-422 KJ  REF=TSIV 1979  Max Lst Sq Error Cp @
1300 K 0.38%.
CHBRF2              RUS 79C   1H   1F   2BR  1G   200.000  6000.000  B 130.91975 1
 0.79956377E+01 0.46809168E-02-0.17376628E-05 0.28678947E-09-0.17435780E-13    2
-0.53795363E+05-0.12434624E+02 0.33173655E+01 0.13144058E-01 0.17756615E-05    3
-0.14547464E-07 0.75186250E-11-0.52318418E+05 0.12722668E+02-0.50754645E+05    4

CHCL RADICAL  SIGMA=1 STATWT=1 NU=3000,1201,815  IAIBIC=3.96E 117  T0=8000
SIGMA=1 STATWT=3  T0=12270 SIGMA=1 STATWT=1  REF=TSIV  MAX LST SQ ERROR CP @
2000 K 0.33% HF298=308.28 KJ
CHCL                L 3/84C  1H   1CL  1     0G   300.000  5000.000  C  48.47189 1
 0.50468426E 01 0.66806213E-03 0.31887100E-06-0.10470093E-09 0.76054614E-14    2
 0.35351730E 05-0.11610727E 01 0.31592255E 01 0.46576671E-02-0.77836523E-06    3
-0.26889417E-08 0.15871107E-11 0.35940453E 05 0.89036818E 01 0.37077792E 05    4
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CHClF  CHLOROFLUOROMETHYL RADICAL  SIGMA=1 STATWT=2  IAIBIC=370E-117  NU=3000,
1150,760,1300,1200,380  REF=TSIV  HF298=-83.14 KJ
CHCLF              L 4/86C  1.H  1.CL 1.F  1.G   298.150  5000.000  C  67.47030 1
 0.65730400E 01 0.29733933E-02-0.10222593E-05 0.15512820E-09-0.85432759E-14    2
-0.12409480E 05-0.51201038E 01 0.33409529E 01 0.10670263E-01-0.39450997E-05    3
-0.48872693E-08 0.34919463E-11-0.11491043E 05 0.11776594E 02-0.10064453E 05    4

CHClF2  CLORODIFLUOROMETHANE  (HCFC-22)   SIGMA=1   STATWT=1  IAIBIC=3419.E-117
NU=3024,1312,1178,809,595,422,1347,1116,365   HF298=-475.+/-15. KJ  REF=TSIV 79
Max Lst Sq Error Cp @ 1300 K 0.41%
CHCLF2  HCFC-22   RUS 79C   1F   2H   1CL  1G   200.000  6000.000  B  86.46845 1
 0.77564079E+01 0.49188408E-02-0.18293348E-05 0.30228522E-09-0.18393251E-13    2
-0.60143678E+05-0.12941733E+02 0.26028998E+01 0.14767611E-01 0.26568017E-06    3
-0.14000683E-07 0.74942979E-11-0.58539689E+05 0.14650645E+02-0.57129043E+05    4

CHCL2  RADICAL      SIGMA=2 STATWT=2 NU=757,902,3000,300,1226,360
IAIBIC=15100E-117  REF=TSIV  HF298=73.9 KJ   MAX LST SQ ERROR CP @ 1300 K 0.35%
CHCL2              L 3/84C  1H   1CL  2     0G   300.000  5000.000  C  83.92487 1
 0.68659325E 01 0.26912021E-02-0.91447470E-06 0.13676213E-09-0.73845654E-14    2
 0.64878789E 04-0.70413742E 01 0.36568127E 01 0.10666471E-01-0.44123180E-05    3
-0.47082409E-08 0.35693497E-11 0.73712227E 04 0.96209192E 01 0.88877011E 04    4

CHCl2F DICHLOROFLUOROMETHANE FC-21  TRC DATA EXTRAPOLATED TO 5000 K USING
WILHOIT'S  POLYNOMIALS.  HF298=-68.1 Kcal
CHCL2F   FC-21    P12/75C  1.H  1.CL 2.F  1.G   298.150  5000.000  C 102.92330 1
 0.85083923E 01 0.40345713E-02-0.14268226E-05 0.22247303E-09-0.12630173E-13    2
-0.37427910E 05-0.15411654E 02 0.31107159E 01 0.16295891E-01-0.47331187E-05    3
-0.94798160E-08 0.61323750E-11-0.35862211E 05 0.12963858E 02-0.34269462E 05    4

CHCl3  (CHLOROFORM) TRICHLOROETHANE  TRC DATA EXTRAPOLATED TO 5000 K USING
WILHOIT'S POLYNOMIALS. HF298=-24.6 Kcal
CHCL3              P 6/81C  1.H  1.CL 3.   0.G   298.150  5000.000  C 119.37790 1
 0.89938030E 01 0.35652192E-02-0.12537648E-05 0.19479131E-09-0.11032021E-13    2
-0.15609000E 05-0.17631689E 02 0.36819801E 01 0.16611021E-01-0.66180801E-05    3
-0.81291560E-08 0.59433135E-11-0.14141844E 05 0.99835104E 01-0.12379277E 05    4

CHD2NO2 Nitro-Methane D2   STATWT = 1  SUMNO = 1 IA = 6.76188 IB = 9.55869
IC = 15.2841    I(red) = 0.754032  V(2) = 0.125 kcal/mole  NU= 443,577,643,896,
923,977,1060,1285,1285,1405,1554,2187,2313,3000  REF=McKean & Watt J. Molec.
Struct. 61,(1976),164.    HF298=  -13.795 kcal/mole   REF = A. BURCAT TAE
Report # 824a, 1998   Max Lst Sq Error Cp @ 1300 K 0.58%
NITRO-METHANE D2  T04/98C  1.H  1.D  2.O  2.G   200.000  6000.000  B  63.05268 1
 8.08961148E+00 9.83765066E-03-3.67240992E-06 6.08123340E-10-3.70523025E-14    2
-1.05585014E+04-1.58799705E+01 2.86575841E+00 9.70884039E-03 2.98575468E-05    3
-4.74818909E-08 1.98756686E-11-8.40693607E+03 1.46207846E+01-6.94164250E+03    4

CHD3  METHANE-D3  STATWT=1.  SIGMA=3.  AE=CE=2.62  BE=3.27  NU=2993,2142,1003,
2263(2),1291(2),1036(2)  REF=BURCAT  MAX LST SQ ERROR CP @ 1300K 0.94% .
HF298=-85.29 KJ.
CHD3               T05/79C  1H   1D   3     0G   300.000  5000.000  B  19.0612  1
 0.40764599E+01 0.79434291E-02-0.27834194E-05 0.42990389E-09-0.24151396E-13    2
-0.12245391E+05-0.13486305E+01 0.21469107E+01 0.74287578E-02 0.56749586E-05    3
-0.77548528E-08 0.21464679E-11-0.11265895E+05 0.10451311E+02-0.10257971E+05    4

CHF RADICAL  STATWT=2  SIGMA=1  IA=0.172  IB=2.240  IC=2.412  NU=1189,1404,2733
HF298=39.0 kcal  REF=Zachariah,Westmoreland,Burgess,Tsang&Melius JPC,100,(1996),
8737-8747  Max Lst Sq. Error Cp @ 6000 K 0.51%
CHF RADICAL        T 8/99C  1.H  1.F  1.   0.G   200.000  6000.000  B  32.01734 1
 3.81407171E+00 2.91531169E-03-1.06577623E-06 1.74013614E-10-1.04973609E-14    2
 1.82312890E+04 4.65785213E+00 4.41475567E+00-5.51349381E-03 2.18470808E-05    3
-2.34089450E-08 8.48772577E-12 1.84034839E+04 3.21728174E+00 1.96254500E+04    4
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CHF2 RADICAL  STATWT=2  IAIBIC=92.E 117  NU=1165,1175,3000,600,1316,500
REF=TSIV 1979  HF298=-254. KJ  Max Lst Sq Error Cp @ 6000 K 0.38%
CHF2              RUS 79C   1H   1F   2    0G   200.000  6000.000  C  51.01575 1
 0.58958702E+01 0.37705626E-02-0.13837102E-05 0.22663348E-09-0.13705690E-13    2
-0.32778360E+05-0.42892918E+01 0.30342605E+01 0.75276516E-02 0.55750157E-05    3
-0.14409464E-07 0.67681867E-11-0.31812224E+05 0.11424782E+02-0.30549004E+05    4

CHF3  (FLUOROFORM) TRIFLUOROMETHANE (HFC-23)  SIGMA=1  IA=IB=7.898  IC=14.403
NU=507(2),700,1117,1152(2),1372(2),3036  REF=Zachariah, Westmoreland, Burgess,
Tsang & Melius JPC 100,(1996),8737-8747  HF298=-165.7 Kcal  REF=TRC/81  Max Lst
Sq Error Cp @ 1300 K 0.45%.
CHF3  FLUOROFORM  T 9/99C  1.H  1.F  3.   0.G   200.000  6000.000  B  70.01415 1
 7.24608934E+00 5.42386589E-03-2.02314469E-06 3.34946550E-10-2.04067622E-14    2
-8.63258021E+04-1.17996156E+01 2.73539118E+00 8.72479733E-03 1.74821274E-05    3
-3.21504458E-08 1.41694802E-11-8.46839563E+04 1.35866083E+01-8.33830015E+04    4

HCN   STATWT=1  SIGMA=1  BE=1.478211  NU=2096,713.5(2),3311  X11=-70741
X12=-2.5265  X13=-10.4434  X22=-2.6533  X23=-19.0055  X33=-52.4901  G22=5.160
Y111=-.1889  Y112=-.0012  Y113=-.7723  Y122=-.0747  Y123=.1240    Y133=-1.1010
Y222=.0285   Y223=-.0375  Y233=-.1230  Y=333=.2702  ALFAB1=.009975
ALFAB2=-.0035616   ALFAB3=.010446  D000=.000002909  HF298=135. KJ  REF=TSIV 79 +
Wagman et al JPCRD 1982 Suppl. 1, 11. (Gurvich 1991 HF298=132+/-4 kJ)
HCN               L 7/88H  1C   1N   1     0G   200.000  6000.000  A  27.02568 1
 0.38022392E+01 0.31464227E-02-0.10632185E-05 0.16619757E-09-0.97997567E-14    2
 0.14910512E+05 0.15754601E+01 0.22589885E+01 0.10051170E-01-0.13351763E-04    3
 0.10092349E-07-0.30089029E-11 0.15215853E+05 0.89164418E+01 0.16236675E+05    4

HNC  STATWT=1  SIGMA=1  B0=1.512  NU=3653,464(2),2024  REF=M. JACOX 88
HF0=194.+/-9. KJ  REF=Gurvich 1991
HNC               L11/92H  1.N  1.C  1.   0.G   200.000  6000.000     27.02568 1
 4.22248103E+00 2.59458278E-03-8.58480969E-07 1.30745002E-10-7.50339765E-15    2
 2.20127593E+04-7.79447358E-02 2.30186735E+00 1.54157529E-02-3.13262156E-05    3
 3.08816551E-08-1.11912353E-11 2.22277183E+04 8.14751135E+00 2.33781812E+04    4

HNCO HYDROGEN ISOCYANATE STATWT=1 SIGMA=1 IAIBIC=5.3166E-117 NU=3531,2274,1327,
660,578,777 REF=JANAF12/70 HF298=-27.9 KCAL REF=East & Allen J. Chem. Phys. 99
(1993), 4638. Max Least Sq Error Cp @ 6000 0.44%
HNCO              T 6/94H   1N   1C   1O   1G   200.000  6000.000  B  43.02508 1
 0.52936894E+01 0.40307770E-02-0.14130589E-05 0.22445562E-09-0.13287683E-13    2
-0.15973489E+05-0.30864710E+01 0.22432188E+01 0.14491349E-01-0.15236174E-04    3
 0.83345851E-08-0.17104033E-11-0.15233708E+05 0.12157321E+02-0.14039745E+05    4

CHN2 CYANAMIDE RADICAL HN*-CN  SIGMA=1   STATWT=2    IA=0.130787   IB=7.4960529
IC=7.626847  NU=3308,1738,1101,1026,437,392  HF298=76.433 Kcal
REF=BAC/MP4 Calculations by C. Melius Private Communication.    Max Lst Sq Error
Cp @ 6000 K 0.33%
CHN2              T 3/93C   1H   1N   2    0G   200.000  6000.000  B  41.03242 1
 0.58470159E+01 0.36667998E-02-0.13120636E-05 0.21135472E-09-0.12636470E-13    2
 0.36343577E+05-0.49756817E+01 0.31861199E+01 0.10792062E-01-0.74954818E-05    3
 0.14780067E-08 0.43976323E-12 0.37095838E+05 0.88362660E+01 0.38462359E+05    4
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CH(NO2)3 Tri-Nitro Methane STATWT = 1 SYMNO = 3  IA = 50.830948  IB = 68.4055572
IC = 99.2098743       (Ir(NO2)= 5.96    ROSYM = 2  V(2) = 0.1 kcal/mole)3
NU = 2749,1962,1572,1261,1232,1167,1135,1064,993,884,724,708,670,619,563,490,
449,421,368,347,335,210,170,157. REF = A.BURCAT TAE Report # 824 1998
HF(298)=-3.2 kcal/mole  REF=Carpenter et. al. J. Chem. Eng. Data 15, (1970),535
Max Lst Sq Error Cp @ 1300 K 0.50%
CH(NO2)3          T04/98C  1.H  1.O  6.N  3.G   200.000  6000.000  B 151.03556 1
 1.96645029E+01 9.80273423E-03-3.99278141E-06 6.90498702E-10-4.31223139E-14    2
-9.12328532E+03-6.52887368E+01 1.66436817E+00 6.81055678E-02-7.81450689E-05    3
 4.46832013E-08-1.01862362E-11-4.52669105E+03 2.56966436E+01-1.61029333E+03    4

CHO SIGMA=1 STATWT=2 A0=24.329 B0=1.494 C0=1.39882 NU=1868,1081,2434 T0=9297
NU=1812,805(2),3319 B0=1.34 STATWT=2  T0=38691  STATWT=2.  A0=16.7  B0=1.149
C0=2.604  NU=1035,1375,2435 REF=TSIV + M. JACOX 88 HF298=42. KJ
HCO               L12/89H  1.C  1.O  1.   0.G   200.000  6000.000  A  29.01834 1
 3.64896209E+00 3.08090819E-03-1.12429876E-06 1.86308085E-10-1.13951828E-14    2
 3.71209048E+03 5.06147406E+00 4.22118584E+00-3.24392532E-03 1.37799446E-05    3
-1.33144093E-08 4.33768865E-12 3.83956496E+03 3.39437243E+00 5.05141013E+03    4

CHO+ FORMYL ION  B0=1.367073  NU=3223,707(2),2088  HF298=833. KJ  REF=JANAF
CHO+              J12/70H  1C   1O   1E   -1G   300.000  5000.000  C  29.0178  1
 0.37411880E+01 0.33441517E-02-0.12397121E-05 0.21189388E-09-0.13704150E-13    2
 0.98884078E+05 0.20654768E+01 0.24739736E+01 0.86715590E-02-0.10031500E-04    3
 0.67170527E-08-0.17872674E-11 0.99146608E+05 0.81625751E+01 0.10019345E+06    4

COOH  CARBOXYL RADICAL SIGMA=1 STATWT=2 IAIBIC=35. NU=3316,1797,1261,1088,620,
615 REF=TSIV HF298=-213. KJ
COOH              RUS 79C  1O   2H   1     0G   200.000  6000.000  B  45.01774 1
 0.53920264E+01 0.41122622E-02-0.14819726E-05 0.23988016E-09-0.14390635E-13    2
-0.27670863E+05-0.22350810E+01 0.29220825E+01 0.76245184E-02 0.32988630E-05    3
-0.10713524E-07 0.51158655E-11-0.26838359E+05 0.11292583E+02-0.25617866E+05    4

HCOO   RADICAL   CALCULATED FROM GROUP THEORY  REF=Benson 1976  HF298=-36.0 kcal
Max Lst Sq Error Cp @ 1500 K 0.40%.
HCOO*  Radical    T04/97H  1.C  1.O  2.   0.G   298.150  5000.000  E  45.01774 1
 5.97791811E+00 3.24247847E-03-1.46666291E-06 2.91808902E-10-2.10704956E-14    2
-2.04910217E+04-7.12854015E+00-3.01936623E+01 2.54607495E-01-6.43484728E-04    3
 6.92943698E-07-2.65871657E-10-1.59887826E+04 1.47958586E+02-1.81158000E+04    4

HCS RADICAL    STATWT=2   A0=0.657   B0=0.671  C0=30.500     NU=2983,1096,816
T0=3063.  STATWT=2  HF0=71.7 kcal  REF=ab-initio calc by Ching-Len Yu & S.H.
Bauer Private Communication    Max Lst Sq Error Cp @ 6000 K 0.58%
HCS               T05/97H  1.C  1.S  1.   0.G   200.000  6000.000  B  45.08494 1
 3.61707294E+00 3.87413811E-03-1.52693796E-06 2.56534366E-10-1.56455118E-14    2
 3.48552427E+04 6.60648943E+00 3.51963223E+00 2.08544960E-03 6.12130414E-06    3
-9.93060979E-09 4.40938577E-12 3.49593934E+04 7.53361036E+00 3.61380016E+04    4

CH2 RAD STATWT=3 SIGMA=2 IAIBIC=.006 E-117 NU=3000,1362,3200  T0=3500  SIGMA=2
STATWT=1  T0=10600 SIGMA=2 STATWT=1  HF298=390 KJ REF=TSIV
CH2(3) TRIPLET    RUS 79C  1H   2    0     0G   200.000  6000.000  B  14.02688 1
 0.25387122E+01 0.38225491E-02-0.12861304E-05 0.19800308E-09-0.11465743E-13    2
 0.46129253E+05 0.81054648E+01 0.41793655E+01-0.22178553E-02 0.79653602E-05    3
-0.69127339E-08 0.22475318E-11 0.45750857E+05-0.76113703E-02 0.46956131E+05    4
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CH2 RAD SINGLET   SIGMA=2  IA=0.1335  IB=0.2469  IC=0.38043  NU=1397,2794,2850
REF= C. Melius BAC-MP4 Database. Polynomial from CHEMKIN THERMODYNAMIC DATABASE.
HF298=101.5 KCAL
CH2(1) SINGLET    C12/87C   1H   2    0    0G   300.00   4000.00   B  14.02688 1
 0.03552888E+02 0.02066788E-01-0.01914116E-05-0.11046733E-09 0.02021349E-12    2
 0.04984975E+06 0.01686570E+02 0.03971265E+02-0.01699088E-02 0.10253689E-05    3
 0.02492550E-07-0.01981266E-10 0.04989367E+06 0.05753207E+00 0.51077663E+05    4

CH2BrCl  Halon 1011  SIGMA=1 IAIBIC=469.E-116  NU=3001,1421,1232,743,608,236,
3065,1136,852  HF298=-45+/-15 KJ REF=TSIV 1979 Max Lst Sq Error Cp @ 6000 K .41%
CH2BRCL HALON1011 RUS 79C   1H   2BR  1CL  1G   200.000  6000.000  B 129.38358 1
 0.65082153E+01 0.57744846E-02-0.20744896E-05 0.33492192E-09-0.20051184E-13    2
-0.79549405E+04-0.49946731E+01 0.30310057E+01 0.10607707E-01 0.63407360E-05    3
-0.18341110E-07 0.88847421E-11-0.68113680E+04 0.13983350E+02-0.54122251E+04    4

CH2CL RADICAL REF=TSIV HF298=116.87 KJ SIGMA=2 STATWT=2 NU=2950,3050,826.3,1391,
1250,396.6  IAIBIC=11.E-117 MAX LST SQ ERROR CP @ 1300 K 0.52%
CH2CL             L 8/84C  1H   2CL  1     0G   300.000  5000.000  B  49.47979 1
 0.47707529E 01 0.43237582E-02-0.14223033E-05 0.20599472E-09-0.10714865E-13    2
 0.12277027E 05 0.46459579E 00 0.33185844E 01 0.65915734E-02 0.10332604E-06    3
-0.43136268E-08 0.21676541E-11 0.12780980E 05 0.84271412E 01 0.14056558E 05    4

CH2C1F  CLOROFLUOROMETHANE FC-31 TRC DATA EXTRAPOLATED TO 5000 K USING WILHOIT'S
POLYNOMIALS. HF298=-63.2 Kcal
CH2CLF  GC-31     P12/75C  1.H  2.CL 1.F  1.G   298.150  5000.000  C  68.47820 1
 0.59572783E 01 0.60879700E-02-0.20813759E-05 0.31346215E-09-0.17084878E-13    2
-0.34280781E 05-0.48930445E 01 0.20975533E 01 0.12551896E-01 0.27147036E-06    3
-0.91319841E-08 0.44713573E-11-0.32973617E 05 0.16155014E 02-0.31803671E 05    4

CH2C12  DICHLOROMETHANE  TRC DATA EXTRAPOLATED TO 5000 K USING WILHOIT'S
POLYNOMIALS.  HF298=-22.8 Kcal
CH2CL2            P12/81C  1.H  2.CL 2.   0.G   298.150  5000.000  C  84.93280 1
 0.64991283E 01 0.55672340E-02-0.18887449E-05 0.28233393E-09-0.15256869E-13    2
-0.14048813E 05-0.70247154E 01 0.23626127E 01 0.13885532E-01-0.20872167E-05    3
-0.86656158E-08 0.49494315E-11-0.12761230E 05 0.15071752E 02-0.11473476E 05    4

CH2DNO2 Nitro-Methane D    STATWT = 1  SYMNO = 1  IA = 6.60202  IB = 8.90396
IC = 14.75046   I(red) = 0.619102   ROSYM = 2    V(2) = 0.104 kcal/mole
NU = 463,579,651,893,957,1099,1254,1304,1338,1480,1557,2221,2997,3082.
REF = McKee JACS 107,(1985),1900.   HF298=  -12.555 kcal   REF =A. BURCAT
TAE Report # 824a, 1998   Max Lst Sq Error Cp @ 1300 K 0.60%
NITRO-METHANE D   T04/98C  1.H  2.D  1.O  2.G   200.000  6000.000  B  62.04652 1
 7.42983565E+00 1.02242244E-02-3.76339564E-06 6.17531100E-10-3.73902847E-14    2
-9.68557204E+03-1.23529524E+01 3.23582229E+00 6.54117396E-03 3.47848512E-05    3
-5.08832580E-08 2.07922157E-11-7.79017302E+03 1.29867207E+01-6.31809439E+03    4

CH2D2  METHANE-D2  STATWT=1.  SIGMA=2.     A0=4.303  B0=3.506  C0=3.05  NU=2974,
2202,1435,1033,1331,3013,1090,2234,1234  REF=BURCAT  MAX LST SQ ERROR CP @ 1300K
0.95% . HF298=-81.75 KJ
CH2D2             T05/79C  1H   2D   2     0G   300.000  5000.000  B  18.0551  1
 0.35087013E+01 0.81863180E-02-0.27852266E-05 0.41648370E-09-0.22470558E-13    2
-0.11595125E+05 0.18880228E+01 0.23866291E+01 0.57553649E-02 0.64751221E-05    3
-0.67107635E-08 0.13974620E-11-0.10846535E+05 0.94605669E+01-0.98322090E+04    4

CH2F RADICAL  STATWT=2  IAIBIC=2.8E-117  NU=2900,3000,1163,1500,1350,500
REF=TSIV 1979  HF298=-32. KJ  Max Lst Sq Error Cp @ 6000 K 0.47%
CH2F              RUS 79C   1H   2F   1     0G   200.000  6000.000  C  33.02528 1
 0.40610825E+01 0.52432553E-02-0.18726751E-05 0.30101543E-09-0.17961659E-13    2
-0.54531615E+04 0.34407775E+01 0.39006976E+01 0.18878812E-03 0.14670620E-04    3
-0.17625373E-07 0.65799837E-11-0.51179668E+04 0.56574728E+01-0.38486934E+04    4
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CH2F2  DIFLUOROMETHANE  FC-32    SIGMA=2   IA=1.650    IB=7.720    IC=8.832
NU=529,1090,1116,1176,1262,1435,1508,2949,3012   REF=Zachariah, Westmoreland,
Burgess, Tsang& Melius JPC 100,(1996),8737-8747   HF298=-108.2 Kcal  REF=TRC/81
Max Lst Sq Error Cp @ 6000 K 0.55%.
CH2F2   FC-32     T 9/99C  1.H  2.F  2.   0.G   200.000  6000.000  B  52.02369 1
 5.06948195E+00 7.23193135E-03-2.64021025E-06 4.30854708E-10-2.59873096E-14    2
-5.67270077E+04-2.34590394E+00 4.25023157E+00-6.84861262E-03 4.85583334E-05    3
-5.83442752E-08 2.24503933E-11-5.57351602E+04 5.76716418E+00-5.44480432E+04    4

CH2N  (H2C=N*) RADICAL  SIGMA=2  T0(STATWT)=0(2)  A0=1.140   B0=1.31   C0=9.48
NU=3103,2820,1725,1337,954,913  T0(STATWT)=35075(4)  HF298=57.4 kcal
REF= REF=Ching-Len Yu & S.H. Bauer Private Communication  Max Lst Sq Error Cp @
400 K 0.59%.
H2CN RADICAL      T05/97H  2.C  1.N  1.   0.G   200.000  6000.000  B  28.03362 1
 3.80315523E+00 5.47197456E-03-1.95314927E-06 3.13362513E-10-1.86249463E-14    2
 2.73218196E+04 3.31721893E+00 3.97799541E+00-3.43275678E-03 2.59134226E-05    3
-3.04692133E-08 1.16272702E-11 2.76769528E+04 4.43029598E+00 2.88846366E+04    4

CH2N  (H*C=NH) RADICAL trans  SIGMA=1  T0(STATWT)=0(2)  A0=1.150   B0=1.26
C0=12.75   NU=3304,2873,1584,1194,977,913  T0(STATWT)=30000(2)  HF298=71.4 kcal
REF= REF=Ching-Len Yu & S.H. Bauer Private Communication  Max Lst Sq Error Cp @
400 K 0.54%
HCNH trans        T05/97H  2.C  1.N  1.   0.G   200.000  6000.000  B  28.03362 1
 4.04014620E+00 5.16591818E-03-1.82276886E-06 2.90299166E-10-1.71614663E-14    2
 3.42988370E+04 2.58896150E+00 3.97114548E+00-3.88875657E-03 2.92918929E-05    3
-3.57482385E-08 1.40303899E-11 3.47237453E+04 5.06390351E+00 3.59296699E+04    4

CH2N  (H*C=NH) RADICAL cis  SIGMA=1  T0(STATWT)=0(2)  A0=1.150   B0=1.27
C0=12.08   NU=3295,2845,1567,1099,924,873  T0(STATWT)=30000(2)  HF298=76.4 kcal
REF= REF=Ching-Len Yu & S.H. Bauer Private Communication  Max Lst Sq Error Cp @
400 K 0.55
HCNH cis          T05/97H  2.C  1.N  1.   0.G   200.000  6000.000  B  28.03362 1
 4.21964804E+00 5.00385006E-03-1.76392053E-06 2.80725924E-10-1.65851919E-14    2
 3.67706419E+04 1.67138658E+00 3.68324269E+00-1.38553482E-03 2.40042191E-05    3
-3.11573905E-08 1.25791818E-11 3.72527355E+04 6.21248890E+00 3.84457533E+04    4

CH2NO  H2N-C(*)=O RADICAL   STATWT=2  SIGMA=2  IA=0.6363  IB=7.397796  IC=8.0341
NU=3539,3390,1839,1589,1207,1060,593,520,188.7  HF298=-5.57 +/-2.37 KCAL
REF= C. Melius Database BAC/MP4 C37 Max Lst Sq Error Cp @ 6000 K 0.37%
H2NCO             T09/96H   2N   1C   1O   1G   200.000  6000.000  B  44.03302 1
 0.57886741D+01 0.60938325D-02-0.21165797D-05 0.33404486D-09-0.19684582D-13    2
-0.50210948D+04-0.44063740D+01 0.35677914D+01 0.10193381D-01-0.15289951D-05    3
-0.47571551D-08 0.26052647D-11-0.42980380D+04 0.75824281D+01-0.28029168D+04    4

CH2NO CH2=N-O* RADICAL  STATWT=2  SIGMA=2  IA=0.8304  IB=6.6914  IC=7.5218
NU=3095,2977,1469,1301,1112,1035,835,712,360.8  HF298=41.45+/-5 KCAL
REF=C. MELIUS DATABASE BAC/MP4 C42   Max Lst Sq Error Cp @ 6000 K 0.44 %.
CH2NO CH2=N-O*    T 9/96C   1H   2N   1O   1G   200.000  6000.000  C  44.03302 1
 0.61088065E+01 0.61700384E-02-0.22263482E-05 0.36051980E-09-0.21629499E-13    2
 0.18374401E+05-0.74217824E+01 0.31022300E+01 0.63256777E-02 0.18394585E-04    3
-0.30856607E-07 0.13425502E-10 0.19544369E+05 0.99247330E+01 0.20858331E+05    4

CH2NO H2C*N=O RADICAL  STATWT=2  SIGMA=2  IA=2.596  IB=3.041  IC=5.0754
NU=3040,2952,1505,1304,1188,1111,983,897,846   HF298=53.52+/-2 KCAL
REF=C. MELIUS DATABASE BAC/MP4 D93X  Max Lst Sq Error Cp @ 200 K 0.82%.
H2CNO H2C*N=O     T 9/96H   2C   1N   1O   1G   200.000  6000.000  C  44.03302 1
 0.54028152E+01 0.69057001E-02-0.25162977E-05 0.41014066E-09-0.24718300E-13    2
 0.24528690E+05-0.44574262E+01 0.38781858E+01-0.66530886E-02 0.53947610E-04    3
-0.68176813E-07 0.27181746E-10 0.25716857E+05 0.74618774E+01 0.26932156E+05    4
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*CH2NO2 Nitro Methylene Radical   SYMNO = 1  STATWT = 2 IA = 6.34509
IB = 6.7566103  IC = 13.1017  IRED=0.3267  V(2)= 0.08 kcal/mole  ROSYM = 2
NU = (457,555),693,719,986,1095,1297,1419,1461,3055,3200   HF298= 36.44 kcal
REF=McKee, J. Am. Chem. Soc. 107,(1985),1900  Max Lst Sq Error Cp @ 6000 K 0.44%
*CH2NO2  RADICAL  T04/98C  1.H  2.N  1.O  2.G   200.000  6000.000  B  60.03242 1
 7.67214886E+00 7.04674142E-03-2.55301211E-06 4.14646979E-10-2.49316782E-14    2
 1.52307521E+04-1.22510821E+01 2.46754293E+00 1.56130407E-02 4.71686464E-06    3
-2.05123642E-08 1.02705094E-11 1.69015807E+04 1.59016345E+01 1.83372153E+04    4

*CH2ONO2  METHYL-NITRATE-RADICAL   STATWT = 2  SYMNO = 1  IA = 6.5230882
IB = 16.246015   IC = 22.69382   Ir(NO2) = 5.96  ROSYM = 2  V(2) = 9.1 kcal
Ir(CH2) = 0.345711   ROSYM = 2  V(2) = 2.3 kcal   NU= 3142,3009,1727,1412,
1306,1165,1120,921,766,718,683,608,364.   HF298 = 23.65 kcal
REF = Melius Database 1988 P73BJ  Max Lst Sq Error Cp @ 1300 K 0.56%
*CH2ONO2 RADICAL  T05/98C  1.H  2.O  3.N  1.G   200.000  6000.000  B  76.03182 1
 1.03913885E+01 7.66103917E-03-3.02728077E-06 5.16124915E-10-3.19767406E-14    2
 7.78486241E+03-2.54151556E+01 2.98654023E+00 2.47990510E-02-1.17175684E-05    3
-5.36820166E-09 4.80947389E-12 1.00202588E+04 1.36939353E+01 1.19010741E+04    4

CH2N2  CYANAMIDE H2N-CN  SIGMA=1  STATWT=1    IA=0.2674823    IB=8.1221516
IC=8.319017  NU =412,475,615,1035,1182,1611,2324,3380,3473
HF298= 32.478+/-4.8 KCAL   REF=C. MELIUS, BAC/MP4 Database N62Z     Max Lst Sq
Error Cp @ 6000 K 0.38%
CH2N2 CYANAMIDE   T 3/93C   1H   2N   2    0G   200.000  6000.000  B  42.04036 1
 0.54262217E+01 0.63845441E-02-0.22119323E-05 0.34832646E-09-0.20489145E-13    2
 0.14263617E+05-0.33915332E+01 0.24205497E+01 0.17026593E-01-0.17728435E-04    3
 0.11218736E-07-0.30107729E-11 0.15000886E+05 0.11611217E+02 0.16343471E+05    4

CH2N2 CARBODIIMIDE HN=C=NH   SIGMA=2  STATWT=1   IA=0.2246383    IB=7.89834
IC=7.903817    IR=0.05859    INT. ROTATION BARRIER V(3)=1601.8 cm-1
NU=3416,3412,2102,1241,913,905,746,511   HF298=35.613+/-3.56 Kcal
REF=C.MELIUS BAC/MP4 Database N62Y     Max Lst Sq Error Cp @ 200 K 0.5%
H2CN2 HN=C=NH     T 3/93H   2C   1N   2    0G   200.000  6000.000  B  42.04036 1
 0.64734743E+01 0.51023160E-02-0.17738598E-05 0.28010178E-09-0.16511234E-13    2
 0.15445903E+05-0.93929437E+01 0.16502481E+01 0.17225336E-01-0.62645743E-05    3
-0.90652062E-08 0.65197171E-11 0.16733605E+05 0.15528105E+02 0.17921055E+05    4

CH2N2 DIAZOMETHANE H2C=N=N  STATWT=1  SIGMA=2  IA=0.2985  IB=7.179138
IC=7.47764  NU= 405,532,595,1115,1181,1419,2061,3024,3139
HF298=68.447+/-5.85 KCAL REF= C. MELIUS BAC/MP4 Database N62X    MAX LST SQ
ERROR CP @ 6000 K 0.45%
CH2N2 H2C=N=N     T 3/93C   1H   2N   2    0G   200.000  6000.000  B  42.04036 1
 0.56157835E+01 0.65328561E-02-0.23376828E-05 0.37633930E-09-0.22483577E-13    2
 0.32222744E+05-0.54835013E+01 0.25553699E+01 0.15039976E-01-0.11279972E-04    3
 0.45140426E-08-0.66460339E-12 0.33104359E+05 0.10402408E+02 0.34443671E+05    4

CH2N2 CYCLO DIAZIRENE H2(CNN)  STATWT=1  SIGMA=2  IA=1.94049  IB=3.39497
IC=4.76825  NU=879,980,1050,1054,1127,1478,1789,2964,3061
HF298=76.516+/-4.54 KCAL REF= C. MELIUS BAC/MP4 Database N62     MAX LST SQ
ERROR CP @ 200 K 0.75%
H2CN2 CY          T 3/93H   2C   1N   2    0G   200.000  6000.000  B  42.04036 1
 0.49500072E+01 0.73057703E-02-0.26589670E-05 0.43302613E-09-0.26081126E-13    2
 0.36251846E+05-0.28322509E+01 0.40367917E+01-0.75951605E-02 0.53236385E-04    3
-0.65261005E-07 0.25586745E-10 0.37284686E+05 0.59240768E+01 0.38504126E+05    4
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CH2(NO2)2 Di Nitro Methane  STATWT = 1 SYMNO = 2  IA = 13.497367 IB = 49.930024
IC = 50.708   (Ir(NO2) = 5.96  ROSYM = 2  V(2) = 0.08 kcal/mole)2
NU = 2962,2875,1959,1951,1602,1555,1358,1275,1063,971,915,895,746,638,585,568,
430,412,194.   REF = A.BURCAT TAE Report # 824 1998    HF298= -14.7 kcal
REF=Knobel et.al., Bull Acad. Sci. USSR Div. Chem. Sci. (1971),425.  Max Lst Sq
Error Cp @ 1300 K 0.62%
CH2(NO2)2          T10/98C  1.H  2.N  2.O  4.G   200.000  6000.000  B 106.03796 1
 1.14912019E+01 1.18834901E-02-4.59405883E-06 7.73301202E-10-4.75226143E-14    2
-1.22791660E+04-2.79393135E+01 2.13762234E+00 3.16667350E-02-1.09883048E-05    3
-1.02396987E-08 6.93005788E-12-9.32805967E+03 2.20134081E+01-7.39728499E+03    4

FORMALDEHYDE CH2O SIGMA=2 A0=9.40546 B0=1.295407 C0=1.134216 NU=2782.4,1746.1,
1500.1,1167.2,2843.2,1249.1 HF298=-108.7 KJ REF=TSIV
CH2O               L 8/88H  2C   1O   1     0G   200.000  6000.000  B  30.02628 1
 0.31694807E+01 0.61932742E-02-0.22505981E-05 0.36598245E-09-0.22015410E-13    2
-0.14478425E+05 0.60423533E+01 0.47937036E+01-0.99081518E-02 0.37321459E-04    3
-0.37927902E-07 0.13177015E-10-0.14308955E+05 0.60288702E+00-0.13059098E+05    4

CH2O2  METHANOIC(FORMIC) ACID  HCOOH MONOMER  STATWT=1 SIGMA=1  IA=1.0953
IB=6.9125  IC=8.0078  BROT=24.96  POT BARRIER V(1)=2011.  V(2)=3123. V(3)=192.
NU=3570,2943,1770,1387,1229,1105,625,1033      NEL=100      HF298=-90.48KCAL
REF=CHAO & ZWOLINSKI 78  Max Lst Sq Error Cp @ 6000 K 0.47%
HCOOH FORMIC ACID L 8/88H   2C   1O   2    0G   200.000  6000.000  B  46.02568 1
 0.46138316E+01 0.64496364E-02-0.22908251E-05 0.36716047E-09-0.21873675E-13    2
-0.47514850E+05 0.84788383E+00 0.38983616E+01-0.35587795E-02 0.35520538E-04    3
-0.43849959E-07 0.17107769E-10-0.46770609E+05 0.73495397E+01-0.45531246E+05    4

CH2S  SIGMA=2  T0(STATWT)=0(1)  A0=0.555  B0=0.59  C0=9.27  NU=3025,2971,1456,
1059,991,990  T0(STATWT)=14507.(3)  REF=JACOX HF0=28.3 kcal  REF=Ching-Len Yu &
S.H. Bauer Private Communication  Max Lst Sq Error Cp @ 400 K 0.59%.
H2CS               T05/97H  2.C  1.S  1.   0.G   200.000  6000.000  B  46.09288 1
 4.18881491E+00 5.12826276E-03-1.86326118E-06 3.12838130E-10-1.93704551E-14    2
 1.20948373E+04 2.65102700E+00 3.98890561E+00-4.48092826E-03 3.23152359E-05    3
-3.98563874E-08 1.57804583E-11 1.25888504E+04 5.99167863E+00 1.37931688E+04    4

CH3 METHYL-RAD   STATWT=1.  SIGMA=6. IA=IB=.2923  IC=.5846  NU=3044,607,3162(2),
1396(2) REF=PAMIDIMUKALA, ROGERS & SKINNER HF298=146.85 KJ
CH3                L 8/88C  1H   3    0     0G   200.000  6000.000  B  15.03482 1
 0.29669735E+01 0.57936672E-02-0.19694809E-05 0.30556936E-09-0.17767843E-13    2
 0.16537116E+05 0.47918803E+01 0.36733375E+01 0.20020559E-02 0.57853135E-05    3
-0.69873054E-08 0.26055599E-11 0.16440180E+05 0.16018315E+01 0.17662905E+05    4

CH3Br METHYL-BROMIDE  DATA EXTRAPOLATED FROM STULL WESTRUM & SINKE TO 5000 K
USING WILHOIT'S POLYNOMIALS HF298=-9.0 KCAL Max Lst Sq Error Cp @ 1200 K 0.16%.
CH3BR              T 2/94C   1H   3BR  1    0G   298.150  5000.000  B  94.93882 1
 0.40606801E+01 0.77232597E-02-0.26266985E-05 0.43354587E-09-0.27981235E-13    2
-0.62955892E+04 0.37017937E+01 0.20747857E+01 0.10566677E-01 0.19067030E-06    3
-0.61144695E-08 0.28451422E-11-0.56081473E+04 0.14632155E+02-0.45289500E+04    4

CH3CL  METHYL CHLORIDE  EXTRAPOLATED FROM TRC DATA USING WILHOIT'S POLYNOMIALS.
HF298=-81.96 KJ
CH3CL              P12/81C  1.H  3.CL 1.   0.G   298.150  5000.000  C  50.48770 1
 0.42952986E 01 0.72846822E-02-0.24161191E-05 0.35205838E-09-0.18406185E-13    2
-0.11793465E 05 0.84613889E 00 0.20672445E 01 0.92091523E-02 0.30426054E-05    3
-0.80342062E-08 0.32127443E-11-0.10896883E 05 0.13570794E 02-0.98581315E 04    4
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CH3F  METHYL FLUORIDE     FC-41      SIGMA=1    IA=0.525    IB=3.184     IC=3.184
NU=1149,1182(2),1464,1467(2),2930,3006(2) REF=Zachariah, Westmoreland, Burgess,
Tsang& Melius JPC 100,(1996),8737-8747    HF298=-237.66 KJ      REF=TRC/81    Max
Lst Sq. Error Cp @ 6000 K 0.60%
CH3F  FC-41        T 9/99C  1.H  3.F  1.    0.G   200.000  6000.000      34.03322 1
 3.31347981E+00 8.60493589E-03-3.08660894E-06 4.97647344E-10-2.97594910E-14    2
-3.02697942E+04 5.79751939E+00 5.03608987E+00-1.46102699E-02 6.05960722E-05    3
-6.59416863E-08 2.42194887E-11-2.98523780E+04 1.35614834E+00-2.85837650E+04    4

CH3I METHYL-IODIDE  DATA EXTRAPOLATED FROM STULL WESTRUM & SINKE TO 5000 K
USING WILHOIT'S POLYNOMIALS HF298=50.4 KCAL Max Lst Sq Error Cp @ 5000 K 0.11%.
CH3I               T 2/94C   1H   3I   1    0G   298.150  5000.000  B 141.93929 1
 0.95866778E+01 0.32097636E-02-0.12670098E-05 0.23134689E-09-0.15935166E-13    2
 0.22120136E+05-0.13346332E+02 0.40063651E+01 0.25850488E-01-0.38017768E-04    3
 0.28016824E-07-0.81110652E-11 0.23302996E+05 0.13697714E+02 0.25362120E+05    4

CH3N METHANIMINE (CH2NH) SIGMA=2 A0=6.545  B0=1.156 C0=0.979  NU=3263,3024,2914,
1638,1452,1344,1058,1127,1061  REF=M.E. Jacox JPCRD 1988, 17, p.418  HF298=20.08
KCAL   REF=Bauer & Wilcox B3LYP/6-31G(d) calculations, private communication
(Melius MP4/G2 1997 HF298=20.35+/-1.03 KCAL) Max Lst Sq Error Cp @ 6000 K 0.57%.
CH3N  (H2C=NH)     T04/98H  3.C  1.N  1.    0.G   200.000  6000.000  B  29.04156 1
 3.44258520E+01 8.37599775E-03-2.97818940E-06 4.77352575E-10-2.84294848E-14    2
 8.40771881E+03 3.95614590E+00 4.79302570E+00-1.26841686E-02 5.69766502E-05    3
-6.34985226E-08 2.37023319E-11 8.85023147E+04 1.10298133E+00 1.01045906E+04    4

CH3NO  NITROSOMETHYL or METHYL-NITROSYL SIGMA=1 IA=1.317537  IB=7.1010932
IC=7.9046  IR=0.3863 NU=2970,2943,2874,1760,1437,1435,1389,1154,983,891,567
ROSYM=3  V(3)=412.7cm-1   HF298=18.882+/-1.74 KCAL.   REF=C.Melius BAC/MP4
Database C47Y   Max Lst Sq Error Cp @ 6000 K 0.58%
CH3NO              T12/92C   1H   3N   1O   1G   200.000  6000.000  B  45.04096 1
 0.50677397E+01 0.93871079E-02-0.33958317E-05 0.55076729E-09-0.33095301E-13    2
 0.71852464E+04-0.10709779E+01 0.52463494E+01-0.68175691E-02 0.46713959E-04    3
-0.53482743E-07 0.19916692E-10 0.79241319E+04 0.18687355E+01 0.95017371E+04    4

CH3NO  FORMAMIDE O=CH-NH2   SIGMA=1  IA=1.1101014 IB= 7.2322785 IC=8.34238
IR=0.21065  NU=3547,3426,2870,1784,1597,1396,1231,1056,1036,602,552
INTERNAL ROTOR  ROSYM=2  V(3)=7998.3 cm-1    HF298=-46.669+/-2.5 KCAL.
REF=C.Melius BAC/MP4 Database C47X    Max Lst Sq Error Cp @ 200 K 0.46%
OCHNH2             T12/92N   1C   1H   3O   1G   200.000  6000.000  B  45.04096 1
 0.50996641E+01 0.96197778E-02-0.33675100E-05 0.52625772E-09-0.30639100E-13    2
-0.25835964E+05-0.22514334E+01 0.31136723E+01 0.29491209E-02 0.32396676E-04    3
-0.44756760E-07 0.18144841E-10-0.24750380E+05 0.10806345E+02-0.23484619E+05    4

CH3NO  FORMALDEHYDE-OXIME  CH2=N-OH  NU=3650,3110,2973,1647,1410,1318,1166,893,
530,953,774,400  A0=2.258  B0=0.396  C0=0.336  SIGMA=2  REF= M.E. JACOX JPCRD 19
(1990) P.1485  Max Lst Sq Error Cp @ 6000 K .45%  HF298=~7. KCAL  REF=NIST 1991.
CH2NOH             T12/92C   1H   3N   1O   1G   200.000  6000.000  B  45.04096 1
 0.61695525E+01 0.84795279E-02-0.29867632E-05 0.47595261E-09-0.28239453E-13    2
 0.88797203E+03-0.86718905E+01 0.25862255E+01 0.10725212E-01 0.14452581E-04    3
-0.28351956E-07 0.12697967E-10 0.21970777E+04 0.11543250E+02 0.35225167E+04    4

CH3NO  FORMIMIDIC-ACID  HN-CH-OH  SIGMA=1  IA=1.137793  IB=7.1567938  IC=829458
IR=0.11946  NU=3614,3381,2988,1718,1394,1335,1175,1067,1049,819
INT ROT (-NH) ROSYM=2 V(3)=4189.8 cm-1 INT ROT (OH) ROSYM=2 IR=0.126761
V(3)=8897. cm-1    HF298=-35.477+/-2.6 Kcal    REF=C.Melius BAC/MP4 Database C47
Max Lst Sq Error Cp @ 200 K 0.89%
NCH3O              T12/92N   1C   1H   3O   1G   200.000  6000.000  B  45.04096 1
 0.47124724E+01 0.10365763E-01-0.37841833E-05 0.60778864E-09-0.36085700E-13    2
-0.20246735E+05-0.47729078E+00 0.43010649E+01-0.11793465E-01 0.73237860E-04    3
-0.88185655E-07 0.34305951E-10-0.19099774E+05 0.70251243E+01-0.17852618E+05    4
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CH3NO  CH2-NH=O  SIGMA=1  IA=1.0784185  IB=6.89888  IC=7.977299  IR=0.2474
V(3)=13234. cm-1  ROSYM=2  NU=3283,3130,3020,1663,1406,1382,1244,1030,1028,888,
715    HF298=14.109+/-2.73 Kcal  REF=C.Melius BAC/MP4 Database D45  Max Lst Sq
Error Cp @ 200 K 0.84%
H3CNO              T12/92H   3C   1N   1O   1G   200.000  6000.000  B  45.04096 1
 0.51586790E+01 0.95358020E-02-0.33500983E-05 0.53311574E-09-0.31736144E-13    2
 0.45908024E+04-0.32378122E+01 0.39607020E+01-0.82834871E-02 0.64408406E-04    3
-0.79465373E-07 0.31225515E-10 0.58604280E+04 0.78294069E+01 0.70998839E+04    4

CH3NO2 Nitro-Methane  STATWT =1  SYNMO = 3 IA = 6.45024  IB = 8.24944
IC = 14.181  I(red)=0.47695   V(2) = 0.0 kcal/mole  ROSYM =2  NU= 598,639,666,
928,1083,1157,1380,1400,1440,1481,1561,2484,2767,2962.  REF=McKean & Watt J. Mol
Struct. 61(1976),164   HF(298)= -19.3 kcal/mole   REF=Knobel, Mirishnichenko
& Lebedev, Bull.Acad Sci USSR  Div. Chem Sci 1971,425  Max Lst Sq Error Cp @
1300 K 0.56%
CH3NO2             T01/00C  1.H  3.N  1.O  2.G   200.000  6000.000  B  61.04036 1
 6.73034758E+00 1.09601272E-02-4.05357875E-06 6.67102246E-10-4.04686823E-14    2
-1.29143475E+04-1.01800883E+01 3.54053638E+00 1.86559899E-03 4.44946580E-05    3
-5.87057133E-08 2.30684496E-11-1.11385976E+04 1.06884657E+01-9.71208165E+03    4

CH3ONO2 Methyl-Nitrate    SYMNO = 1 STATWT = 1  IA = 6.67244  IB = 17.20275
IC =  23.3497    Ir (NO2) = 5.96  ROSYM = 2  V(2) = 9.1 kcal/mole
Ir (CH3) = 0.53436 ROSYM = 3 V(3) = 2.32 kcal/mole    NU=3008,2940,2907,1672,
1468,1435,1434,1287,1176,1136,1017,854,759,657,578,340.    REF =Brand & Cawthon
JACS 77,(1955),319.  HF298=-29.16 kcal REF = Roy & Ogg J. Phys. Chem. 63(1959),
1522.   Max Lst Sq Error Cp @ 1300 K 0.66%
CH3ONO2            T05/98C  1.H  3.N  1.O  3.G   200.000  6000.000  B  77.03976 1
 9.77845489E+00 1.10069541E-02-4.25928645E-06 7.18198185E-10-4.42041793E-14    2
-1.88804487E+04-2.39163197E+01 3.91363583E+00 1.52137945E-02 1.73479131E-05    3
-3.37074473E-08 1.44322204E-11-1.66103232E+04 9.44208392E+00-1.46737980E+04    4

CH3N2  CH3N=N* METHYL DIAZINE RADICAL  STATWT=2  SIGMA=3  IA=1.20736  IB=7.14898
IC=7.83945  NU=2972,2971,2888,1507,1453,1449,1375,1096,1035,821,445,147.9
HF298=247.7+/-12. KJ REF=C. MELIUS DATABASE BACMP4 #840 A67F Max Lst Sq Error Cp
@ 6000 K 0.58%
CH3N2 CH3N=N*      T 9/96C   1H   3N   2    0G   200.000  6000.000  B  43.04830 1
 0.57393539D+01 0.92314020D-02-0.33396566D-05 0.54160230D-09-0.32522545D-13    2
 0.27235968D+05-0.53905119D+01 0.46506054D+01-0.14932994D-02 0.37619849D-04    3
-0.46522472D-07 0.17885496D-10 0.28216313D+05 0.35837652D+01 0.29785394D+05    4

CH3O  METHYLOXIDE  STATWT=2.  SIGMA=3.     A0=5.21  B0=C0=0.932 NU=2840,1362,1047,
2774(2),1487(2),653(2) T0=31614.5  NU=3079,1315,660,2962(2),1407(2),595(2)
REF=M. JACOX JPCRD 17 (1988), 419 Max Lst Sq Error Cp @ 1300 K 0.57%.
HF298=16.3 kJ  REF=Burcat & Kudchadker (1979).
CH3O               L 8/88C  1H   3O   1    0G   200.000  6000.000  B  31.03422 1
 0.42653308E+01 0.78576406E-02-0.28410438E-05 0.46045190E-09-0.27631906E-13    2
 0.59351066E+02 0.39309947E+00 0.32652337E+01 0.33031665E-02 0.17048801E-04    3
-0.22709630E-07 0.88071768E-11 0.73229580E+03 0.74257357E+01 0.19625450E+04    4

H3CO HYDROXYMETHYLENE RAD (CH2OH)   STATWT=2.  SIGMA=1.  IA=.4443  IB=2.8205
IC=32251 IR=0.982  NU=3650,2844,1459,1334,1048,1183,2960,607   ROSYM=2 POTENTIAL
BARRIER  V(2)=700  T0=41064  IA=.4041  IB=3.0848  IC=3.1518 NU=3650,2844,
1459, 1091,1351,1623,2960,950,573  STATWT=2    REF=M. JACOX JPCRD 17 (1988) 420
+ BURCAT & KUDCHADKER  Max Lst Sq Error Cp @ 6000 K 0.4%  HF298=-17.8+/-1.3 KJ.
REF= Atkinson et al. JPCRD 29,(2000),167.
CH2OH              T12/00C  1H   3O   1    0G   200.000  6000.000  B  31.03422 1
 4.72398695E+00 6.50832540E-03-2.24240605E-06 3.51742805E-10-2.06424726E-14    2
-3.95577100E+03 1.47350104E+00 4.73864580E+00 1.27132491E-03 1.46005656E-05    3
-1.83666166E-08 7.07708694E-12-3.70620951E+03 2.65277676E+00-2.14083572E+03    4
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CH3O2  METHYLPEROXIDE RAD (CH3OO)  SIGMA=1  STATWT=2  IA*IB*IC=7.203 E-116
NU=2930(3),1400(2),1350,1100,960,900(2),450,300 (FREE INTERNAL ROTATION).
REF=W. TSANG  JPCRD 15 (1986) 1087.  MAX LST SQ ERROR CP @ 1300 K .72 %
HF300=6.7 KCAL REF=Benson
CH3O2              L 1/84C  1H   3O   2     0G   300.000  5000.00   C  47.034   1
 0.66812963E 01 0.80057271E-02-0.27188507E-05 0.40631365E-09-0.21927725E-13    2
 0.52621851E 03-0.99423847E 01 0.20986490E 01 0.15786357E-01 0.75683261E-07    3
-0.11274587E-07 0.56665133E-11 0.20695879E 04 0.15007068E 02 0.33715510E+04    4

CH3S RADICAL  SIGMA=3  STATWT=2  IA=0.53164  IB=6.02619  IC=6.04473  REF=BURCAT
NU=2776,1313,727,2706,1496,586,[1098,401,635] REF= Chiang & Lee J.Chem. Phys. 95
(1991), 66. HF298=29.78 KCAL  REF=Nicovich et al. J. Chem. Phys. 96,(1992),2518
Max Lst Sq. Erroe Cp @ 1300 0.47%.
CH3S               T 5/93C   1H   3S   1     0G   200.000  6000.000  D  47.10082 1
 0.65678714E+01 0.59142537E-02-0.21696985E-05 0.35515294E-09-0.21464598E-13    2
 0.12405931E+05-0.10366792E+02 0.19296246E+01 0.19284464E-01-0.16194139E-04    3
 0.61734966E-08-0.54733095E-12 0.13684473E+05 0.13507111E+02 0.14985792E+05    4

CH4    RRHO        J 5/61C  1H   4    0     0G   300.000  5000.000  B  16.0428  1
 0.23594046E 01 0.87309405E-02-0.28397053E-05 0.40459835E-09-0.20527095E-13    2
-0.10288820E 05 0.60290012E 01 0.29283962E 01 0.25691092E-02 0.78437060E-05    3
-0.49102979E-08 0.20380030E-12-0.10054172E 05 0.46342220E 01-0.89722666E+04    4

CH4 METHANE  STATWT=1. SIGMA=12.  IA=IB=IC=0.52410356  NU=2916.7,1533.295(2),
3019.491(3),1310.756(3)  X11=-26,X12=-3,X13=-75,X14=-4,X22=-.4,X23=-9,X24=-20,
X33=-17,X34=-17,X44=-11  ALFA1=.01,ALFA2=-.09,ALFA3=.04,ALFA4=.07 D0=1.10864E-4
REF=TSIV  MAX LST SQ ERROR CP @ 1300K 0.84% . HF298=-74.6 KJ
CH4   ANHARMONIC  L 8/88C  1H   4    0     0G   200.000  6000.000  A  16.04276 1
 0.16354256E+01 0.10084431E-01-0.33692369E-05 0.53497280E-09-0.31552817E-13    2
-0.10005603E+05 0.99936953E+01 0.51498792E+01-0.13671008E-01 0.49180130E-04    3
-0.48474403E-07 0.16669441E-10-0.10246648E+05-0.46413244E+01-0.89722666E+04    4

CH4N  CH3NH* METHYL AMINO RADICAL  STATWT=2  SIGMA=3    IA=0.6587  IB=3.3113
IC=3.4543  NU=3257,2937,2871,2830,1468,1458,1406,1303,1016,966,965,252.6
HF298=187.6+/-4.77 KJ  REF=C. MELIUS DATABASE BACMP4 #999 N38X  Max Lst Sq Error
Cp @ 6000 K 0.57 %
CH4N CH3NH*        T 9/96C   1H   4N   1     0G   200.000  6000.000  B  30.04950 1
 0.43023153D+01 0.10277337D-01-0.36593760D-05 0.58702457D-09-0.34979453D-13    2
 0.20473126D+05 0.13025403D+00 0.47462749D+01-0.71705198D-02 0.50242579D-04    3
-0.58589231D-07 0.22243219D-10 0.21124201D+05 0.17162390D+01 0.22559203D+05    4

CH4N2O  Urea  (NH2)2C=O  IAIBIC=936.8E-117  SIGMA=2  NU=3548,3448,3440(2),1734,
1594(2),1394,1014,1000,790,618,600,578,542,410,233,228      HF298=-235.5 kJ
REF=Dorofeeva & Tolmach Thermochim. Acta 240, (1994),47-66. Max Lst Sq Error
Cp @ 6000 K  0.38 %
(NH2)2C=O Urea     T10/99C  1.H  4.N  2.O  1.G   200.000  6000.000  B  60.05564 1
 8.96505812E+00 1.08623207E-02-3.73612748E-06 5.85618314E-10-3.43401569E-14    2
-3.19075377E+04-2.11968192E+01 1.27019759E+00 3.79235458E-02-4.13652154E-05    3
 2.49128013E-08-6.09879982E-12-3.00691642E+04 1.71177671E+01-2.83239782E+04    4

CH4N4O2 NITROGUANIDINE (PICRITE) (NH2)2C=N-NO2  REF= Dorofeeva & Tolmach
Thermochim. Acta 240, (1994),47-66. Data estimated by Dorofeeva and extrapolated
to 5000 K using Wilhoit's polynomials. HF298=1.+/-20. kJ    Max Lst Sq
Error Cp @ 1200 K 0.49%
Nitroguanidine     T10/99C  1.H  4.N  4.O  2.G   298.150  5000.000  D 104.06852 1
 1.38288509E+01 1.52703007E-02-5.55748705E-06 9.62860873E-10-6.41418016E-14    2
-5.38226605E+03-4.25512674E+01 5.74393403E-01 6.18916652E-02-7.09491928E-05    3
 4.52102784E-08-1.22867606E-11-2.25858616E+03 2.33882854E+01 1.20271670E+02    4
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CH3OH liquid METHANOL DATA TAKEN FROM TRC 12/87 HF298=-57.101 kcal
CH3OH(L)          P12/87C  1.H  4.O  1.   0.L   200.000   468.000  C  32.04216 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00 5.88066591E+00 5.00819112E-02-3.53131418E-04    3
 1.00311460E-06-7.91670649E-10-3.12023523E+04-2.47332972E+01-2.87341748E+04    4

CH4O  METHANOL (CH3OH)   STATWT=1.  SIGMA=3.  SIGMA BARRIER=3. IA=.6578
IB=3.4004  IC=3.5306  IR=.0993 NU=3681,3000,2844,1477,1455,1345,1060,1033,2960,
1477,1165,298  POTENTIAL BARRIER  V3=373.21  V6=-0.521   REF=CHEN WILHOIT &
ZWOLINSKI  MAX LST SQ ERROR CP @ 1300 K  0.82%. HF298=-200.94 KJ
CH3OH             L 8/88C  1H   4O   1     0G   200.000  6000.000  B  32.04216 1
 0.36012593E+01 0.10243223E-01-0.35999217E-05 0.57251951E-09-0.33912719E-13    2
-0.25997155E+05 0.47056025E+01 0.57153948E+01-0.15230920E-01 0.65244182E-04    3
-0.71080873E-07 0.26135383E-10-0.25642765E+05-0.15040970E+01-0.24167389E+05    4

CH4O2 PEROXYMETHANE (CH3OOH) SIGMA=1  STATWT=1 IA=1.8264 IB=7.73148 IC=8.8279
IR(OH)0.12964 IR(CH3)=0.4352 POTENTIAL BARRIER V3(OH)=447.7 V3(CH3)=1164.7 cm-1
NU=3650,2961,2938,2873,1434,1453,1440,1379,1201,1155,1107,926,445  REF= BAC/MP4
Melius Database 1993  HF298=-33.4+/-1.2 Kcal REF=Lay et.al JPC 100 (1996),8240
Max Lst Sq Error Cp @ 6000 0.48%
CH4O2             T11/96C   1H   4O   2     0G   200.000  6000.000  B  48.04156 1
 6.86907934E+00 1.00840883E-02-3.66515947E-06 5.96302681E-10-3.58894156E-14    2
-1.98402231E+04-1.24951986E+01 3.72654981E+00 7.51851847E-03 2.35970425E-05    3
-3.52694507E-08 1.42757614E-11-1.83982011E+04 6.52443362E+00-1.68074366E+04    4

CH3SH METHANETHIOL  SIGMA=1  IA=0.797364  IB=6.4954022  IC=6.76794  IR=0.181954
NU=2970(2),2892,2599,1460,1449,1358,1088,964,778,692 POT BARRIER V(3)=454.7cm-1
ROSYM=2  HF298=-5.38+/-1 KCAL  REF=C. Melius BAC/MP4 Database, S6B   Max Lst Sq
Error Cp @ 6000 K 0.55%
CH4S              T 4/93C   1H   4S   1     0G   200.000  6000.000  B  48.10876 1
 0.46777426E+01 0.95699729E-02-0.34209825E-05 0.55016476E-09-0.32838372E-13    2
-0.48206134E+04 0.10108699E+01 0.42867053E+01-0.12993254E-04 0.29820894E-04    3
-0.37118619E-07 0.14368072E-10-0.41817048E+04 0.56301215E+01-0.27073057E+04    4

CH5N  METHYLAMINE (CH3NH2)  STATWT=1.  SIGMA=1.  IA=.81375  IB=3.8663  IC=3.7089
IR=0.5288  POT BARRIER V(3)=1980.  ROSYM=6   NU=3361,2961,2820,1623,1473,1430,
1130,1044,780,3427,2985,1485,1419,1195      REF=Dewar & Rzepa  Max Lst Sq Error
Cp @ 1300K 0.83% .HF298=-5.5 KCAL  REF=Stull, Westrum & Sinke
CH5N              T09/81C  1H   5N   1     0G   300.000  5000.000  C  31.0574  1
 0.44235811E+01 0.11449948E-01-0.36999727E-05 0.52389848E-09-0.26375054E-13    2
-0.49847539E+04-0.41469345E+00 0.27267694E+01 0.10014653E-01 0.67409546E-05    3
-0.98750093E-08 0.30637376E-11-0.40688989E+04 0.10215076E+02-0.27676911E+04    4

CH5N2  METHYL HYDRAZINE RADICAL CH3N*NH2  SIGMA=6  STATWT=2  IA=1.779  IB=7.9946
IC=9.1582  NU=3442,3308,2951,2880,2822,1647,1464,1455,1414,1316,1230,1073,1031,
932,755,453,385,143.9    HF298=51.43+/-1.3 kcal    REF=C.MELIUS DATABASE  N86A
Max Lst Sq Error Cp @ 6000 K 0.54%
CH5N2 CH3N*NH2    T 9/96C   1H   5N   2     0G   200.000  6000.000  B  45.06418 1
 0.62727186D+01 0.13750206D-01-0.48829875D-05 0.78213769D-09-0.46564024D-13    2
 0.22861878D+05-0.96381311D+01 0.42113439D+01 0.34130124D-02 0.41788037D-04    3
-0.55495848D-07 0.21958966D-10 0.24203232D+05 0.48609693D+01 0.25880433D+05    4

CH5N4 GUANIDINE  (NH2)2C=NH  SIGMA=4 IAIBIC=1010.E-117   NU=3450,3400(3),3260,
1670,1640,1611,1450,1300,1284,1000(2),800(2),600,550,400(2),230(2)
REF= Dorofeeva & Tolmach  Thermochim. Acta 240, (1994),47-66.
HF298=15.+/-10. kJ    Max Lst Sq Error Cp @ 1200 K 0.49%
CH5N4 GUANIDINE   T10/99C  1.H  5.N  3.   0.G   200.000  6000.000  B  59.07092 1
 8.64673050E+00 1.38037583E-02-4.78895966E-06 7.55059297E-10-4.44582536E-14    2
-5.52365417E+03-2.09594729E+01 2.30997765E+00 2.84093787E-02-1.07395307E-05    3
-7.11224938E-09 5.50455394E-12-3.64916310E+03 1.24181134E+01-1.80407504E+03    4
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CH6N2 METHYLHYDRAZINE CH3-NH-NH2 SIGMA=1  IA=2.198  IB=8.775  IC=9.981  NU=3316,
3304,3258,2962,2782,1622,1469,2938,1445,1412,1305,1200,1118,1137,1104,992,888,
821,447,315 CH3-ROTOR IR=0.432 ROSYM=3 POT BARRIER V(3)=1283.    REF=Durig,
Harris & Wertz J. Chem. Phys 50, (1969), 1449  HF298=22.6 KCAL  REF=Stein et.al
NIST PROGRAM 1991. Max Lst Sq Error Cp @ 6000 K 0.54%
CH6N2             T 2/92C   1H   6N   2    0G   200.000  6000.000  B  46.07212 1
 0.75413086E+01 0.14079165E-01-0.50307978E-05 0.80927230E-09-0.48327049E-13    2
 0.77794950E+04-0.16320371E+02 0.37698582E+01 0.41854649E-02 0.53726419E-04    3
-0.75016804E-07 0.30685682E-10 0.97217733E+04 0.78388323E+01 0.11372697E+05    4

CN  CYANID RADICAL  REF=TSIV  T0=0 WE=2068.435 WEXE=12.9765 WEYE=-3.082E-2
WEZE=-1.228E-3 BE=1.89931 ALFAB1=1.72786E-2 ALFAB2=-4.74E-5 ALFAB3=-4.512E-7
ALFAB4=3.533E-10 ALFAB5=-7.87E-12 DE=6.3782E-6 BETA1=-4.39E-8 BETA2=-9.65E-9
BETA3=-6.9E-10 T0=9240.041 WE=1813.474 WEXE=12.8272 WEYE=5.61E-3 WEZE=4.192E-4
BE=1.71547 ALFAB1=1.73452E-2 ALFAB2= 9.583E-6 ALFAB3=2.756E-6 ALFAB4=4.323E-8
ALFAB5=3.324E-9 ALFAB6=1.6E-10 ALFAB7=-3E-12 DE=6.1534E-6 BETA1=-0.781E-8
BETA2=6.83E-10 BETA3=-1.164E-10   T0=25752. WE=2163.9 WEXE=20.2 BE=1.985
ALFAB1=2.3E-2 DE=6.543 BETA1=8.7E-8  T0=32400. WE=1249  T0=43000. WE=873.
T0=47700. WE=1274. T0=53800. WE=1286. T0=54486. WE=1004.7 WEXE=8.78 BE=1.162
ALFAB1=1.3E-2 T0=59151.18 WE=1681. WEXE=3.6 WEYE=-1.02 BE=1.4871 ALFAB1=0.643
DE=5.E-6 T0=60095.5 WE=1243. WEXE=14. BE=1.384 ALFAB1=2.E-2 T0=61154.96 WE=1651.3
WEXE=43.84 BE=1.521 ALFAB1=0.21E-2  T0=62400. WE=950.7  T0=63700. T0=64223.98
WE=1121.76 WEXE=14.203 WEYE=0.18 BE=1.306 ALFAB1=2.1E-2 DE=5.8E+6  T0=64400
WE=1225.5 T0=69500. WE=651.5   T0=70200. WE=1183.2  T0=70700. WE=1446.4
HF298=104.47+/-1.5 KCAL REF=Huang, Barts & Halpern J.Phys.Chem. 96, (1992), 425.
CN                T 6/94C   1N  1    0     0G   200.000  6000.000  A  26.01774 1
 0.37459804E+01 0.43450773E-04 0.29705984E-06-0.68651804E-10 0.44134174E-14    2
 0.52353188E+05 0.27867600E+01 0.36129350E+01-0.95551327E-03 0.21442976E-05    3
-0.31516324E-09-0.46430356E-12 0.52525340E+05 0.39804995E+01 0.52571034E+05    4

NCO  SIGMA=1 STATWT=2 IB=7.18666  NU=1275,532.7(2),1922 T0=95.2 SIGMA=1 STATWT=2
REF=TSIV  HF298=31.5 Kcal  REF= East & Allen J.Phys.Chem. 99 (1993), 4638   Max
Lst Sq Error Cp @ 1300 K 0.31%
CNO               T 6/94C   1N   1O   1    0G   200.000  6000.000  B  42.01714 1
 0.51075979E+01 0.23371500E-02-0.88984637E-06 0.14920037E-09-0.91663122E-14    2
 0.14024945E+05-0.22908127E+01 0.27405490E+01 0.95089992E-02-0.10338762E-04    3
 0.68805052E-08-0.20963552E-11 0.14690320E+05 0.98908197E+01 0.15851325E+05    4

CNN  SIGMA=1  STATWT=3  IB=6.5  NU=1241,393(2),2847  T0=3000  SIGMA=1  STATWT=2
T0=4000  SIGMA=1 STATWT=1 REF=TSIV  HF298=400.65 KJ
CNN               RUS 79C  1N   2    0     0G   200.000  6000.000  B  40.02448 1
 0.41398983E+01 0.38071002E-02-0.14753456E-05 0.24441991E-09-0.14746300E-13    2
 0.46790796E+05 0.32444306E+01 0.27584988E+01 0.12901042E-01-0.22802003E-04    3
 0.21393697E-07-0.75499090E-11 0.46953824E+05 0.91902188E+01 0.48186940E+05    4

CN2  NCN  SIGMA=2  STATWT=3  B0=.397  NU=1197,370(2),1475  T0=30383.74  B0=.396
STATWT=6  NU=1154,460(2),1475  REF=JACOX JPCRD (1988)  HF0=500. KJ
REF=Gurvich 1991
NCN     (NCN)     L12/89N  2.C  1.   0.   0.G   200.000  6000.000  B  40.02448 1
 5.73815514E+00 1.77244606E-03-6.85751131E-07 1.15711980E-10-7.07567907E-15    2
 5.82214890E+04-6.30533665E+00 3.24134033E+00 8.50091346E-03-7.61608140E-06    3
 3.64986585E-09-8.42551872E-13 5.89477370E+04 6.70956450E+00 6.02315091E+04    4
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C(NO2)4 Tetra-Nitro-Metane  SYMNO = 4   Ia = 81.178919  Ib = 109.0935512
Ic = 119.96637        (Ir(NO2) = 5.96  ROSYM = 2  V(2)= 0.2 kcal/mole)4
NU = 1985,1565,1213,1192(2),1146,1129,1015,791,701,687,672,646,640,594,562,
491,481,408,378,357,354,344,333,206,191,183,146,138.    REF =A.BURCAT TAE
Report # 824 1998   HF298=19.69  kcal   REF = Lebedev et. al. Russ. J. Phys.
Chem. 49,(1975), 1133 Eng. Transl. Max Lst Sq Error Cp @ 1300 K 0.45%.
C(NO2)4           T10/98C  1.O  8.N  4.   0.G   200.000  6000.000  B 196.03316 1
 2.63028700E+01 9.03437992E-03-3.84962536E-06 6.80136488E-10-4.29929370E-14    2
 2.32054355E+02-9.52181326E+01 1.50837189E+00 9.93550200E-02-1.38531389E-04    3
 9.75231469E-08-2.77303820E-11 6.08687871E+03 2.77172777E+01 9.90833615E+03    4

CO  CARBON-MONOXIDE  CALCULATED FROM TSIV TABLE. REF=TSIV 79  HF298=-110.53 KJ
Max Lst Sq Error Cp @ 1300 K 0.12%.
CO                RUS 79C  1O   1    0     0G   200.000  6000.000  A  28.01040 1
 0.30484859E+01 0.13517281E-02-0.48579405E-06 0.78853644E-10-0.46980746E-14    2
-0.14266117E+05 0.60170977E+01 0.35795335E+01-0.61035369E-03 0.10168143E-05    3
 0.90700586E-09-0.90442449E-12-0.14344086E+05 0.35084093E+01-0.13293628E+05    4

COS CARBON OXIDE SULFIDE  SIGMA=1  B0=0.20287 cm-1  NU=2064,859,524(2)  x11=-4.0
x22=-0.4   x33=-7.0   x12=-6.8   x23=-11.5   x13=-4.5   ALFA1=0.0006044
ALFA2=0.0003539  ALFA3=0.001838 A000=0 C000=0 D000=4.37E-8  HF298=-138.407+/-1.0
KJ  REF=JANAF
COS               J 3/61C  1O   1S   1     0G   300.000  5000.000  A  60.0764  1
 0.52392000E 01 0.24100584E-02-0.96064522E-06 0.17778347E-09-0.12235704E-13    2
-0.18480455E 05-0.30910517E 01 0.24625321E 01 0.11947992E-01-0.13794370E-04    3
 0.80707736E-08-0.18327653E-11-0.17803987E 05 0.10792556E 02-0.16646069E-05    4

CO2  CARBON-DIOXIDE   SIGMA=2   B0=0.39027   NU=1333.5,667(2),2351   X11=-3.014
X12=-5.058   X12=-19.048   X22=1.521   X23=-12.616   X33=-12.597   G22=-1.422
Y111=.0184   Y112=-.0667   Y113=-.0944    Y122=-.0657  Y123=.0880   Y133=.0268
Y222=.0105   Y223=-.0168   Y233=.0320   Y333=.0115   W0=51.834   ALPHA1=.00115
ALPHA2=-.000715   ALPHA3=.00311   D000=.129E-6   T0=30000 STATWT=3;   T0=33000
STATWT=6  T0=36000  STATWT=3;  T0=45000  STATWT=2;  REF=Gurvich Vol 2 1991 p.27
HF298=-393.51 KJ    Max Lst Sq Error Cp @ 1400 K 0.4%
CO2               L 7/88C  1O   2    0     0G   200.000  6000.000  A  44.00980 1
 0.46365111E+01 0.27414569E-02-0.99589759E-06 0.16038666E-09-0.91619857E-14    2
-0.49024904E+05-0.19348955E+01 0.23568130E+01 0.89841299E-02-0.71220632E-05    3
 0.24573008E-08-0.14288548E-12-0.48371971E+05 0.99009035E+01-0.47328105E+05    4

CP  CARBON PHOSPHIDE T0=0 Be=0.7986 WE=1239.67 WEXE=6.86 ALPHAE=0.00597 De=1.33
T0=7053.2  Be=0.7135  WE=1061.99  WEXE=6.035  ALPHAE=0.0058 De=1.3
T0=29100.4 Be=0.6829  WE=836.32  WEXE=5.917  ALPHAE=0.00628  De=1.83
{HF298=449.9+/-9 kJ  REF=JANAF 1985} HF298=72.466 kJ REF=Gurvich 1991
CP                L 9/93C  1.P  1.   0.   0.G   200.000  6000.000  C  42.98476 1
 4.16986061E+00-3.33893154E-04 6.30510095E-07-1.65248916E-10 1.25248542E-14    2
 6.12121016E+04 2.05762288E+00 3.70291400E+00-2.94026330E-03 1.25263783E-05    3
-1.43948287E-08 5.61955320E-12 6.15029332E+04 5.34971467E+00 8.71534000E+03    4

CS  CARBON SULFIDE  SIGMA=1  Be=0.820046  WE=1285.08  WEXE=6.46  ALPHAE=0.005922
T0(STATWT)=0(1),27509(2),27590(2),27607(2),38613.9(6),38797.6(2),38851.8(3),
39160.8(3),39170(2),39950(2)  HF298=280.3+/-25 KJ  REF=JANAF
CS                J12/76C  1S   1   000    0G   300.000  5000.000  A  44.0770  1
 0.36826012E+01 0.90473203E-03-0.36436374E-06 0.63854294E-10-0.36933982E-14    2
 0.32497490E+05 0.38850496E+01 0.34039344E+01-0.65773308E-03 0.61712157E-05    3
-0.73689604E-08 0.27346738E-11 0.32689393E+05 0.58977001E+01 0.33711396E+05    4
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CS2  CARBON DISULFIDE  SIGMA=2  Be=0.109277 cm-1 D0=1.05E-8  g22=-0.74
NU=657.98,395.93(2),1535.35  x11=-0.83  x22=0.82  x33=-6.54  x12=-1.75
x23=-6.49 x13=-7.59  ALFA1=0.0002144 ALFA2=0.000713  ALFA3=-0.0002148
HF298=116.943+/-0.84 KJ  REF=JANAF
CS2                J12/76C  1S   20   00    0G   300.000  5000.000  A  76.1430  1
 0.59252610E+01 0.18252996E-02-0.75585380E-06 0.14605073E-09-0.10438595E-13    2
 0.12048071E+05-0.60723317E+01 0.28326013E+01 0.13290791E-01-0.18144694E-04    3
 0.12831681E-07-0.36800609E-11 0.12766782E+05 0.92087947E+01 0.14064616E+05    4

C2  CALCULATED FROM TSIV TABLES HF298=830.86 KJ
C2                 RUS 79C   2   0    0     0G   200.000  6000.000  A  24.02200 1
 0.37913706E+01 0.51650473E-03-0.25486960E-07-0.82263554E-11 0.10086168E-14    2
 0.99023059E+05 0.28151802E+01 0.86470550E+00 0.39353120E-01-0.11981818E-03    3
 0.13908103E-06-0.55205503E-10 0.98731303E+05 0.11530141E+02 0.99928438E+05    4

C2Br2F4  1,2 DIBROMO TETRAFLUORO ETHANE, HALON 2402  SIGMA=2   IA=39.179
IB=155.14416  IC=163.61  IR=26.4159  NU=(scaled by .89) 1229,1221,1200,1121,
1023,754,631,526,487,333.5,326,306,298.5,264,194,182,121  ROSYM=3 POT BARRIER
V(3)=5141.4 cm-1 (estim).     REF=M.Karni Gaussian 89 calc 5/93 + Burcat
HF298=-189.0+/- 1.0 Kcal    REF=Kolosov & Papina Russ. Chem. Rev 52, (1983),
p.754.  Max Lst Sq Error Cp @ 1300 K 0.34%
C2BR2F4            T 8/95C   2BR  2F   4    0G   200.000  6000.000  C 259.82361 1
 0.16927925D+02 0.52040023D-02-0.21650634D-05 0.37666686D-09-0.23550019D-13    2
-0.10111059D+06-0.69271880D+02 0.43050634D+01 0.50253865D-01-0.66832698D-04    3
 0.44622030D-07-0.12028279D-10-0.98117172D+05-0.65395609D+01-0.95107950D+05    4

C2Cl RADICAL STATWT=2 IB=13.5 NU=800,359(2),2050  REF=TSIV 1979 Max Lst Sq Error
Cp @ 1300 K 0.32 %  HF298=494.09 KJ
C2CL               RUS 79C   2CL  1    0    0G   200.000  6000.000  B  59.47470 1
 0.56234123E+01 0.18105201E-02-0.68417616E-06 0.11416613E-09-0.69911780E-14    2
 0.57535699E+05-0.37681711E+01 0.25669685E+01 0.16082406E-01-0.28879777E-04    3
 0.26238319E-07-0.91509851E-11 0.58152495E+05 0.10748857E+02 0.59425029E+05    4

C2Cl2  DICHLOROACETYLENE  SIGMA=2   B0=0.046368 cm-1    NU=2200,410,925,380(2),
165(2)  HF298=209.6=/-42 KJ  REF=JANAF
C2CL2              J12/68C  2CL  20   00    0G   300.000  5000.000  C  94.9274  1
 0.81728547E 01 0.23659892E-02-0.96552505E-06 0.17736148E-09-0.12135203E-13    2
 0.22510190E 05-0.14916744E 02 0.50229482E 01 0.14082667E-01-0.18095669E-04    3
 0.11610348E-07-0.28817478E-11 0.23227482E 05 0.59684170E 00 0.25208379E+05    4

C2Cl2F4  DICHLOROTETRAFLUOROETHANE  FC-114  SIGMA=2   TRC DATA EXTRAPOLATED TO
6000 K USING WILHOIT'S POLYNOMIALS HF298=-900.4 KJ  Max Lst Sq Error Cp @ 1200 K
0.29%.
C2CL2F4            P 6/89C   2CL  2F   4    0G   200.000  6000.000  C 170.92101 1
 0.18371829E+02 0.35022641E-02-0.14461714E-05 0.25677130E-09-0.16390256E-13    2
-0.11490699E+06-0.64188919E+02 0.15529390E+01 0.61192651E-01-0.77774410E-04    3
 0.46109224E-07-0.10412101E-10-0.11087452E+06 0.19780366E+02-0.10829261E+06    4

C2CL3 TRICHLOROVINYL RADICAL  STATWT=2  IAIBIC=9.9E-113  NU=625,950,850,1600,
300,200(2),400,450  REF=TSIV 1979  Max Lst Sq Error Cp @ 1200 K 0.3%
HF298=190.28 KJ
C2CL3              RUS 79C   2CL  3    0    0G   200.000  6000.000  C 130.38010 1
 0.10595050E+02 0.24399967E-02-0.95037713E-06 0.16169666E-09-0.10033459E-13    2
 0.19234142E+05-0.22503828E+02 0.26913275E+01 0.34419583E-01-0.54507749E-04    3
 0.43131421E-07-0.13498250E-10 0.20955741E+05 0.15941066E+02 0.22885293E+05    4
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C2Cl3F3  TRICHLOROTRIFLUOROETHANE CCl2F-CClF2  FC-113  SIGMA=1 TRC  DATA
EXTRAPOLATED TO 6000 K  USING WILHOIT'S POLYNOMIALS  HF298=-705.8 KJ  Max Lst Sq
Error Cp @ 1300 K 0.36%
CCl2F-CCLF2        P 6/89C   2CL  3F   3    0G   200.000  6000.000  C 187.37531 1
 0.18530350E+02 0.34300395E-02-0.14462044E-05 0.25941090E-09-0.16648746E-13    2
-0.91474377E+05-0.62171585E+02 0.24748737E+01 0.60785666E-01-0.83261974E-04    3
 0.55593237E-07-0.14834855E-10-0.87694606E+05 0.17547918E+02-0.84887744E+05    4

C2Cl3F3  111-TRICHLORO 222-TRIFLUORO ETHANE CF3-CCl3  (FC-113A) SIGMA=9   TRC
DATA EXTRAPOLATED TO 6000 K USING WILHOIT'S POLYNOMIALS  HF298=-740.5 KJ Lst Sq
Error Cp @ 1200 K 0.35%.
C2CL3F3  FC-113A  P 6/89C   2CL  3F   3    0G   200.000  6000.000  C 187.37531 1
 0.18413343E+02 0.35473766E-02-0.15023623E-05 0.27024166E-09-0.17375093E-13    2
-0.95640066E+05-0.63672664E+02 0.29342707E+01 0.56805544E-01-0.73255691E-04    3
 0.45121198E-07-0.10894098E-10-0.91909696E+05 0.13640335E+02-0.89073199E+05    4

C2CL4 TETRACHLOROETHYLENE DATA TAKEN FROM TRC/12/82 EXTRAPOLATED USING WILHOIT'S
POLYNOMIALS.  HF298=-12.13 KJ
C2CL4              L10/87C  2.CL 4.   0.   0.G   298.150  5000.000  C 165.83400 1
 0.12935937E 02 0.34309200E-02-0.15067194E-05 0.29346993E-09-0.21070896E-13    2
-0.58932337E 04-0.34693855E 02 0.41434792E 01 0.37422372E-01-0.54369793E-04    3
 0.39112863E-07-0.11176384E-10-0.39492629E 04 0.83314072E 01-0.14589129E 04    4

C2CL5 PENTACHLOROETHYL RADICAL  STATWT=2  IAIBIC=8.3E-112 NU=550,800,850,725,775
1000,250,300,400,175,300,165,225,250 ROSYM=3 IR=24.6 V(1)=1150 1/CM REF=TSIV 79
Max Lst Sq Error Cp @ 1200 K 0.20%  HF298=39.0 KJ
C2CL5              RUS79 C   2CL  5    0    0G   200.000  6000.000  C 201.28550 1
 0.17153955E+02 0.13960259E-02-0.64226587E-06 0.11840383E-09-0.76901280E-14    2
-0.10091822E+04-0.51540891E+02 0.29430292E+01 0.63377422E-01-0.10845541E-03    3
 0.87020632E-07-0.26867241E-10 0.17951146E+04 0.16297364E+02 0.46905951E+04    4

C2Cl6 HEXACHLOROETHANE   SIGMA=6 SIGMA BARRIER=3 IAIBIC=13.865E-112 IR=24.4
V(3)=14.7 KCAL. NU=975,431,170,675,372,778(2),271(2),114(2),859(2),340(2),223(2)
HF298=-33.2 KCAL REF=Chao, Rodgers, Wilhoit & Zwolinski JPCRD 3, (1974), 141
C2CL6              L10/87C  2.CL 6.   0.   0.G   298.150  5000.000  B 236.74000 1
 0.19034286E 02 0.33956821E-02-0.15115289E-05 0.29700315E-09-0.21453827E-13    2
-0.23103803E 05-0.62866080E 02 0.46383531E 01 0.63365561E-01-0.10080030E-03    3
 0.76636922E-07-0.22646550E-10-0.20156513E 05 0.64616440E 01-0.16706994E 05    4

C2D2  ACETYLENE-D2  STATWT=1.  SIGMA=2.  IB=3.2838  NU=2701,1762,2439,505(2),
537(2) X11=15.43,X12=12.1,X13=58.78,X14=10.87,X15=6.92,X22=6.31,X23=.91,X24=
8.34,X25=.56,X34=5.54,X35=3.13,X44=-3.66,X45=7.7,X55=1.24,X33=14.3,G44=-0.75,
G55=-1.36  REF=SHIMANOUCHI  MAX LST SQ ERROR CP @ 1300K 0.55% . HF0=53.22 KCAL
derived from HF0 of C2H2 in JANAF 1971.
C2D2               T 8/80C  2D   2    0     0G   300.000  5000.000  A  28.0502  1
 0.57631445E+01 0.39823391E-02-0.14399011E-05 0.21952536E-09-0.12146185E-13    2
 0.24641469E+05-0.92791763E+01 0.37629929E+01 0.83192550E-02-0.22101658E-05    3
-0.40820787E-08 0.27229842E-11 0.25258297E+05 0.13356880E+01 2.6723643 E+04    4

C2D2O  KETENE-D2  SIGMA=2  IA=.5974  IB=9.1958   IC=9.7932  NU=2267,2120,1228,
927,2383,855,371,542,432  REF=B.MOORE &PIMENTEL  MAX LST SQ ERROR CP @ 1300 K
0.65 %.  HF298=9.54 KCAL derived from Benson's value for C2H2O
C2D2O              T10/82C  2D   2O   1     0G   300.000  5000.000  B  44.0496  1
 0.68584700E+01 0.55908523E-02-0.19912059E-05 0.31183456E-09-0.17762101E-13    2
 0.21307729E+04-0.11521992E+02 0.34471798E+01 0.11882458E-01-0.17057137E-05    3
-0.64614767E-08 0.35897769E-11 0.32729224E+04 0.69639057E+01 0.48011892E+04    4
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C2D4  ETHYLENE-D4  STATWT=1.  SIGMA=4.   IA=1.1487  IB=3.793  IC=4.942  NU=2247,
1515,981,728,2289,1009,720,780,2345,586,2200,1078  REF=BURCAT  MAX LST SQ ERROR
CP @ 1300K 0.86% . HF298=30.27 KJ.
C2D4              T12/79C  2D   4    0     0G   300.000  5000.000  B  32.0784  1
 0.67207203E 01 0.84912479E-02-0.30327419E-05 0.47564219E-09-0.27109157E-13    2
 0.62753809E 03-0.14424983E 02 0.13294621E 01 0.17719518E-01-0.13082199E-05    3
-0.10431190E-07 0.53182406E-11 0.24874675E 04 0.15025264E 02 0.36406234E+04    4

C2OD4  ETHANAL-D4 (ACETALDEHIDE-D4)   STATWT=1   SIGMA=1  IA=2.4015  IB=9.7752
IC=11.109  IR=.64048  POT BARRIER V(3)=1161.  NU=2265,2130,2060,1737,1045,938,
1028,1151,747,436,2225,1028,573,670  REF=CHAO,WILHOIT & HALL MAX LST SQ ERROR
CP @ 1300 K 0.85 %. HF298=-43.16 KCAL.
C2OD4             T 8/81C  2D   4O   1     0G   300.     5000.     B  48.0778  1
 0.85226345E+01 0.92743672E-02-0.33571869E-05 0.53372684E-09-0.30898383E-13    2
-0.25431613E+05-0.19829504E+02 0.24537258E+01 0.18615011E-01 0.81830109E-06    3
-0.12927025E-07 0.59826883E-11-0.23262375E+05 0.13648181E+02-0.21718827E+05    4

C2D6  ETHANE-D6  STATWT=1.  SIGMA=6.  SIGMA BARRIER=3. IA=2.0942  IB=IC=6.0986
NU=2083,1155,843,2087,1077,2226(2),1041(2),970(2),2235(2),1081(2),594(2)
POTENTIAL BARRIER  V0=2.87  IR=.5235  REF=BURCAT  MAX LST SQ ERROR CP @ 1300 K
0.92 % . HF298=-110.68 KJ.
C2D6              T05/80C  2D   6    0     0G   300.000  4000.000  B  36.1066  1
 0.87366476E+01 0.11772312E-01-0.42297552E-05 0.66704353E-09-0.38247847E-13    2
-0.17392641E 05-0.25919988E 02 0.81539208E 00 0.24633620E-01 0.28606987E-07    3
-0.16559884E-07 0.79903445E-11-0.14620465E 05 0.17542796E 02-0.13311668E+05    4

C2D6N2 AZOMETHANE-D6 (CD3NNCD3)  STATWT=1  SIGMA=2  IA=3.147  IB=24.215
IC=25.133  IR=0.765  POT BARRIER V0=1700.  NU=2234,2127,1569,1122,1044,1034,761,
523,2225,1027,803,2239,1049,896,261,2240,1115,1112,1051,921,900,304,(191,166
TORSIONAL FREQ)  REF=PAMIDIMUKKALA,ROGERS &SKINNER  MAX LST SQ ERROR  CP @ 1300K
0.9 % .  HF298=28.5 KCAL.
C2D6N2            L 8/84C  2D   6N   2     0G   300.000  5000.000  B  64.12001 1
 0.13025591E 02 0.13045497E-01-0.47310468E-05 0.75233886E-09-0.43511835E-13    2
 0.86393672E 04-0.43220398E 02 0.23340378E 01 0.30852020E-01 0.74860048E-06    3
-0.23019155E-07 0.11133473E-10 0.12308605E 05 0.15217487E 02 0.14341845E 05    4

C2D6O  DIMETHYL-ETHER-D6  SIGMA=2  SIGMA BARRIER=3  IA=3.2656  IB=11.2126
IC=12.3437  IR=9.271  V(3)=2500.  NU=2248(2),2054(2),1059(4),1057(2),1033,827,
362,2202,1162,872,2184,931,950 REF=KANAZAWA AND NUKADA  MAX LST SQ ERROR @
1300 K 0.86 %. HF0=-45.9 KCAL derived from HFO of C2H6O by Stull,Westrum & Sinke
C2D6O             T12/82C  2D   6O   1     0G   300.000  5000.0    B  52.10601 1
 0.10630716E+02 0.12416139E-01-0.44895924E-05 0.71285688E-09-0.41213699E-13    2
-0.29983387E+05-0.32492361E+02 0.16130285E+01 0.27251996E-01 0.22420198E-06    3
-0.19127672E-07 0.92674445E-11-0.26856473E+05 0.16893214E+02-0.25195712E+05    4

C2F RADICAL  STATWT=2  IB=7.8  NU=1100,400(2),2175   REF=TSIV 1979  Max Lst Sq
Error Cp @ 1300 K 0.37%  HF298=353.855 KJ
C2F               RUS 79C   2F   1    0     0G   200.000  6000.000  C  43.02040 1
 0.52609167E+01 0.21458355E-02-0.80752800E-06 0.13438298E-09-0.82137530E-14    2
 0.40747737E+05-0.31423716E+01 0.27021656E+01 0.12793323E-01-0.20443809E-04    3
 0.17853370E-07-0.61796555E-11 0.41332714E+05 0.93400394E+01 0.42558732E+05    4

C2F2  DIFLUOROACETYLENE  SIGMA=2  B0=0.117932 cm-1  NU=1050,1900,1149,450(2),
300(2)  HF298=20.9+/-21 KJ  REF=JANAF
C2F2              J12/67C  2.F  2.   0.   0.G   300.000  5000.000  C  62.01881 1
 7.51645810E+00 3.16864620E-03-1.33113850E-06 2.49600490E-10-1.73420720E-14    2
-1.61076550E+02-1.50680621E+01 3.53458370E+00 1.44458450E-02-1.21896920E-05    3
 3.60429850E-09 1.91189510E-13 9.21335620E+02 5.41946520E+00 2.51676233E+03    4
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C2F3  TRIFLUOROVINYL RADICAL  STATWT=2  IAIBIC=5.2E-114  NU=925,1350,1250,1800,
500(2),250,550,300    REF= TSIV 1979   Max Lst Sq Error Cp @ 1300 K 0.42%
HF298=-228.175 KJ
C2F3                RUS 79C   2F   3    0    0G   200.000  6000.000  C  81.01721 1
 0.92799301E+01 0.37264216E-02-0.14403501E-05 0.24385276E-09-0.15080391E-13    2
-0.30844099E+05-0.19232437E+02 0.24146440E+01 0.26829183E-01-0.33928627E-04    3
 0.23191119E-07-0.67115453E-11-0.29098292E+05 0.15357683E+02-0.27442988E+05    4

C2F4  TETRAFLUOROETHYLENE  SIGMA=4 IA=15.3019  IB=25.46  IC=40.7619  NU=1872,
1340,1337,778,551,218,394,406,1186,190,508,558  HF298=-658.56=/-2.9 KJ
REF=JANAF
C2F4    FC-1114   J 6/69C  2.F  4.   0.   0.G   300.000  5000.000  B 100.01561 1
 1.10864680E+01 5.27884290E-03-2.23544000E-06 4.21668460E-10-2.94339140E-14    2
-8.32928840E+04-2.98668810E+01 3.61661830E+00 2.64886180E-02-2.24332660E-05    3
 6.22864450E-09 6.21492440E-13-8.12772420E+04 8.52376403E+00-7.92072049E+04    4

C2F5 PENTAFLOROETHYL RADICAL SIGMA=1 STATWT=2 IA=21.788 IB=33.994 IC=41.428
IR=5.128 ROSYM=3 V(3)=881. 1/CM NU=1398,1273,1227,1184,1117,820,703,604(2),514,
419,366,227,211 REF=Chen Rauk & Tschuikow-Roux J. Chem. Phys. 95 (1991), 2774
Max Lst Sq Error Cp @ 1300 K 0.36%  HF298=-213.0 Kcal
C2F5                T01/92C   2F   5    0    0G   200.000  6000.000  B 119.01402 1
 0.14093289E+02 0.44836847E-02-0.17454011E-05 0.29629851E-09-0.18397296E-13    2
-0.11234658E+06-0.42296047E+02 0.19562988E+01 0.44980179E-01-0.54414843E-04    3
 0.31961057E-07-0.73732181E-11-0.10934658E+06 0.18665321E+02-0.10718515E+06    4

C2F6  HEXAFLUOROETHANE  SIGMA=6  IA=29.3165  IB=IC=45.2602  IR=7.32  INTERNAL
ROTATION BARRIER  V=3.96 KCAL   NU=1228,1117,376(2),807,714,1251(2),348,1243(2),
523(2),619(2),220(2)   HF298=-1343.9=/- 5.0 KJ  REF=JANAF
C2F6    FC-116    J 6/69C   2F   6    0    0G   200.000  6000.000  B 138.01242 1
 0.16719258E+02 0.49437735E-02-0.19391149E-05 0.32877818E-09-0.20351232E-13    2
-0.16782926E+06-0.59061597E+02 0.13474068E+01 0.53054838E-01-0.56195247E-04    3
 0.24584738E-07-0.27593922E-11-0.16394375E+06 0.18739834E+02-0.16163310E+06    4

C2F6O2  CF3-OO-CF3 SIGMA=18 Calculated Using THERM (97) Extrapolated 1000-5000K
Using Wilhoit's Polynomials  HF298=360.2+/-3. kcal REF=Levy & Kennedy JACS 94
(1972) 3302  Max Lst Sq Error Cp @ 1000K 0.30%
CF3-O-O-CF3         T10/97C   2F   6O   2    0G   298.150  5000.000  F 170.01122 1
 1.87994539D+01 8.78358323D-03-3.68712829D-06 6.99609239D-10-4.92829440D-14    2
-1.88252514D+05-5.97973365D+01 9.11006951D+00 2.71182010D-02-1.23579087D-06    3
-2.30183402D-08 1.25085439D-11-1.85129629D+05-7.65920017D+00-1.81258643E+05    4

C2H ETHYNYL RADICAL SIGMA=1  STATWT=2 B0=1.457 NU=3328,372(2),1841  T0=4000
STATWT=4  B0=1.457 NU=3460,560(2),1850  REF=Kiefer, Sidhu, Kern, Xie,Chen,
Harding 1992   HF298=135.88 Kcal REF= NIST Webbook 1999.  MAX LST SQ ERROR CP
@ 400 K 0.34 % .
C2H ETHYNYL RAD   T07/00C  2.H  1.   0.   0.G   200.000  6000.000  B  25.02994 1
 3.66459586E+00 3.82189487E-03-1.36509398E-06 2.13253692E-10-1.23098939E-14    2
 6.72238503E+04 3.91355399E+00 2.90180321E+00 1.32859725E-02-2.80508233E-05    3
 2.89300812E-08-1.07446930E-11 6.71171170E+04 6.17234595E+00 6.83770805E+04    4


C2HCl CHLOROACETYLENE  HF298=213.8+/-42 KJ  B0=0.188645 cm-1 NU=3340,2110,756,
604(2),326(2)  SIGMA=1   REF=JANAF
C2HCL               J12/68C   2H   1CL  1    0G   200.000  6000.000  B  60.48264 1
 0.65309289E+01 0.34106362E-02-0.11975370E-05 0.19036853E-09-0.11274117E-13    2
 0.23483612E+05-0.94114463E+01 0.11110549E+01 0.31070093E-01-0.56793918E-04    3
 0.50648615E-07-0.17112722E-10 0.24411612E+05 0.15622398E+02 0.25714083E+05    4
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C2HClF2 1,1-CHCl=CF2 CLORO-DIFLORO-ETHYLENE  FC-1122 SIGMA=1  IAIBIC=1.2873E 113
NU=1745,3130,1333,1199,845,970,433,579,201,751,572,243  HF298=-334. KJ
REF=TSIV 79  Max Lst sq error Cp @ 1300 K 0.39%
C2HCLF2-1,1       RUS 79C   2F   2H   1CL  1G   200.000  6000.000  B  98.47945 1
 0.99982378E+01 0.56213876E-02-0.20890705E-05 0.34507576E-09-0.20992736E-13    2
-0.43955643E+05-0.23448017E+02 0.20480403E+01 0.29590895E-01-0.28065357E-04    3
 0.11297923E-07-0.10168634E-11-0.41870475E+05 0.17086656E+02-0.40170738E+05    4

C2HClF2 cis-CHF=CFCl cis-CLORO-DIFLORO-ETHYLENE  FC-1131  SIGMA=1
IAIBIC=1.2873E 113   NU=1716,3137,1326,1159,854,1112,361,480,224,776,523,255
T0=850  HF298=-323.569 KJ   REF=TSIV 79  Max Lst sq error Cp @ 1300 K 0.33%
C2HCLF2 cis       RUS 79C   2F   2H   1CL  1G   200.000  6000.000  B  98.47945 1
 0.10773817E+02 0.48843919E-02-0.18135371E-05 0.29944899E-09-0.18214330E-13    2
-0.42909705E+05-0.27423997E+02 0.18766172E+01 0.32753447E-01-0.32851961E-04    3
 0.13358593E-07-0.10107904E-11-0.40667163E+05 0.17580933E+02-0.38916184E+05    4

C2HClF2 trans-CFCl=CHF trans-CLORO-DIFLORO-ETHYLENE  SIGMA=1  IAIBIC=1.2873E 113
NU=1708,3120,1290,1196,696,1150,397,578,200,776,467,310      T0=900
HF298=-323.103 KJ    REF=TSIV 79    Max Lst sq error Cp @ 1300 K 0.33%
C2HCLF2 trans     RUS 79C   2F   2H   1CL  1G   200.000  6000.000  B  98.47945 1
 0.10848435E+02 0.48316495E-02-0.17979829E-05 0.29732063E-09-0.18103369E-13    2
-0.42888036E+05-0.27962648E+02 0.15000194E+01 0.34865481E-01-0.37049162E-04    3
 0.17161874E-07-0.23168944E-11-0.40562524E+05 0.19158855E+02-0.38860137E+05    4

C2HCLF4 1-CHLORO-1,1,2,2-TETRA-FLORO-ETHANE (HCFC-124a)  TRC 1989 DATA TO 1500 K
EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS   HF298=-903.3 KJ    Max Lst
Sq Error Cp @ 1400 K 0.32%.
CF2H-CCLF2 FC-124AP   89C   2F   4H   1CL  1G   200.000  5000.000  C 136.47625 1
 0.14476092E+02 0.77521899E-02-0.34676003E-05 0.68691373E-09-0.49890490E-13    2
-0.11413815E+06-0.44436670E+02 0.25660695E+01 0.40636569E-01-0.30205490E-04    3
 0.15001542E-08 0.49004025E-11-0.11095106E+06 0.16810762E+02-0.10864140E+06    4

C2HClF4  2-CHLORO-1,1,1,2-TETRAFLORO-ETHANE (HCFC-124)  TRC 1989 DATA TO 1500K
EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS  HF298=-924.7 KJ    Max Lst
Sq Error Cp @ 1400 K 0.32%.
CF3-CCLFH HCFC124 P   89C   2F   4H   1CL  1G   200.000  5000.000  C 136.47625 1
 0.14310765E+02 0.77386392E-02-0.33659964E-05 0.65591076E-09-0.47163678E-13    2
-0.11665629E+06-0.43664043E+02 0.25109331E+01 0.39611296E-01-0.26968606E-04    3
-0.22740439E-08 0.64125753E-11-0.11348471E+06 0.17136671E+02-0.11121521E+06    4

C2HCl2F3 2,2-DICHLORO-1,1,1-TRIFLORO-ETHANE  (HCFC-123)  TRC 1989 DATA TO 1500 K
EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS  HF298=-743.9 KJ  Max Lst Sq
Error Cp @ 1400 K 0.3%
CF3-CCL2H HCFC123 P   89C   2F   3H   1CL  2G   200.000  5000.000  C 152.93055 1
 0.15372216E+02 0.65536841E-02-0.28223775E-05 0.54480973E-09-0.38845129E-13    2
-0.95263745E+05-0.49194203E+02 0.24843775E+01 0.41924396E-01-0.29376222E-04    3
-0.37135096E-08 0.82904456E-11-0.91811259E+05 0.17075157E+02-0.89470095E+05    4

C2HCl2F3 1,2-DICHLORO-1,1,2-TRIFLORO-ETHANE  (HCFC-123a)     TRC (1989) DATA TO
1500 K EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS    HF298=-710.0 KJ
Max Lst Sq Error Cp @ 1300 K 0.28%.
CF2CL-CFCLH       P   89C   2F   3H   1CL  2G   200.000  5000.000  C 152.93055 1
 0.15214490E+02 0.68034260E-02-0.29677784E-05 0.57947261E-09-0.41715986E-13    2
-0.91047599E+05-0.46292045E+02 0.22308101E+01 0.46950596E-01-0.46338534E-04    3
 0.17532444E-07-0.78742071E-12-0.87769687E+05 0.19469685E+02-0.85392885E+05    4
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C2HCl2F3 1,1-DICHLORO-1,2,2-TRIFLORO-ETHANE   TRC (1989) DATA TO 1500 K
EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS  HF298=-702.1 KJ   Max Lst Sq
Error Cp @ 800 K 0.29%.
CFCL2-CF2H          P   89C   2F   3H   1CL  2G   200.000  5000.000  C 152.93055 1
 0.15065748E+02 0.70864071E-02-0.30919691E-05 0.60150084E-09-0.43128759E-13    2
-0.90106886E+05-0.46351547E+02 0.28807063E+01 0.42935581E-01-0.38052765E-04    3
 0.94294010E-08 0.24256356E-11-0.86893560E+05 0.15891141E+02-0.84442739E+05    4

C2HCl3   TRICHLOROETHYLENE  SIGMA=1  IAIBIC=928.E-115  NU=3096,1590,1250,933,
859,633,381,274,172,783,452,211   REF=TSIV 1979    Max Lst Sq Error Cp @ 1300 K
0.33%  HF298=-4.1 KJ
C2HCL3              RUS 79C   2H   1CL  3    0G   200.000  6000.000  B 131.38804 1
 0.10888462E+02 0.47583118E-02-0.17617541E-05 0.29031942E-09-0.17633485E-13    2
-0.44243872E+04-0.25439709E+02 0.25996860E+01 0.34238007E-01-0.43577745E-04    3
 0.28199249E-07-0.73014917E-11-0.24572558E+04 0.15763417E+02-0.49311385E+03    4

C2HCl4  TETRACHLOROETHYL RADICAL (CHCl2CCl2*) STATWT=2  SIGMA=1   IA=52.8187
IB=65.056   IC=109.1656   IR=15.4306  ROSYM=3  INT ROT BARRIER V3=2580 1/CM
NU=1023,2984,812,778,706,618,1265,1210,382,326,314,279,231,168  REF=Skinner &
Rabinovich  HF298=45. KJ  REF=BOZZELLI & RITTER's program Max Lst Sq Error Cp @
1300 K 0.34%
C2HCL4              T07/93C   2H   1CL  4    0G   200.000  6000.000  B 166.84074 1
 0.14345153E+02 0.38508430E-02-0.15288445E-05 0.26296252E-09-0.16428120E-13    2
 0.30975111E+03-0.40373922E+02 0.33451714E+01 0.42519471E-01-0.56084672E-04    3
 0.36883667E-07-0.97499515E-11 0.29522231E+04 0.14447025E+02 0.54122251E+04    4

C2HF FLUOROACETYLENE  SIGMA=1  B0=0.323577 cm-1  NU=3360,2250,1060,580(2),367(2)
HF298=125.5+/-63 KJ  REF=JANAF
C2HF                J12/67C  2H   1F   10    0G   300.000  5000.000  B  44.0283  1
 6.09495010E+00 3.94324280E-03-1.47114380E-06 2.52946410E-10-1.64466630E-14    2
 1.29769070E+04-8.31534304E+00 2.69017700E+00 1.76808530E-02-2.27498550E-05    3
 1.49205680E-08-3.73819250E-12 1.36832230E+04 8.14697176E+00 1.50978852E+04    4

C2HF5 PENTAFLOROETHANE  (HFC-125) SIGMA=1  IA=22.7367   IB=34.6826   IC=41.8355
IR=5.5278  NU=3008,1393,1309,1218,1111,867,725,577,523,361,246,1359,1198,1145,
508,413,216  POTENTIAL BARRIER V3=4338 cal HF298=-264. KCAL REF=Chen et al 1975.
Max Lst Sq Error Cp @ 1300 0.39%
C2HF5               T 9/92C   2H   1F   5    0G   200.000  6000.000  B 120.02196 1
 0.14511481E+02 0.67806778E-02-0.25698903E-05 0.42902547E-09-0.26324390E-13    2
-0.13843215E+06-0.46709702E+02 0.26173863E+01 0.35802157E-01-0.17656511E-04    3
-0.10850738E-07 0.92126754E-11-0.13504778E+06 0.15423796E+02-0.13284920E+06    4

HCCN  STATWT=3  SIGMA=1  IB=7.8  NU=3229,1735,1179,458(2),370(2)
HF0=609.241+/-100. KJ   REF=Gurvich 89
HCCN                RUS 91H  1.C  2.N  1.   0.G   200.000  6000.000  B  39.03668 1
 6.56314169E+00 3.48040967E-03-1.24603080E-06 2.00764486E-10-1.20044547E-14    2
 7.11347086E+04-9.86556141E+00 1.87184307E+00 2.60611314E-02-4.62723965E-05    3
 4.18609731E-08-1.45352705E-11 7.20340360E+04 1.22173228E+01 7.34175107E+04    4

C2HO  KETYL RAD  SIGMA=1  STATWT=2  A0=41.5 B0=0363 C0=0359 REF= Endo & Hirota
J. Chem. Phys. 86 (1987),4319  NU=1967,380,1063,730,610,3290 HF298=42.4
+/- 2.1 Kcal REF=Oakes, Jones, Blerbaum & Ellison  J. Phys. Chem. 87 (1983),4810
MAX LST SQ ERROR CP @ 6000 K 0.32%
C2HO                T 6/94C   2H   1O   1    0G   200.000  6000.000  B  41.02934 1
 0.58469006E+01 0.36405960E-02-0.12959007E-05 0.20796919E-09-0.12400022E-13    2
 0.19248496E+05-0.52916533E+01 0.23350118E+01 0.17010083E-01-0.22018867E-04    3
 0.15406447E-07-0.43455097E-11 0.20050299E+05 0.11976729E+02 0.21336387E+05    4
```

Table 4 (continued)

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VINYLIDENE CH2C RADICAL  SIGMA=2  STATWT=1  IA=0.29432 IB=2.17453  IC=2.46885
NU=3344,3239,1710,1288,787,444 REF=OSAMURA, SCHAFER, GRAY & MILER J.A.C.S. 103
(1981) 1904.  Max Lst Sq Error Cp @ 6000 K 0.35% HF0=403.91 KJ REF= Chen, Jonas,
Kinsey & Field J Chem Phys 91 (1989) 3976.
H2C2              L12/89H  2C   2    0     0G   200.000  6000.000  B  26.03788 1
 0.42780340E+01 0.47562804E-02-0.16301009E-05 0.25462806E-09-0.14886379E-13    2
 0.48316688E+05 0.64023701E+00 0.32815483E+01 0.69764791E-02-0.23855244E-05    3
-0.12104432E-08 0.98189545E-12 0.48621794E+05 0.59203910E+01 0.49887266E+05    4

C2H2 ACETYLENE SIGMA=2 B0=1.1766 NU=3372.83,1973.8,3283.83,612.88(2),730.29(2)
X11=-18.57,X12=-13.09 X13=-102.39 X14=-16.54 X15=-10.85 X22=-7.92 X23=-2.83
X24=-12.70 X25=-1.38 X33=-30.95 X34=-8.22 X35=-8.68 X44=3.3 X45=-5.24 X55=-2.27
G44=-1.36 G55=3.45 ALPHA1=6.83E-3 ALPHA2=6.3E-3 ALPHA3=5.6E-3 ALPHA4=-1.3E-3
ALPHA5=-2.2E-3 D0=1.598E-6 T0=25000(3),35000(6),42198(1),50000(3),54116(1)
REF=TSIV HF298=227.4 KJ
C2H2              L 8/88C  2H   2    0     0G   200.000  6000.000  A  26.03788 1
 0.46587047E+01 0.48840949E-02-0.16083563E-05 0.24698787E-09-0.13861505E-13    2
 0.25663218E+05-0.39979074E+01 0.80869108E+00 0.23361395E-01-0.35516636E-04    3
 0.28014566E-07-0.85004459E-11 0.26332764E+05 0.13939671E+02 0.27349778E+05    4

C2H2F2  1,1-C2H2F2 1,1-DIFLUOROETHYLENE (FC-1132a)  SIGMA=2  IAIBIC=963.624E-117
NU=1727.6,3057,3,1393,925.5,549.7,592,3174,1300.8,954.3,437,803.5,609.6   Max
Lst Sq Error Cp @ 6000 0.44%  REF=TSIV 1979  HF298=336.4 KJ
C2H2F2 FC-1132A   RUS 79C   2H   2F   2    0G   200.000  6000.000  B  64.03469 1
 0.79327643E+01 0.72799810E-02-0.26415344E-05 0.42945073E-09-0.25839319E-13    2
 0.37251697E+05-0.16507476E+02 0.91165863E+00 0.26603461E-01-0.18948171E-04    3
 0.19953224E-08 0.24125513E-11 0.39167462E+05 0.19690888E+02 0.40459390E+05    4

C2H2F2  Cis-C2H2F2  Cis-DIFLUOROETHYLENE  SIGMA=2  IAIBIC=1021.74E-117  NU=1716,
3122,1263,1015,237,839,495,3136,1374,1130,769,756   REF=TSIV 1979   Max Lst Sq
Error Cp @ 6000K 0.46%    HF298=313.192 KJ
H2C2F2            RUS 79H   2C   2F   2    0G   200.000  6000.000  B  64.03469 1
 0.76464991E+01 0.75564145E-02-0.27460965E-05 0.44690892E-09-0.26908805E-13    2
 0.34501235E+05-0.14697526E+02 0.26982329E+01 0.12388075E-01 0.15375850E-04    3
-0.32354406E-07 0.14769065E-10 0.36234156E+05 0.12826030E+02 0.37668125E+05    4

C2H2F2 Trans-C2H2F2  Trans-DIFLUOROETHYLENE  FC-1132  SIGMA=2   IAIBIC=671.E-117
NU=1694,3111,1286,1123,548,875,329,788,3144,1274,1159,341  REF=TSIV 1979    Max
Lst Sq Error Cp @ 6000 K 0.45%  HF298=310.038 KJ
F2C2H2  FC-1132   RUS 79F   2C   2H   2    0G   200.000  6000.000  B  64.03469 1
 0.77364716E+01 0.74682715E-02-0.27124152E-05 0.44124475E-09-0.26559965E-13    2
 0.34125364E+05-0.15227976E+02 0.28231827E+01 0.13973974E-01 0.87909744E-05    3
-0.23954877E-07 0.11273758E-10 0.35790306E+05 0.11761385E+02 0.37288788E+05    4

CF3CH2 Beta-TRIFLUOROETHYL RADICAL SIGMA=1. IA=1.4637  IB=15.056  IC=15.413
IR=0.2892 CALCULATED AS FREE ROTOR  NU=3113,3024,1440,1294,1277,1192,940,838,
598,574,523,466,364,319 REF=Chen Rauk & Tschuikow-Roux J. CHEM. PHYS. 93 (1990)
6620  Max Lst Sq Error Cp @ 6000 K 0.36%  HF298=-123.6 Kcal
C2F3H2            T 1/92C   2F   3H   2    0G   200.000  6000.000  B  83.03309 1
 0.10987821E+02 0.68153248E-02-0.24820763E-05 0.40457086E-09-0.24387675E-13    2
-0.66370037E+05-0.29515293E+02 0.54654037E+00 0.42697217E-01-0.49566004E-04    3
 0.27781281E-07-0.57577830E-11-0.63872559E+05 0.22578365E+02-0.62197580E+05    4
```

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C2H2(NO2)2 Di-Nitroethylene-trans     SYMNO = 2  STATWT = 1     IA = 15.0866142
IB = 70.306506   IC = 83.23265   (Ir(NO2)= 5.96  ROSYM = 2
V(2) = 5.04 kcal)x2    NU=3329,3033,2035,1906,1794,1620,1527,1439,1167,
1081,996,943,771,698,676,630,512, 474,418,353,291,140    REF = BURCAT, TAE
Report # 824 1998.   HF298 = 14.2  kcal    REF =Stein et al., NIST Database #25
1994.  Max Lst Sq Error Cp @ 1300 K 0.51%.
DI-NITROETHYLENE  T05/98C  2.H  2.N  2.O  4.G   200.000  6000.000  B 118.04896 1
 1.56460865E+01 1.07958253E-02-4.19362099E-06 7.07938872E-10-4.35902999E-14    2
 9.19140603E+02-5.15469476E+01 2.71427290E+00 4.42404733E-02-3.07593033E-05    3
 3.50616078E-09 3.21103574E-12 4.63337698E+03 1.58746522E+01 7.14567665E+03    4

C2H2O  KETENE SIGMA=2  IA=.299  IB=8.1477 IC=8.4466  NU=3070,2152,1388,1118,
3166,977,438,591,525  REF=MOORE & PIMENTEL  MAX ERROR CP @ 6000 K 0.42%.
HF298=-11.4+/-0.4 KCAL REF= Vogt, Williamson & Beauchamp JACS 100 (1978), 3478
C2H2O KETENE      T 6/94C   2H   2O   1    0G   200.000  6000.000  B  42.03728 1
 0.57577901E+01 0.63496507E-02-0.22584407E-05 0.36208462E-09-0.21569030E-13    2
-0.79786113E+04-0.61064037E+01 0.21401165E+01 0.18088368E-01-0.17324216E-04    3
 0.92767477E-08-0.19915011E-11-0.70430509E+04 0.12198699E+02-0.57366700E+04    4

C2H2O  ETHYNOL  HCC-OH   SIGMA=1  IA=0.121323  IB=8.4583765  IC=8.5796996
NU=346,383,523,600,1072,1232,2198,3339,3501  REF= M. JACOX JPCRD 19,(1990),1469
HF298=22.273 KCAL REF=C. Melius BAC/MP4 Calculations (Private Communication)
Max Lst Sq Error Cp @ 6000 K 0.31%
HCCOH             T 4/93C   2H   2O   1    0G   200.000  6000.000  B  42.03728 1
 0.63660255E+01 0.55038729E-02-0.18851901E-05 0.29446414E-09-0.17218598E-13    2
 0.89184965E+04-0.82504705E+01 0.19654173E+01 0.25585205E-01-0.38773334E-04    3
 0.31566335E-07-0.10081670E-10 0.97694090E+04 0.12602749E+02 0.11207642E+05    4

C2H2O2 (CHO-CHO) Trans-GLYOXAL   SIGMA=2   IA=1.62951  IB=17.33101  IC=18.60038
NU=2843,1745,1352,1065,551,801,1048,2835,1732,1312,339,127     REF= SCUSERIA  &
SCHAEFER JACS 111,(1989),7761 HF298=-212.0 KJ REF=Pedley, Naylor & Kirby 1986
Max Lst Sq Error Cp @ 1300 K 0.56%
C2H2O2 TRANS      T 9/92C   2H   2O   2    0G   200.000  6000.000  C  58.03668 1
 0.70656795E+01 0.82911978E-02-0.30597593E-05 0.50281749E-09-0.30471963E-13    2
-0.28473229E+05-0.11025499E+02 0.41707921E+01 0.64595753E-02 0.19616033E-04    3
-0.29133403E-07 0.11656466E-10-0.27149460E+05 0.64224068E+01-0.25497594E+05    4

C2H2O2 (CHO-CHO) Cis-GLYOXAL SIGMA=4  IA=3.14528  IB=13.51604  IC= 16.66133
NU=2840,1746,1359,827,285,739,1049,2753,1772,1317,766,91  REF=SCUSERIA & SHAEFER
JACS 111,(1989),7761  HF298=-212.0 KJ REF=Pedley, Naylor & Kirby 1986.   Max Lst
Sq Error Cp @ 1300 K 0.55%
C2H2O2 CIS        T 9/92C   2H   2O   2    0G   200.000  6000.000  C  58.03668 1
 0.71660908E+01 0.82156532E-02-0.30357804E-05 0.49928280E-09-0.30274243E-13    2
-0.28502158E+05-0.11724463E+02 0.41659627E+01 0.65590466E-02 0.20251392E-04    3
-0.30590514E-07 0.12429084E-10-0.27155540E+05 0.62611341E+01-0.25497594E+05    4

C2H3  VINYL-RAD  STATWT=2.  SIGMA=1.  IA=0.35825   IB=2.61   IC=2.9682544
NU=749.6,803,872.4,1076.4,1257.6,1454.5,2895,2976.7,3038 REF=Ab-Initio Calc. by
Karni, Oref and Burcat TAE #643 1989. HF298=299.74 KJ  REF=Ervin JACS 112 (1990)
5750 Max Lst Sq Error Cp @ 40 K 0.63
C2H3              T06/93C   2H   3    0    0G   200.000  6000.000  B  27.04582 1
 0.47025310E+01 0.72642283E-02-0.25801992E-05 0.41319944E-09-0.24591492E-13    2
 0.34029675E+05-0.14293714E+01 0.30019602E+01 0.30304354E-02 0.24444315E-04    3
-0.35810242E-07 0.15108700E-10 0.34868173E+05 0.93304495E+01 0.36050230E+05    4
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C2H3CL CHLOROETHYLENE  STATWT=1.  SIGMA=1.  IAIBIC=3.20E-115  NU=3120.6,3086.4,
3034.3,1610.9,1370,1280,1030,720.5,395,942.5,896.5,620.4    REF=TSIV 1979    Max
Lst Sq Error Cp @ 6000 K 0.47%     HF298=23. KJ
C2H3CL            RUS 79C   2H   3CL  1    0G   200.000  6000.000  B  62.49852 1
 0.63232954E+01 0.85236086E-02-0.30420698E-05 0.48893443E-09-0.29178872E-13    2
 0.61799473E+02-0.77489330E+01 0.22718917E+01 0.12508882E-01 0.12133827E-04    3
-0.27307119E-07 0.12657108E-10 0.14736901E+04 0.14757729E+02 0.27662484E+04    4

C2H3F2 Alfa DIFLUOROETHYL RADICAL (CH3CF2) SIGMA=1. STATWT=2. IA=8.1022
IB=9.064  IC=10.2057  ROSYM=3.  IR=0.50451 ROT BARR V3=790. 1/CM  NU=2989,2959,
2886,1461,1458,1419,1260,1259,1089,981,843,524,447,357  REF=CHEN, RAUK, &
TSCHUIKOW-ROUX 93 1990, 1187 MAX LST SQ ERROR CP 1300 K 0.51 % HF298=-72.3 KCAL
C2H3F2            T12/91C   2H   3F   2    0G   200.000  6000.000  B  65.04263 1
 0.79153881E+01 0.95796027E-02-0.34798118E-05 0.56594378E-09-0.34053931E-13    2
-0.39692403E+05-0.14382963E+02 0.33232137E+01 0.16181070E-01 0.34104446E-05    3
-0.15893036E-07 0.75253769E-11-0.38094855E+05 0.10888528E+02-0.36382565E+05    4

1,1,1-C2H3F3  1,1,1-TRIFLUOROETHANE  (FC-143A)   DATA FROM Stull Westrum & Sinke
EXTRAPOLATED THROUGH WILHOIT'S POLYNOMIALS  Max Lst Sq Error H-H298 @ 300K 0.67%
HF298=-178.2 Kcal
C2H3F3  FC-143A   T 1/92C   2H   3F   3    0G   298.150  6000.000  B  84.04103 1
 0.10557160E+02 0.93524968E-02-0.30011296E-05 0.45429289E-09-0.26247438E-13    2
-0.93951864E+05-0.29976755E+02 0.19057753E+00 0.41471773E-01-0.40881127E-04    3
 0.20598737E-07-0.40433877E-11-0.91250937E+05 0.22743253E+02-0.89673210E+05    4

C2H3N  METHYLCYANIDE (CH3CN)  STATWT=1.  SIGMA=3.  A0=5.289  B0=C0=.3068
NU=2954,2268,1389,920,3009(2),1453(2),1041(2),362(2) T0=55000  REF=SPANGENBERG
&BORGER  MAX LST SQ ERROR CP @ 1300K 0.79% .HF298=21 KCAL Stull, Westrum & Sinke
C2H3N             T04/80C  2H   3N   1    0G   300.000  5000.000  C  41.0526  1
 0.54956026E 01 0.89018531E-02-0.29834273E-05 0.43930859E-09-0.23263757E-13    2
 0.81332734E 04-0.54995676E 01 0.28112087E 01 0.11668280E-01 0.18374703E-05    3
-0.75577553E-08 0.30708968E-11 0.92079258E 04 0.97588467E 01 0.10567430E+05    4

C2H3NO2 Nitroethylene   STATWT =1  IA = 6.77795  IB = 17.4725  IC = 24.2505
Ir = 5.96   ROSYM = 2   V(2) = 5.04 kcal/mole   NU=3103,3094,3013,1699,1628,
1479,1378,1264,1066,1026,966,904,828,654,544,536,323.       HF298 = 7.955 kcal
REF = Melius Database 1988 D39 Max Lst Sq Error Cp @ 6000 0.52%
NITROETHYLENE     T11/97C  2.H  3.N  1.O  2.G   200.000  6000.000  B  73.05136 1
 1.00660026E+01 1.04932532E-02-3.92096997E-06 6.47758885E-10-3.93529661E-14    2
-3.10704319E+02-2.61804452E+01 2.75930739E+00 1.70703761E-02 2.37349272E-05    3
-4.77968933E-08 2.14789743E-11 2.29629458E+03 1.46559809E+01 4.00308858E+03    4

C2H3O  CH3CO RAD  SIGMA=1  STATWT=2  A=2.9436   B=0.334  C=0.3186  BROT=10.51589
INT ROT SYM=3  V(3)=92 1/cm NU=2904,2903,2826,1886,1405,1402,1325,1025,925,817,
454  REF=NIMLOS SODERQUIST & ELLISON JACS 111,(1989),7675  MAX LST SQ ERROR CP @
1300 K 0.55%. HF298=-10.0 KJ  REF=Niiaranen, Gutman & Krasnoperov J. Phys. Chem.
96 (1992) 5881.
C2H3O (CH3CO)     T 9/92C   2H   3O   1    0G   200.000  6000.000  B  43.04522 1
 0.59447731E+01 0.78667205E-02-0.28865882E-05 0.47270875E-09-0.28599861E-13    2
-0.37873075E+04-0.50136751E+01 0.41634257E+01-0.23261610E-03 0.34267820E-04    3
-0.44105227E-07 0.17275612E-10-0.26574529E+04 0.73468280E+01-0.12027167E+04    4

C2H3O  (CH2CHO) RADICAL  SIGMA=1  SIGMA ROT=2  STATWT=2  IA=1.226  IB=7.7552
IC=8.7646  IR=.2902    INT ROT POTENTIAL  V(2)=2000.  NU=3005,2822,1743,1441,
1400,1352,1113,509,2967,867,763  REF= BURCAT,MILLER & GARDINER  MAX LST SQ ERROR
CP @ 1300 K  0.74 %. HF298=6.22 KCAL derived from Benson & O'Neal NSRDS-NBS 1970
CH2CHO            T04/83O   1H   3C   2    0G   300.     5000.     B  43.0451  1
 0.59756699E+01 0.81305914E-02-0.27436245E-05 0.40703041E-09-0.21760171E-13    2
 0.49032178E+03-0.50320879E+01 0.34090624E+01 0.10738574E-01 0.18914925E-05    3
-0.71585831E-08 0.28673851E-11 0.15214766E+04 0.95714535E+01 0.30474436E+04    4
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C2H3O  OXIRANE (ETHYLENE OXIDE) RADICAL ROUGH ESTIMATION MADE USING BOZZELLI &
RITTER'S PROGRAM FROM JANAF'S ETHYLENE OXIDE DATA OF 9/1965 MINUS A SECONDARY
PROTON AND EXTRAPOLATED TO 3000 K USING WILHOIT'S POLYNOMIALS. HF298 = 139.83 KJ
C2H3O             T 9/92C   2H   3O   1    0G   298.150  3000.000  F  43.04522 1
 0.48131470E+00 0.20711914E-01-0.12693155E-04 0.34579642E-08-0.35399703E-12    2
 0.15648642E+05 0.34629876E+02 0.10854772E+01 0.12845259E-01 0.24138660E-05    3
-0.44642672E-08-0.29381916E-12 0.15910655E+05 0.33395312E+02 0.16817588E+05    4

C2H4  ETHYLENE      STATWT=1.  SIGMA=4.  IA=.5752  IB=2.802  IC=3.372  NU=3021,1623,
1342,1023,3083,1236,949,943,3106,826,2989,1444    REF=CHAO&ZWOLINSKY,BURCAT
MAX LST SQ ERROR CP @ 1300K 0.83% . HF298=52.3 KJ
ETHYLENE          L 4/85C  2.H 4.   0.    0.G   300.000  5000.000  B  28.05360 1
 0.43985453E 01 0.96228607E-02-0.31663776E-05 0.45747628E-09-0.23659406E-13    2
 0.41153203E 04-0.24627438E 01 0.12176600E 01 0.13002675E-01 0.35037447E-05    3
-0.11155514E-07 0.47203222E-11 0.53373828E 04 0.15480169E 02 0.62902830E 04    4

C2H4F  Alfa-FLUOROETHYL RADICAL (CH3CHF) STATWT=2. SIGMA=1. IA=1.7795  IB=8.7444
IC=9.927  ROSYM=3. IR=0.48875 INT ROT BARRIER V3=587. 1/CM  NU=3023,2958,2926,
2862,1469,1454,1416,1349,1162,1096,1031,887,647,392     REF=CHEN, RAUK &
TSCHUIKOW-ROUX 1990  MAX LST SQ ERROR CP @ 6000 K 0.55%  HF298=-17.26 KCAL.
C2H4F             T12/91C   2H   4F   1    0G   200.000  6000.000  B  47.05216 1
 0.60065274E+01 0.11133004E-01-0.40017964E-05 0.64613341E-09-0.38678848E-13    2
-0.11429867E+05-0.55288750E+01 0.46163442E+01 0.74570459E-03 0.37958220E-04    3
-0.48405526E-07 0.18830447E-10-0.10343617E+05 0.51147332E+01-0.86855197E+04    4

C2H4Cl  Beta-CHLOREETHYL RADICAL  (CH2ClCH2)  STATWT=2  SIGMA=1 IA=2.61729
IB=14.31277  IC= 15.9312  IR=0.292687  NU=1006,3002,2992,2946,2921,676,1446,
1444,1368,1324,1236,1140,954,336  POTENTIAL BARRIER V3=650 cm-1    ROSYM=3
REF=Skinner & Rabinovitch  HF298=90.12 KJ REF=Bozzelli & Ritter's program
Max Lst Sq Error Cp @ 6000 K 0.54%
C2H4CL            T 7/93C   2H   4CL  1    0G   200.000  6000.000  B  63.50646 1
 0.59979919E+01 0.11113997E-01-0.39890576E-05 0.64350472E-09-0.38503835E-13    2
 0.80972298E+04-0.45621917E+01 0.45895607E+01 0.64757653E-03 0.38470903E-04    3
-0.49101872E-07 0.19121765E-10 0.91898417E+04 0.61950714E+01 0.10838883E+05    4

C2H4O Vinyl Alcohol IA=1.363243 IB=7.9930197 IC=9.3562625  NU=412,470.5,693.4,
922,926.3,1029,1054.3,1293,1315.3,1434.7,1645.4,2964.6,3022,3050,3461
BROT=6.414 INT ROT POTENTIAL V(3)=1067. V(6)=-1.49 Ref= Ab-Initio Calc Karni,
Oref & Burcat TAE Report 643 1989. HF298=-29.8 KCAL REF=Holm & Losing JACS 104
(1982) 2648. Max Lst Sq Error Cp @ 6000 K 0.5%
C2H4O             L 8/89C   2H  4O   1     0G   200.000  6000.000  B  44.05316 1
 0.68220305E+01 0.11059739E-01-0.39224574E-05 0.62778505E-09-0.37355714E-13    2
-0.18038769E+05-0.83716090E+01 0.30137746E+01 0.10203771E-01 0.25405637E-04    3
-0.42341002E-07 0.18267561E-10-0.16497347E+05 0.13873511E+02-0.14995857E+05    4

C2H4O  OXYRANE (ETHYLENE OXIDE)    SIGMA=2  IA=3.2793  IB=3.8059  IC=5.9511
NU=3006,1498,1271,1120,877,3063,1300,860,3006,1472,1151,892,3065,1142,822
REF=SHIMANOUCHI  HF298=-52.635 KJ FROM JANAF 1985.
C2H4O OXYRANE     L 8/88C   2H  4O   1     0G   200.000  6000.000  B  44.05316 1
 0.54887641E+01 0.12046190E-01-0.43336931E-05 0.70028311E-09-0.41949088E-13    2
-0.91804251E+04-0.70799605E+01 0.37590532E+01-0.94412180E-02 0.80309721E-04    3
-0.10080788E-06 0.40039921E-10-0.75608143E+04 0.78497475E+01-0.63304657E+04    4

C2OH4  ACETALDEHYDE (CH3CHO)  STATWT=1.  SIGMA=1.  IA=2.76748  IB=6.9781  IR=.44
IC=9.03498  NU=3005,2917,2822,1743,1441,1400,1352,1113,919,509,2967,1420,867,
1113,919,509,2967,1420,867,763 Int Rot Potential V3=412.3 ROSYM=3  REF=CHAO,
HALL,MARSH & WILHOIT JCPRD 15, (1986) p.1369 HF298=-166.19 KJ
CH3CHO            L 8/88C   2H  4O   1     0G   200.000  6000.000  B  44.05316 1
 0.54041108E+01 0.11723059E-01-0.42263137E-05 0.68372451E-09-0.40984863E-13    2
-0.22593122E+05-0.34807917E+01 0.47294595E+01-0.31932858E-02 0.47534921E-04    3
-0.57458611E-07 0.21931112E-10-0.21572878E+05 0.41030159E+01-0.19987949E+05    4
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C2H4O2 ETHANOIC (ACETIC) ACID  STATWT=1  SIGMA=1  IA=7.40342  IB=8.85376
IC=15.7599  IR(CH3)=.0253924  IR(OH)=.095545  POT BARRIER V(OH)=12200.  V(CH3) =
481   NU=3583,3051,2944,1788,1430,1382,1264,1182,989,847,657,581,2996,1430,1048,
642,(565,75 TORSION)  REF=CHAO & ZWOLINSKI  HF298=-432.25 KJ.
ACETIC ACID        L 4/85C   2.H  4.O  2.   0.G   300.000  5000.000  B  60.05240 1
 0.80064869E 01 0.12856044E-01-0.48697575E-05 0.80440143E-09-0.48353330E-13    2
-0.55868555E 05-0.17297928E 02 0.11682196E 01 0.22342462E-01 0.18119208E-05    3
-0.15536841E-07 0.69631271E-11-0.53317695E 05 0.20806107E 02-0.51987931E 05    4

C2H4O2Cl2 Alfa CHLOROPEROXYETHANE CH3CCl2O-OH  SIGMA=3   IA=46.623  IB=38.942
IC=35.485  IR(C-C)=0.5163539 IR(C-O)=4.310  IR(O-O)=0.144446   V(3)(C-C)=1601.9
cm-1  V(3)(C-O)=2973. cm-1  V(3)(O-O)=1916.7 cm-1 NU=3651,3009,2995,2922,1465,
1462,1439,1413,1194,1132,1099,1066,924,734,563,549,406,352,299,288,269
HF298=-55.3 KCAL REF=Lay et al JPC 100,(1996),8240  Max Lst Sq Error Cp @ 1300 K
0.44%
C2H4O2CL2          T01/97C  2.H  4.O  2.CL 2.G   200.000  6000.000  B 130.95796 1
 1.55129087E+01 1.03537432E-02-3.85668118E-06 6.37648016E-10-3.88430532E-14    2
-3.39225403E+04-5.01703472E+01 2.43416999E+00 4.58166561E-02-3.41051998E-05    3
 5.34704665E-09 3.11610278E-12-3.03007573E+04 1.74771898E+01-2.78278816E+04    4

C2H4O4 METHANOIC(FORMIC) ACID  (HCOOH)2 DIMER    STATWT=1  SIGMA=2  IA=13.615
IB=37.724  IC=51.340  NU=3200,2956,1672,1395,1350,1204,675,232,215,1063,677,519,
1073,917,164,68,3110,2957,1754,1450,1365,1218,697,248  REF=CHAO & ZWOLINSKI
HF298=-820.94 KJ.
(FORMIC ACID)2     L 4/85C  2.H   4.O  4.   0.G   300.000  5000.000  B  92.05120 1
 0.12207371E 02 0.13688851E-01-0.46840369E-05 0.70511663E-09-0.38369285E-13    2
-0.10395938E 06-0.35709808E 02 0.37692385E 01 0.27224716E-01 0.17238053E-05    3
-0.20776724E-07 0.99379949E-11-0.10104988E 06 0.10505494E 02-0.98737314E 05    4

C2H5  ETHYL RAD.  STATWT=2  SIGMA=1  IA=0.8005  IB=3.7134  IC=3.9931  IR=0.1846
SIGMAR=3.  POT BARRIER V3=53 1/CM NU=3112,3033,2987,2920,2842,1440(3),1366,1175,
1138,975,784,540, HF298=28.36 Kcal. REF= Chen, Rauk & Tschuikow-Roux (1990)
Max Lst Sq Error Cp & 6000 K 0.58%
C2H5               T12/91C   2H   5    0    0G   200.000  6000.000  B  29.06170 1
 0.42878814E+01 0.12433893E-01-0.44139119E-05 0.70654102E-09-0.42035136E-13    2
 0.12056455E+05 0.84602583E+00 0.43058580E+01-0.41833638E-02 0.49707270E-04    3
-0.59905874E-07 0.23048478E-10 0.12841714E+05 0.47100236E+01 0.14271225E+05    4

C2H5Br ETHYL-BROMIDE  DATA EXTRAPOLATED FROM STULL WESTRUM & SINKE TO 5000 K
USING WILHOIT'S POLYNOMIALS HF298=-15.3 KCAL Max Lst Sq Error Cp @ 1200 K 0.24%.
C2H5BR             T 2/94C   2H   5BR  1    0G   298.150  5000.000  B 108.96570 1
 0.80623575E+01 0.97420119E-02-0.21617179E-05 0.27251396E-09-0.15792222E-13    2
-0.11170246E+05-0.15671607E+02 0.15211477E+01 0.23000029E-01-0.43918084E-05    3
-0.96809477E-08 0.54509524E-11-0.91196650E+04 0.19321632E+02-0.76992150E+04    4

C2H5CL  CHLOROETHANE  DATA TAKEN FROM STULL WESTRUM & SINKE  EXTRAPOLATED USING
WILHOIT'S POLYNOMIALS  Max Lst Sq Error Cp @ 1200 K 0.31% HF298=-26.70 KCAL
C2H5CL             T 1/92C   2H   5CL  1    0G   298.150  6000.000  B  64.51440 1
 0.74917510E+01 0.10851018E-01-0.28560673E-05 0.37702526E-09-0.20026431E-13    2
-0.16769890E+05-0.14093344E+02 0.10325328E+01 0.24358172E-01-0.65945967E-05    3
-0.76422532E-08 0.46898451E-11-0.14755228E+05 0.20383089E+02-0.13435885E+05    4

C2H5F ETHYL-FLUORIDE  SIGMA=1 IA=2.284  IB=8.806   IC=10.054  NU=243,415,810,
880,1048(2),1108,1277,1365,1395,1449,1479,2915,2941,3003(3)   REF=Zachariah,
Westmoreland, Burgess, Tsang & Melius JPC 100,(1996),8737-8747  HF298=-62.5 KCAL
REF=Stull, Westrum & Sinke 1969. Max Lst Sq Error Cp @ 6000 K 0.60%.
C2H5F FLUOROETHANET 9/99C  2.H  5.F  1.   0.G   200.000  6000.000  B  48.06010 1
 5.83367491E+00 1.44137229E-02-5.18362602E-06 8.37285904E-10-5.01372486E-14    2
-3.44770328E+04-7.07133327E+00 4.39565497E+00-4.45282690E-03 6.55884290E-05    3
-8.12718783E-08 3.15915417E-11-3.29974677E+04 5.80198053E+00-3.14510416E+04    4
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Table 4 (continued)

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C2H5I ETHYL-IODIDE  DATA EXTRAPOLATED FROM STULL WESTRUM & SINKE TO 5000 K
USING WILHOIT'S POLYNOMIALS HF298=-2.0 KCAL Max Lst Sq Error Cp @ 1200 K 0.25%.
C2H5I             T 2/94C   2H   5I   1    0G   298.150  5000.000  B 155.96617 1
 0.64809111E+01 0.13447817E-01-0.47579710E-05 0.81008580E-09-0.53421203E-13    2
-0.39662060E+04-0.61701523E+01 0.13957728E+01 0.25801118E-01-0.13368068E-04    3
 0.75631068E-09 0.13422883E-11-0.24533839E+04 0.20577483E+02-0.10064333E+04    4

C2H5NO2 Nitro-Ethane  STATWT = 1  IA = 7.4804  IB = 19.8289  IC = 26.2826
Ir(NO2) = 5.97   ROSYM = 2 V(2) = 0.08 kcal/mole  Ir(CH3) = 0.51666  ROSYM = 3
V(3) = 3.5 kcal/mole   NU=3003,(2961),2956,(2929),2754,1582,1561,(1465),1460,
(1447),1400,1386,1252,1141,1117,996,881,774,(639,591,501,286).  HF298=-24.8 kcal
REF = Melius Database 1988 D74B    Max Lst Sq Error Cp @ 1300 K 0.64%
NITROETHANE       T04/98C  2.H  5.N  1.O  2.G   200.000  6000.000  B  75.06724 1
 9.21849299E+00 1.62001532E-02-5.98159944E-06 9.81277173E-10-5.93455530E-14    2
-1.68676292E+04-2.07232926E+01 3.37137598E+00 1.37914267E-02 3.84687528E-05    3
-6.02380553E-08 2.49654782E-11-1.43330647E+04 1.40009494E+01-1.24822894E+04    4

C2H5ONO2 Ethyl Nitrate  STATWT = 1  IA = 9.9190168  IB = 32.356995  IC = 36.4527
Ir(NO2) = 5.96   ROSYM =2  V(2) = 9.1 kcal/mole   Ir(CH3) = 0.5166 ROSYM = 3
V(3) = 3.5 kcal    NU= 3003,2959,2946,2933,2877,1703,1481,1468,1455,1427,
1403,1355,1296,1172,1086,1066,968,878,815,790,692,589,396,342,207.
REF = Melius Database 1988 P73BN    HF298 = -37.04 kcal   REF = Gray, Pratt
& Larkin J. Chem. Soc (1956),210   Max Lst Sq Error Cp @ 1300 K 0.65%
ETHYL-NITRATE     T05/98C  2.H  5.N  1.O  3.G   200.000  6000.000  B  91.06664 1
 1.21360953E+01 1.70091385E-02-6.43739515E-06 1.07219880E-09-6.54950920E-14    2
-2.41902070E+04-3.71640527E+01 3.75721604E+00 1.93623098E-02 3.87534117E-05    3
-6.64089530E-08 2.82505579E-11-2.08444383E+04 1.11813240E+01-1.86391453E+04    4

C2H5O  ETHYL-OXIDE RAD   (CH3CH2O) SIGMA=1  SIGMA BARRIER=3  STATWT=2  IA=2.327
IB=8.395  IC=9.693  IR=0.4331  V(3)=3300.  NU=2989(3),1456(2),1391,1320,1126,
1040,868,423,2989,1456,1270,1104,801  REF=BURCAT,MILLER AND GARDINER  MAX LST SQ
ERROR @ 1300 K 0.84 % . HF300=-4.0 KCAL REF=Benson
OC2H5             T11/82O  1C   2H   5     0G   300.000  5000.0    B  45.0609  1
 0.60114346E+01 0.12165219E-01-0.40449604E-05 0.59076588E-09-0.30969595E-13    2
-0.49366992E+04-0.67901798E+01 0.17302504E+01 0.16908489E-01 0.39996221E-05    3
-0.13711180E-07 0.57643603E-11-0.32922483E+04 0.17336115E+02-0.20138288E+04    4

C2H5O  (CH2CH2OH) RADICAL  SIGMA=1  STATWT=2  IA=2.359 IB=8.08  IC=9.935
IR(CH2)=0.79  IR(OH)=.1363  INT ROT POTENTIAL  SIGMA ROT(OH)=2     V(2)=201,
SIGMA ROT(CH2)=3  V(3)=3000.  NU=3689,2989(3),1320,1242,1067,1040,877,427,1456,
1270,1104,801  REF=BURCAT,MILLER & GARDINER  MAX LST SQ ERROR CP @ 1300 K 0.65 %
HF298=-5.0 KCAL estinated according to Benson.
H5C2O             T 4/83H   5C  2O   1     0G   300.000  5000.     B  45.0609  1
 0.75944014E+01 0.93229339E-02-0.30303854E-05 0.43216319E-09-0.21970039E-13    2
-0.57727852E+04-0.13955572E+02 0.14019508E+01 0.21543175E-01-0.22326512E-05    3
-0.14464092E-07 0.80488420E-11-0.38464519E+04 0.19148981E+02-0.25154820E+04    4

C2H5O  (CH3CHOH)    RADICAL  SIGMA =1  STATWT=2  IA=1941  IB=9.542  IC=10.916
IR(CH3)=.4331  IR(OH)=.1363  INT ROT POTENTIAL   SIGMA ROT(CH3)=3  V(3)=3300.
SIGMA ROT(OH)=2  V(2)=800.  NU=3689,2989(4),1456(3),1391,1242,1067,1040,877,427,
1270 1104  REF=BURCAT,MILLER & GARDINER  MAX LST SQ ERROR CP @ 1300 K  0.75 % .
HF298=-5.0 KCAL estimated according to Benson.
C2OH5             T 4/83C   2O  1H   5     0G   300.000  5000.     B  45.0609  1
 0.67665424E+01 0.11634436E-01-0.37790651E-05 0.53828875E-09-0.27315345E-13    2
-0.56092969E+04-0.93980442E+01 0.24813328E+01 0.16790036E-01 0.37755499E-05    3
-0.13923497E-07 0.60095193E-11-0.40120054E+04 0.14581622E+02-0.25172860E+04    4
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Table 4 (continued)

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C2H5O  CH2-O-CH3 RAD   SIGMA=1 SIGMA BARRIER=2.,3.  STATWT=2.      IA=2.15  IB=7.91
IC=9.558  IR(CH2)=3.335  V(2)=2000  IR(CH3)=4.787  V(3)=2720  NU=2996(2),2817,
1464(3),1452,1244,928,418,2952,1150,1227,1102,2925,1179  REF=BURCAT,MILLER AND
GARDINER   MAX LST SQ ERROR @ 1300 K 0.83 % . HF300=-2.0 kcal  REF=Benson
C2H5O              T11/82C  2H   5O   1     0G   300.000  5000.0    B  45.0609  1
 0.65567484E+01 0.12180723E-01-0.40628420E-05 0.59495830E-09-0.31276214E-13    2
-0.40282515E+04-0.81302772E+01 0.35953999E+01 0.13379216E-01 0.53914910E-05    3
-0.10947097E-07 0.38193320E-11-0.27021975E+04 0.92850365E+01-0.10077563E+04    4

C2H5O2Cl Alfa-CHLORO-PEROXYETHANE CH3CHClO-OH  SIGMA=3   IA=39.142  IB=24.814
IC=16.91   IR(C-C)=0.511373  IR(C-O)=4.14245  IR(O-O)=0.144446  V(3)(C-C)=1490.
cm-1  V(3)(C-O)=1479.46 cm-1  V(3)(O-O)=2427.3 cm-1 NU=3652,3019,2989,2977,2909,
1469,1464,1428,1416,1359,1300,1167,1122,1068,1009,890,632,518,430,316,305
HF298=-50.9 KCAL REF=Lay et al JPC 100,(1996),8240  Max Lst Sq Error Cp @ 6000 K
0.6%
C2H5O2CL           T01/97C  2.H  5.O  2.CL 1.G   200.000  6000.000  B  96.51320 1
 1.15961106E+01 1.46988166E-02-5.56315884E-06 9.24997440E-10-5.64231971E-14    2
-3.06724523E+04-3.20337220E+01 3.19878206E+00 2.50806853E-02 1.51506919E-05    3
-4.08074392E-08 1.89776224E-11-2.77443750E+04 1.43864750E+01-2.56137283E+04    4

C2H5OO PEROXYETHYL RADICAL  STATWT=2  IA=2.4505  IB=18.5705  Ic=19.984
NU=2955,2936,2934,2901,2874,1493,1467,1454,1410,1371,1259,1152,1145,1129,1006,
860,786,491,300,231,91.9  REF=Melius MP4 A40 1988   HF298=-6.86 kcal  REF=
Atkinson et. al, JPCRD 28 (1999),191 {Hf298= -2.32 kcal REF=Melius 1988}
{HF298=-4. kcal REF=NIST 1994 estimate} Max Lst sq Error Cp @ 1300 K 0.58%
C2H5OO PEROXYETH   T08/00C  2.H  5.O  2.   0.G   200.000  6000.000  C  61.06050 1
 8.05957692E+00 1.52921019E-02-5.54442603E-06 9.00496195E-10-5.41302799E-14    2
-7.31028500E+03-1.59992904E+01 5.21694144E+00 1.24160003E-04 6.15529492E-05    3
-7.94505636E-08 3.12101317E-11-5.41455775E+03 4.22381533E+00-3.45206633E+03    4

C2H6  ETHANE  STATWT=1.  SIGMA=6.  SIGMA BARRIER=3.  IA=1.0481     IB=IC=4.22486
IR=.26203  NU=2954,1388,995,2896,1379,2969(2),1468(2),1190(2),2985(2),1469(2),
822(2)  POTENTIAL BARRIER V0=2.96  REF=CHAO WILHOIT&ZWOLINSKI  MAX LST SQ ERROR
CP @ 1300K 0.95% . HF298=-20.04 KCAL
ETHANE             L 5/84C  2.H 6.   0.    0.G   300.000  5000.000  B  30.06940 1
 0.47028847E 01 0.14042635E-01-0.46469377E-05 0.67473738E-09-0.35089312E-13    2
-0.12671988E 05-0.45433950E 01 0.15395260E 01 0.15040841E-01 0.66847115E-05    3
-0.13382948E-07 0.48561398E-11-0.11248766E 05 0.14107375E 02-0.10085085E 05    4

(CH3)2N DIMETHYLAZIDE RADICAL ESTIMATED BY NIST 1994 to 1500 K and extrapolated
using Wilhoit's Method. SIGMA=6  HF298=159.1 kJ. Max Lst Sq Error Cp @ 1500 K
0.33 %.
C2H6N              T 7/95C   2H   6N   1     0G   298.150  5000.000  E  44.07638 1
 0.66265845E+01 0.15639689E-01-0.58042716E-05 0.10101047E-08-0.66950103E-13    2
 0.15809048E+05-0.10849938E+02 0.17521819E+01 0.22097412E-01 0.15576120E-06    3
-0.12281567E-07 0.56327749E-11 0.17650884E+05 0.16389129E+02 0.19135223E+05    4

C2H6N2 AZOMETHANE (CH3NNCH3)  STATWT=1  SYGMA=2  IA=2.063  IB=19.082  IC=20.029
IR=0.425  POT BARRIER V0=1700. NU=2989,2926,1583,1437,1381,1179,919,591,2977,
1416,1027,2981,1440,1111,312,2988,2925,1447,1384,1112,1008,353,(2148222 TORSION)
REF=PAMIDIMUKKALA, ROGERS & SKINNER  MAX LST SQ  ERROR CP @ 1300. 0.9%.
HF298=35.54 KCAL.
C2H6N2             T 8/81C  2.H  6.N  2.   0.G   300.000  5000.000  B  58.08280 1
 0.81902246E 01 0.15981115E-01-0.53652748E-05 0.79098639E-09-0.41925359E-13    2
 0.13938773E 05-0.18192831E 02 0.34860029E 01 0.18514410E-01 0.86240079E-05    3
-0.17172741E-07 0.61034997E-11 0.15975109E 05 0.92264036E 01 0.17884533E 05    4
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C2H6N2O2 N-methyl N-nitromethanamine (CH3)2N-NO2 SIGMA=2   IAIBIC=11752E-117
IR(CH3)=0.59  IR(NO2)=3.94 ROSYM(CH3)=3  ROSYM(NO2)=2  V3(CH3)=1050 cm-1
V2(NO2)=2800 cm-1   NU=3033(2),2948(2),2993(2),1528,1462,1456,1454,1450,1441,
1411,1304,1292,1248,1144,1110,1050,1023,838,762,626,619,427,350,225  HF298=-4.8
kJ  REF=Dorofeeva & Tolmach Thermochim Acta 240,(1994),47-66  Max Lst Sq Error
Cp @ 1300 K 0.60 %.
(CH3)2N-NO2        T10/99C  2.H  6.N  2.O  2.G   200.000  6000.000  B  90.08192 1
 1.24703937E+01 1.86034893E-02-6.89301702E-06 1.13154966E-09-6.84339128E-14    2
-6.24684007E+03-3.95039089E+01 4.22510053E+00 2.24381715E-02 3.20605902E-05    3
-5.84889497E-08 2.50090693E-11-3.01379947E+03 7.74519704E+00-5.77304014E+02    4

C2H5OH liquid Ethanol (L)DATA TAKEN FROM TRC 12/87 HF298=-66.326 kcal
C2H5OH(L) McBrid  P12/87C  2.H  6.O  1.   0.L   200.000   468.000  C  46.06904 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00 7.27370930E+00 6.43852436E-02-4.77630118E-04    3
 1.44382308E-06-1.11087366E-09-3.65159272E+04-3.07153973E+01-3.33763486E+04    4

C2H6O  ETHANOL (C2H5OH)    STATWT=1.  SIGMA=3  SIGMA BARRIER CH3=3.  ROSYM OH=1
REF=CHAO, HALL, MARSH & WILHOIT JPCRD 15 (1986) P.1369. This is an equilibrium
mixture of one trans and two gauche isomers, therefore sigma was set artificialy
to 3. The two gauche isomers are equal. The trans values are: IAIBIC=218.459
BROT CH3=6.4144 V(3)CH3=1166. BROT OH=21.07 V(OH) (1)=57 (2)=8.025 (3)=395.
NU=3659,2985,2939,2900,1460,1430,1395,1320,1245,1055,1026,883,422,2887(2),1460,
1270,1117,801 The cis values are: IAIBIC=233.455E-117 BROT CH3=6.416 OH=20.94
V(3) CH3=1331 V(OH) as for trans NU=3675,2985,2939,2900,1460(2),1430,1395,1320,
1245,1055,1026,887,596,2887(2)1270,1070,801  HF298=-234.95 KJ
C2H5OH             L 8/88C  2H   6O   1     0G   200.000  6000.000  B  46.06904 1
 0.65624365E+01 0.15204222E-01-0.53896795E-05 0.86225011E-09-0.51289787E-13    2
-0.31525621E+05-0.94730202E+01 0.48586957E+01-0.37401726E-02 0.69555378E-04    3
-0.88654796E-07 0.35168835E-10-0.29996132E+05 0.48018545E+01-0.28257829E+05    4

C2H6O  DIMETHYL-ETHER SIGMA=2  SIGMA BARRIER=3   IAIBIC=170.493    IR=0.4291
V(3)=903.4 NU=2999(2),2935,2920,2820(2),1485,1467,1463,1459,1449,1432,1250,
1179,1178,1148,1104,931,424  REF=CHAO, HALL, MARSH & WILHOIT JPCRD 15, (1986)
P.1369 HF298=-184.05 KJ
CH3OCH3            L 9/88C  2H   6O   1     0G   200.000  6000.000  B  46.06904 1
 0.56483880E+01 0.16338220E-01-0.58680268E-05 0.94683462E-09-0.56650169E-13    2
-0.25100722E+05-0.59623267E+01 0.53055789E+01-0.21421160E-02 0.53085949E-04    3
-0.62313044E-07 0.23072397E-10-0.23979910E+05 0.71342649E+00-0.22136501E+05    4

C2H6O2 PEROXYETHANE C2H5O-OH  SIGMA=3   IA=21.607  IB=20.135  IC=2.7509
IR(C-C)=0.49484   IR(C-O)=2.859  IR(O-O)=0.1428  V(3)(C-C)=1143.7 cm-1
V(3)(C-O)=1479.46 cm-1  V(3)(O-O)=2427.3 cm-1 NU=3661,2966,2955,2936,2898,2892,
1484,1481,1466,1423,1405,1383,1263,1174,1153,1087,1002,868,804,481,293
HF298=-41.5 Kcal REF=Lay et al JPC 100,(1996),8240  Max Lst Sq Error Cp @ 6000 K
0.6%
C2H6O2             T10/96C  2.H  6.O  2.   0.G   200.000  6000.000  B  62.06844 1
 9.99511555E+00 1.47311626E-02-5.30621235E-06 8.58442516E-10-5.14814807E-14    2
-2.53850722E+04-2.53504050E+01 4.37310002E+00 1.04422436E-02 4.63854723E-05    3
-7.02772770E-08 2.93034879E-11-2.29362227E+04 8.30134323E+00-2.08834916E+04    4

C2H5SH ETHANETHIOL DATA FROM STULL WESTRUM & SINKE  1969, EXTRAPOLATED
TO 5000 K USING WILHOIT'S POLYNOMIALS. HF298=-11.02 KCAL Max Lst Sq Error H-Href
@ 300 K *6.7%*.
C2H6S              T 4/93C   2H   6S   1     0G   298.150  5000.000  B  62.13564 1
 0.64687045E+01 0.16391622E-01-0.60377275E-05 0.10524727E-08-0.70286890E-13    2
-0.86436726E+04-0.69816273E+01 0.21847425E+01 0.24139946E-01-0.54359062E-05    3
-0.71826248E-08 0.40986272E-11-0.72094881E+04 0.16264503E+02-0.55454477E+04    4
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C2H6S  METHYL SULFIDE CH3-S-CH3  DATA FROM STULL WESTRUM & SINKE EXTRAPOLATED
TO 5000 K USING WILHOIT'S POLYNOMIALS. HF298=-8.97 KCAL Max Lst Sq Error H-Href
@ 300 K *6.4%*
C2H6S (CH3SCH3)    T 4/93C   2H   6S   1    0G   298.150  5000.000  B  62.13564 1
 0.61189311E+01 0.16882055E-01-0.63478415E-05 0.11172322E-08-0.74890322E-13    2
-0.74615078E+04-0.61902955E+01 0.19139966E+01 0.29420442E-01-0.24128528E-04    3
 0.15495718E-07-0.50061422E-11-0.62072425E+04 0.15648303E+02-0.45138535E+04    4

C2H6S2  METHYL DISULFIDE CH3-S-S-CH3  DATA FROM STULL WESTRUM & SINKE EXTRAPO-
LATED TO 5000 K USING WILHOIT'S POLYNOMIALS. HF298=-5.77 KCAL  Max Lst Sq Error
H-Href @ 300 K *7.8%*
C2H6S2             T 4/93C   2H   6S   2    0G   298.150  5000.000  B  94.20164 1
 0.91856110E+01 0.17160184E-01-0.66808919E-05 0.12071229E-08-0.82458844E-13    2
-0.69404925E+04-0.17999496E+02 0.51094624E+01 0.20928434E-01 0.43660805E-05    3
-0.17144491E-07 0.75300808E-11-0.53653977E+04 0.50798739E+01-0.29035602E+04    4

(CH3)2N-NH* UNSYMETRICAL DIMETHYL HYDRAZINE RADICAL VERY ROUGH ESTIMATE BASED ON
BOZZELLI & RITTER AND STEIN'S METHOD 1985 AND EXTRAPOLATED USING BOZZELLI &
RITTER POLYNOMIALS HF298=40.2+/-2. KCAL Max Lst Sq Error Cp @ 500 K 0.87%
C2H7N2             T 3/92C   2H   7N   2    0G   298.150  5000.000  F  59.09106 1
 0.73869042E+01 0.20545002E-01-0.76539338E-05 0.12996130E-08-0.82822039E-13    2
 0.16598849E+05-0.16520462E+02-0.11327504E+01 0.50235285E-01-0.52323994E-04    3
 0.35809697E-07-0.11058376E-10 0.18730972E+05 0.26216502E+02 0.20229310E+05    4

CH3NH-NHCH3 SYMETRICAL DIMETHYL HYDRAZINE SIGMA=4 IA=4.593949  IB=17.1057
IC=18.565859  NU=3378,3294,2948,2936,2902,2900,2827,2799,1508.5,1491,1474,1471,
1465,1457,1432,1421,1222.5,1190,1157,1119,1113,1011,900.5,863,757,442,404
N-CH3 Rotation IR=0.488 Potential Barrier V(3)=1049 cm-1 ROSYM=3  N-N Rotation
IR=1.53152  Potential Barrier V(2)=3778 cm-1 ROSYM=2  REF=C. Melius BAC/MP4
Calculations, Private Communication  HF298=22.584+/-1.8 KCAL  Max Lst Sq Error
Cp @ 1300 K 0.65%
C2H8N2 SYM         T 7/93C   2H   8N   2    0G   200.000  6000.000  B  60.09900 1
 0.80414886E+01 0.21261224E-01-0.77211118E-05 0.12549260E-08-0.75477198E-13    2
 0.70952651E+04-0.19466398E+02 0.52268579E+01 0.75034124E-03 0.75377281E-04    3
-0.95913660E-07 0.37320229E-10 0.92788780E+04 0.19786705E+01 0.11364645E+05    4

(CH3)2N-NH2 UNSYMETRICAL DIMETHYL HYDRAZINE SIGMA=18. STATWT=1 IAIBIC=14.95E-115
NU=3338,3315,2980(2),2961(2),2816,2777,1587,1464(2),1449(2),1402(2),1319,1246,
1215,1144,1060,1032,966,908,808,459,441,411 IR(CH3)=0.503 IR(NH2)=0.303 ROT
INT BARRIER V3(CH3)=4.69 KCAL V3(NH2)=3. KCAL REF=J.R. Durig & W.C. Harris  J.
CHEM. Phys. 51 (1969), 4457. MAX LST SQ ERROR Cp @ 6000 K 0.30%  HF298=53.33 KJ
C2H8N2 UNSYM       T09/91C   2H   8N   2    0G   200.000  6000.000  B  60.09900 1
 0.95884921E+01 0.20043079E-01-0.71185025E-05 0.11401487E-08-0.67870741E-13    2
 0.18116417E+04-0.25995709E+02 0.30395710E+01 0.22043065E-01 0.30487429E-04    3
-0.57055204E-07 0.25070487E-10 0.43464264E+04 0.11553546E+02 0.64008583E+04    4

CCN RADICAL  SIGMA=1 STATWT=2 IB=7.0317 NU=1717,325(2),1066  Te=40.34 STATWT=2
T0=10600.  STATWT=4  T0=21259.15 STATWT=4  T0=22413. STATWT=2  T0=26661.73
STATWT=2   REF=TSIV  HF298=604.85 KJ
CCN                RUS 79C  2N   1    0     0G   200.000  6000.000  B  38.02874 1
 0.58067399E+01 0.15990703E-02-0.59490513E-06 0.10618890E-09-0.68989867E-14    2
 0.70740102E+05-0.52450773E+01 0.37445392E+01 0.70577131E-02-0.64588927E-05    3
 0.35772165E-08-0.10103810E-11 0.71360584E+05 0.55673126E+01 0.72740240E+05    4

CNC RADICAL  SIGMA=2 STATWT=2  IB=6.173  NU=1100,321(2),1453  Te=26.41 SIGMA=2
STATWT=2  REF=TSIV  HF298=654.94 KJ
CNC                RUS 79C  2N   1    0     0G   200.000  6000.000  B  38.02874 1
 0.59325578E+01 0.15792030E-02-0.61235866E-06 0.10387387E-09-0.64318698E-14    2
 0.76724556E+05-0.66018499E+01 0.39895547E+01 0.52201058E-02-0.58212323E-06    3
-0.33928816E-08 0.17621885E-11 0.77357494E+05 0.38873499E+01 0.78767981E+05    4
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C2N2    REF= TSIV  HF298=309.1 KJ
C2N2               RUS 79C  2N   2    0     0G   200.000  6000.000  B  52.03548 1
 0.67055078E+01 0.36425829E-02-0.13094063E-05 0.21643797E-09-0.13121437E-13    2
 0.34860766E+05-0.10493904E+02 0.23292532E+01 0.26153785E-01-0.49000399E-04    3
 0.46191748E-07-0.16432385E-10 0.35668442E+05 0.98501993E+01 0.37175973E+05    4

C2N6O12 HEXANITROETHANE C2(NO2)6 SIGMA=6 IAIBIC=6364500.E-117  (IR(NO2)=59.6)x6
IR(C(NO2)3)=684   V(2)-NO2=2800 cm-1  V(3)-C(NO2)3=1000 cm-1   NU=1627,1353,
1143,858,375,335,113,1630(2),1268(2),1003(2),665(2),391(4),238(2),103(2),1621,
1333,888,582,376,240,1639(2),1285(2),820(2),633(2),383(2),347(2),155(2),92(2),
642,774  REF= Olga Dorofeeva Unpublished Results 1999   HF298=179.+/-5.9 kJ
REF= Pepekin Miroshichenko, Lebedev, Aspin Rus J. Phys. Chem. Eng. Trans. 42,
(1968),1583-1584  Max Lst Sq Error Cp @ 1200 K 0.58%
Hexanitroethane   T11/99C  2.N  6.O 12.   0.G   200.000  6000.000  C 300.05524 1
 4.21870612E+01 1.23800129E-02-5.52306964E-06 1.00910711E-09-6.53407906E-14    2
 5.66970453E+03-1.69918944E+02 1.06751275E+01 1.00230936E-01-1.00773651E-04    3
 5.18003948E-08-1.19450365E-11 1.46844877E+04-6.42835467E+00 2.15286289E+04    4

C2O  SIGMA=1  STATWT=3  IB=7.269 NU=1978,379.4(2),1074   T0=4000.   STATWT=2
T0=6500.  STATWT=1  T0=11651.  STATWT=6   REF=TSIV   HF298=291.04 KJ
C2O                RUS 79C   2O  1    0     0G   200.000  6000.000  B  40.02140 1
 0.51512722E+01 0.23726722E-02-0.76135971E-06 0.11706415E-09-0.70257804E-14    2
 0.33241888E+05-0.22183135E+01 0.28648610E+01 0.11990216E-01-0.18362448E-04    3
 0.15769739E-07-0.53897452E-11 0.33749932E+05 0.88867772E+01 0.35003406E+05    4

C3  CALCULATED FROM TSIV TABLES HF298=839.96 KJ
C3                 RUS 79C  3    0    0     0G   200.000  6000.000  B  36.03300 1
 0.48035776E+01 0.21451125E-02-0.10729208E-05 0.26073528E-09-0.20163197E-13    2
 0.99396542E+05 0.38936985E+00 0.54328396E+01-0.44675438E-02 0.14932148E-04    3
-0.14795314E-07 0.50142111E-11 0.99495722E+05-0.15872071E+01 0.10102201E+06    4

C3D4  CYCLOPROPENE-D4  STATWT=1.  SIGMA=2.  IA=3.861  IB=4.9423  IC=7.826
NU=2435,2142,1548,1147,1023,639,749,640,2313,885,863(2),637,2262,424
REF=BURCAT(1982)  MAX LST SQ ERROR CP @ 1300 K 0.79 % .HF298=63.0 KCAL
C3D4               T 2/82C  3D   4    0     0G   300.000  5000.000  B  44.0894  1
 0.89251080E+01 0.92740692E-02-0.33307069E-05 0.52548144E-09-0.30162352E-13    2
 0.27717801E+05-0.24771932E+02 0.87993717E+00 0.25426447E-01-0.47690091E-05    3
-0.14818401E-07 0.86449008E-11 0.30267191E+05 0.18314783E+02 0.31592361E+05    4

C3D6  CYCLOPROPANE-D6  STATWT=1.  SIGMA=6  IA=IB=6.0672  IC=8.75747  NU=2236,
1274,956,800,870,2336,614,2211(2),1072(2),855(2),717(2),2329(2),940(2),528(2)
REF=DUNCAN & BURNS  MAX LST SQ ERROR @ 1300 K 0.85 % . HF298=32.85 KJ. REF= C3H6
C3D6               T12/81C  3D   6    0     0G   300.000  5000.000  B  48.1176  1
 0.10402956E+02 0.12471735E-01-0.44642438E-05 0.70182371E-09-0.40115975E-13    2
-0.77593262E+03-0.35093755E+02-0.79611647E+00 0.35631880E-01-0.75448597E-05    3
-0.20582778E-07 0.12364153E-10 0.27102590E+04 0.24640681E+02 0.39509243E+04    4

C3F6 HEXAFLUORO PROPENE  IA=32.62   IB=67.0   IC=89.46  IR=7.99  ROSYM=3
POTENTIAL BARRIER V(3)=524.6 cm-1  REF=BRINKMANN & BURCAT FROM LOWREY et.al,
J MOL. STRUCT 53 (1979),189   NU=1797,1399,1333,1211,1179,1122,1037,767,655,
609,559(2),513,462,370,364,250(2),171,134    REF=NIELSEN CLAASSEN & SMITH JCP
20 (1952),1916   HF298=-268.9 KCAL Max Lst Sq Error Cp @ 1300 K 0.43%.
C3F6               T 3/95C   3F   6    0     0G   200.000  6000.000  B 150.02342 1
 0.17044075E+02 0.70305647E-02-0.27319665E-05 0.46409607E-09-0.28766698E-13    2
-0.14174864E+06-0.58929196E+02 0.12094279E+01 0.59383698E-01-0.71616083E-04    3
 0.43686588E-07-0.10885628E-10-0.13776344E+06 0.20848317E+02-0.13531496E+06    4
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C3F7 RADICAL CF3CF*CF3  SIGMA=18   STATWT=2 IA=38.9352  IB=80.40703 IC=91.12589
NU=1393,1370,1290,1243,1238,1204,1182,969,769,687,684,598,534,522,492,443,335,
311,286.5,241,167,132,50.3,16.8   HF298=-321.91 kcal  REF=Melius database 1987
AB1W  Max Lst Sq Error Cp @ 1300 K 0.40%
C3F7 CF3CF*CF3 M  T12/99C  3.F  7.   0.   0.G   200.000  6000.000  C 169.02182 1
 2.05301132E+01 7.60062764E-03-2.96491015E-06 5.04882378E-10-3.13452721E-14    2
-1.69702083E+05-7.19281430E+01 3.14241614E+00 6.03443070E-02-6.17598017E-05    3
 2.79379580E-08-4.02551172E-12-1.65147364E+05 1.66897624E+01-1.62020670E+05    4

C3F8  OCTAFLUOROPROPANE (FC-218)   SIGMA=18  CALCULATED AND EXTRAPOLATED USING
BOZZELLI & RITTER'S PROGRAM. HF298=-1760.12 KJ. REF=DOMALSKI & HEARING   JPCRD
22 (1993), p. 1065.
C3F8 FC-218       T 1/94C   3F   8    0    0G   298.150  5000.000  D 188.02023 1
 0.23380508E+02 0.71509045E-02-0.30004329E-05 0.55566723E-09-0.37865981E-13    2
-0.22034342E+06-0.89673706E+02 0.16732611E+01 0.72542284E-01-0.70291850E-04    3
 0.25054365E-07-0.94876882E-12-0.21484389E+06 0.20590469E+02-0.21169268E+06    4

C3H RAD  STATWT=3.  SIGMA=1.  B0=.4047     NU=3312,2089(2),1230,630(2),2040
REF=SPANGENBERG & BORGER  MAX LST SQ ERROR CP @ 1300K 0.6%. HF298=163.5 KCAL
REF=Estimated from C2H C4H and C6H by Kiefer et al 1992
C3H               T07/93C   3H   1    0    0G   200.000  6000.000  C  37.04094 1
 0.34671283E+01 0.62969122E-02-0.22708676E-05 0.36749291E-09-0.22034692E-13    2
 0.80801495E+05 0.53527629E+01 0.24726647E+01 0.85316627E-02-0.63505996E-05    3
 0.56681332E-08-0.24832298E-11 0.81205573E+05 0.10875808E+02 0.82275925E+05    4

C3HF7 2-HEPTAFLUORO-PROPANE CF3-CHF-CF3 (FC-227ea) SIGMA=2 STATWT=1  IA=38.9667
IB=78.08525  IC=88.49144  NU=2966,1428,1392,1324,1296,1280,1242,1224,1150,1131,
896,853,725,669,593,535,519,502,442,335,314,283,232,214,152,89.7.26.9
HF298=-1564.8. KJ REF=Melius Database 1987 AB1V  Max Lst Sq Error Cp @
1300 K 0.44%.
C3F7H  FC227EA    T12/99C  3.H  1.F  7.   0.G   200.000  6000.000  C 170.02976 1
 2.03195617E+01 1.04618873E-02-3.99351610E-06 6.70976809E-10-4.12886922E-14    2
-1.96070480E+05-7.39087817E+01 3.19381844E+00 5.64358210E-02-4.24435538E-05    3
 6.01422805E-09 4.21730731E-12-1.91302556E+05 1.47970140E+01-1.88203033E+05    4

C3HN CYANO-ACETYLENE HCC-CN ESTIMATED BY MACKIE & COLKET 22nd COMBUST SYMP 1990
EXTRAPOLATED 2000-3000 K USING WILHOIT'S POLYNOMIALS  HF298=84.6 KCAL Max Lst Sq
Error Cp @ 1500 K 0.68%
C3HN              T 6/92C   3H   1N   1    0G   298.150  3000.000  E  51.04768 1
 0.88772204E+01 0.29716427E-02-0.54197830E-06 0.00000000E+00 0.00000000E+00    2
 0.39418987E+05-0.23891571E+02 0.45374481E+01 0.12685759E-01-0.59612178E-05    3
 0.00000000E+00 0.00000000E+00 0.40708114E+05-0.91798142E+00 0.42572130E+05    4

C3H2 CYCLOPROPENYLIDENE BI-RADICAL SINGLET SIGMA=2 STATWT=1 Ia=2.35340 Ib=2.4065
Ic=4.8941  Nu=788,887,[898,979],1063,1277,[1588,3080,3114] REF=Webbook NIST2000
+[]Vereecken, et al 108,(1998),1068   HF298=114 kcal  REF= Kiefer et.al.
J. Phys. Chem 101, (1997), 4057   {HF298=121.63+/-6.3 kcal REF=Melius 1988 P60V}
{HF298=136 kcal   REF=PM3 RHF calculation}   Max Lst Sq  Error Cp @ 200 K 0.82%
C3H2(1) Cyclo     T12/00C  3.H  2.   0.   0.G   200.000  6000.000  B  38.04888 1
 5.69445684E+00 6.53821902E-03-2.35907266E-06 3.82037385E-10-2.29227460E-14    2
 5.49264274E+04-6.96163733E+00 3.18167129E+00-3.37611741E-04 3.95343765E-05    3
-5.49792422E-08 2.28335240E-11 5.61816758E+04 9.06482468E+00 5.73666999E+04    4

C3H2 (3) RAD having a structure H2CCC**. TRIPLET  SIGMA=1  STATWT=2 Ia=0.2852
Ib=7.9457  Ic=8.23089  REF=Melius A69E   Nu=3116,3030,1409,1320,956,913,615,437,
344  HF298=155.6 kcal REF=Vereecken et al, 108,(1998),1068 {HF298=160.7 kcal.
REF=Melius Database 1988 A69D}    Max Lst Sq Error Cp @ 6000 K 0.47%
C3H2 H2C=C=C**    T12/00C  3.H  2.   0.   0.G   200.000  6000.000  B  38.04888 1
 6.67324760E+00 5.57728847E-03-1.99180164E-06 3.20289158E-10-1.91216274E-14    2
 7.57571184E+04-9.72894405E+00 2.43417332E+00 1.73013063E-02-1.18294047E-05    3
 1.02756397E-09 1.62626314E-12 7.69074892E+04 1.21012230E+01 7.83005132E+04    4
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```
C3H2(3) RAD   *HC=C=CH* PROP-2-YNYLIDENE TRIPLET  SIGMA=2   STATWT=2   Ia=0.075
Ib=8.2828   Ic=8.3057  {HF298=129.39 kcal} REF=Melius 1988 A69K
Nu=[3318],3265,1621,[1238,434],401,[337],246,[209] REF=Webbook NIST 2000
+[]Vereecken, et al 108,(1998),1068     HF298=123.6 kcal  REF=Kiefer
et. al. J. PHYS. Chem 101, (1997),4057     Max Lst Sq Error Cp @ 6000 K 0.38%
C3H2 *HC=C=C** (3)T12/00C  3.H  2.   0.   0.G   200.000  6000.000  B  38.04888 1
 7.47247828E+00 4.57765158E-03-1.56482124E-06 2.43991963E-10-1.42462923E-14    2
 5.96940836E+04-1.27113314E+01 3.74356467E+00 2.51955211E-02-4.62608277E-05    3
 4.34360520E-08-1.53992558E-11 6.02917182E+04 4.22612394E+00 6.21975799E+04    4

C3H2(1) RAD  *HC=C=CH* PROP-2-YNYLIDENE SINGLET  SIGMA=2   STATWT=1   Ia=0.15205
Ib=8.0709   Ic=8.22298 {HF298=141.43+/-2.67 kcal}  REF=Melius Database 1988 A69G
Nu=3120,3115,1769,1195,936,784,436,319,285  HF298=138.6+/-10 kcal  REF=Vereecken,
et al 108,(1998),1068   {HF298=127.5 kcal  REF=Kiefer et. al. J. PHYS. Chem 101,
(1997),4057}      Max Lst Sq Error Cp @ 6000 K 0.36%
C3H2 *HC=C=CH* (1)T12/00C  3.H  2.   0.   0.G   200.000  6000.000  B  38.04888 1
 6.74647933E+00 5.43300692E-03-1.92072372E-06 3.06675627E-10-1.82157003E-14    2
 6.72827137E+04-1.09202302E+01 2.87526884E+00 1.99235625E-02-2.41971222E-05    3
 1.66378231E-08-4.69230978E-12 6.81861445E+04 8.19359597E+00 6.97458299E+04    4

C3H2N CYANO-ETHYLENE RADICAL HC*=CH-CN ESTIMATED BY MACKIE & COLKET 22nd COMBUST
SYMP. 1990 EXTRAPOLATED 2000-3000 K USING WILHOIT's POLYNOMIALS.  HF298=97 KCAL
Max Lst Sq Error Cp @ 1500 0.64%
C3H2N            T 6/92C   3H   2N   1    0G   298.150  3000.000  E  52.05562 1
 0.96001313E+01 0.38148554E-02-0.63228547E-06 0.00000000E+00 0.00000000E+00    2
 0.45134563E+05-0.24709525E+02 0.42128781E+01 0.14484744E-01-0.59662404E-05    3
 0.00000000E+00 0.00000000E+00 0.46964857E+05 0.45013912E+01 0.48812017E+05    4

C3H3 RAD  STATWT=2.  SIGMA=2.  IA=.29055  IB=8.8826  IC=9.16487    NU=3264,3081,
2990,1912,1390,1007,930,607,585,449,364,331  REF=Kumaran et.al. Israel J. Chem,
36, (1996),223  HF298=346. kJ  REF=TSANG, Int. J. Chem. Kinet 10 (1978),687
Max Lst Sq Error Cp @ 6000 K 0.39%
C3H3 PROPARGYL    T 5/97C  3.H  3.   0.   0.G   200.000  6000.000  B  39.05682 1
 7.14221880E+00 7.61902005E-03-2.67459950E-06 4.24914801E-10-2.51475415E-14    2
 3.89087427E+04-1.25848435E+01 1.35110927E+00 3.27411223E-02-4.73827135E-05    3
 3.76309808E-08-1.18540923E-11 4.01057783E+04 1.52058924E+01 4.16139977E+04    4

C3H3Cl  1-CHLORO,1-PROPYNE Cl-CC-CH3 ESTIMATED VALUES BY NIST 94 TO 1000 K AND
EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS  S298=67.87 CAL. FROM STULL
WESTRUM & SINKE  SIGMA=3  HF298=35.2 KCAL   Max Lst Sq Error Cp @ 1000 K 0.48%
CLC3H3 1ClPROPYNE T 1/96CL  1C   3H   3    0G   298.150  5000.000  F  74.50952 1
 0.81343956E+01 0.98453550E-02-0.38027919E-05 0.68016167E-09-0.45987715E-13    2
 0.14316797E+05-0.16188642E+02 0.42197737E+01 0.15755283E-01-0.15018964E-05    3
-0.72933170E-08 0.35641684E-11 0.15780828E+05 0.55475193E+01 0.17713227E+05    4

C3H3Cl  3-CHLORO,1-PROPYNE H-CC-CH2Cl   SIGMA=1  IA=3.42022  IB=27.5776
IC=30.49975  NU=3339,3048,2990,2051,1442,1283,1174,937,898,727,553,533,407,229,
151  HF0=40.10 KCAL  REF=Kumaran et.al. ISRAEL J. Chem 36,(1996),223   Max Lst
Sq Error Cp @ 6000 K 0.43%
C3H3Cl CH2Cl-CCH  T 5/97C  3.H  3.CL 1.   0.G   200.000  6000.000  B  74.50952 1
 8.60964894E+00 9.12088266E-03-3.24810521E-06 5.21296691E-10-3.10793797E-14    2
 1.61738376E+04-1.69659939E+01 2.49757092E+00 2.75585732E-02-2.33670745E-05    3
 8.99167349E-09-7.08099389E-13 1.77912033E+04 1.42223355E+01 1.95717345E+04    4
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C3H3Cl 3-CHLOROCYCLOPROPENE  SIGMA=1  IA=3.9183  IB=21.13565  IC=22.3311
NU=3201,3161,3061,1602,1289,1164,1036,1025,916,854,804,708,572,348,344
HF0=53.88 kcal  REF=Kumaran et.al. ISRAEL J. Chem 36,(1996),223  Max  Lst Sq
Error Cp @ 200 K 0.54%
3-C3H3Cl  CY      T 5/97C  3.H  3.CL 1.   0.G   200.000  6000.000  B  74.50952 1
 8.70661016E+00 9.10661478E-03-3.26153884E-06 5.25606764E-10-3.14309766E-14    2
 2.26426992E+04-1.98513212E+01 1.38549419E+00 2.36867059E-02 4.57822305E-07    3
-2.34745441E-08 1.29903835E-11 2.48296574E+04 1.90259812E+01 2.62593301E+04    4

C3H3Cl CHLOROALLENE  CHCl=C=CH2  SIGMA=1  IA=2.57347  IB=29.7692  IC=31.7616
NU=3130,3111,3041,1954,1428,1260,1085,985,858,833,766,550,490,294,175  HF0=39.86
kcal  REF=Kumaran et.al. ISRAEL J Chem 36,(1996),223  Max Lst Sq Error Cp @
6000 K 0.48%
C3H3Cl CHCl=C=CH2 T 5/97C  3.H  3.CL 1.   0.G   200.000  6000.000  B  74.50952 1
 8.48868205E+00 9.30781907E-03-3.33392517E-06 5.37178372E-10-3.21149115E-14    2
 1.58981402E+04-1.72834335E+01 2.17876528E+00 2.46488928E-02-1.08872907E-05    3
-6.58963705E-09 5.61690902E-12 1.77072077E+04 1.57028855E+01 1.93458135E+04    4

C3H3N CYANO ETHYLENE (ACRYLONITRILE) H2C=CH-CN DATA FROM STULL, WESTRUM & SINKE
EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS   HF298=43.9 KCAL REF=MACKIE
& COLKET 22nd COMBUSTION SYMP 1990  Max Lst Sq Error Cp @ 1200 0.22%
C3H3N             T 3/93C   3H   3N   1    0G   298.150  5000.000  B  53.06356 1
 0.69065705E+01 0.10800137E-01-0.37628658E-05 0.63163169E-09-0.41239008E-13    2
 0.19145754E+05-0.10479364E+02 0.11375668E+01 0.27608666E-01-0.21536835E-04    3
 0.84150703E-08-0.10902334E-11 0.20699089E+05 0.19117727E+02 0.22091212E+05    4

C3H3O ACROLEIN RADICAL CH2=CH-C*=O  STATWT=2  SIGMA=1  IA=0.6266  IB=8.44834
IC=9.0738  Nu=3138,3127,3058,2188,1844,1333,1250,1184,1101,1012,922,717,560,301,
258  REF=Burcat (MOPAC6 PM3)  HF298=17.3 kcal  REF=McMillan & Golden Ann Rev.
Phys. Chem 33,(1982),493.  Max Lst Sq Error Cp @ 6000 K 0.52%
C3H3O CH2=CHC*=O  T05/99C  3.H  3.O  1.   0.G   200.000  6000.000  C  55.05622 1
 6.95842227E+00 1.07193211E-02-3.85218494E-06 6.22009064E-10-3.72401640E-14    2
 5.64826498E+03-1.14745786E+01 3.21169467E+00 1.18422105E-02 1.67462582E-05    3
-3.06947176E-08 1.33048816E-11 7.12815750E+03 1.00881663E+01 8.70564832E+03    4


H4C3  PROPYNE  STATWT=1.  SIGMA=3.  IA=.5283  IB=IC=9.8172  NU=3334,2918,2142,
1382,931,3008(2),1452(2),1053(2),633(2),328(2)   REF=SHIMANOUCHI  MAX LST SQ
ERROR CP @ 1300K 0.59% . HF298=44.319 KCAL REF=TRC(API #44).
H4C3 PROPYNE      T 2/90H   4C   3    0    0G   200.000  6000.000  B  40.06476 1
 0.60252400E+01 0.11336542E-01-0.40223391E-05 0.64376063E-09-0.38299635E-13    2
 0.19620942E+05-0.86043785E+01 0.26803869E+01 0.15799651E-01 0.25070596E-05    3
-0.13657623E-07 0.66154285E-11 0.20802374E+05 0.98769351E+01 0.22302059E+05    4

C3H4  ALLENE  STATWT=1.  SIGMA=4.  IA=.555  IB=IC=9.4389  NU=3015,1443,1073,
865,3007,1957,1398,3086(2),999(2),841(2),355(2)  REF SHIMANOUCHI  MAX LST SQ
ERROR CP @ 1300K 0.3% . HF298=190.92 KJ REF=TRC(1988).
C3H4 ALLENE       L 8/89C   3H  4    0     0G   200.000  6000.000  B  40.06476 1
 0.63168722E+01 0.11133728E-01-0.39629378E-05 0.63564238E-09-0.37875540E-13    2
 0.20117495E+05-0.10995766E+02 0.26130445E+01 0.12122575E-01 0.18539880E-04    3
-0.34525149E-07 0.15335079E-10 0.21541567E+05 0.10226139E+02 0.22962267E+05    4

C3H4  CYCLOPROPENE  STATWT=1  SIGMA=2  IA=2.792  IB=3.846  IC=6.085  NU=3152,
2909,1653,1483,1105,905,996,815,3116,1043,1011,769,2995,1088,569  REF=YUM &
EGGERS MAX LST SQ ERROR CP @ 1300 K 0.78 % . HF298=277.1 KJ   REF=Dorofeeva,
Gurvich & Jorish JPCRD 15 (1986) 437.
C3H4 CYCLOPROPENE T12/81C   3H  4    0     0G   300.000  5000.000  B  40.0648  1
 0.66999931E+01 0.10357372E-01-0.34551167E-05 0.50652949E-09-0.26682276E-13    2
 0.30199051E+05-0.13378770E+02-0.24621047E-01 0.23197215E-01-0.18474357E-05    3
-0.15927593E-07 0.86846155E-11 0.32334137E+05 0.22729762E+02 0.3332728 E+05    4
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C3H4CL 3-CHLOROPROPENYL-1 (*CH=CH-CH2CL) VERY ROUGH ESTIMATE MADE BY Weisman &
Benson (1989) EXTRAPOLATED BY WILHOIT'S POLYNOMIALS Max Lst Sq Error Cp @ 1200 K
**2.43%**   HF298=56.3 KCAL
C3H4CL            T 2/92C   3H   4CL  1    0G   298.150  5000.000  F  75.51746 1
 0.12647329E+02 0.48590959E-02-0.50757043E-06 0.00000000E+00 0.00000000E+00    2
 0.22783329E+05-0.39359537E+02 0.31710019E+01 0.21669817E-01-0.87210576E-05    3
 0.00000000E+00 0.00000000E+00 0.26499558E+05 0.13298996E+02 0.28331098E+05    4

C3H4CL 1-CHLOROALLYL (CHCL-C*H-CH2) VERY ROUGH ESTIMATE MADE BY Weisman & Benson
(1989) EXTRAPOLATED BY WILHOIT'S POLYNOMIALS Max Lst Sq Error Cp @ 1200 K **4.3%
HF298=25.6 KCAL.
CLC3H4            T 2/92CL  1C   3H   4    0G   298.150  5000.000  F  75.51746 1
 0.15465487E+02 0.25924820E-02-0.29662608E-06 0.00000000E+00 0.00000000E+00    2
 0.58619120E+04-0.56125312E+02 0.32384832E+01 0.21320222E-01-0.75151082E-05    3
 0.00000000E+00 0.00000000E+00 0.11035572E+05 0.13116111E+02 0.12882347E+05    4

C3H4N 2-PROPIONITRILE RADICAL CH3-CH*CN  STATWT=2  SIGMA=3 ESTIMATED USING NIST
1994 PROGRAM FROM [C-(H)3];[C.-(C)(CN)(H)]  HF298=195 KJ Max Lst Sq Error Cp @
400 K 0.46%
C3H4N             T10/94C   3H   4N   1    0G   298.150  5000.000  E  54.07150 1
 0.10231862E+02 0.71400760E-02-0.13133923E-05 0.13292440E-09-0.66022531E-14    2
 0.19025810E+05-0.28440556E+02-0.33826965E+00 0.32723744E-01-0.20997746E-04    3
 0.32049909E-08 0.15921475E-11 0.22277791E+05 0.27410122E+02 0.23452976E+05    4

C3H4N2 1,3-DIAZOLE, IMIDAZOLE, GLYOXALINE   SYMNO=1    IA=8.4525  IB=8.7054
IC=17.1579  NU=3501,3103,3077,3075,1558,1487,1418,1344,1260,1123,1102,1064,1034,
912,892,879,862,749,655,619,478      HF298=33.69 KCAL  REF=C. MELIUS DATABASE
BACMP22  #38 P1TZ  Max Lst Sq Error Cp @ 6000 K **1.04%**
C3H4N2 1,3-DIAZOLET 9/96C   3H   4N   2    0G   200.000  6000.000  B  68.07824 1
 0.92025957E+01 0.14142668E-01-0.51071395E-05 0.82778679E-09-0.49706044E-13    2
 0.12518192E+05-0.26079671E+02 0.13020933E+01 0.11479286E-01 0.60444678E-04    3
-0.95013016E-07 0.40803163E-10 0.15689407E+05 0.20116256E+02 0.16953369E+05    4

C3H4N4O6  1,3,3-Tri-Nitro-Azetidine    SYMNO = 2  STATWT = 1   IA = 60.59091
IB = 147.3316 IC = 169.6545    Ir(NO2) = 5.96  ROSYM =2   V(2)=12.5 kcal/mole
3036,3021,2973,2900,1589(2),1538,1510,1428,1403,1380,1365,1340,1325,1280,
1216,1200,1183,1172,1113,1085,1057(2),906,865(2),843(2),816,761(2),712,662(2),
626(3),601,564(3),480(2),162.   REF =Yu, Zhang & Bauer, (THEOCHEM)15,(1998),...
HF298= 30.7 kcal  REF = Politzer et al J. Molec Struct (THEOCHEM)338,(1995),249.
Max Lst Sq Error Cp @ 200 K 0.98%
1,3,3 TRI-NITRO-  T05/98C  3.H  4.N  4.O  6.G   200.000  6000.000  B 192.08812 1
 2.22004023E+01 2.61448557E-02-1.00734632E-05 1.69575778E-09-1.04302158E-13    2
 4.95227016E+03-9.72924159E+01-3.22895573E+00 6.02068540E-02 4.89990294E-05    3
-1.24714696E-07 5.86010192E-11 1.35213474E+04 4.22296092E+01 1.54487516E+04    4

C3H4O  2-PROPENAL, ACROLEIN, ACRYLALDEHYDE    SIGMA=1   IA=0.828   IB=8.3686
IC=9.17905 REF=Burcat (MOPAC6 PM3) NU=3103,3028,3000,2800,1724,1625,1420,1360,
1275,1158,912,564,327,993,980,959,593,157  REF=Shimanuchi, NBS 1972 HF298=-17.8
+/- 0.3 kcal  REF=Stein, NIST 1994    Max Lst Sq Error Cp @ 6000 K 0.56%
C3H4O ACROLEIN    T05/99C  3.H  4.O  1.   0.G   200.000  6000.000  B  56.06416 1
 7.65585747E+00 1.29138634E-02-4.67510310E-06 7.58623343E-10-4.55761782E-14    2
-1.25007135E+04-1.64463335E+01 3.51513293E+00 8.76497333E-03 3.56361100E-05    3
-5.33123832E-08 2.20038319E-11-1.06147449E+04 8.66137871E+00-8.95725665E+03    4
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Table 4 (continued)

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C3H5 ALLYL RAD SYMMETRIC STABILIZED BY RESONANCE CH2-C*H-CH2   STATWT=2  SIGMA=2
IA=1.52057 IB=8.20036 IC=9.70572  REF=Nicolaides & Borden JACS 114,(1992), 8682
NU=3107(2),3051,3021,3019,1477,1463,1389,1242,1184,1005,983,913,801,738,517,510,
418   REF=Sim, Shaub, Chin, Dupuis JCP 95,(1991),4315  HF298=39.1 Kcal
REF=Wu & Kern JPC 91 (1987),6291  Max Lst Sq Error Cp @ 200 K 0.57%.
C3H5 SYMMETRIC    T 9/96C   3H   5    0    0G   200.000  6000.000  B  41.07270 1
 0.70094568D+01 0.13106629D-01-0.46533442D-05 0.74514323D-09-0.44350051D-13    2
 0.16412909D+05-0.13946114D+02 0.14698036D+01 0.19034365D-01 0.14480425D-04    3
-0.35468652D-07 0.16647594D-10 0.18325831D+05 0.16724114D+02 0.19675772D+05    4

C3H5 TERTIARY NONSYMMETRIC RAD  (CH2=C*CH3) STATWT=2.  SIGMA=1. IA=1.2558815
IB=10.379297 IC=11.08304 NU=315,470.8,834.5,836,911.6,1018.8,1090.8,1356,1390,
1435,1448,1507,2830,2888,2902.5,2906.8,2999.7 IR=0.3945E-39 (INT ROT POTENTIAL
V3=17.7 Kcal. REF= Nicolaides & Borden JACS 114 (1992),8682)  ROSYM=3.
REF=Ab-Initio Calculat. Karni, Oref & Burcat TAE #643 1989. HF298=56.8 Kcal
REF=Wo & Kern JPC 91 (1987),6291   Max Lst Sq Error Cp @ 6000 K 0.61%.
T-C3H5 CH3C*=CH2  T 6/96C   3H   5    0    0G   200.000  6000.000  B  41.07270 1
 0.61101805E+01 0.14673395E-01-0.53676822E-05 0.86904932E-09-0.51932006E-13    2
 0.25532442E+05-0.83555712E+01 0.25544033E+01 0.10986798E-01 0.30174305E-04    3
-0.47253568E-07 0.19771073E-10 0.27150242E+05 0.13207592E+02 0.28582707E+05    4

C3H5 SECONDARY RAD (CH3-CH=CH*) ALLYL RADICAL ROSIM=3  STATWT=2  VERY ROUGH
ESTIMATION USING BENSON'S & STEINS GROUP ADDITIVITY METHODS REF=TAN et.al Comb.
Sci. Tech. 102 (1994),21  EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS
HF298=62.8 Kcal  REF=Wo & Kern JPC 91 (1992),6291  Max Lst Sq Error Cp @ 1500 K
0.48%.
S-C3H5 CH3CH=CH*  T 6/96C   3H   5    0    0G   298.150  5000.000  F  41.07270 1
 0.61342175E+01 0.13325025E-01-0.48645230E-05 0.83773904E-09-0.55161424E-13    2
 0.28626198E+05-0.74112134E+01 0.22361012E+01 0.16387245E-01 0.76639733E-05    3
-0.19364818E-07 0.84155468E-11 0.30173536E+05 0.14806060E+02 0.31602007E+05    4

C3H5CL 3-CHLOROPROPENE-1 ESTIMATED BY Weissman & Benson 1989 EXTRAPOLATED USING
WILHOIT'S POLYNOMIALS HF298=-6.4 KCAL Max Lst Sq Error Cp @ 1200 K **3.0%**
C3H5CL            T 2/92C   3H   5CL  1    0G   298.150  5000.000  F  76.52540 1
 0.15793139E+02 0.39014273E-02-0.35641112E-06 0.00000000E+00 0.00000000E+00    2
-0.10235421E+05-0.58909374E+02 0.13873502E+01 0.29378119E-01-0.11679320E-04    3
 0.00000000E+00 0.00000000E+00-0.48368046E+04 0.20741241E+02-0.32205867E+04    4

C3H5N  ETHYL-CYANIDE (PROPIONITRILE) C2H5CN  DATA TAKEN FROM STULL WESTRUM &
SINKE EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS HF298=12.1 Kcal Max Lst
Sq Error Cp @ 1300 K 0.38%
C3H5N             T 3/93C   3H   5N   1    0G   298.150  5000.000  B  55.07944 1
 0.66453492E+01 0.16602435E-01-0.63295389E-05 0.11244907E-08-0.75837066E-13    2
 0.28684940E+04-0.93133221E+01 0.23948965E+01 0.22916966E-01-0.26286823E-05    3
-0.91651662E-08 0.44488849E-11 0.43955322E+04 0.14181511E+02 0.60889217E+04    4

C3H5NO2 Nitro-Propylene  STATWT = 1  IA = 9.5524  IB = 30.9429  IC = 39.9889
Ir(NO2) = 5.96    ROSYM = 2   V(2) = 1.5 kcal  Ir(CH3)= 0.5166  ROSYM = 3
V(3) = 8.8 kcal    NU = 3091,3001,2954,2954,2888,1696,1629,1477,1457,1448,
1400,1354,1228,1081,1072,971,955,887,831,762.655,575,382,362,223.
HF298 = 2.387 kcal   REF = Melius Database 1988  D85J     Max Lst Sq Error Cp
@ 1300 K  0.67%
NITROPROPYLENE C  T11/97C  3.H  5.N  1.O  2.G   200.000  6000.000  B  87.07824 1
 1.16044034E+01 1.73925254E-02-6.55603780E-06 1.08945442E-09-6.64543040E-14    2
-4.17082639E+03-3.40158247E+01 3.65175571E+00 2.01896036E-02 3.27504513E-05    3
-5.72328212E-08 2.41049017E-11-9.72583112E+02 1.18667163E+01 1.20117818E+03    4
```

```
C3H5NO2  Nitro-Cyclo-Propane   STATWT = 1  SYMNO =2  IA = 10.5515  IB = 28.5698
IC = 32.4822   Ir(NO2) = 5.96  ROSYM = 2  V(2) = 4.7 kcal/mole   NU = 3103,3095,
3019(2),2934,1571,1443,1407,1373,1325,1202,1118,1110,1075,1042,936,921,880,854,
828,770,645,483,309,289,730.   REF = Holtzclaw, Harris & Bush +Mochel, Britt &
Boggs J. Chem. Phys. 58,(1973),3221    HF298= 4.2 kcal   REF = Stein, NIST 94
Max Lst Sq Error Cp @ 200 K 0.91%.
NITRO-CYCLO-PROP  T05/98C  3.H  5.N  1.O  2.G   200.000  6000.000  B  87.07824 1
 1.28562217E+01 1.60380202E-02-5.91815923E-06 9.70786323E-10-5.87171694E-14    2
-3.71800893E+03-4.27122315E+01 2.06472972E+00 2.06839369E-02 5.54644460E-05    3
-9.75050004E-08 4.31800396E-11 2.60851586E+02 1.85111076E+01 2.11351000E+03    4

C3H5N3O9 NG  Nitroglycerine      STATWT = 1  SYMNO = 2     IA = 113.023087
IB = 216.411718  IC = 260.003555   (Ir(NO2) = 5.96  ROSYM = 2
V(2) = 9.1 kcal/mole)x3    NU = 3024,3014,2953,2941,2831,2142,3132,1537,1522,
1363,1359,1329,1318,1303,1231,1209,1160,1151,1145,1118,1093,1085,971,928,915,798,
701,676,654,639,627,622,582,478,470,463,409,379,348,317,312,276, 264,232,188,173,
97.7,62,60,54.1,44.4    REF = BURCAT, TAE Report # 824, 1998  HF298 =-66.7 kcal
REF = Miroshnichenko et al, Bul Acad. Sci. USSR, Chem Sci. (1988),1778.
Max Lst Sq Error Cp @ 1300 K 0.59%
NITROGLICERINE    T05/98C  3.H  5.N  3.O  9.G   200.000  6000.000  B 227.08752 1
 3.24464077E+01 2.44149769E-02-9.67605267E-06 1.65298018E-09-1.02555476E-13    2
-4.65896112E+04-1.31431034E+02 5.70797625E+00 9.52017978E-02-7.18228583E-05    3
 1.66304815E-08 3.01835927E-12-3.88975467E+04 7.78535957E+00-3.35645516E+04    4


C3H5O  C2H5CO RADICAL ESTIMATION MADE USING BOZZELLI & RITTER'S PROGRAM.BASED ON
PROPIONALDEHYDE FROM Chao et al 1986 MINUS H FROM ALDEHYDE GROUP   SIGMA=3
EXTRAPOLATED USING WILHOIT's POLYNOMIALS    HF298 = -36.02 KJ Max Lst Sq Error
Cp @ 1500 K 0.62%  **NIST 94 HF298 value of -46.86 kJ probably erroneous **
C2H5CO            T 9/92C   3H   5O   1    0G   298.150  5000.000  D  57.07210 1
 0.30445698E+01 0.23236429E-01-0.86317936E-05 0.14799550E-08-0.96860829E-13    2
-0.61787211E+04 0.13122302E+02 0.67368294E+01-0.26945299E-02 0.49927017E-04    3
-0.50025808E-07 0.15011503E-10-0.65703366E+04-0.23398732E+01-0.43321855E+04    4

C3H5O RADICAL *CH2COCH3 STATWT=2 SYMNO=1. IAIBIC=1290.63E-117  IR=0.4888
NU=3019(2),2972,2963,1731,1454,1435,1426,1410,1364,1216,1091,1066,891,877,777,
530,484,385 POT BARRIER V3=272 cm-1 REF=ACETONE JPCRD 15 (1986), 1369 MAX LST SQ
ERROR Cp @ 6000 0.59%. HF298=-3.36+/-0.5 KCAL REF= BOZZELLI & RITTER's PROGRAM
CH2COCH3          T 5/92C   3H   5O   1    0G   200.000  6000.000  C  57.07210 1
 0.72554278E+01 0.15458520E-01-0.55798138E-05 0.90356727E-09-0.54203987E-13    2
-0.52833268E+04-0.11180177E+02 0.39944373E+01 0.40814746E-02 0.52034636E-04    3
-0.70009530E-07 0.27882479E-10-0.33976925E+04 0.10569296E+02-0.16908080E+04    4

C3H5O  *CH2-CH O CH2 PROPYLENE OXIDE RADICAL ESTIMATED BY BOZZELLI & RITTER'S
PROGRAM FROM Stull & all 1969 DATA FOR PROPYLENE OXIDE - A PROTON. EXTRAPOLATED
TO 3000 K USING WILHOIT'S POLYNOMIALS. HF298=110.33 KJ
C3H5O             T 9/92C   3H   5O   1    0G   298.150  3000.000  F  57.07210 1
 0.91206991E+01 0.12196117E-01-0.42929777E-05 0.12616892E-08-0.15705367E-12    2
 0.91765012E+04-0.22071447E+02 0.70599393E+00 0.25629797E-01 0.71080411E-05    3
-0.29693495E-07 0.14360721E-10 0.11909268E+05 0.23610039E+02 0.13269823E+05    4

C3H6  PROPYLENE  STATWT=1  SIGMA=3  IA=1.8133  IB=9.0187  IC=10.317   IR=0.3945
POT BARRIER V3=1997.  NU=3091,3022,2991,2973,2932,1653,1459,1414,1378,1298,1178,
935,919,428,2953,1443,1045,990,912,575,  REF=CHAO&ZWOLINSKI MAX LST SQR ERROR
CP @ 1300 K 0.88 % .HF298=4.88 KCAL REF=TRC(API #44)
PROPYLENE         L 4/85C  3.H  6.   0.   0.G   300.000  5000.000  B  42.08060 1
 0.67213974E 01 0.14931757E-01-0.49652353E-05 0.72510753E-09-0.38001476E-13    2
-0.92453149E 03-0.12155617E 02 0.14575157E 01 0.21142263E-01 0.40468012E-05    3
-0.16319003E-07 0.70475153E-11 0.10740208E 04 0.17399460E 02 0.24557265E 04    4
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C3H6  CYCLOPROPANE  STATWT=1  SIGMA=6  IA=IB=4.1766  IC=6.6358     NU=3038,1479,
1188,1126,1070,3102,854,3024(2),1438(2),1029(2),867(2),3082(2),1188(2),739(2)
REF=SHIMANOUCHI  HF298=53.3 KJ REF=Dorofeeva, Gurvich & Jorish JPCRD 15 (1986),
437.    MAX LST SQ ERROR CP @ 1300 K 0.88 %
C3H6CY            T12/81C  3H   6    0     0G   300.000  5000.000  B  42.0806  1
 0.68271122E+01 0.15246719E-01-0.50710187E-05 0.74134521E-09-0.38929339E-13    2
 0.27764282E+04-0.16856832E+02-0.17865782E+01 0.29799264E-01 0.13068729E-05    3
-0.23190996E-07 0.11576777E-10 0.56478437E+04 0.29976481E+02 0.64108408E+04    4

C3H6N2O2 n-Nitro-Azetidine   SYMNO = 2  STATWT = 1  IA = 17.7086  IB = 36.1404
IC = 47.502    Ir(NO2) = 5.96  ROSYM =2  V(2)=12.5 kcal     NU =2982,2973,
2964,2925,2914,2911,1641,1507,1481,1464,1431,1318,1284,1263,1214,1188,1182,1148,
1131,1113,946,902,900,827,822,806,722,593,475,247,241.7,136.7  HF298= 27.28 kcal
REF = Melius Database 1988  D90A      Max Lst Sq Error Cp @ 200 K 0.78%
N-NITRO-AZETIDIN  T11/97C  3.H  6.N  2.O  2.G   200.000  6000.000  B 102.09292 1
 1.28386051E+01 2.27540814E-02-8.59766661E-06 1.42856214E-09-8.70663456E-14    2
 7.35548462E+03-4.36199680E+01 4.36363512E+00 7.73075634E-03 9.68585080E-05    3
-1.36307741E-07 5.56913572E-11 1.14684500E+04 9.18578377E+00 1.37257378E+04    4

C3H6N6O6  RDX  1,3,5-Triazine Solid Cp 290-345 REF= Engineering Design Hanbook
Military Pirotechnics Series Part One AMCP 706-185 (1967)  S298=33.94 cal
Graphic Integ  HF298(solid)=18.9 Kcal REF=NIST 98 (Krien, Licht, Zierath,
Thermochim. Acta,6,(1973),465-472)  Max Lst Sq Error Cp @ 293 K 0.22 %
RDX Solid         T 4/99C  3.H  6.N  6.O  6.S   293.000   478.500  D 222.11748 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00-2.26955822E+02 2.10620186E+00-6.38009038E-03    3
 8.94180990E-06-4.63001831E-09 2.44460154E+04 8.96445093E+02 9.51079498E+03    4

C3H6N6O6  RDX  1,3,5-Triazine     STATWT = 1    SYMNO = 6    IA = 137.8906
IB = 137.8906  IC = 245.5315 (Ir(NO2) = 5.97 ROSYM = 2 V(2)= 16.7 kcal)x3
NU = 2770,2767(2),2688,2684(2),1337,1332(2),1295(2),1280,1218(2),1207,1181,1180,
1104(2),1097,1081,1042,1027,1012(2),907(2),818,807,806,762,702(2),638,590,583,
581,554(2),528,501(2),320,307, 303,302,273,266(2),154,152,91.3,90.2,79.03
REF = Wu & Fried J Chem Phys 101,(1997),8675   HF298=  45.89 kcal
REF =Pepekin et al, Bull Acad Sci USSR Chem Sci (1974),1707  Max Lst Sq Error
Cp @ 6000 K 0.54%
RDX 135 Triazine  T 6/98C  3.H  6.N  6.O  6.G   200.000  6000.000  B 222.11748 1
 3.27884812E+01 2.84393334E-02-1.11821531E-05 1.88280824E-09-1.15260232E-13    2
 9.54327013E+03-1.42802148E+02 1.46580269E+00 1.05297168E-01-5.23365036E-05    3
-2.70780427E-08 2.44647856E-11 1.84793520E+04 2.07951964E+01 2.30921606E+04    4

C3H6O  PROPIONALDEHYDE  DATA FROM Chao et al 1986 EXTRAPOLATED TO 5000 K USING
WILHOIT'S POLYNOMIALS. HF298 = -45.90 KCAL REF=Stull Westrum & Sinke 1969  Max
Lst Sq Error Cp @ 5000 K 0.37%
C2H5CHO           T 9/92C   3H   6O   1    0G   273.150  5000.000  B  58.08004 1
 0.33137982E+01 0.26619606E-01-0.10475596E-04 0.18815334E-08-0.12761310E-12    2
-0.25459603E+05 0.96608447E+01 0.76044596E+01-0.86403564E-02 0.73930097E-04    3
-0.79687398E-07 0.28004927E-10-0.25489789E+05-0.67643691E+01-0.23097645E+05    4

C3H6O  ACETONE (CH3-CO-CH3) STATWT=1  SIGMA=2  IAIBIC=1390.63E-117 IR=0.4888
NU=3019(2),2972,2963,2937(2),1731,1454,1435,1426,1410,1364(2),1216,1091,1066,
891,877,777,530,484,385  POT BARRIER V3=272 cm-1 REF=CHAO et. al., JPCRD 15,
(1986),1369 Max Lst Sq Error Cp @ 6000 0.6%  HF298=-51.9 KCAL REF=CHAO &
ZWOLINSKI JPCRD 5 (1976), 319.
CH3COCH3          T 5/92C   3H   6O   1    0G   200.000  6000.000  B  58.08004 1
 0.72975991E+01 0.17566207E-01-0.63170456E-05 0.10203086E-08-0.61094016E-13    2
-0.29817680E+05-0.12756981E+02 0.55557943E+01-0.28365428E-02 0.70568945E-04    3
-0.87810488E-07 0.34028266E-10-0.28113337E+05 0.23226600E+01-0.26116945E+05    4
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C3H6O  PROPYLENEOXIDE  STATWT=1.  SIGMA=1.  IA=4.657  IB=12.561  IC=14.103
IR=.53 NU=3065(2),3006,2975,2929,2846,1500,1456(2),1406,1368,1263,1166,1142,
1132,1102,1023,950,896,828,745,416,371 POT BARRIER V3=2560 REF=SWALEN & HERSHBAC
MAX LST SQ ERROE CP @ 1300 K 0.86 % HF298=-92.76 KJ. REF=Stull, Westrum & Sinke.
PROPYLENE OXIDE   L 9/85C  3.H   6.O  1.    0.G   300.000  5000.000  B  58.07980 1
 0.86900558E 01 0.16020987E-01-0.53971753E-05 0.79941542E-09-0.42656366E-13    2
-0.15420691E 05-0.22485016E 02 0.48733836E 00 0.28519690E-01 0.30096162E-05    3
-0.22652642E-07 0.10706728E-10-0.12556434E 05 0.22605270E 02-0.11156446E 05    4

C3H6O  TRIMETHYLENE OXIDE (CYCLO) DATA ESTIMATED FROM BENSON'S GROUP VALUES BY
NIST PROGRAM 1991. EXTRAPOLATED TO 5000 K BY WILHOIT'S POLYNOMIALS. SIGMA=2
HF298=-19.25 KCAL and S298=65.46 CAL REF=STULL WESTRUM & SINKE  Max Lst Sq Error
Cp @ 1000 K *1.14%*
C3H6O CY          T 4/93C   3H   6O   1    0G   298.150  5000.000  E  58.08004 1
 0.88240924E+01 0.27857309E-02 0.12226227E-04-0.32987121E-08 0.25680945E-12    2
-0.12836680E+05-0.19638899E+02-0.11087750E+01 0.24207901E-01 0.25376282E-04    3
-0.54511280E-07 0.27089100E-10-0.10561565E+05 0.31340504E+02-0.96869208E+04    4

C3H6O VINYL METHYL ETHER C2H3-O-CH3 REF= Cp VALUES FROM Reid, Prausnitz & Poling
S298 & HF298 ESTIMATED BY NIST 93. EXTRAPOLATED USING WILHOIT'S POLYNOMIALS
HF298=-108.+/-8.4 KJ   Max Lst Sq Error Cp @ 1000 K 0.8%
C3H6O vme         T07/95C   3H   6O   1    0G   200.000  3000.000  D  58.08004 1
 0.77424945E+01 0.18725649E-01-0.80536180E-05 0.14957685E-08-0.10210991E-12    2
-0.17089284E+05-0.14520440E+02 0.20961609E+01 0.26090818E-01-0.56331528E-05    3
-0.56841781E-08 0.27833886E-11-0.14714469E+05 0.17579590E+02-0.12989532E+05    4

C3H6O CYCLOPROPANOL FROM NIST 93 EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNO-
MIALS   HF298=-114.3 KJ  Max Lst Sq Error Cp @ 500 K 0.6%
C3H6O CYPROPANOL  T07/95C   3H   6O   1    0G   298.150  5000.000  E  58.08004 1
 0.14304260E+02 0.13325578E-02 0.59393097E-05-0.15599729E-08 0.11892706E-12    2
-0.19370199E+05-0.50395683E+02-0.24991982E+01 0.42273270E-01-0.13523613E-04    3
-0.19409961E-07 0.13330563E-10-0.14729286E+05 0.37116329E+02-0.13747052E+05    4

C3H6S  THIETHANE CY-C3H6S  SIGMA=2  STATWT=1  A0=0.148  B0=0.222  C0=0.337
REF= C.J.Nielsen Acta Chem. Scan. A 31,(1977), 31.  NU=2994(2),2972,2950,2946,
2903,1470,1454,1452,1281,1229,1224,1183,1165,1011,986,974,933,845,823,700,677,
529,114   REF=Shaw et.al. JPC 92,(1988), 6528     T0(STATWT)=3063(2)
HF298=14.48 kcal REF=Pedley & Naylor 1986  REF=Ching-Len Yu & S.H.Bauer Private
Communication  Max Lst Sq. Error Cp @ 200 K ***1.10%***.
C3H6S  THIETHANE  T05/97C  3.H  6.S  1.   0.G   200.000  6000.000  B  74.14664 1
 8.39851867E+00 1.75807579E-02-6.34783803E-06 1.02801267E-09-6.16584833E-14    2
 2.99017716E+03-2.17569867E+01 2.83653731E+00 4.35820504E-03 7.71681730E-05    3
-1.08731256E-07 4.49661338E-11 5.75902343E+03 1.34578417E+01 7.28657732E+03    4

C3H7  N-C3H7  HF298= 100.5 KJ  REF= WING TSANG  NBS  1984  NU=3100(2),2960(5),
1440(5),1390,1100,990(4),980,960,530,330 STATWT=2 IAIBIC=254.E-117 FIRST ROTOR
ROSYM=3, V(3)=3585., IB=4.2E-40  SECOND ROTOR ROSYM=2  V(2)=.1 IB=4.2E-40
N-C3H7          N-L 9/84C  3H   7    0     0G   300.000  5000.000  C  43.08830 1
 0.77026987E 01 0.16044203E-01-0.52833220E-05 0.76298590E-09-0.39392284E-13    2
 0.82984336E 04-0.15480180E 02 0.10515518E 01 0.25991980E-01 0.23800540E-05    3
-0.19609569E-07 0.93732470E-11 0.10631863E 05 0.21122559E 02 0.12087447E 05    4

C3H7  ISO-C3H7     HF298= 93.3  KJ.  REFN:  WING  TSANG NBS 1984
NU=3100,2960(6),1440(6),1300,1200,990(4),950,397,367, STATWT=2, IAIBIC=267.E-117
SYMNO=2, ROSYM=3,V(3)=.1 IB=4.2E-40
I-C3H7          I-L 9/84C  3H   7    0     0G   300.000  5000.000  C  43.08830 1
 0.65294638E 01 0.17193288E-01-0.57153220E-05 0.83408080E-09-0.43663532E-13    2
 0.77179102E 04-0.91399021E 01 0.14461584E 01 0.20988975E-01 0.77172672E-05    3
-0.18481391E-07 0.71269024E-11 0.98206094E 04 0.20108200E 02 0.11221480E 05    4
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C3H7I  1-IODOPROPANE        SIGMA=1  IA=8.29  IB=38.9476  IC=45.962  IR=6.27
POTENTIAL BARRIER V3= 698.5 cm-1 ROSYM=3  REF=BRINKMAN & BURCAT  NU=2998,2963,
2962(2),2904,2880,2868,1460,1456(2),1433,1380,1344,1279,1195,1167,1075,1036,
1012,880,816,764,503,390,263,189  REF=SHIMANOUCHI JPCRD 9 (1980) 1221  HF0=-10.2
+/-2. KJ REF= BRAND & al. Chem Phys 76 (1983),114   Max Lst Sq Error Cp @ 6000 K
0.613 %.
1-C3H7I            T 5/97C   3H   7I   1    0G   200.000  6000.000  C 169.99305 1
 8.75274672E+00 1.93877662E-02-6.96410211E-06 1.12226927E-09-6.71103091E-14    2
-8.16015913E+03-1.73406686E+01 4.99662911E+00 7.01218575E-03 5.68773142E-05    3
-7.77001229E-08 3.10455636E-11-6.01366014E+03 7.55650710E+00-3.84863125E+03    4

C3H7I  2-IODOPROPANE    SIGMA=1  IA=10.31   IB=38.2149   IC=45.6879  IR=0.5292
TWO EQUAL CH3 ROTORS ROSYM=3 POTENTIAL BARRIER V3=698.5 cm-1  REF=BRINKMAN &
BURCAT NU=2997,2978,2961,2937,2925,2890,2882,1468(2)1459,1428,1389,1378,1325,
1210,1153,1113,1020,937,925,879,409,398,230,217 REF=KLABOE SPECTRACHIMICA ACTA
26A (1970), 87   HF0=-20.1+/-2.   KJ REF=BRAND & al Chem Phys 76 (1983), 114
Max Lst Sq Error Cp @ 1300 K 0.613 %.
2-C3H7I            T 5/97C   3H   7I   1    0G   200.000  6000.000  C 169.99305 1
 8.75725833E+00 1.88631159E-02-6.76401581E-06 1.09030360E-09-6.51918852E-14    2
-9.05136717E+03-1.66958638E+01 6.01588010E+00 8.83549699E-03 4.05024381E-05    3
-5.47331103E-08 2.12607652E-11-7.36100208E+03 1.91161348E+00-4.91494664E+03    4

C3H7N CYCLOPROPYLAMINE (C3H5NH2)  REF=DRAEGER HARRISON AND GOOD   DATA EXTRAPO-
LATED THROUGH WILHOIT'S POLYNOMIALS   HF298=77.37 KJ  MAX LST SQ ERROR CP @
1400 K 0.95 % .
C3H5NH2            L 2/84C  3H    7N   1    0G   300.000  5000.00   B  57.09499 1
 0.11077434E 02 0.15626516E-01-0.52517407E-05 0.79408302E-09-0.43887471E-13    2
 0.43691211E 04-0.35471283E 02 0.92693955E 00 0.35704415E-01-0.35520043E-05    3
-0.24779276E-07 0.13902465E-10 0.75181836E 04 0.18755966E 02 0.93077042E+04    4

C3H7N  CY -C3H6N:-H  AZETIDINE  SiGMA=2  STATWT=1  A0=0.220  B0=0.378  C0=0.382
NU=3358,3003,2961,2932,2920,2871,2862,1499,1458,1450,1341,1321,1252,1244,1196,
1180,1146,1088,1028,990,949,920,910,815,736,648,217  REF=Shaw et.al JPC 94,
(1990),118  HF298=23.47 kcal REF=Kamo et al Nippon Kagaknkai Shi 8, (1987),1560
REF TOTAL=Ching-Len Yu & S.H.Bauer Private Communication  Max Lst Sq Error Cp @
200 K ***1.43%***.
C3H7N AZETIDINE   T05/97C  3.H  7.N  1.   0.G   200.000  6000.000  B  57.09532 1
 7.71995188E+00 2.08359439E-02-7.51341908E-06 1.21565468E-09-7.28540548E-14    2
 7.40055773E+03-2.05389040E+01 3.72047052E+00-9.49272901E-03 1.21925375E-04    3
-1.56493514E-07 6.25256744E-11 1.03256972E+04 9.61790101E+00 1.18104951E+04    4

C3H7NO2 1-Nitro-Propane     STATWT = 1    IA = 13.094016  IB = 35.457574
IC = 37.3826884   Ir(NO2) = 5.96  ROSYM = 2    V(2) = 0.08 kcal/mole
Ir(CH3) = 0.51666 ROSYM =3   V(3) = 3.5 kcal/mole    Ir(C2H5) = 2.104  ROSYM = 2
V(2)= 9.0 kcal  NU = (3187,3088,3080,3031),2981,2905,2280,(1907),1567,1447,
(1415,1403,1392),1377,1232,1225,(1155,1140,1134,1068,1052),885,796,727,619,601,
569,(474,417,268)*. In Parenthesis values added to IR bands.  REF = NIST 97
HF298=-29.7 kcal  REF= Pedley & Rylance 1977  Max Lst Sq Error Cp @ 1300 K 0.65%
C3H7NO2            T05/98C  3.H  7.N  1.O  2.G   200.000  6000.000  B  89.09412 1
 1.27038541E+01 2.12000123E-02-7.88951874E-06 1.29872564E-09-7.87331819E-14    2
-2.09708557E+04-3.93362344E+01 2.45041896E+00 2.99807749E-02 2.82471382E-05    3
-6.00704031E-08 2.66264111E-11-1.71521009E+04 1.84229851E+01-1.49455350E+04    4
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C3H7ONO2 NPN  n-Propyl-Nitrate    STATWT = 1  IA = 15.235443  IB = 51.655271
IC = 55.1180418   Ir(NO2) = 5.96    ROSYM = 2      V(2) = 9.1 kcal/mole
Ir(CH3) = 0.51666 ROSYM = 3  V(3) = 3.5 kcal/mole    Ir(C2H5) = 3.027  ROSYM = 2
V(2) = 9.0 kcal/mole     NU= 3182,3088,3077,3049,3027,2955,2948,2099,1537,1430,
1413,1403,1401,1359,1341,1300,1161,1155,1129,1108,1105,1025,941,917,815,641,609,
541,461,359,301,244,179.    REF = BURCAT TAE # 824 (1998)   HF298 = -41.6 kcal
REF = Sull Westrum & Sinke   Max Lst Sq Error Cp @ 1300 K 0.64%
C3H7NO3 NPN       T05/98C  3.H  7.N  1.O  3.G   200.000  6000.000  B 105.09352 1
 1.52256437E+01 2.22034122E-02-8.38746793E-06 1.39150880E-09-8.47131095E-14    2
-2.78718897E+04-5.27407711E+01 4.46362749E+00 2.95649058E-02 3.53085312E-05    3
-6.91816807E-08 3.01929999E-11-2.37681986E+04 8.34607830E+00-2.09338133E+04    4

C3H7O N-PROPOXY RADICAL  SIGMA=3  ESTIMATED USING THE NIST 1994 PROGRAM TO 1500K
EXTRAPOLATED USING WILHOIT'S POLYNOMIALS  HF298=-9.0 KCAL Max Lst Sq Error Cp @
500 K 0.44%.
C3H7O N-PROPOXY   T 3/96C   3H   7O   1    0G   298.150  5000.000  F  59.08798 1
 0.84124958E+01 0.19520193E-01-0.71317071E-05 0.12393621E-08-0.82483889E-13    2
-0.87750718E+04-0.18293360E+02 0.91452571E+00 0.33601264E-01-0.12282254E-04    3
-0.10739947E-08 0.72924952E-12-0.61847956E+04 0.22563171E+02-0.45289500E+04    4

C3H8  PROPANE  STATWT=1. SIGMA=6.   SIGMA BARRIER=3. IA=2.8899     IB=IC=10.5472
IR=.44202  NU=2977,2962,2887,1476,1462,1392,1158,869,369,2967,1451,1278,940,
2968,2887,1464,1378,1338,1054,922,2973,2968,1472,1192,748  POT BARRIER V0=3.29
REF=CHAO WILHOIT&ZWOLINSKI  MAX LST SQ ERROR CP @ 1300K 0.94% HF298=-25.02 KCAL.
PROPANE           L 4/85C  3.H  8.   0.   0.G   300.000  5000.000  B  44.09620 1
 0.75341368E 01 0.18872239E-01-0.62718491E-05 0.91475649E-09-0.47838069E-13    2
-0.16467516E 05-0.17892349E 02 0.93355381E 00 0.26424579E-01 0.61059727E-05    3
-0.21977499E-07 0.95149253E-11-0.13958520E 05 0.19201691E 02-0.12489986E 05    4

1-C3H8O    1-PROPANOL  C3H7OH VALUES FROM TRC TABLES UP TO 1500 K MATCHED WITH
DATA CALCULATED FROM CONSTANTS BY CHAO et. al. JPCRD 15 (1986) P.1369
HF298=-255.2 KJ
C3H7OH PROPANOL   L 9/88C   3H   8O   1    0G   200.000  6000.000  B  60.09592 1
 0.87109009E+01 0.20803801E-01-0.73841230E-05 0.11817484E-08-0.70349614E-13    2
-0.35124716E+05-0.18900965E+02 0.52779942E+01 0.80866061E-03 0.82154818E-04    3
-0.10848818E-06 0.43488690E-10-0.32834877E+05 0.57052684E+01-0.30693330E+05    4

2-PROPANOL (CH3)2CHOH  SIGMA=3 IAIBIC=1831.0E-117  NU=3650,2940(6),2875,1475(2),
1460(2),1387,1367,1340,1256(2),1153,1130,1072,955(2),940,818,488,427,373
TWO EQUIVALENT METYL ROTORS IR=0.5036 POTENTIAL BARRIER V(3)=1399 cm-1 ROSYM=3
OH ROTOR IR=0.1281 POTENTIAL BARRIER V(1)=0.03 cm-1 V(2)=-0.086 cm-1 V(3)=0.40
cm-1  ROSYM=2   REF=CHAO et. al. JCPRD 15 (1986)  P.1369     HF298=-272.7 KJ
(CH3)2CHOH        L 9/88C   3H   8O   1    0G   200.000  6000.000  B  60.09592 1
 0.96426813E+01 0.20022483E-01-0.71195450E-05 0.11413813E-08-0.67993688E-13    2
-0.37484005E+05-0.25634465E+02 0.43079906E+01 0.10250203E-01 0.61984404E-04    3
-0.90329571E-07 0.37405980E-10-0.34924881E+05 0.75584028E+01-0.32798084E+05    4

C3O2   HF298=-93.64 KJ  REF=TRC (API) April 30 1984
C3O2              L 7/88C  3O   2    0     0G   200.000  6000.000  B  68.03180 1
 0.84617494E+01 0.48155296E-02-0.18093067E-05 0.30078642E-09-0.18372137E-13    2
-0.14327160E+05-0.17060508E+02 0.21966949E+01 0.31455190E-01-0.50745522E-04    3
 0.43579038E-07-0.14735014E-10-0.12946099E+05 0.13298479E+02-0.11262239E+05    4

C4  SIGMA=2 STATWT=3 IB=16.3  NU=2570,1100,2170,440(2),200(2)  T0=4000. STATWT=2
T0=6000. STATWT=6  T0=8000. STATWT=1  T0=14000.  STATWT=2  T0=19564.  STATWT=6
T0=24000.  STATWT=8  T0=28000.  STATWT=2  REF=TSIV  HF298=1033.9 KJ
C4                R 79  C   4   0    0     0G   200.000  6000.000  B  48.04400 1
 0.56307710E+01 0.48313818E-02-0.15041681E-05 0.20289460E-09-0.10036092E-13    2
 0.12250094E+06-0.29887309E+01 0.33227750E+01 0.20259234E-01-0.37345213E-04    3
 0.35685909E-07-0.12771861E-10 0.12272364E+06 0.68097958E+01 0.12434933E+06    4
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C4Cl6 Perchloro-1,3-butadiene   SIGMA=2   Ia=102.47612  Ib=201.1241
Ic=265.3158 Nu=1832,1764,1309,879,859,787,784,691,605,574,414,378,366,365,274,
271.5,227.7,180.4,168.4,129.15,111.7,68.47,61.56,29.2  REF=MOPAC6 PM3 calc.
HF298=-23.1 kcal REF=THERGAS est. { HF298=-2.55 kcal PM3 est}  Max Lst Sq Error
Cp @ 1200 K 0.32%   ** Internal rotation not considered. Estimated HF **
C4CL6 Butadiene   T08/00C  4.CL 6.   0.   0.G   200.000  6000.000  D 260.76020 1
 2.21980993E+01 5.83006041E-03-2.25806563E-06 3.82826576E-10-2.36983327E-14    2
-1.93181619E+04-7.45658167E+01 5.11650693E+00 7.63368754E-02-1.23398475E-04    3
 1.00027196E-07-3.19528806E-11-1.56350963E+04 8.26053886E+00-1.16243050E+04    4

C4F6  PERFLUORO 1-3 BUTADIENE  SIGMA=1     SIGMAR=2  IA=42.1018  IB=80.1264
IC=116.0475  IR=132.823  V(2)=2850.  NU=1796,1381,1138,933,702,660,529,464,396,
375,329,181,1765,1329,1189,972,633,547,520,422,293,259,204    REF=WURREY, BUCY
AND DURIG  MAX LST SQ ERROR @ 1300 K 0.44 % . HF298=-240. KCAL   REF= Atkinson &
Stedman J. Chem. Soc (1962), 512
C4F6              T12/82C  4F   6    0     0G   300.000  5000.0    B  162.034391
 0.20649826E+02 0.63778609E-02-0.24356023E-05 0.40486192E-09-0.24477111E-13    2
-0.12834769E+06-0.75434682E+02 0.61921721E+01 0.40591445E-01-0.14628447E-04    3
-0.22981666E-07 0.15799126E-10-0.12425062E+06 0.15772644E+00-0.12077197E+06    4

C4F6  PERFLUOROCYCLOBUTENE  SIGMA=2  IA=53.90  IB=64.95  IC=87.73  NU=1799,1418,
1387,1136,966,684,469.2,286,1182,493,337,174,98,1282,638,187,146,1259,1171,983,
579,429,238,217  REF=NIELSEN AND EL-SABEN     MAX LST SQ ERROR @ 1300 K 0.53 %
HF298=-289.4 KCAL  REF= Atkinson & Stedmann J. Chem. Soc (1962), 512.
F6C4              T12/82F  6C   4    0     0G   300.000  5000.000  B 162.03439 1
 0.19723373E+02 0.81368275E-02-0.30685842E-05 0.50541860E-09-0.30311613E-13    2
-0.15313506E+06-0.72023473E+02 0.60944862E+01 0.36527760E-01-0.68788740E-05    3
-0.24970031E-07 0.14493539E-10-0.14896744E+06 0.49672994E+00-0.14563498E+06    4

C4F8 PERFLUOROCYCLOBUTANE  ESTIMATED USING NIST 1994 TO 1000 K, EXTRAPOLATED TO
5000 K USING WILHOIT'S POLYNOMIALS  HF298=-1513.6 KJ Max Lst Sq Error Cp @ 500 K
*1.25%*
C4F8 CY           T11/94C   4F   8    0     0G   298.150  5000.000  F 200.03123 1
 0.25859659E+02 0.14057850E-01-0.86342611E-05 0.18743110E-08-0.13985280E-12    2
-0.19308325E+06-0.10861981E+03-0.64087603E+01 0.11778844E+00-0.15735373E-03    3
 0.11577968E-06-0.37112295E-10-0.18418883E+06 0.56186329E+02-0.18204320E+06    4

C4F10 PERFLUOROBUTANE (FC-3-1-10)  SIGMA=18  CALCULATED and EXTRAPOLATED USING
NIST 94 AND BOZZELLI & RITTER'S PROGRAM. HF298=-510.85 KCAL   Max Lst Sq Error
Cp @ 1400 K 0.19%.
C4F10             T12/94C   4F  10    0     0G   298.150  5000.000  E 238.02803 1
 0.30442529E+02 0.87222991E-02-0.36625862E-05 0.67841011E-09-0.46225435E-13    2
-0.26830628E+06-0.12239409E+03-0.43510861E+00 0.11003166E+00-0.12712106E-03    3
 0.66741713E-07-0.13106885E-10-0.26083419E+06 0.32565014E+02-0.25707075E+06    4

C4H  RAD  T0=0 STATWT=4. SIGMA=1.  B0=0.1558  NU=3485,2283,2116,910,565(2),
473(2),204(2)  T0=350. STATWT=2. NU=3474,2129,1864,889,695,424,186,565,473,204
REF=Kiefer, Sidhu, Kern, Xie, Chen & Harding (1992) LST SQ ERROR CP @ 1300 K
0.34% . HF298=192.0 KCAL
C4H               T12/91C   4H   1    0     0G   200.000  6000.000  B  49.05194 1
 0.77680939E+01 0.49850386E-02-0.17648839E-05 0.28217408E-09-0.16779623E-13    2
 0.93912126E+05-0.14159577E+02 0.13210657E+01 0.38562824E-01-0.71343174E-04    3
 0.65319977E-07-0.22607050E-10 0.95021629E+05 0.15554575E+02 0.96617600E+05    4
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C4H2  BUTADIYNE  STATWT=1.  SIGMA=2.  IB=19.054  NU=3329(2),2184,874,2020,627(2)
483(2),630(2),220(2)  REF=DUFF&BAUER  ALSO KOOPS et al., J.MOLEC. STRUCT. 125
(1984) 179. MAX LST SQ ERROR CP @ 6000 K 0.33%. HF298=440.5 KJ  REF= STEIN et al
NIST PROGRAM 1991.
C4H2                L 9/89C  4H   2    0     0G   200.000  6000.000  C  50.05988 1
 0.86670035E+01 0.67166371E-02-0.23544995E-05 0.37383079E-09-0.22118914E-13    2
 0.49856933E+05-0.21114205E+02-0.39518508E+00 0.51955813E-01-0.91786616E-04    3
 0.80523929E-07-0.26917088E-10 0.51451709E+05 0.20969101E+02 0.52978651E+05    4

C4H3 RAD  STATWT=1.  SIGMA=2. CALCULATED BY REMOVING A STABILIZED VINYL-H FROM
C4H4 (1-BUTEN-3YN) USING STEIN'S COEFFICIENTS METHOD. ESTIMATED HF298=115.5 KCAL
C4H3                L 9/89C   4H   3    0    0G   298.150  6000.000  D  51.06782 1
 0.84762079E+01 0.88782327E-02-0.30328412E-05 0.47358302E-09-0.27716627E-13    2
 0.54756540E+05-0.17170551E+02 0.24173247E+01 0.24104782E-01-0.12813470E-04    3
-0.28606237E-08 0.39194527E-11 0.56506476E+05 0.14471107E+02 0.58181574E+05    4

C4H4  1-BUTEN-3YN  STATWT=1.  SIGMA=1. A0=1.678094245 B0=.158273884 C0=.14442624
DJ=6.4E-08 DJK=-277.5E-08 DK=8499.2E-8 NU=3330,3116,3068,3030,2111,1599,1415,
1312,1096,874,625,539,217,974,927,677,618,304 REF=TORNENG et al., SPECTROCHIM.
ACTA 36A (1989) 975.  MAX LST SQ ERROR CP @ 6000 K 0.48%. HF0=75.3 kcal
C4H4                L 9/89C  4H   4    0     0G   200.000  6000.000  B  52.07576 1
 0.82948104E+01 0.11994381E-01-0.42624075E-05 0.68306978E-09-0.40680631E-13    2
 0.33550866E+05-0.18426826E+02 0.14049083E+01 0.29531073E-01-0.15596302E-04    3
-0.32142002E-08 0.45436937E-11 0.35507830E+05 0.17450183E+02 0.37097268E+05    4

CYCLOBUTADIENE      SIGMA=4  STATWT=1 IAIBIC=360.E-117  NU=3050,1510,1120,900(3),
1100,570(2),1235,770,3030(2),1240,720,3040,1520,990 REF=DOROFEEVA, GURVICH &
JORISH JCPRD 15 (1986), 437. HF298=385 KJ MAX LST SQ ERROR Cp @ 6000 K 0.54%.
C4H4 CY             T 2/90C   4H   4    0     0G   200.000  6000.000  B  52.07576 1
 0.80419352E+01 0.12520407E-01-0.45234623E-05 0.73313766E-09-0.44012214E-13    2
 0.42510913E+05-0.21127639E+02 0.12789207E+01 0.13420710E-01 0.41197797E-04    3
-0.69893781E-07 0.30724360E-10 0.45086412E+05 0.17678892E+02 0.46304593E+05    4

C4H4N2 PYRAZINE (SIX MEMBERED RING WITH N IN PARA POSITION)   SIGMA=4  STATWT=1
IA=12.8266  IB=13.8011  IC=26.6277  NU= 3037,3031,3015,3014,1615,1579,1493,1404,
1337,1215,1227,1074,1010,1003,1001,995,982,935,801,748,695,584,435.7,380.6
REF= C. Melius Database #PJ11 HF298=46.8+-0.3 Kcal   REF=Pedley, Nylor & Kirby
Max Lst Sq Error Cp @ 200 K **1.06 %**.
C4H4N2 PYRAZINE   T 9/96C   4H   4N   2    0G   200.000  6000.000  B  80.08924 1
 0.10551339D+02 0.16036746D-01-0.58863657D-05 0.96422235D-09-0.58315531D-13    2
 0.18418344D+05-0.33943388D+02 0.13116930D+01 0.14100415D-01 0.64443831D-04    3
-0.10163885D-06 0.43390536D-10 0.22143754D+05 0.19991866D+02 0.23550540D+05    4

C4H4N2 PYRIMIDINE (SIX MEMBERED RING WITH N IN ORTO POSITION) SIGMA=2  STATWT=1
IA=13.10379  IB=13.46  IC=26.57  NU=3045,3033,3015,3010,1608,1607.5,1466,1405,
1357,1214,1126,1083,1040,1039,1032,1010,985,978,813.7,704,671,610,411.7,371.3
REF=C.Melius Database #PI11  HF298=47.0+-0.2 Kcal REF=Pedley, Naylor & Kirby
Max Lst Sq Error Cp @ 200 K **1.08 %**.
C4H4N2 PYRIMIDINE T 9/96C   4H   4N   2    0G   200.000  6000.000  B  80.08924 1
 0.10431658D+02 0.16150995D-01-0.59292286D-05 0.97133853D-09-0.58749686D-13    2
 0.18552038D+05-0.33249214D+02 0.16371390D+01 0.11977423D-01 0.68383238D-04    3
-0.10465037D-06 0.44218587D-10 0.22212482D+05 0.18656416D+02 0.23651183D+05    4

C4H4O FURAN (CY)  SIGMA=2   IAIBIC=1448.6   NU=3167,3161,3140,3129,1556,1491,
1384,1267,1180,1140,1066,1040,995,873,871,863,838,745,728,613,603  REF= Chao
et. al, JPCRD 15,(1986),1369  HF298=-8.29 KCAL  REF=STULL WESTRUN & SINKE
Max Lst Sq Error Cp @ 200 K **1.24%**.
C4H4O FURAN         T03/97C  4.H  4.O  1.   0.G   200.000  6000.000  B  68.07516 1
 9.38935003E+00 1.40291241E-02-5.07755110E-06 8.24137332E-10-4.95319963E-14    2
-8.68241814E+03-2.79162920E+01 8.47469463E-01 1.31773796E-02 5.99735901E-05    3
-9.71562904E-08 4.22733796E-11-5.36785445E+03 2.14945172E+01-4.17166616E+03    4
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Table 4 (continued)

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C4H4O  VINYL-KETENE   H2C=CHCH=C=O     ESTIMATED FROM GROUP ADDITIVITY DATA
AND EXTRAPOLATED FROM 2000 to 5000 K USING Wilhoit's POLYNOMIALS
REF=Zhong & Bozzelli JPC-A 102 (1998), 3537.  HF298=1.82 kcal.
C4H4O VIN-KETENE  T 8/99C  4.H  4.O  1.   0.G   298.150  5000.000  E  68.07516 1
 1.23643838E+01 1.06418956E-02-3.86206756E-06 6.59950397E-10-4.31365036E-14    2
-4.13532125E+03-3.93260231E+01-8.42448203E-01 4.99696552E-02-3.75384323E-05    3
-2.31300014E-09 1.04518708E-11-7.22677920E+02 2.77811950E+01 9.15854332E+02    4

C4H4O2 1,4-Dioxin (Hexa-diene-ring) REF=Dorofeeva Thermochim Acta 200,(1992),121
-150  Data from Dorofeeva extrapolated to 5000 K using Wilhoit's polynomials.
HF298=-140.0 kJ Max Lst Sq Error Cp @ 200 K 0.86%
C4H4O2 1,4DIOXIN  T11/99C  4.H  4.O  2.   0.G   200.000  5000.000  B  84.07456 1
 1.01212024E+01 1.75021756E-02-7.25353136E-06 1.37001596E-09-9.65875016E-14    2
-2.16035452E+04-3.00246825E+01 6.10172295E-01 2.69946560E-02 2.96882541E-05    3
-6.66919493E-08 3.10421420E-11-1.83649383E+04 2.26144524E+01-1.68380338E+04    4

C4H4S THIOPHENE (CY)  SIGMA=2 IAIBIC=4192.  NU=3126,3125,3098(2),1507,1409,1360,
1256,1085,1083,1036,898,872,867,839,751,712,683,608,565,452  HF298=114.9 KJ
REF=Dorofeeva and Gurvich 1995  Max Lst Sq Error Cp @ 200 K 0.99%
C4H4S Thiophene   T03/97C  4.H  4.S  1.   0.G   200.000  6000.000  B  84.14176 1
 1.03361791E+01 1.31485110E-02-4.75133660E-06 7.70341282E-10-4.62623029E-14    2
 9.14755147E+03-3.14959122E+01-5.33958016E-01 3.04279440E-02 1.57128681E-05    3
-5.21636175E-08 2.60141958E-11 1.25779686E+04 2.72103378E+01 1.38192148E+04    4


N-C4H5  CH2=CHCH=CH RADICAL  CALCULATED USING BENSON'S GROUP ADITIVITY METHOD.
EXTRAPOLATED AND ESTIMATED BY M.B.COLKET (UNPUBLISHED). HF298=345.1+/-6.0 KJ
N-C4H5          N-A 8/83C  4H   5    0     0G   300.     3000.     E  53.0835  1
 0.72559180E 01 0.17141310E-01-0.74350450E-05 0.16410520E-08-0.15360780E-12    2
 0.38227410E 05-0.12422830E 02-0.20329280E 01 0.53630530E-01-0.63382690E-04    3
 0.40641440E-07-0.10398020E-10 0.40219650E 05 0.32787830E 02 0.41505750E+05    4

I-C4H5  CH2=CHC=CH2 RADICAL  CALCULATED USING BENSON'S GROUP ADDITIVITY METHOD.
EXTRAPOLATED AND ESTIMATED BY M.B.COLKET (UNPUBLISHED). HF298=330.8 KJ
I-C4H5          I-A 8/83C   4H  5    0     0G   300.    3000.      E  53.0835  1
 0.72559180E 01 0.17141310E-01-0.74350450E-05 0.16410520E-08-0.15360780E-12    2
 0.36339860E 05-0.13420580E 02 0.10251400E 02-0.25627670E-01 0.10715090E-03    3
-0.11090190E-06 0.37550050E-10 0.37128550E 05-0.20574530E 02 0.39785870E+05    4

T-C4H5  CH2CH=C=CH2 RADICAL  CALCULATED USING BENSON'S GROUP ADDITIVITY METHOD.
EXTRAPOLATED AND ESTIMATED BY M.B.COLKET (UNPUBLISHED). HF298=302.2 KJ
T-C4H5          T-A 8/83C   4H   5    0    0G   300.    3000.      E  53.0835  1
 0.40734210E 01 0.24907370E-01-0.13229540E-04 0.34159060E-08-0.34874460E-12    2
 0.33975420E 05 0.43252930E 01-0.19509230E 01 0.53281440E-01-0.65306770E-04    3
 0.46994220E-07-0.14204880E-10 0.35048460E 05 0.32542460E 02 0.36346100E+05    4

C4H5N PYRROLE (CY) (AZOLE, IMIDOLE)  SIGMA=2  IAIBIC=1586.5  NU=3527,3148,3140,
3125,3116,1530,1467,1422,1382,1287,1144,1134,1074,1048,1016,881,869,865,826,721,
710,618,601,474  HF298=108.18+/-0.81 KJ REF= Das et.al JPCRD 22,(1993),659  Max
Lst Sq Error Cp @ 200 **2.1%**
C4H5N PYRROLE     T 8/95C   4H   5N   1    0G   200.000  6000.000  B  67.09044 1
 0.97727000E+01 0.16111112E-01-0.57690298E-05 0.92973976E-09-0.55604978E-13    2
 0.82631988E+04-0.30359085E+02 0.38558756E+00 0.18943518E-01 0.52673009E-04    3
-0.91458921E-07 0.40445724E-10 0.11750328E+05 0.23102254E+02 0.13010989E+05    4
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C4H5N  CYCLOPROPANE CARBONITRILE C3H5-CN  ESTIMATED USING NIST 1994 EXTRAPOLATED
USING WILHOIT'S POLYNOMIALS  HF298=44.0+/-0.2 kcal  REF=Fuchs Hallman Perlman
Canad. J. Chem. 60 (1982),1832. Max Lst Sq Error Cp @ 1200 K 0.15%.
C4H5N  CY          T05/97C  4.H  5.N  1.   0.G   298.150  5000.000  F  67.09044 1
 1.52373018E+01 1.72183181E-03 5.28844337E-06-1.33654754E-09 9.80870879E-14    2
 1.60781873E+04-5.52187990E+01-8.84377903E-02 3.45352161E-02-1.98537057E-06    3
-2.58387099E-08 1.43612783E-11 2.06947417E+04 2.60727715E+01 2.21415333E+04    4

C4H6  2-BUTAYN (DIMETHYLACETYLENE) STATWT=1  SIGMA=6  IA=1.0605  IB=IC=25.0029
IR=.530  V(3)=500. (ONE ROTATION ONLY)      NU=371(2),725,1029(2),1050(2),1380(2),
1126,1448(2),1468(2),2270,2916,2966(2),2976(3),213(2)  REF=YOST OSBORNE &GARNER
MAX LST SQ ERROR CP # 1300 K  0.87 % .HF298=34.97 KCAL REF= Stull, Westrum &
Sinke
C4H6               T12/82C  4H   6    0     0G   300.000  5000.000  B  54.091   1
 0.80465832E+01 0.16485251E-01-0.55222272E-05 0.81235929E-09-0.42950784E-13    2
 0.13701305E+05-0.18017740E+02 0.31971083E+01 0.20255916E-01 0.65101922E-05    3
-0.16584423E-07 0.64002822E-11 0.15715203E+05 0.99088230E+01 0.17597979E+05    4

1,3-C4H6  1,3-BUTADIENE  CALCULATED USING BENSON'S GROUP ADDITIVITY METHOD.
EXTRAPOLATED AND ESTIMATED BY M.B.COLKET (UNPUBLISHED). HF298=26.5 KCAL
REF= Weisman & Benson 1989
1,3-C4H6           A 8/83C  4H   6    0     0G   300.     3000.     E  54.0914  1
 0.71309430E 01 0.20640080E-01-0.93239060E-05 0.21473070E-08-0.20613610E-12    2
 0.96126540E 04-0.14172220E 02-0.25309000E 01 0.53879690E-01-0.51739330E-04    3
 0.25107200E-07-0.43247260E-11 0.11876910E 05 0.33913880E 02 0.13335620E+05    4

1,2-C4H6  1,2-BUTADIENE  CALCULATED USING BENSON'S GROUP ADDITIVITY METHOD.
EXTRAPOLATED AND ESTIMATED BY M.B.COLKET (UNPUBLISHED). HF298=162.2 KJ  REF=
Stull Westrum & Sinke 1969.
1,2-C4H6           A 8/83C  4H   6    0     0G   300.     3000.     E  54.0914  1
 0.17815570E 02-0.42575020E-02 0.10511850E-04-0.44738440E-08 0.58481380E-12    2
 0.12673420E 05-0.69826620E 02 0.10234670E 01 0.34959190E-01-0.22009050E-04    3
 0.69422720E-08-0.78791870E-12 0.18117990E 05 0.19750660E 02 0.19508070E+05    4

C4H6 CYCLOBUTENE  STATWT=1  SIGMA=2 IA*IB*IC=550*10E-117  NU=3063,2941,1564,
1448,1185,1113,981,883,2955,1142,1000,909,327,3056,2934,1430,1294,1212,1013,890,
2961,1074,846,636 HF298=156.7 KJ REF=Dorofeeva, Gurvich & Jorish JPCRD 15(1986)
437. Max Lst Sq Error Cp @ 6000 K 0.61%
C4H6 CY            T 1/90C   4H  6    0     0G   200.000  6000.000  B  54.09164 1
 0.78484947E+01 0.18081385E-01-0.65319179E-05 0.10584303E-08-0.63525891E-13    2
 0.14615386E+05-0.20897529E+02 0.29163222E+01-0.32056882E-02 0.10026293E-03    3
-0.13424741E-06 0.54666711E-10 0.17473224E+05 0.12481748E+02 0.18846571E+05    4

C4H6CL2  1,4-DICHLOROBUTENE-1 CALCULATED BY Weissman & Benson 1989 EXTRAPOLATED
BY WILHOIT'S POLYNOMIALS  HF298=-13.9 KCAL Max Lst Sq Error Cp @ 1200 K 0.5%.
C4H6CL2            T 2/92C   4H   6CL  2    0G   298.150  3000.000  E 124.99704 1
 0.16127633E+02 0.11072718E-01-0.15344777E-05 0.00000000E+00 0.00000000E+00    2
-0.13626543E+05-0.52374678E+02 0.37922774E+01 0.37246319E-01-0.15873622E-04    3
 0.00000000E+00 0.00000000E+00-0.96406196E+04 0.13786390E+02-0.69947117E+04    4

C4H6CL2  3,4-DICHLOROBUTENE-1 CALCULATED BY Weismann & Benson 1989 EXTRAPOLATED
BY WILHOIT'S POLYNOMIALS  HF298=-16.5 KCAL Max Lst Sq Error Cp @ 1200 K 0.52%.
CL2C4H6            T 2/92CL  2C   4H   6    0G   298.150  3000.000  E 124.99704 1
 0.15561772E+02 0.10650244E-01-0.15071115E-05 0.00000000E+00 0.00000000E+00    2
-0.14529573E+05-0.48539789E+02 0.49444570E+01 0.33489486E-01-0.14196579E-04    3
 0.00000000E+00 0.00000000E+00-0.11140342E+05 0.82672959E+01-0.83030750E+04    4
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Table 4 (continued)

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C4H6O 2,5-DIHYDROFURAN  (1- OXOLENE CY)   REF=Chao et. al. JPCRD 15,(1986),1369
EXTRAPOLATED 1600-5000 K USING WILHOIT'S POLYNOMIALS    HF298=-108.78 KJ
 REF=Kudchadker, Kudchadker & Wilhoit TRC 1978 Key Chemicals Data Book- Furan,
Dihydrofuran, Tetrahydrofuran  Max Lst Sq Error Cp @ 200 K 0.10%.
C4H6O 2,5DHFURAN  T 3/97C   4H   6O   1    0G   200.000  5000.000  B  70.09104 1
 8.60658242E+00 2.08310051E-02-8.42229481E-06 1.56717640E-09-1.09391202E-13    2
-1.76177415E+04-2.32464750E+01 2.67053463E+00 4.92586420E-03 8.86967406E-05    3
-1.26219194E-07 5.23991321E-11-1.46572472E+04 1.45722395E+01-1.30831522E+04    4

C4H6S  2,5-DIHYDROTHIOPHEN  REF=DOROFEEVA & GURVICH JPCRD 24,(1995),1351 EXTRA-
POLATED USING WILHOIT'S POLYNOMIALS  HF298=86.9 KJ Max Lst Sq Error Cp @ 200 K
0.85%.
2,5 C4H6S         T 3/97C  4.H  6.S  1.   0.G   200.000  5000.000  B  86.15764 1
 1.00854835E+01 1.90975958E-02-7.20771905E-06 1.28890804E-09-8.80278600E-14    2
 5.53885520E+03-2.96760237E+01 1.04681536E+00 2.39100306E-02 4.05153733E-05    3
-7.65294400E-08 3.42334612E-11 8.85389773E+03 2.14459803E+01 1.04516081E+04    4

N-C4H7  3 BUTEN 1-YL CH2=CHCH2CH2 RADICAL  ESTIMATED USING NIST 1994 PROGRAM
(BENSON'S GROUP ADDITIVITY METHOD). EXTRAPOLATED USING WILHOIT'S POLYNOMIALS.
SIGMA=2  HF298=46.0 KCAL. Max List Sq Error Cp @ 500 K 0.63%.
N-C4H7            T 2/96C   4H   7    0    0G   298.150  5000.000  E  55.09958 1
 0.11184356E+02 0.14457868E-01-0.44852630E-05 0.73693834E-09-0.48752824E-13    2
 0.17987671E+05-0.32095703E+02 0.21544552E+01 0.21568453E-01 0.29077822E-04    3
-0.54719830E-07 0.23710092E-10 0.21387008E+05 0.18934394E+02 0.23147967E+05    4

I-C4H7  CH2=CHCHCH3 RADICAL  CALCULATED USING BENSON'S GROUP ADDITIVITY METHOD.
EXTRAPOLATED AND ESTIMATED BY M.B. COLKET (UNPUBLISHED). HF298=126.5 KJ
I-C4H7            A 8/83C   4H  7    0    0G     300.    3000.     E  55.0993  1
 0.5521420E 01  0.2683684E-01 -0.1286430E-04  0.3088640E-08 -0.3030856E-12     2
 0.1198044E 05 -0.4482447E 01 -0.1080514E 01  0.4638686E-01 -0.3464697E-04     3
 0.1401374E-07 -0.2395040E-11  0.1375538E 05  0.2934466E 02  0.1521437E+05     4

T-C4H7  CH2CH=CHCH3 RADICAL  CALCULATED USING BENSON'S GROUP ADDITIVITY METHOD.
EXTRAPOLATED AND ESTIMATED BY M.B. COLKET (UNPUBLISHED). HF298=128.3 KJ
T-C4H7            A 8/83C   4H  7    0    0G     300.    3000.     E  55.0993  1
 0.4219753E 01  0.2882451E-01 -0.1399213E-04  0.3340718E-08 -0.3226427E-12     2
 0.1266295E 05  0.3253111E 01 -0.2152314E+01  0.5547424E-01 -0.6226715E-04     3
 0.4593056E-07 -0.1492297E-10  0.1407443E 05  0.3421103E 02  0.1543086E+05     4

C4H7   2-METHYL-ALLYL  *CH2C(CH3)=CH2 RADICAL  ESTIMATED USING NIST 1994 PROGRAM
(BENSON'S GROUP ADDITIVITY METHOD). EXTRAPOLATED USING WILHOIT'S POLYNOMIALS.
SIGMA=6  HF298=29.0 KCAL. Max List Sq Error Cp @ 1500 K  0.33%
C4H7 ME-ALL       T 2/96C   4H   7    0    0G   298.150  5000.000  E  55.09958 1
 0.90657617E+01 0.19477743E-01-0.73385554E-05 0.12863733E-08-0.85601393E-13    2
 0.10187905E+05-0.24022063E+02-0.34391326E+01 0.67889035E-01-0.92118162E-04    3
 0.75423011E-07-0.25411345E-10 0.13278011E+05 0.37956421E+02 0.14593283E+05    4

C4H7  CYCLOBUTYL RADICAL  ESTIMATED USING NIST 1994 PROGRAM (BENSON'S GROUP
ADDITIVITY METHOD). EXTRAPOLATED USING WILHOIT'S POLYNOMIALS.   SIGMA=2
HF298=51.2 KCAL. Max List Sq Error Cp @ 500 K 0.51%.
C4H7 CY           T02/96C   4H   7    0    0G   298.150  5000.000  E  55.09958 1
 0.89828490E+01 0.18434133E-01-0.61712552E-05 0.10133543E-08-0.65253450E-13    2
 0.20938022E+05-0.24329659E+02 0.86697607E+00 0.10779112E-01 0.74653141E-04    3
-0.11106766E-06 0.46911251E-10 0.24564894E+05 0.24591843E+02 0.25764693E+05    4

C4H7O 2-BUTANONE RAD CH3-CH*CO-CH3 ESTIMATED USING BOZELLI & RITTER'S PROGRAM
2-BUTANONE MINUS ALKOXY BOND HF298=-4.92 KCAL
C4H7O             T 6/92C   4H   7O   1    0G   298.150  5000.000  E  71.09898 1
 0.89768844E+01 0.22749346E-01-0.86722034E-05 0.15338364E-08-0.10284024E-12    2
-0.21339874E+04-0.18032447E+02 0.67110277E+00 0.45702301E-01-0.40527985E-04    3
 0.28517489E-07-0.10017095E-10-0.55084866E+03 0.25800808E+02-0.24758260E+04    4
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Table 4 (continued)

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C4H7O 2-METYL,ALLYL OXY RADICAL H2C=C(CH3)CH2O*  SIGMA=3 ROUGH ESTIMATE USING
BOZZELLI & RITTER'S PROGRAM TO 1000 K FROM 2 METHYL ALLYL ALCOHOL. EXTRAPOLATED
USING WILHOIT'S POLYNOMIALS TO 5000 K. GROUPS USED C/CD/H3;  CD/H2;  CD/C2;
O/C/H;  C/CD/H2/O - ALKOXY BOND. HF298=12.35 KCAL   Max Lst Sq Error Cp @ 1000 K
0.53%.
C4H7O 2MALLYLOXY  T 1/96C   4H   7O   1    0G   298.150  5000.000  F  71.09898 1
 0.10201164E+02 0.20773985E-01-0.78691839E-05 0.13913117E-08-0.93376086E-13    2
 0.12268093E+04-0.26399888E+02 0.45826315E+01 0.19154338E-01 0.27729464E-04    3
-0.45646819E-07 0.18456024E-10 0.38386017E+04 0.72739076E+01 0.62197580E+04    4

C4H8  1-BUTENE CH2=CH-CH2-CH3 SPECTROSCOPIC DATA NOT AVAILABLE. REF= CHAO & HALL
Private Communication   MAX LST SQ ERROR CP @ 4500 K  1.45 % . HF298=-0.54 KJ
C4H8              T 6/83C   4H   8    0    0G   300.000  5000.     B  56.104   1
 0.20535841E+01 0.34350507E-01-0.15883197E-04 0.33089662E-08-0.25361045E-12    2
-0.21397231E+04 0.15556360E+02 0.11811380E+01 0.30853380E-01 0.50865247E-05    3
-0.24654888E-07 0.11110193E-10-0.17904004E+04 0.21075639E+02-0.06494670E+03    4

ISOBUTENE  CH2=C(CH3)2   SPECTROSCOPIC DATA NOT AVAILABLE    REF=CHAO & HALL
Private Communication  MAX LST SQ ERROR CP @ 4500 K 1.27 % . HF298=-17.15 KJ
H8C4              T 6/83H   8C   4    0    0G   300.000  5000.0    B  56.104   1
 0.44609470E+01 0.29611487E-01-0.13077129E-04 0.26571934E-08-0.20134713E-12    2
-0.50066758E+04 0.10803180E+01 0.26471405E+01 0.25902957E-01 0.81985354E-05    3
-0.22193259E-07 0.88958580E-11-0.40373069E+04 0.12689550E+02-0.20626591E+04    4

C4H8  2-BUTENE-TRANS  CH3-CH=CH-CH3  SPECTROSCOPIC DATA NOT AVAILABLE  REF= CHAO
& HALL  Private Communication  MAX LST SQ ERROR CP @ 4500 K  1.52 % .
HF298=-10.96 KJ
C4H8TRANS         T 6/83C   4H   8    0    0G   300.000  5000.00   B  56.104   1
 0.82797676E+00 0.35864539E-01-0.16634498E-04 0.34732759E-08-0.26657398E-12    2
-0.30521033E+04 0.21355710E+02 0.12594252E+01 0.27808424E-01 0.87013932E-05    3
-0.24402205E-07 0.98977710E-11-0.29647742E+04 0.20514290E+02-0.13181775E+04    4

C4H8  2-BUTENE-CIS  CH3-CH=CH-CH3   SPECTROSCOPIC DATA NOT AVAILABLE  REF= CHAO
& HALL  Private Commun.  MAX LST SQ ERROR CP @ 4500 K 1.5 %. HF298=-7.41 KJ
C4H8CIS           T 6/83C   4H   8    0    0G   300.000  5000.     B  56.104   1
 0.11097383E+01 0.35542578E-01-0.16481703E-04 0.34412202E-08-0.26411468E-12    2
-0.26507607E+04 0.19366680E+02 0.24108791E+01 0.25147773E-01 0.98473047E-05    3
-0.22716758E-07 0.86585895E-11-0.27758694E+04 0.14097700E+02-0.89121300E+03    4

C4H8  CYCLOBUTANE  VALUES FROM Dorofeeva, Gurvich & Jorish JPCRD 15 (1986), 437.
EXTRAPOLATED USING WILHOIT'S METHOD. HF298=28.4 KJ  Max Lst Sq Error Cp @ 1300 K
0.48 %.
C4H8 CY           T 1/90C   4H   8    0    0G   200.000  5000.000  B  56.10752 1
 0.59858453E+01 0.26809962E-01-0.10846260E-04 0.20133589E-08-0.14020730E-12    2
-0.56733861E+03-0.12313076E+02 0.38114076E+01-0.96804077E-02 0.12791623E-03    3
-0.16305543E-06 0.64830904E-10 0.18710969E+04 0.85966860E+01 0.34157154E+04    4

C4H8N8O8 HMX Octogen Solid-beta   Cp 290-345 REF= Yin,Ziru,Ganghe,Chengyun
17th Internat. Pyrotech. Seminar 1991 Vol 1, 515-521 S298=33.94 cal Graphic
Integ  HF298(solid)=17.9 Kcal/mol REF=NIST 98  Max Lst Sq Error Cp @ 293 K 0.22 %
beta HMX          HF298 C  4.H  8.N  8.O  8.S   273.000   544.000  D 296.15664 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00 1.98869800E+01-1.81294708E-01 1.61616631E-03    3
-3.42368773E-06 2.30310099E-09 2.53647933E+03-8.79398440E+01 9.00757832E+03    4
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Table 4 (continued)

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C4H8N8O8 HMX Octogen   SIGMA= 128. STATWT = 1.  Ia = 166.71154 Ib = 333.65031
Ic = 355.174455   4 (Ir(NO2) = 5.96    V2 = 16.7 kcal/mole)    NU = 3110,3076,
3034,2992,2979,2977,2914,2912,2076,2062,2051,1968,1892,1747,1726,1706,1464,1412,
1406,1397,1385,1382,1367,1366,1356,1338,1312,1271,1258,1224,1179,1167,1141,1127,
1109,1071,1046,1021,1005,1004,990,963,819,776,758,736,714,696,676,662,638,625,
624,608,544,494,471,434,358,348,338,312,256,218,143,130,122,108,97.1,80.3,74.6,
64.6,55.5,393.    HF298= 44.9 kcal   REF = BURCAT TAE Report # 824 1998
{HF298=65.7+/-7.2 kcal REF=o. Dorofeeva & P. Tolmach, Thermochim Acta 240,(1994)
47-66}  Max Lst Sq Error Cp @ 6000 K 0.63%
C4H8N8O8 HMX      T 6/98C  4.H  8.N  8.O  8.G   200.000  6000.000  F 296.15664 1
 3.44746335E+01 4.64515729E-02-1.79061365E-05 2.98652447E-09-1.81854443E-13    2
 7.27250557E+03-1.48183270E+02 8.14013076E+00 8.33153720E-02 2.72627839E-05    3
-9.98161338E-08 4.69225870E-11 1.63985782E+04-3.22778664E+00 2.25944283E+04    4

C4H8O  2-METHYL,ALLYL ALCOHOL  H2C=C(CH3)CH2OH SIGMA=3 ESTIMATED USING NIST 94
FROM GROUPS C/CD/H2/O; CD/C2;  C/CD/H3; CD/H2  HF298=-39.6 KCAL Max Lst Sq Error
Cp @ 1000 K 0.49%
C4H8O 2MALLYL ALC T 1/96C   4H   8O   1    0G   298.150  5000.000  E  72.10692 1
 0.10660322E+02 0.22030010E-01-0.81853385E-05 0.14316220E-08-0.95435662E-13    2
-0.25097783E+05-0.28060034E+02 0.30802185E+01 0.32417908E-01 0.11903228E-05    3
-0.20853567E-07 0.98797594E-11-0.22260591E+05 0.14160332E+02-0.19927380E+05    4

C4H8O  2-BUTANONE C2H5-CO-CH3  IAIBIC=6268.4E-117  SIGMA=1  NU=2983(4),2941,
2910(2),2884,1716,1460(2),1422,1413(2),1373,1346,1263(2),1182,1108,1089,997,952,
934,768,760,590,460,413,260  IR(C2H5)=2.621 ROSYM=1 POTENTIAL BARRIER C2H5
V(1)=667.8 cm-1 V(3)=334.2 cm-1 IR(CH3-CH2)=0.5119 ROSYM=3 POTENTIAL BARRIER
V(3)=919.2 cm-1  IR(CH3)=0.5071 ROSYM=3 POTENTIAL BARRIER V(3))=181.3 cm-1
NEL=60 REF=CHAO et al JPCRD 15, (1986) 1369 Max Lst Sq Error Cp @ 1300 K 0.63%
HF298=-56.97 KCAL REF=Stull, Sinke & Westrum
C4H8O             T 5/92C   4H   8O   1    0G   200.000  6000.000  B  72.10692 1
 0.10155224E+02 0.22543521E-01-0.81766338E-05 0.13266807E-08-0.79735407E-13    2
-0.33635513E+05-0.25571125E+02 0.63433693E+01 0.94237046E-02 0.55004487E-04    3
-0.73507239E-07 0.28504736E-10-0.31332537E+05 0.88015186E-01-0.28668253E+05    4

C4H8O trans-2,3-DIMETHYL-OXYRANE (trans-DIMETHYL-ETHYLENE-OXIDE)   HF298=-31.0
KCAL  REF=NIST (1991) EXTRAPOLATED FROM 1000 K to 5000 K USING WILHOIT'S
POLYNOMIALS
H8C4O             T 8/93C   4H   8O   1    0G   298.150  5000.000  E  72.10692 1
 0.12941058E+02 0.19981990E-01-0.75877303E-05 0.13521897E-08-0.91405872E-13    2
-0.21867511E+05-0.45899493E+02-0.14293192E+01 0.50569206E-01-0.18756927E-04    3
-0.14736866E-07 0.10838963E-10-0.17231486E+05 0.30995365E+02-0.15599717E+05    4

C4H8O  ETHYL -OXYRANE HF298=-28.0 KCAL REF=NIST (1991) EXTRAPOLATED FROM 1000K
TO 5000 K USING WILHOIT'S POLYNOMIALS
OC4H8             T 9/93C   4H   8O   1    0G   298.150  5000.000  E  72.10692 1
 0.12428338E+02 0.16728392E-01-0.31572488E-05 0.26966084E-09-0.84291614E-14    2
-0.19657838E+05-0.39576992E+02-0.42610481E+01 0.70714327E-01-0.72542161E-04    3
 0.43463849E-07-0.11154810E-10-0.15402386E+05 0.44804255E+02-0.14090067E+05    4

C4H8O TETRAHYDROFURAN (OXOLAN CY) SIGMA=2   REF=Chao et.al JPCRD 15,(1986), 1369
EXTRAPOLATED 1600-5000 K USING WILHOIT'S POLYNOMIALS HF298=-184.18 KJ
REF=Kudchadker, Kudchadker & Wilhoit TRC 1978 Key Chemicals Data Book- Furan,
Dihydrofuran, Tetrahydrofuran  Max Lst Sq Error Cp @ 200 K 0.12%.
C4H8O T.H.FURAN   T 3/97C   4H   8O   1    0G   200.000  5000.000  B  72.10692 1
 6.97323971E+00 2.88949921E-02-1.16992973E-05 2.17090268E-09-1.51075478E-13    2
-2.67236416E+04-1.44239686E+01 4.08780471E+00-1.16647870E-02 1.44507977E-04    3
-1.83315676E-07 7.25734431E-11-2.38006675E+04 1.16117821E+01-2.21516361E+04    4
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C4H8O2 1,4-DIOXANE SIGMA=4 IA=16.3132  IB=17.4452  IC=30.0912  NU=2934,2933.5,
2931,2930.7,2855,2850,2847,2841,1485,1479,1471,1465,1419,1398,1382,1342,1302,
1293,1260,1216,1158,1150,1135,1094,1038,1003,887,871,849,829,598,475.7,418.6,
397,258.4,237 HF298=-75.15+/-1.6 kcal  REF=C. MELIUS DATABASE D94T  Max Lst Sq
Error Cp @ 200 K 0.86%.
C4H8O2 DIOXANE    T03/97C  4.H  8.O  2.   0.G   200.000  6000.000  B  88.10632 1
 1.09080022E+01 2.65730193E-02-9.70934955E-06 1.58519471E-09-9.56379521E-14    2
-4.38420203E+04-3.79862937E+01 3.64975602E+00 3.21199783E-03 1.12973931E-04    3
-1.50581748E-07 6.00072918E-11-3.97765405E+04 9.86785750E+00-3.78167324E+04    4

C4H8O4 ETHANOIC (ACETIC) ACID DIMER (CH3COOH)2  IA*IB*IC=1.6141 E-112    IR=0.522
POT BARRIER  V(3)=481  NU=3193,3032,2949,1675,1436,1436,1370,1283,1018,886,624,
448,196,110,3140,3028,2956,1715,1413,1413,1359,1295,1013,886,624,480,188,2990,
1413,1050,934,635,67,47,3000,1436,1112,912,623,115 REF=CHAO ,& ZWOLINSKI
HF298=-222.04 KCAL.
(ACETIC ACID)2    L 4/85C  4.H  8.O  4.   0.G   300.000  5000.000  B 120.10480 1
 0.16889709E 02 0.24042282E-01-0.81198195E-05 0.12043047E-08-0.64287172E-13    2
-0.11939869E 06-0.56889542E 02 0.38098164E 01 0.43781001E-01 0.49562641E-05    3
-0.34783344E-07 0.16188592E-10-0.11480044E 06 0.15119080E 02-0.11173555E 06    4

C4H8O4 1,3,5,7 Tetra-Oxocane (Octahedron-ring)  REF=Dorofeeva Thermochim Acta
200,(1992),121-150  Data from Dorofeeva extrapolated to 5000 K using Wilhoit's
polynomials.  SIGMA=8   HF298=-620.2 kJ   Max Lst Sq Error Cp @ 200 K 0.63%
C4H8O4 Tetraoxoca T11/99C  4.H  8.O  4.   0.G   200.000  5000.000  B 120.10512 1
 1.23990610E+01 3.33828188E-02-1.36133532E-05 2.53106627E-09-1.76207962E-13    2
-8.13386934E+04-4.28948598E+01 3.51394172E+00 1.62812222E-02 1.01537862E-04    3
-1.46551354E-07 5.97417135E-11-7.69994933E+04 1.27220188E+01-7.45924895E+04    4

C4H8S TETRAHYDROTHIOPHEN  SIGMA=2 REF=Dorofeeva & Gurvich JPCRD 25,(1995),1351
EXTRAPOLATED USING WILHOIT'S POLYNOMIALS  HF298=-34.1 KJ  Max Lst Sq Error Cp @
200 K 0.86 %.
C4H8S T.H.THIOPHE T 3/97C  4.H  8.S  1.   0.G   200.000  5000.000  B  88.17352 1
 1.05353487E+01 2.35320902E-02-8.77376230E-06 1.56515072E-09-1.06979035E-13    2
-9.48200844E+03-3.23144630E+01 1.55153937E+00 2.25556797E-02 5.70166001E-05    3
-9.59127084E-08 4.15407376E-11-5.90019315E+03 1.99054134E+01-4.10126393E+03    4

C4H8S2 1,4 DITHIANE  SIGMA=2 IAIBIC=51450.  NU=2944,2936,2905(2),2955(2),
2919(2),1418,1410,1408,1404,1297,1283,1275,1206(2),1156,1152,1110,999,994,944,
904,894,821,694,669,653,628,480,374,333,253,277,169  HF298=0.0 KJ
REF=Dorofeeva & Gurvich JPCRD 24,(1995),1351 Max Lst Sq Error Cp @ 200 K 0.65%
1,4-C4H8S2        T03/97C  4.H  8.S  2.   0.G   200.000  6000.000  B 120.23952 1
 1.36035997E+01 2.38171520E-02-8.63455848E-06 1.40243589E-09-8.43096867E-14    2
-6.54885251E+03-4.84322813E+01 1.50684634E+00 3.27456314E-02 4.42731895E-05    3
-8.78680150E-08 3.94466672E-11-2.14083750E+03 1.96208497E+01 0.00000000E+00    4

C4H8S2 1,3 DITHIANE  SIGMA=1 IAIBIC=51236.  NU=2958,2936,2905,2900(2),2860,2838,
2818,1432,1426,1417,1387,1285,1272,1244,1210,1180,1175,1152,1090,1010,1009,921,
887,815,792,748,679,672,636,470,336,315,312,217,167  HF298=-10.0 KJ
REF=Dorofeeva & Gurvich JPCRD 24,(1995),1351 Max Lst Sq Error Cp @ 200 K 0.66%
1,3-C4H8S2        T03/97C  4.H  8.S  2.   0.G   200.000  6000.000  B 120.23952 1
 1.37583597E+01 2.38041270E-02-8.65896154E-06 1.40951445E-09-8.48640095E-14    2
-7.81751735E+03-4.84750572E+01 1.60889846E+00 3.27014397E-02 4.42707028E-05    3
-8.76314400E-08 3.92785746E-11-3.37238305E+03 1.99277613E+01-1.20271670E+03    4

N-C4H9 N-BUTYL RADICAL.  TRC 10/84 DATA TO 3000K EXTRAPOLATED USING WILHOIT'S
POLYNOMIALS TO 6000K. MAX LST SQ ERROR CP @ 1300 0.57% . HF298 66.53 KJ.
C4H9,n-butyl      P10/84C  4.H  9.   0.   0.G   200.000  6000.000  B  57.11546 1
 9.18975615E+00 2.36322267E-02-8.64270985E-06 1.42770515E-09-8.70203716E-14    2
 3.37702909E+03-2.15600560E+01 5.82430540E+00 5.50309080E-03 7.49300330E-05    3
-1.02085943E-07 4.13484714E-11 5.54078049E+03 2.17609509E+00 8.00167418E+03    4
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I-C4H9 ISO-BUTYL RADICAL. CH3C(CH3)(H)CH2*  TRC 10/84 DATA TO 3000K EXTRAPOLATED
USING WILHOIT'S POLYNOMIALS TO 6000K. MAX LST SQ ERROR CP @ 1300 0.57% .
HF298=57.32  KJ.
C4H9,i-butyl       P10/84C  4.H  9.   0.   0.G   200.000  6000.000  B  57.11546 1
 9.43040607E+00 2.34271349E-02-8.53599182E-06 1.39748355E-09-8.44057456E-14    2
 2.14214862E+03-2.42207994E+01 3.54885235E+00 1.78747638E-02 5.00782825E-05    3
-7.94475071E-08 3.35802354E-11 4.74011588E+03 1.11849382E+01 6.89397210E+03    4

C4H9  S-C4H9,  2-BUTYL RADICAL IAIBIC=1920. E-117 STATWT=2 NU=3020(2),2950(6),
2820,1460(5),1377(2),1355(2),1200,1172,1098,965(2),921(2),799,371(2),550,437.
FIRST ROTOR ROSYM=2, V(1)=1253.8 cm-1 IR=.35  SECOND ROTOR=THIRD ROTOR  ROSYM=3
V(1)=.035 cm-1  IR=0.49  REF=Wing Tsang JPCRD 19 (1990) p.86  Max Lst Sq Error
Cp @ 200 K 0.56% HF298=70. KJ
S-C4H9             T07/95C   4H   9    0    0G   200.000  6000.000  B  57.11546 1
 0.88057265E+01 0.23630381E-01-0.84564737E-05 0.13612584E-08-0.81313232E-13    2
 0.37941169E+04-0.19996770E+02 0.46457042E+01 0.79313214E-02 0.70027013E-04    3
-0.95973349E-07 0.38628890E-10 0.62341181E+04 0.79642808E+01 0.84190169E+04    4

C4H9 T-C4H9 HF298=51.7 KJ. REF= W.TSANG JACS 107,(1985),2872  STATWT=2  SIGMA=3
NU=2931(6),2825(3),1455(6),1370(3),1279,1252(2),1189(2),1126,992(2),733,541(2),
200   IAIBIC=2240.E-117, THREE EQUIV ROTORS (ROSYM=3,  V(3)=2400., IR=4.7E-40)
C4H9,t-butyl       L 1/93C  4.H  9.   0.   0.G   200.000  6000.000  B  57.11546 1
 6.63074656E+00 2.59353745E-02-9.37163111E-06 1.51845890E-09-9.11190863E-14    2
 2.00861323E+03-9.20581440E+00 6.87327133E+00-1.85146306E-02 1.30560116E-04    3
-1.50832755E-07 5.65358282E-11 4.10958938E+03 2.30016604E-01 6.21804532E+03    4

C4H9N PYRROLIDINE (TETRAHYDROPYRROLE, TETRAMETHYLENEIMINE)  IAIBIC=3330.5
IR=1.119  ROSYM=2. V(2)=280. cm-1    NU=3367,2970(2),2882(4),2818(2),1480(2),
1468(2),1418,1348,1299,1284,1239,1220,1205,1171,1136,1105,1080,1053,1025,980,
925,909,872,844,792,612,570,145   HF298=-3.59+/-0.80 KJ  REF=Das et. al JPCRD 22
(1993), 659  Max Lst Sq Error Cp @ 200 K **1.47%**
C4H9N PYRROLIDINE T 3/95C   4H   9N   1    0G   200.000  6000.000  B  71.12220 1
 0.91914472E+01 0.27301993E-01-0.98874802E-05 0.16049052E-08-0.96462592E-13    2
-0.59280463E+04-0.26546544E+02 0.55475933E+01-0.20299796E-01 0.17343060E-03    3
-0.21528524E-06 0.84721240E-10-0.23303304E+04 0.56593427E+01-0.43177529E+03    4

C4H9NO2 1-Nitro-Butane    STATWT = 1     IA = 17.914472     IB = 52.800976
IC = 57.4685911     Ir (NO2) = 5.96  ROSYM =2  V(2) = 0.08 kcal/mole
Ir(CH3)= 0.51666 ROSYM =3 V(3) = 3.5 kcal/mole  Ir(C2H5) = 2.104   ROSYM =2
V(2) = 9.0 kcal    Ir(C3H7) = 2.22    ROSYM = 3 V(3) =13.64 kcal
NU = (3157,3092,3083,3062,3060,3056),2970,2889,2760,2276,1568,1440,(1425,1408,
1405,1400,1394),1379,(1374,1346,1278,1241),1211,(1191,1160),1123,(1088,1054,
1033),900,860,752,712,611,(535,446,368,243).     HF298 = -34.4 kcal
REF=Stein, NIST 94   Max Lst Sq Error Cp @ 6000 K 0.70%
NITRO-BUTANE       T05/98C  4.H  9.N  1.O  2.G   200.000  6000.000  B 103.12100 1
 1.27918861E+01 2.96302599E-02-1.10618131E-05 1.81914243E-09-1.10094356E-13    2
-2.40186756E+04-4.05022397E+01 4.50296897E+00 1.41859282E-02 9.14552906E-05    3
-1.29431188E-07 5.23563809E-11-1.98606730E+04 1.15748426E+01-1.73106533E+04    4

C4H9O N-BUTOXY RADICAL    SIGMA=3   FROM NIST 94 EXTRAPOLATED TO 5000 K USING
WILHOIT'S POLYNOMIALS   HF298=-13.9 KCAL  Max Lst Sq Error Cp @ 500 K 0.85%.
C4H9O n-BUTOXY RA T 1/96C   4H   9O   1    0G   298.150  5000.000  E  73.11486 1
 0.10935015E+02 0.25158441E-01-0.94963023E-05 0.16741723E-08-0.11205595E-12    2
-0.12551934E+05-0.30200127E+02 0.30817760E+01 0.29308668E-01 0.18141677E-04    3
-0.35949223E-07 0.13544117E-10-0.93118541E+04 0.15205995E+02-0.69947117E+04    4
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Table 4 (continued)

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C4H9O  I-BUTOXY RADICAL 2 METHYL PROPOXY RADICAL (CH3)2CHCH2O* SIGMA=9 ESTIMATED
BY NIST 94 AND EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS.   HF298=-16.2
KCAL  Max Lst Sq Error Cp @ 1500 K 0.83%.
C4H9O I-BUTOXY RA T 1/96C   4H   9O   1    0G   298.150  5000.000  F  73.11486 1
 0.11090141E+02 0.24629071E-01-0.89642503E-05 0.15541428E-08-0.10329922E-12    2
-0.13712316E+05-0.32289483E+02 0.52100434E+00 0.45705123E-01-0.20150863E-04    3
 0.32366878E-08-0.11345219E-11-0.10166726E+05 0.24933738E+02-0.81521100E+04    4

C4H9O  S-BUTOXY-2 RADICAL CH3CH(O*)CH2CH3  SIGMA=9 ESTIMATED USING NIST 94
EXTRAPOLATED USING WILHOIT'S POLYNOMIALS  HF298=-17.5 KCAL  Max Lst Sq Error Cp
@ 500 K 0.78%.
C4H9O S-BUTOXY    T 3/96C   4H   9O   1    0G   298.150  5000.000  F  73.11486 1
 0.10756600E+02 0.25885126E-01-0.97716354E-05 0.17188651E-08-0.11479370E-12    2
-0.14234397E+05-0.29914852E+02 0.28407105E+01 0.30613523E-01 0.21594868E-04    3
-0.45479217E-07 0.18810365E-10-0.11123719E+05 0.15355928E+02-0.88062917E+04    4

C4H9O  T-BUTOXY RADICAL (CH3)3CO*  SIGMA=27  FROM NIST 94  EXTRAPOLATED USING
WILHOIT'S POLYNOMIALS  HF298=-22.0 KCAL  Max Lst Sq Error Cp @ 500 K 0.78%.
C4H9O T-BUTOXY RA T 1/96C   4H   9O   1    0G   298.150  5000.000  E  73.11486 1
 0.14224104E+02 0.20801076E-01-0.78104966E-05 0.13814543E-08-0.92815320E-13    2
-0.17860714E+05-0.52945574E+02 0.51084723E+00 0.47429062E-01-0.18776241E-04    3
-0.36631132E-08 0.29790315E-11-0.13159430E+05 0.21550692E+02-0.11070767E+05    4

N-C4H10  N-BUTANE   STATWT=1  SIGMA=18       IA=3.6865  IB=23.093  IC=24.704
IR=3*.52483  SIGMA ROT=1  POTENTIAL BARRIER V(3)=3300 *3  NU=2965,2872,2853,
1460,1442,1382,1361,1151,1059,842,432,2968,2930,1461,1257,948,731,2965,2912,
1460,1300,1180,803,2968,2780,2853,1461(2),1379,1290,1009,964,271  REF = CHEN,
WILHOIT &ZWOLINSKI   MAX LST SQ ERROR CP @ 1300 K O.91 % .HF298=-30.06 KCAL
N-C4H10          N-L 4/85C  4.H 10.   0.   0.G   300.000  5000.000  B  58.12300 1
 0.10525002E 02 0.23590874E-01-0.78538906E-05 0.11456114E-08-0.59930956E-13    2
-0.20495137E 05-0.32192017E 02 0.15764151E 01 0.34589723E-01 0.69701609E-05    3
-0.28163637E-07 0.12375117E-10-0.17147004E 05 0.17872742E 02-0.15126872E 05    4

I-C4H10  ISOBUTANE  (2-METHYLPROPANE) STATWT=1  SIGMA=81  IA=18.648  IB=10.777
IC=10.777  IR=3X(0.51364)  POT BARRIER V3=3851. V6=-150.  NU=2962(2),2904(2),
2880(2),1477(2),1394(2),1177(2),797(2),433(2),2958(2),1450(2),981(2),2962,2962,
2894,1477,1475,1371,1330,1166,966,367,(TORSION 256,220(2))  REF=CHEN,WILHOIT
& ZWOLINSKI   MAX LST SQ ERROR CP @ 1300 K 0.89 % . HF298=-32.18 KCAL.
I-C4H10          I-L 4/85C  4.H 10.   0.   0.G   300.000  5000.000  B  58.12300 1
 0.10854125E 02 0.23317061E-01-0.77685427E-05 0.11348074E-08-0.59397203E-13    2
-0.21728570E 05-0.35915939E 02 0.54559016E 00 0.37825324E-01 0.56197796E-05    3
-0.30570963E-07 0.14058456E-10-0.18034047E 05 0.21129608E 02-0.16193704E 05    4

C4H10FO2P SARIN CH(CH3)2OP(O)FCH3  SIGMA=1  IA=30.7204  IB=67.1005  IC=73.1898
NU=2962,2959,2958,2947,2941,2927,2921,2885,2878,2872,1475,1467,1460,1456,1435,
1431,1411,1399,1372,1355,1352,1287,1167,1143,1123,1024,922,917,908,904,842,827,
751,636,511,457,413,382,353,309,276,255,244,223,192,146.8,82,40.1  REF=C.MELIUS
DATABASE BACMP4 #2417 Q2U HF298=-230.2+/-9.57 KCAL Max Lst Sq Error Cp @ 1300 K
0.56%.
C4H10FO2P SARIN   T 9/96C   4H  10F   1O   2G   200.000  6000.000  D 140.09437 1
 0.18578606E+02 0.30137329E-01-0.10920099E-04 0.17729267E-08-0.10654834E-12    2
-0.12429242E+06-0.68579536E+02 0.52448929E+01 0.45868801E-01 0.21805453E-04    3
-0.61857475E-07 0.28400543E-10-0.11952678E+06 0.55156043E+01-0.11584048E+06    4
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Table 4 (continued)

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C4H10O-N 1-BUTANOL SYMNO=3  STATWT=1 IAIBIC=8444.0E-117 NU=3300,2290(9),1470,
1450(4),1294(7),1250,1070,1050,955(4),890(3),446,392,350 INTERNAL ROTATIONS
CH3-C3H6OH  ROSYM=1 IR=0.485 POTENTIAL BARRIER V(3)=1140 cm-1 NEL=60
C2H5-C2H4OH ROSYM=1 IR=2.038 POTENTIAL BARRIER V(3)=1140 cm-1 NEL=60
C3H7-CH2OH  ROSYM=1 IR=1.835 POTENTIAL BARRIER V(3)=1140 cm-1 NEL=60
C4H9-OH     ROSYM=1 IR=0.127 POTENTIAL BARRIER V(3)=258.8 cm-1 NEL=60
HF298=-274.68 kJ   REF=Chao et. al, JCPRD 15, (1986), 1369    Max Lst Sq Error
Cp @ 1300 K 0.77%
C4H10O-N          T07/96C   4H  10O   1    0G   200.000  6000.000  B  74.12280 1
 0.13084060E+02 0.26489386E-01-0.10030766E-04 0.16703993E-08-0.10204842E-12    2
-0.39853115E+05-0.42581058E+02 0.59455772E+01 0.23216158E-02 0.10865741E-03    3
-0.14026051E-06 0.54446937E-10-0.35620542E+05 0.52265747E+01-0.33036174E+05    4

C4H10O-S 2-BUTANOL (D,L) SYMNO=3  STATWT=1 IAIBIC=7910.E-117 NU=3682,2980(6),
2943(2),2891,1450(4),1394,1380(2),1350,1314,1290,1250,1145,1110,1080,1034,992,
970,912,820,780,500,435,382,274     INTERNAL ROTATIONS
CH3-C2H4OHCH3  ROSYM=1 IR=0.5043 POTENTIAL BARRIER V(3)=1084.2 cm-1 NEL=60
C2H5CHOH-CH3   ROSYM=1 IR=0.5043 POTENTIAL BARRIER V(3)=1399.3 cm-1 NEL=60
C2H5-CHOHCH3   ROSYM=1 IR=3.027  POTENTIAL BARRIER V(3)= 752.3 cm-1 NEL=60
C4H9-OH        ROSYM=1 IR=0.127  POTENTIAL BARRIER V(3)= 279.7 cm-1 NEL=60
HF298=-292.63 kJ   REF=Chao et. al, JCPRD 15, (1986), 1369  Max Lst Sq Error
Cp @ 6000 K 0.57%
C4H10O-S          T07/96C   4H  10O   1    0G   200.000  6000.000  B  74.12280 1
 0.11644218E+02 0.25565041E-01-0.91441752E-05 0.14708132E-08-0.87878387E-13    2
-0.40944516E+05-0.32554307E+02 0.52699764E+01 0.14103965E-01 0.70685163E-04    3
-0.10285799E-06 0.42246905E-10-0.37834271E+05 0.72163727E+01-0.35194974E+05    4

C4H10O-T 2METHYL-2PROPANOL  SYMNO=54   IAIBIC=5961.7E-117 NU=3643,2980(6),
2910(2),2880,1472(5),1450,1395,1374(2),1330,1230,1215,1140,1106(2),1013(3),919,
748,462(2),424,356,344     INTERNAL ROTATIONS THREE EQUIVALENT ROTATIONS + 1
CH3-COH(CH3)2  ROSYM=1 IR=0.5145 POTENTIAL BARRIER V(3)=1329.1 cm-1 NEL=60
C4H9-OH        ROSYM=1 IR=0.1291 POTENTIAL BARRIER V(3)= 314.8 cm-1 NEL=60
HF298=-312.63 kJ  REF=Chao et. al, JCPRD 15, (1986), 1369   Max Lst Sq Error Cp
@ 6000 K 0.547%
C4H10O-T          T07/96C   4H  10O   1    0G   200.000  6000.000  B  74.12280 1
 0.12195905E+02 0.25213437E-01-0.89531088E-05 0.14332117E-08-0.85400239E-13    2
-0.43495400E+05-0.39715527E+02 0.41048907E+01 0.23022720E-01 0.53016433E-04    3
-0.87928571E-07 0.37588572E-10-0.40159890E+05 0.77499347E+01-0.37600349E+05    4

C4N2  CARBON SUBNITRID (2-BUTYNEDINITRILE)  SIGMA=2  STATWT=1  B0=0.045397 cm-1
nu=2290,2241,2119,1154,692,504(2),472(2),263(2),107(2)  HF298=533.46+/-0.8 kJ
REF=JANAF
C4N2              J 3/61C  4.N  2.   0.   0.G   300.000  5000.000  B  76.05740 1
 0.10042150E 02 0.66359589E-02-0.27599729E-05 0.51846134E-09-0.36297628E-13    2
 0.60605931E 05-0.24861763E 02 0.42279276E 01 0.31558920E-01-0.47552144E-04    3
 0.38601109E-07-0.12435513E-10 0.61848577E 05 0.31801730E 01 0.64158691E-05    4

C5  CALCULATED FROM TSIV TABLES  HF298=1050.94 KJ
C5                R 79  C   5    0    0    0G   200.000  6000.000  B  60.05500 1
 0.95745339E+01 0.38602096E-02-0.14755973E-05 0.24805134E-09-0.15266141E-13    2
 0.12305353E+06-0.23713600E+02 0.33587697E+01 0.32434654E-01-0.59304509E-04    3
 0.56009855E-07-0.20306838E-10 0.12437624E+06 0.60490139E+01 0.12639642E+06    4

C5F12 PERFLUOROPENTANE (FC-4-1-12)  SIGMA=18  CALCULATED and EXTRAPOLATED USING
NIST 93 AND BOZZELLI & RITTER'S PROGRAM. HF298=-607.86 KCAL Max Lst Sq Error Cp
@ 1400 K 0.18%
C5F12  FC 41-12   T12/94C   5F  12    0    0G   298.150  5000.000  E 288.03584 1
 0.36667427E+02 0.11143649E-01-0.46707310E-05 0.86434283E-09-0.58866364E-13    2
-0.31952055E+06-0.15059131E+03 0.41651260E+00 0.12785646E+00-0.14464730E-03    3
 0.74809522E-07-0.14534599E-10-0.31055833E+06 0.32067147E+02-0.30588830E+06    4
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Table 4 (continued)

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C5H RAD   T0=0.  STATWT=4.  IB=35.5335  NU=712.(2),557.(2),637.(2),843.,3329.,
2290.,586.(2),2200.,1570.   SIGMA=1.   T0=4000.  STATWT=2.   REF=DUFF & BAUER
MAX LST SQ ERROR CP @  400 K 0.88 % . HF0=185.4 KCAL.
C5H                T12/81C   5H   1    0    0G   300.000  5000.000  C  61.0629  1
 0.86957493E+01 0.60543008E-02-0.20160105E-05 0.28928926E-09-0.14700995E-13    2
 0.90310687E+05-0.21029110E+02 0.16348248E+01 0.25095381E-01-0.12066364E-04    3
-0.10465111E-07 0.88099883E-11 0.92124875E+05 0.15135100E+02 0.93598280E+05    4

C5H2 RAD    SIGMA=2.  T0=0  STATWT=3.  IB=37.7286  NU=627(2),350(2),1900,630(2),
3329(2),1800,550(2),1570,450(2),843  T0=1576.4   STATWT=2.  T0=2624.  STATWT=1.
REF=DUFF & BAUER  MAX LST SQ ERROR CP @ 400 K 0.62 % .HF0=165. KCAL
C5H2               T12/81C   5H   2    0    0G   300.000  5000.000  C  62.0709  1
 0.11329175E+02 0.74240565E-02-0.26281887E-05 0.40825410E-09-0.23013326E-13    2
 0.78787062E+05-0.36184340E+02 0.30623217E+01 0.27099982E-01-0.10091697E-04    3
-0.12727451E-07 0.91672191E-11 0.81149687E+05 0.70842413E+01 0.83156537E+05    4

C5H3 1,3PENTADIYNE-5-YL RAD  SIGMA=2  STATWT=2  IA=.2813  IB=39.0398  IC=39.3211
NU=3012,3102,1410,1090,935,3005,615,629,870,1950,2100,1200,480,220,530,350,200,
300  REF=DUFF & BAUER  MAX LST SQ ERROR CP @ 1300 K 0.47 %.  HF298=602.58 KJ
ESTIMATED BY USING BOZZELLI & RITTER'S PROGRAM FROM 1,3 PENTADIYINE
C5H3               T 2/92C   5H   3    0    0G   200.000  6000.000  C  63.07882 1
 0.10296658E+02 0.10470124E-01-0.37746103E-05 0.61077326E-09-0.36621089E-13    2
 0.68439389E+05-0.27338507E+02 0.15946538E+01 0.43378369E-01-0.56253789E-04    3
 0.41304029E-07-0.12456939E-10 0.70491079E+05 0.15644812E+02 0.72473303E+05    4

C5H3 1,4-PENTADIYNE-3-YL RADICAL (HCCCH*CCH)   SIGMA=2   STATWT=2   IA=2.8885
IB=30.7707  IC=33.659  NU=138,330(2),347,483,484,560,612,644,645,886,1058,1324,
1718,1817,2993,3242,3245 REF=Sandia BAC/MP4 Database by C. Melius, Private Commu
HF298=134.945+/-10.3 KCAL Max Lst Sq Error Cp @ 1300 K 0.39%
C5H3 1,4DIYNE3YL  T 3/94C   5H   3    0    0G   200.000  6000.000  B  63.07882 1
 0.11453917E+02 0.92730586E-02-0.33071124E-05 0.53138989E-09-0.31710350E-13    2
 0.63604544E+05-0.32238569E+02-0.32458342E-01 0.59449660E-01-0.93606717E-04    3
 0.76931684E-07-0.24822627E-10 0.65960596E+05 0.22810663E+02 0.67906573E+05    4

C5H3 CYCLOPENTATRIENE-YL (RADICAL OF 1,2,4-CYCLOPENTATRIENE NONSYM) STATWT=2
SIGMA=1 IA=7.56527  IB=9.649169  IC=17.21444  NU=464,481,685,687,768,770,864,
965,1001,1136,1161,1241,1345,1366,3047,3063,3084 REF=Sandia BAC/MP4 Database
of C. Melius Private Communication  HF298=166.771+/-17.8 KCAL  Max Lst Sq Error
Cp @ 200 K 0.81%
C5H3 CY            T 3/94C   5H   3    0    0G   200.000  6000.000  B  63.07882 1
 0.10397501E+02 0.10548283E-01-0.38462526E-05 0.62738447E-09-0.37836482E-13    2
 0.79435481E+05-0.30539213E+02-0.30279743E+00 0.31376032E-01 0.30789383E-05    3
-0.35937535E-07 0.19474441E-10 0.82652282E+05 0.26395722E+02 0.83921947E+05    4

C5H3N  CYANO VINYL ACETYLENE HCC-CH=CH-CN ESTIMATED BY MACKIE & COLKET  22 COMB.
SYMP. 1990   HF298=99.5 KCAL  Max Lst Sq Error Cp @ 1500 1.02%
C5H3N              T 6/92C   5H   3N   1    0G   298.150  3000.000  E  77.08556 1
 0.14806620E+02 0.62822470E-02-0.10688211E-05 0.00000000E+00 0.00000000E+00    2
 0.44230048E+05-0.50142232E+02 0.36182825E+01 0.29971121E-01-0.13687184E-04    3
 0.00000000E+00 0.00000000E+00 0.47780069E+05 0.97643721E+01 0.50070058E+05    4

1,3 PENTADIYNE CALCULATED BY STEIN et. al., NIST PROGRAM 1991 BY BENSON'S GROUPS
SIGMA=3 HF298=95.5 KCAL. Max Lst Sq Error Cp @ 1500 K 0.46%
C5H4 1,3-diyne     T 2/92C   5H   4    0    0G   298.150  5000.000  E  64.08676 1
 0.94095519E+01 0.13173708E-01-0.40061435E-05 0.59642775E-09-0.35402340E-13    2
 0.44336639E+05-0.22571166E+02 0.22059680E+01 0.39193876E-01-0.40875017E-04    3
 0.25229634E-07-0.65871791E-11 0.45971817E+05 0.13030572E+02 0.48057192E+05    4
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C5H4 1,4 PENTADIYNE SIGMA=2   IA=4.3175  IB=29.34052  IC= 33.15  NU=140,322,344,
347,549,714,715,729,731,863,929,945,1215,1323,1438,2165,2166,2878,2910,3272,3273
HF298=111.083+/-4.34 KCAL. REF=Sandia BAC/MP4 Database by C. Melius, Private
Communication.  Max Lst Sq Error Cp @ 6000 K 0.47%
C5H4 1,4-DIYNE    T 3/94C   5H   4    0    0G   200.000  6000.000  B  64.08676 1
 0.10173103E+02 0.13101600E-01-0.46855312E-05 0.75410582E-09-0.45046300E-13    2
 0.51670259E+05-0.27484672E+02 0.67637785E+00 0.43825713E-01-0.42484124E-04    3
 0.20857349E-07-0.35770854E-11 0.54085055E+05 0.20473491E+02 0.55898817E+05    4

C5H4 PENTATETRAENE CH2=C=C=C=CH2 CALCULATED BY STEIN et. al., NIST PROGRAM 1991
BY BENSON'S GROUPS EXTRAPOLATED USING WILHOIT'S POLYNOMIALS  SIGMA=4 HF298=115.1
kcal    Max Lst Sq Error Cp @ 1500 K 0.62%
C5H4 TETRAENE     T 2/92C   5H   4    0    0G   298.150  5000.000  E  64.08676 1
 0.11124165E+02 0.12235837E-01-0.44730391E-05 0.76946188E-09-0.50645655E-13    2
 0.53338819E+05-0.33179944E+02 0.26856814E+01 0.33957442E-01-0.21163041E-04    3
 0.78588129E-09 0.33578153E-11 0.55794036E+05 0.10876842E+02 0.57920238E+05    4

C5H4 1,2-PENTADIENE-4-YNE CH2=C=CHCCH    SIGMA=1   IA=3.19788  IB=31.756333
IC=34.3861  NU=140,305,355,360,587,628,690,727,877,905,910,995,1097,1320,1440,
1978,2154,2971,2991,3042,3273  HF298=106.107+/-5.88 KCAL REF= Sandia BAC/MP4
Database By C. Melius Private Communication.  Max Lst Sq Error Cp @ 6000 K .48%.
H4C5              T 3/94H   4C   5    0    0G   200.000  6000.000  B  64.08676 1
 0.10270189E+02 0.13073162E-01-0.46889368E-05 0.75613521E-09-0.45229670E-13    2
 0.49102428E+05-0.27545396E+02 0.87018870E+00 0.41493544E-01-0.35400870E-04    3
 0.13012008E-07-0.60955029E-12 0.51578444E+05 0.20378880E+02 0.53394811E+05    4

C5H4 1,2,4-CYCLOPENTATRIENE NOSYM  SIGMA=1   IA=7.8241  IB=10.128436  IC=17.642
NU=344,378,613,627,803,808,878,934,935,958,1070,1091,1098,1276,1339,1443,1548,
3022,3034,3070,3073  REF=Sandia BAC/MP4 Database of C. Melius, Private Commun.
HF298=131.808+/-5.6 KCAL  Max Lst Sq Error Cp @ 200 K 0.9%
C5H4 CY           T 3/94C   5H   4    0    0G   200.000  6000.000  B  64.08676 1
 0.10106809E+02 0.13457466E-01-0.48862383E-05 0.79465424E-09-0.47821691E-13    2
 0.61714735E+05-0.30155332E+02 0.98338482E+00 0.21429446E-01 0.33390071E-04    3
-0.66941379E-07 0.30563346E-10 0.64905174E+05 0.20682801E+02 0.66327982E+05    4

C5H4N CHAIN RADICAL *CH=CH-CH=CH-CN ESTIMATED BY Mackie & Colket, 22 COMB. Symp
1990. EXTRAPOLATED TO 3000 K USING WILHOIT'S METHOD. HF298=114+/-3 KCAL  Max Lst
Sq Error Cp @ 1500 K 1.15%
C5H4N CHAIN       T 7/92C   5H   4N   1    0G   298.150  3000.000  E  78.09350 1
 0.15596313E+02 0.75129941E-02-0.12797594E-05 0.00000000E+00 0.00000000E+00    2
 0.51193603E+05-0.54112281E+02 0.26651107E+01 0.35935483E-01-0.16911955E-04    3
 0.00000000E+00 0.00000000E+00 0.55124292E+05 0.14606907E+02 0.57366700E+05    4

C5H4N META PYRIDYL RADICAL ESTIMATED BY Mackie & Colket, 22 COMB. SYMP 1990.
EXTRAPOLATED TO 3000 K USING WILHOIT'S METHOD. HF298=91.6 KCAL   (FOR ORTHO AND
PARA RADICALS ADD -1.5 KCAL) Max Lst Sq Error Cp @ 1500 K 1.56%
C5H4N CY          T 6/92C   5H   4N   1    0G   298.150  3000.000  E  78.09350 1
 0.15000314E+02 0.85494897E-02-0.15120770E-05 0.00000000E+00 0.00000000E+00    2
 0.39253830E+05-0.57218867E+02-0.18358976E+01 0.42242509E-01-0.18567008E-04    3
 0.00000000E+00 0.00000000E+00 0.44928510E+05 0.33916009E+02 0.46094647E+05    4

C5H4O CYCLOPENTADIENE-1-ONE SIGMA=2  A=0.273  B=0.131   C=0.088  NU=209,448,
(458),640,(632),714,729,(822),839,943,945,949,(1068,1136,1332,1678,1724,1727,
1789,1870),3161,3171,3204,3206  HF298=13.2 kcal  REF=(in parenthesis EXPERIM.
M. JACOX JPCRD 19,(1990),1532) + Wang & Brezinsky JPC-A 102,(1998),1530.
Max Lst Sq Error Cp @ 400 K 0.55%
C5H4O CY CPD-ONE  T 8/99C  5.H  4.O  1.   0.G   200.000  6000.000  B  80.08616 1
 1.00806824E+01 1.61143465E-02-5.83314509E-06 9.46759320E-10-5.68972206E-14    2
 1.94364771E+03-2.94521623E+01 2.64576497E-01 3.34873827E-02 1.67738470E-06    3
-2.96207455E-08 1.54431476E-11 5.11159287E+03 2.35409513E+01 6.64245999E+03    4
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C5H4O2 3 ketene 2 propylene aldehyde O=CHCH=CHCH=C=O ESTIMATED FROM GROUP
ADDITIVITY DATA AND EXTRAPOLATED FROM 2000 to 5000 K USING Wilhoit's POLYNO-
MIALS   REF=Zhong & Bozzelli JPC-A 102 (1998), 3537.  HF298=-31.02 kcal.
C5H4O2 3 ketene   T 8/99C  5.H  4.O  2.   0.G   298.150  5000.000  E  96.08556 1
 1.70051783E+01 1.18777410E-02-4.42932164E-06 7.73145824E-10-5.13171774E-14    2
-2.23799192E+04-6.06575687E+01-2.49445917E+00 7.89809618E-02-8.99756000E-05    3
 4.41706654E-08-5.54927126E-12-1.76662551E+04 3.66197220E+01-1.56097810E+04    4

C5H5 3-PENTENE-1-YNE-5-YL RADICAL ESTIMATED USING NIST 1994 PROGRAM STRUCTURES &
PROPERTIES.  EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS. SIGMA=2
HF298=97.1+/-2.0 KCAL   Max Lst Sq Error Cp @ 500 K **1.23%**
C5H5 3en1-yne5-yl T 4/94C   5H   5    0    0G   298.150  5000.000  E  65.09470 1
 0.14889675E+02 0.82161004E-02-0.15178062E-05 0.16268184E-09-0.88052708E-14    2
 0.42719249E+05-0.53382883E+02-0.26085299E+01 0.65236909E-01-0.82191379E-04    3
 0.60364270E-07-0.19071607E-10 0.47360405E+05 0.35504920E+02 0.48866379E+05    4

C5H5  CYCLOPENTADIENYL RADICAL Ab-Initio Calc Karni,Oref & Burcat JPCRD 20
(1991), 665  SIGMA=2 STATWT=2 IA=9.06849 IB=9.9295 IC=18.998 NU=484,496.6,652.7,
702.3,709.7,766.7,814.5,833.6,893.5,902.6,917.3,954.9,982,1080,1201,1275.3,
1337,1364,1404,3024.4,3029.4,3039,3048,3061 HF298=266.1 KJ Max Lst Sq Error
Cp @ 6000 K 0.52%  HF298=63.6 KCAL
C5H5 CY           T12/89C   5H   5    0    0G   200.000  6000.000  B  65.09470 1
 0.10844072E+02 0.15392831E-01-0.55630422E-05 0.90189440E-09-0.54156619E-13    2
 0.26950886E+05-0.35254983E+02-0.95902849E+00 0.31396777E-01 0.26724050E-04    3
-0.68942183E-07 0.33301983E-10 0.30779441E+05 0.29072780E+02 0.32004580E+05    4

C5H5N PYRIDINE (AZINE) SIGMA=2  IAIBIC=5696.6  NU=3094.2,3086.9,3072.8,3042.4,
3030.1,1583.9,1580.5,1483.4,1441.9,1362.3,1227,1218,1143.3,1079,1071.9,1031.7,
1007,991.4,980,936.6,880,744,700.3,652,601.4,403.3,373  HF298=140.37+/-0.54 KJ
REF=Das et al. 1993  Max Lst Sq Error Cp @ 200 K **1.2%**
C5H5N PYRIDINE    T 3/95C   5H   5N   1    0G   200.000  6000.000  B  79.10144 1
 0.10737274E+02 0.18411346E-01-0.67089960E-05 0.10937092E-08-0.65928113E-13    2
 0.11511982E+05-0.35580435E+02 0.12333682E+01 0.14084676E-01 0.73775044E-04    3
-0.11405870E-06 0.48433017E-10 0.15439523E+05 0.20414274E+02 0.16882534E+05    4

1-HYDROXY-2,4-CYCLOPENTADIENE-1-YL RADICAL 2,4-C5H4OH Ab-Initio Calculations by
Karni Oref & Burcat JPCRD 20 (1991), 665. SIGMA=1  STATWT=2   IA=10.736637
IB=24.951617   IC=35.688254    ROSYM=2  INT ROT POTENTIAL V2=1213. IR=0.1336
NU=295.6,365.8,510.4,593.4,615.4,680.6,717.3,724.5,831.7,884.8,897.6,905.5,939,
1060.8,1087,1208.5,1272.6,1284.8,1365,1503.8,1467,3028,3043.8,3054,3074.5,
3482.6   HF298=15.9 kcal REF=Wang&Brezinsky JPC,102,(1998),1530.  Max. List Sq
Error Cp @ 200 K 0.71%
C5H4OH CYCLO RAD  T 8/99C  5.H  5.O  1.   0.G   200.000  6000.000  B  81.09410 1
 1.33741248E+01 1.51996469E-02-5.45685046E-06 8.80944866E-10-5.27493258E-14    2
 2.20358027E+03-4.59569069E+01-1.28398054E+00 4.90298511E-02-1.35844414E-05    3
-2.92983743E-08 1.90820619E-11 6.37364803E+03 3.08073591E+01 8.00114499E+03    4

1-OXYL-1,3-CYCLOPENTADIENE RADICAL 1,3-C5H5O Ab-Initio Calculations Karni,Oref &
Burcat JPCRD 20 (1991) 665. SIGMA=1 STATWT=2 IA=11.147244  IB=21.976487
IC=35.267015 NU=191.35,386.3,417.8,520.8,607,637,774.7,867.7,899.5,925.6,989,
1024.4,1129,1150,1218,1267.4,1321.6,1341.6,1375.4,1422,2868,2900.7,3025.4,3037,
3051,787.6,797  HF298=59.8 KJ Max Lst Sq Error Cp @ 6000 0.53%.
1,3C5H5O RADICAL  T 4/91C   5H   5O   1    0G   200.000  6000.000  B  81.09410 1
 0.12606535E+02 0.16747067E-01-0.61097587E-05 0.99674576E-09-0.60111834E-13    2
 0.14114657E+04-0.42604911E+02 0.23043601E+00 0.32322572E-01 0.28900908E-04    3
-0.70680613E-07 0.33407174E-10 0.55554724E+04 0.25330946E+02 0.71922458E+04    4
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Table 4 (continued)

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1-OXYL-1,4-CYCLOPENTADIENE RADICAL 1,4-C5H5O Ab-Initio calculations Karni,Oref &
Burcat JPCRD 20(1991) 665. SIGMA=1 STATWT=2 IA=11.180668  IB=24.926636
IC=35.551016 NU=224.8,338.5,410,562.5,620,653,729,751,826,862,896,920.6,939,
1038,1144.4,1145,1197.6,1243,1285.4,1337,1385.7,1433,2854,2881.6,3027,3046,
3055.8 HF298=103.3 KJ Max Lst Sq Error Cp @ 6000 K 0.53%
1,4C5H5O RADICAL  T 4/91C   5H   5O   1    0G   200.000  6000.000  B  81.09410 1
 0.12711510E+02 0.16650171E-01-0.60741189E-05 0.99090150E-09-0.59758183E-13    2
 0.66172961E+04-0.43161680E+02 0.45438248E-01 0.33871750E-01 0.25637288E-04    3
-0.67844135E-07 0.32508364E-10 0.10797244E+05 0.26058142E+02 0.12424063E+05    4

1-OXYL-2,4-CYCLOPENTADIENE RADICAL 2,4-C5H5O Ab-Initio Calculations Wang &
Brezinsky JPC, 102,(1998),1530. SIGMA=2 STATWT=2  A=0.245  B=0.132  C=0.094
Nu=176,397,523,626,690,766,798,804,878,947,968(2),1055,1066,1090,1118,1276,1311,
1363,1574,1603,1871,2843,3030,3038,3062,3068  HF298=52.8 kcal
2,4-c-C5H5O       D 9/97C   5H   5O   1   00G   300.000  3000.000  B  81.09410 1
 0.85405312E+01 0.22989510E-01-0.95437563E-05 0.17061612E-08-0.97459360E-13    2
 0.22263699E+05-0.20818825E+02-0.30777600E+01 0.52581679E-01-0.28856513E-04    3
-0.33885479E-08 0.63361399E-11 0.25510455E+05 0.39591522E+02 0.26570048E+05    4

C5H5O2 2-pentenedialdehyde-1-yl radical O=C*CH=CHCH2CHO    ESTIMATED FROM GROUP
ADDITIVITY DATA AND EXTRAPOLATED FROM 2000 to 5000 K USING Wilhoit's POLYNO-
MIALS   REF=Zhong & Bozzelli JPC-A 102 (1998), 3537.  HF298=-19.99 kcal.
C5H5O2 2-pentene  T 8/99C  5.H  5.O  2.   0.G   298.150  5000.000  E  97.09350 1
 1.46629817E+01 1.65541793E-02-6.29149065E-06 1.11259736E-09-7.44617493E-14    2
-1.63990894E+04-4.40514968E+01-3.53400779E+00 8.32842318E-02-1.14653205E-04    3
 9.02774159E-08-2.94687646E-11-1.18588987E+04 4.67266279E+01-1.00593011E+04    4

C5H5O2 2-pentenedialdehyde-4-yl radical O=CHCH=CHCH*CHO    ESTIMATED FROM GROUP
ADDITIVITY DATA AND EXTRAPOLATED FROM 2000 to 5000 K USING Wilhoit's POLYNO-
MIALS   REF=Zhong & Bozzelli JPC-A 102 (1998), 3537.  HF298=-17.89 kcal.
C5H5O2 2-pentene  T 8/99C  5.H  5.O  2.   0.G   298.150  5000.000  E  97.09350 1
 1.56927684E+01 1.57719181E-02-6.01048812E-06 1.06457071E-09-7.13241582E-14    2
-1.54871075E+04-5.03606092E+01-3.16128127E+00 8.34432454E-02-1.14264559E-04    3
 8.92804044E-08-2.89089773E-11-1.06704590E+04 4.41383953E+01-8.75093782E+03    4

C5H6 1-PENTEN-3-YNE SIGMA=3 HF298=59.6 KCAL REF=NIST 1991 TO 1500 K EXTRAPOLATED
TO 5000 K USING WILHOIT'S POLYNOMIALS  Max Lst Sq Error Cp @ 500 K **1.3%**
C5H6 1en-2yne     T 4/94C   5H   6    0    0G   298.150  5000.000  E  66.10264 1
 0.11961729E+02 0.14213107E-01-0.37135572E-05 0.53054857E-09-0.32337040E-13    2
 0.24700248E+05-0.36324258E+02 0.18057462E+01 0.29748651E-01 0.88584433E-05    3
-0.31819540E-07 0.14349539E-10 0.28108939E+05 0.19197135E+02 0.29991713E+05    4

C5H6 3-PENTEN-1-YNE SIGMA=3 HF298=61.3 KCAL REF=NIST 1991 TO 1500 K EXTRAPOLATED
TO 5000 K USING WILHOIT'S POLYNOMIALS  Max Lst Sq Error Cp @ 500 K **1.6%**
The metod does not differentiate between the Cis and the Trans isomers.
C5H6 3en-1yne     T 4/94C   5H   6    0    0G   298.150  5000.000  E  66.10264 1
 0.12461757E+02 0.14686414E-01-0.48422257E-05 0.80222734E-09-0.52391736E-13    2
 0.25378034E+05-0.39930098E+02 0.16581871E+01 0.36047209E-01-0.79525384E-05    3
-0.15547159E-07 0.88371326E-11 0.28847420E+05 0.18120095E+02 0.30847182E+05    4

C5H6  CYCLOPENTADIENE  STATWT=1  SIGMA=2  IA*IB*IC=1996*10E-117    NU=3091,3075,
2886,1500,1378,1365,1106,994,915,802,1100,941,700,516,3105,3043,1580,1292,1239,
11090,959,805,2900,925,891,664,350   REF=Dorofeeva, Gurvich & Jorish JPCRD 15,
(1986) 437.  HF298=134.3 KJ from Pedley, Naylor and Kirby.   Max Lst Sq Error
Cp @ 6000 K 0.58 %.
CYCLOPENTADIENE   T 1/90C   5H   6    0    0G     200.000  6000.000  B  66.10264 1
 0.99757848E+01 0.18905543E-01-0.68411461E-05 0.11099340E-08-0.66680236E-13    2
 0.11081693E+05-0.32209454E+02 0.86108957E+00 0.14804031E-01 0.72108895E-04    3
-0.11338055E-06 0.48689972E-10 0.14801755E+05 0.21353453E+02 0.16152485E+05    4
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C5H6N2 2-AMINO-PYRIDINE   SIGMA=2   STATWT=1  IA=14.22  IB=30.312  IC=44.465
NU=3499,3399,3036,3019,3005,3000,1631,1612,1594,1486,1439,1314,1290,1193,1122,
1091,1027,1023,1001,989,967,855,824,775,744,615,589,541,497,411,385,331,207.5
HF298=28.35 KCAL REF=C.MELIUS DATABASE BACMP4 PF11 Binkerton,Pilcher,Al-Takhin
J.Chem.Thermodyn 16 (1984) 373 HF298=28.0+/-0.2 KCAL  Max Lst Sq Error Cp @ 200
K 0.6 %
C5H6N2            T 9/96C   5H   6N   2    0G   200.000  6000.000  B  94.11612 1
 0.13806658D+02 0.20732346D-01-0.74781249D-05 0.12110605D-08-0.72674834D-13    2
 0.78210347D+04-0.50686216D+02-0.37783801D+00 0.42946164D-01 0.15869990D-04    3
-0.59636577D-07 0.29397526D-10 0.12433786D+05 0.26323931D+02 0.14266192D+05    4

2,4-CYCLOPENTADIENE-1-OL C5H5OH Ab-Initio Calculations Karni, Oref & Burcat JPCR
20(1991) 665. SIGMA=1  STATWT=1  IA=12.53933  IB=24.829069  IC=33.91959  NU=300,
368.4,520.3,542.6,705.8,768.6,791.7,809.5,842.3,888.6,979.6,1012.8,1018,1019,
1096.8,1117.8,1206.6,1241.3,1290.5,1343.8,1334.5,1540,1603,1889.8,3021.5,3030,
3048.6,3057.6,3436.6  ROSYM=1  BROT=21.07 INT ROT POTTENTIAL BARRIER V1=30.4
V2=86.14 V3=401. Max Lst Sq Error Cp @ 6000 K 0.54%. HF298=7.9 KJ.
2,4-C5H5OH        T 4/91C   5H   6O   1    0G   200.000  6000.000  B  82.10204 1
 0.12073957E+02 0.19167781E-01-0.69148807E-05 0.11197648E-08-0.67186779E-13    2
-0.47916482E+04-0.40662174E+02 0.15607391E+01 0.22274522E-01 0.57195791E-04    3
-0.99408942E-07 0.43757325E-10-0.83475005E+03 0.19351929E+02 0.95014619E+03    4

1,3-CYCLOPENTADIENE-1-OL C5H5OH Ab-Initio Calculations Karni, Oref & Burcat JPCR
20(1991) 665.  SIGMA=1 STATWT=1  IA=10.761122 IB=26.5896 IC=36.79168  NU=341.8,
363,424,527.4,603,714,793,865.4,874.7,887.3,928.3,935,1001.6,1089,1119,1151.4,
1206.8,1254,1312,1383.4,1412,1545,1606,2866.5,2899.5,3021.5,3032.6,3053,3466
ROSYM=2  IR=0.1336  INT ROT POTENTIAL BARRIER V2=1213. HF298=-24.3 KJ
Max Lst Sq Error Cp @ 6000 K 0.6%
1,3-C5H5OH        T 4/91O   1C   5H   6    0G   200.000  6000.000  B  82.10204 1
 0.12696134E+02 0.18618412E-01-0.67184339E-05 0.10881502E-08-0.65298439E-13    2
-0.88025224E+04-0.44039241E+02-0.22499411E-01 0.36512400E-01 0.22970166E-04    3
-0.65452226E-07 0.31611123E-10-0.46272736E+04 0.25340697E+02-0.29226016E+04    4

1,4-CYCLOPENTADIENE-1-OL  C5H5OH  Ab-Initio Calculation by Karni, Oref & Burcat
JPCRD 20 (1991) 665. SIGMA=1  STATWT=1  IA=10.995026  IB=26.446161  IC=36.88101
NU=335,369.3,379,607,616,742.7,795,795.4,850.3,889.3,926,935,999,1074.5,1112,
1147.6,1195.5,1252,1298,1387,1421.8,1550,1626,2851.6,2880,3030.3,3036.5,3057.6,
3472 ROSYM=2 IR=0.1336 INT ROT POTENTIAL BARRIER V2=1213. HF298=-27.2 KJ.  Max
Lst Sq Error Cp @ 6000 K 0.6%
1,4 C5H5OH        T 4/91O   1C   5H   6    0G   200.000  6000.000  B  82.10204 1
 0.12734997E+02 0.18582251E-01-0.67050926E-05 0.10859592E-08-0.65165720E-13    2
-0.91625548E+04-0.44227527E+02-0.84687145E-01 0.36826867E-01 0.22761297E-04    3
-0.65709925E-07 0.31839396E-10-0.49692504E+04 0.25639055E+02-0.32713894E+04    4

C5H7  1,3-PENTADIENYL-5 RADICAL  CALCULATED BY Weissman & Benson 1989  EXTRAPO-
LATED USING WILHOIT'S POLYNOMIALS TO 3000 K TO GET BETTER FIT. HF298=53. KCAL
Max Lst Sq Error Cp @ 1200 K 0.67%
C5H7              T 2/92C   5H   7    0    0G   298.150  3000.000  F  67.11058 1
 0.18941353E+02 0.85102411E-02-0.14014643E-05 0.00000000E+00 0.00000000E+00    2
 0.18109184E+05-0.78403470E+02-0.56457147E+00 0.48115796E-01-0.23131123E-04    3
 0.00000000E+00 0.00000000E+00 0.24904574E+05 0.27439042E+02 0.26670483E+05    4

C5H7 CYCLOPENTENYL RADICAL ESTIMATED USING BOZZELLI'S PROGRAM FROM DOROFEVA'S
C5H8 CYCLOPENTENE - CYPENE bond. EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNO-
MIALS. HF298=166.88 KJ Max Lst Sq Error Cp @ 1500 K 0.26%.
C5H7 CY           T 4/94C   5H   7    0    0G   298.150  5000.000  E  67.11058 1
 0.12785659E+02 0.16457862E-01-0.48399641E-05 0.73814083E-09-0.46000369E-13    2
 0.13869296E+05-0.44346243E+02-0.27323095E+01 0.40890569E-01 0.16006014E-04    3
-0.56085466E-07 0.26970736E-10 0.19024806E+05 0.40179407E+02 0.20070936E+05    4
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C5H7CL 5-CHLOROPENTADIENE-1,3 (CH2=CHCH=CHCH2CL) CALCULATED BY Weissman & Benson
1989. EXTRAPOLATED USING WILHOIT'S POLYNOMIALS. HF298=17.0 KCAL Max Lst Sq Error
CP @ 1200 K **1.8%**
C5H7CL            T 2/92C   5H   7CL  1    0G   298.150  5000.000  F 102.56328 1
 0.25397667E+02 0.22132288E-02-0.18399465E-06 0.00000000E+00 0.00000000E+00    2
-0.29035978E+04-0.10856612E+03 0.30282986E+01 0.39111282E-01-0.15685560E-04    3
 0.00000000E+00 0.00000000E+00 0.60520027E+04 0.16669045E+02 0.85546833E+04    4

C5H7Cl2  1,5-DICHLOROPENTENE-1-YL-3 (*ClCHCH2CH=CHCH2Cl) CALCULATED BY Weissman
& Benson 1989. EXTRAPOLATED USING WILHOIT'S POLYNOMIALS.  HF298=14.7 KCAL
Max Lst Sq Error Cp @ 1200 K  0.57%
C5H7CL2           T 7/95C   5H   7CL  2    0G   298.150  5000.000  F 138.01598 1
 0.20682058E+02 0.97162863E-02-0.88311605E-06 0.00000000E+00 0.00000000E+00    2
-0.10994753E+04-0.88530581E+02 0.17386362E+01 0.51281909E-01-0.24336075E-04    3
 0.00000000E+00 0.00000000E+00 0.48145961E+04 0.12419440E+02 0.73972850E+04    4

C5H7NO 2-METHYL-3-OXO-BUTYRO-NITRYL CH3-C=O-CH(CH3)-CN  ROSYM=2x3  ESTIMATED
USING NIST 1994 FROM [C-(C)(CN)(CO)(H)]=[C-(C)2(CN)(H)]; [CO-(C)2]; 2x[C-(H)3]
HF298=-108.7 KJ Max Lst Sq Error H-H298 @ 300 K 0.69%
C5H7NO            T10/94C   5H   7N   1O   1G   298.150  5000.000  E  97.11672 1
 0.11348162E+02 0.26153783E-01-0.10147863E-04 0.18274196E-08-0.12448116E-12    2
-0.18497976E+05-0.27546501E+02 0.70321296E+01 0.17114461E-01 0.43753706E-04    3
-0.64537212E-07 0.25693936E-10-0.16201998E+05 0.23072915E-01-0.13073530E+05    4

C5H8 1,3-PENTADIENE CALCULATED BY Weissman & Benson 1989 EXTRAPOLATED TO 3000 K
USING WILHOIT'S POLYNOMIALS TO GET BETTER FIT. HF298=18.2 KCAL  Max Lst Sq Error
Cp @ 1200 K 0.67%.
C5H8              T 2/92C   5H   8    0    0G   298.150  3000.000  F  68.11852 1
 0.19403114E+02 0.96325407E-02-0.15683147E-05 0.00000000E+00 0.00000000E+00    2
 0.20635571E+03-0.80798713E+02-0.30882087E+00 0.48355898E-01-0.22284758E-04    3
 0.00000000E+00 0.00000000E+00 0.72982329E+04 0.26828785E+02 0.91585433E+04    4

C5H8 ISOPRENE, 2-METHYL 1,3-BUTADIENE   SIGMA=3   REF=Stull Westrum & Sinke
EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS HF298=18.1 KCAL Max Lst Sq
Error H-Href @ 300 K 0.82%
C5H8 ISOPRENE     T 5/96C   5H   8    0    0G   298.150  5000.000  B  68.11852 1
 0.10991663E+02 0.22439484E-01-0.81159626E-05 0.13948336E-08-0.92194080E-13    2
 0.40581428E+04-0.32980170E+02-0.36106649E+01 0.74856698E-01-0.83303221E-04    3
 0.52256651E-07-0.13581639E-10 0.74967178E+04 0.39483975E+02 0.91082217E+04    4

C5H8  CYCLOPENTENE  REF=DOROFEEVA GURVICH & JORISH JPCRD 15 (1986) 437.    DATA
EXTRAPOLATED USING WILHOIT POLYNOMIALS. HF298= 32.7 KJ  Max Lst Sq Error Cp @
1300 K 0.46%.
C5H8 CY           T 2/90C   5H   8    0    0G   200.000  5000.000  B  68.11852 1
 0.77244792E+01 0.28322316E-01-0.11545236E-04 0.21540815E-08-0.15054178E-12    2
-0.78261573E+03-0.19769698E+02 0.26898140E+01 0.20954550E-02 0.11303687E-03    3
-0.15408070E-06 0.62763658E-10 0.23139663E+04 0.15294056E+02 0.39328836E+04    4

C5H8CL 5-CHLOROPENTENE-1YL-3 (*CH2CH2CH=CHCH2CL) CALCULATED BY Weissman & Benson
1989. EXTRAPOLATED USING WILHOIT'S POLYNOMIALS. HF298=18.9 KCAL Max Lst Sq Error
Cp @ 1200 K **2.0%**
C5H8CL            T 2/92C   5H   8CL  1    0G   298.150  5000.000  F 103.57122 1
 0.21008537E+02 0.10412247E-01-0.10360547E-05 0.00000000E+00 0.00000000E+00    2
 0.11221103E+03-0.83375603E+02 0.18765490E+01 0.47421032E-01-0.20297237E-04    3
 0.00000000E+00 0.00000000E+00 0.70229095E+04 0.21260602E+02 0.95107950E+04    4
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C5H8N4O12 PENTA ERITHRITOL TETRA NITRATE PETN C(CH2ONO2)4 Solid   Cp 293-333
REF= Yin,Ziru,Ganghe,Chengyun 17th Internat. Pyrotech. Seminar 1991 Vol 1,
515-521 S298=24.37 cal  Graphic Integ  HF298(solid)=-128.7+/-0.2 Kcal
REF=NIST 98 (Ornelas et al Rev. Sci. Instrum. 37,(1966) 907-912    Max Lst Sq
Error Cp @ 293 K 0.05 %
PETN   Solid      T 4/99C  5.H  8.N  4.O 12.S   293.000   550.000  D 316.13828 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00 2.77774680E+02-1.73349082E+00 3.09926721E-03    3
 8.72626335E-07-2.15382459E-09-9.86240953E+04-1.19475100E+03-6.47639849E+04    4

C5H8N4O12 PENTA ERITHRITOL TETRA NITRATE PETN C(CH2ONO2)4  SIGMA=4    IA=172.42
IB=461.12  IC=462.62  (IR(NO2)=5.96  ROSYM=2  V(2)=9.1 kcal/mole )x4 rotors
NU=3029,3028,3006,2999,2972,2971,2936,2929,1735,1730,1711,1710,1494,1485,1473,
1469,1445,1435,1424,1417,1390,1380,1363,1362,1334,1325,1288,1256,1199,1198,
1128,1098,1079,1072,1055,1022,988,974,969,962,923,918,865,810.3(2),807(2),773,
764,724,696,694,667,663,645,590,541,462,409,408,372,284,274,249,222,218,199,184,
166,139,114,112.5,75.4,67.8,65.1,60,57  REF=C. MELIUS DATABASE BACMP22 #86  AA9A
HF298=-92.5 kcal REF=Cox & Pilcher 1970  Max Lst Sq Error Cp @ 1300 k 0.67%
C5H8N4O12 PETN    T11/97C  5.H  8.N  4.O 12.G   200.000  6000.000    316.13828 1
 4.20349983E+01 4.16412378E-02-1.62923542E-05 2.75856914E-09-1.70123449E-13    2
-6.48342117E+04-1.86444303E+02 1.01315796E+01 7.43819642E-02 7.88205030E-05    3
-1.68073189E-07 7.47114699E-11-5.32738211E+04-8.13692751E+00-4.65475416E+04    4

C5H9 CYCLOPENTYL RADICAL CALCULATED USING BOZELLI & RITTER'S COEFICIENT METHOD
USING BENSON'S GROUPS AND EXTRAPOLATED BY WILHOIT'S POLYNOMIALS     SIGMA=2
HF298=27.5 KCAL  REF=Stein et. al., NIST PROGRAM 1991.
C5H9 CY           T 2/92C   5H   9    0    0G   298.150  5000.000  F  69.12646 1
 0.11406802E+02 0.22563988E-01-0.70235595E-05 0.11321968E-08-0.73438204E-13    2
 0.75268769E+04-0.39636280E+02 0.29427128E+00 0.13823374E-01 0.90847653E-04    3
-0.13008694E-06 0.53051811E-10 0.12565712E+05 0.27389773E+02 0.13838458E+05    4

C5H9 PENTEN-2-YL-5 CH3CH=CHCH2CH2*  CALCULATED BY Weismann & Benson 1989. EXTRA-
POLATED USING WILHOIT'S POLYNOMIALS  HF298=38.0 KCAL
C5H9              T 2/92C   5H   9    0    0G   298.150  3000.000  F  69.12646 1
 0.20313000E+02 0.10869880E-01-0.19063805E-05 0.00000000E+00 0.00000000E+00    2
 0.94061603E+04-0.82533815E+02 0.11430827E+01 0.44350789E-01-0.17825470E-04    3
 0.00000000E+00 0.00000000E+00 0.16967656E+05 0.24181940E+02 0.19122233E+05    4

C5H9 PENTEN-2-YL-1 *CH2CH=CHCH2CH3  CALCULATED BY Weismann & Benson 1989. EXTRA-
POLATED USING WILHOIT'S POLYNOMIALS  HF298=27. KCAL
H9C5              T 2/92C   5H   9    0    0G   298.150  3000.000  F  69.12646 1
 0.20445128E+02 0.10907665E-01-0.17916513E-05 0.00000000E+00 0.00000000E+00    2
 0.37740200E+04-0.84800566E+02 0.34671311E+00 0.46758622E-01-0.19207040E-04    3
 0.00000000E+00 0.00000000E+00 0.11574896E+05 0.26704158E+02 0.13586850E+05    4

C5H9 3-METHYL-1-BUTEN-3-YL H2C=CH-C*(CH3)-CH3 SIGMA=18 ESTIMATED BY NIST PROGRAM
(1994) EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS. HF298=19.3 KCAL  Max
Lst Sq Error Cp @ 1500 K 0.43%.
C5H9 3M1BUTEN3YL  T 5/96C   5H   9    0    0G   298.150  5000.000  F  69.12646 1
 0.10525096E+02 0.26132390E-01-0.98482454E-05 0.17295482E-08-0.11536188E-12    2
 0.43545451E+04-0.31794253E+02 0.41170174E+01 0.21052833E-01 0.46247772E-04    3
-0.72799250E-07 0.29713776E-10 0.72701012E+04 0.68883799E+01 0.97120817E+04    4

C5H9 3-METHYL-1-BUTEN-1-YL *HC=CH-CH(CH3)-CH3 SIGMA=9  ESTIMATED BY NIST PROGRAM
(1994) EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS. HF298=50.7 KCAL  Max
Lst Sq Error Cp @ 1500 K 0.19%.
C5H9 3M1BUTEN1YL  T 5/96C   5H   9    0    0G   298.150  5000.000  E  69.12646 1
 0.12467494E+02 0.22329954E-01-0.76869307E-05 0.12651997E-08-0.80609456E-13    2
 0.19913799E+05-0.38859739E+02 0.19660139E+01 0.45617488E-01-0.92039963E-05    3
-0.28501148E-07 0.18371669E-10 0.23028331E+05 0.16461958E+02 0.25513085E+05    4
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C5H9 3-METHYL-1-BUTEN-4-YL H2C=CH-CH(CH3)-CH2* SIGMA=9 ESTIMATED BY NIST PROGRAM
(1994) EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS. HF298=42.3 KCAL  Max
Lst Sq Error Cp @ 1500 K 0.43%.
C5H9 3M1BUTEN4YL  T 5/96C   5H   9    0    0G   298.150  5000.000  E  69.12646 1
 0.13126454E+02 0.20337031E-01-0.63441521E-05 0.99697655E-09-0.62523110E-13    2
 0.15559475E+05-0.41449511E+02-0.17838437E+01 0.72924194E-01-0.86508640E-04    3
 0.64737446E-07-0.21365264E-10 0.19223118E+05 0.33121120E+02 0.21286065E+05    4

C5H9N 1,2,3,6-TERAHYDRO-PYRIDINE SIGMA=1. IA=2.57  IB=2.86  IC=0.43  NU=3420,
3050,3040,2929,2925,2860,2850(2),2840,1600,1455,1454,1448,1438,1425,1369,1357,
1278,1250,1220,1215,1150,1124,1084,1054,965,950,890,885,815,811,770,700,630,521,
474,399,285,186  REF=Sidhu et. al., 1991   HF298=18.+/-2 KCAL ESTIMATED USING
BENSON'S GROUP ADDITIVITY. Max Lst Sq Error Cp @ 200 K 0.96%
C5H9N             T 2/92C   5H   9N   1    0G   200.000  6000.000  B  83.13320 1
 0.11833534E+02 0.28098151E-01-0.10182947E-04 0.16536607E-08-0.99405120E-13    2
 0.26418000E+04-0.46192454E+02 0.17693067E+01 0.16923937E-01 0.94000576E-04    3
-0.13916857E-06 0.57777745E-10 0.71954216E+04 0.14882677E+02 0.90579000E+04    4

1-PENTENE EXTRAPOLATED FROM API PROJECT #44 DATA USING WILHOIT'S POLYNOMIALS
HF298=-5.0 KCAL
C5H10 1-PENTENE 1-P12/52C   5H  10    0    0G   300.000  5000.000  C  70.13400 1
 0.12541454E 02 0.23941070E-01-0.77445529E-05 0.11157970E-08-0.57968116E-13    2
-0.87175352E 04-0.39854187E 02 0.17627859E 01 0.38902789E-01 0.58380774E-05    3
-0.30547188E-07 0.13839465E-10-0.48109883E 04 0.19929169E 02-0.25594116E 04    4

C5H10 2-PENTENE-Trans  EXTRAPOLATED FROM API PROJECT #44 DATA USING WILHOIT'S
POLYNOMIALS  HF298=-7.59 KCAL  Max Lst Sq Error Cp @ 1200 K 0.35%
C5H10 2-PENTENE 2-P12/52C   5H  10    0    0G   298.150  5000.000  C  70.13440 1
 0.94842492E+01 0.29600248E-01-0.11393033E-04 0.20468617E-08-0.13936013E-12    2
-0.89116325E+04-0.23775434E+02 0.18750517E+01 0.37994733E-01 0.57083514E-05    3
-0.29082134E-07 0.13102964E-10-0.60663547E+04 0.18907614E+02-0.38194145E+04    4

C5H10  2METHYL-1-BUTENE EXTRAPOLATED FROM STULL WESTRUM & SINKE USING WILHOIT'S
POLYNOMIALS HF298=-8.68 KCAL Max Lst Sq Error H @ 300 K 0.5%.
C5H10 2MB-1ene    T11/95C   5H  10    0    0G   298.150  5000.000  B  70.13440 1
 0.10169614E+02 0.29142736E-01-0.11304015E-04 0.20426202E-08-0.13964602E-12    2
-0.97185802E+04-0.27826511E+02 0.15343285E+01 0.40535723E-01 0.26841152E-05    3
-0.27784359E-07 0.12941501E-10-0.66019829E+04 0.20108917E+02-0.43679207E+04    4

C5H10  2METHYL-2-BUTENE EXTRAPOLATED FROM STULL WESTRUM & SINKE USING WILHOIT'S
POLYNOMIALS HF298=-10.17 KCAL Max Lst Sq Error Cp @ 1200 K 0.35%.
C5H10 2MB-2ene    T11/95C   5H  10    0    0G   298.150  5000.000  B  70.13440 1
 0.86980441E+01 0.30551374E-01-0.11746424E-04 0.21071085E-08-0.14329275E-12    2
-0.99867755E+04-0.19723898E+02 0.12618252E+01 0.39178857E-01 0.31182431E-05    3
-0.25702067E-07 0.11609951E-10-0.72175421E+04 0.21915280E+02-0.51177135E+04    4

C5H10  2METHYL-3-BUTENE EXTRAPOLATED FROM STULL WESTRUM & SINKE USING WILHOIT'S
POLYNOMIALS HF298=-6.92 KCAL Max Lst Sq Error H @ 300 K 0.8%.
C5H10 2MB-3ene    T 5/96C   5H  10    0    0G   298.150  5000.000  B  70.13440 1
 0.10712560E+02 0.28487570E-01-0.10916621E-04 0.19543209E-08-0.13271736E-12    2
-0.87445219E+04-0.30984943E+02-0.13221471E+00 0.61756848E-01-0.53167981E-04    3
 0.29073931E-07-0.74254711E-11-0.57719514E+04 0.24567827E+02-0.34822593E+04    4

C5H10  CYCLOPENTANE  REF=DOROFEEVA GURVICH & JORISH JPCRD 15 (1986) 437   DATA
EXTRAPOLATED FROM 1600 K USING WILHOIT'S POLYNOMIALS. HF298=-78.4 KJ  Max Lst
Sq Error Cp @ 1300 K 0.46 %.
C5H10 (CYCLO)     T 2/10C   5H  10    0    0G   200.000  5000.000  B  70.13440 1
 0.69545862E+01 0.34646557E-01-0.14029265E-04 0.26044187E-08-0.18133788E-12    2
-0.14403923E+05-0.17468548E+02 0.37037372E+01-0.11558026E-01 0.16410400E-03    3
-0.20935073E-06 0.83095982E-10-0.11095213E+05 0.11957860E+02-0.94292989E+04    4
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C5H10O TETRAHYDRO-PYRAN (CYCLO) ESTIMATED FROM BENSON'S GROUP VALUES BY NIST
1991. EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS.      SIGMA=2
HF298=-53.5 +/- 0.2 KCAL  REF=STULL WESTRUM & SINKE       Max Lst Sq Error
Cp @ 1000 K 0.50 %.
C5H10O            T 4/93C   5H  10O   1    0G   298.150  5000.000  E  86.13380 1
 0.13194934E+02 0.29686076E-01-0.11181511E-04 0.19599388E-08-0.13057603E-12    2
-0.33510327E+05-0.49486514E+02-0.56123960E+01 0.96754751E-01-0.11576165E-03    3
 0.83446868E-07-0.25479016E-10-0.28679331E+05 0.44826119E+02-0.26922092E+05    4

N-C5H11 N-PENTYL RADICAL  REF=N.Cohen JPC,96 (1992),9052  EXTRAPOLATED FROM 1600
K TO 5000 K WITH WILHOIT'S POLYNOMIALS.  HF298=13.29 KCAL   MAX LST SQ ERROR CP
@ 1500 K 0.4%.
N-C5H11 n-pentyl  T03/97C  5.H 11.   0.   0.G   298.150  5000.000  D  71.14234 1
 1.13309915E+01 3.03697959E-02-1.13963838E-05 1.99610398E-09-1.32881065E-13    2
 7.35080645E+02-3.13492414E+01 3.57937980E+00 3.04191686E-02 3.27870896E-05    3
-5.86554303E-08 2.39351280E-11 4.08346324E+03 1.42560613E+01 6.68774949E+03    4

S-C5H11 S-PENTYL RADICAL    REF=N.Cohen JPC,96 (1992),9052   EXTRAPOLATED USING
WILHOIT'S POLYNOMIALS.  HF298= 10.89 Kcal Max Lst Sq Error Cp @ 1500 K 0.43%
S-C5H11 1m-butyl  T03/97C  5.H 11.   0.   0.G   298.150  5000.000  D  71.14234 1
 1.05838403E+01 3.11018862E-02-1.17149660E-05 2.05728548E-09-1.37198647E-13    2
-1.80355565E+02-2.72603116E+01 7.53834570E+00 7.11191190E-03 7.97981697E-05    3
-1.00325084E-07 3.76603045E-11 2.39183947E+03-3.31129273E+00 5.48002949E+03    4

C5H11  T-C5H11 RADICAL HF298=32.6 KJ,  REFN:  WING TSANG JACS (1985) p.2872
NU=2931(9),2825(2),1455(8),1370(3),1279,1252(2),1189(2),1126,992(3),733,541(2),
380,200,990(9)      STATWT=2 IAIBIC =8590.E-117  FIRST ROTOR  ROSYM=3  V(3)=3585.,
IB=4.8E-40 SECOND ROTOR  ROSYM=1,V(2)=.1, IB=21.E-40  THIRD ROTOR
ROSYM=3,V(2)=.1,IB=4.8E-40
T-C5H11           T-L 5/87C  5.H 11.   0.   0.G   298.150  5000.000  B  71.14190 1
 0.67232314E 01 0.36074004E-01-0.14425089E-04 0.26385814E-08-0.18130546E-12    2
-0.66929018E 03-0.68507985E 01 0.18160004E 01 0.25384068E-01 0.46807718E-04    3
-0.70666410E-07 0.27488045E-10 0.19643507E 04 0.24638344E 02 0.39209036E 04    4

C5H11 2,2,M,M-PROPYL (NEOPENTYL) RADICAL SIGMA=54     REF=N.Cohen JPC,96 (1992),
9052  EXTRAPOLATED USING WILHOIT POLYNOMIALS. HF298=8.22 KCAL  Max Lst Sq Error
Cp @ 1500 K **1.12%.**
C5H11  neopentyl  T03/97C  5.H 11.   0.   0.G   298.150  5000.000  D  71.14234 1
 2.60303371E+01-3.89073388E-03 1.18835338E-05-2.05929731E-09 1.06754076E-13    2
-5.66523187E+03-1.12796509E+02-4.46503561E+00 9.32367831E-02-1.41121240E-04    3
 1.52613544E-07-6.83999414E-11 2.30110241E+03 4.28019931E+01 4.13644099E+03    4

C5H11NO2  1-Nitro-Pentane    STATWT=1  SYMNO=2 IA=21.264770  IB = 85.889716
IC = 100.4047696   Ir (NO2) = 5.96  ROSYM =2  V(2) = 0.08 kcal/mole
Ir(CH3)= 0.51666  ROSYM =3  V(3) = 3.5 kcal    Ir(C2H5) = 2.104  ROSYM =2
V(2) = 9.0 kcal    Ir(C3H7) = 2.22  ROSYM = 2 V(2) =13.64 kcal
NU = 3183,3088,3069,3034,3027,3024,2992,2955,2949,2947,2893,1901,1611,1474,1421,
1410,1403,1402,1398,1386,1367,1341,1300,1253,1173,1167,1153,1146,1129,1121,1081,
1039,1020,990,965,926,866,830,805,691,615, 480,470,394,315,295,214   REF = NIST
97 WEBBOOK  HF298 =-39.3 kcal   REF =BURCAT TAE # 824 (1998).  Max Lst Sq Error
Cp @ 200 & 6000 K 0.68%
NITRO-PENTANE     T06/98C  5.H 11.N  1.O  2.G   200.000  6000.000  B 117.14788 1
 1.59382106E+01 3.48884183E-02-1.29633850E-05 2.12755256E-09-1.28618354E-13    2
-2.80406921E+04-5.83080492E+01 4.00703926E+00 2.29727394E-02 1.04023119E-04    3
-1.55573589E-07 6.44328697E-11-2.26341947E+04 1.39586649E+01-1.97764150E+04    4
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C5H12  N-PENTANE   SIGMA=18  API DATA EXTRAPOLATED THROUGH WILHOIT'S POLYNOMIALS.
MAX LST SQ ERROR CP @  1300 K 1.1 %. HF298=-35 KCAL.
PENTANE          N-P10/85C  5.H 12.   0.   0.G   298.150  5000.000  C  72.14980 1
 0.13546998E 02 0.28421786E-01-0.94174648E-05 0.13893589E-08-0.74212609E-13    2
-0.24577680E 05-0.47034348E 02 0.18983679E 01 0.41203037E-01 0.12312175E-04    3
-0.36589501E-07 0.15042509E-10-0.20091500E 05 0.18665909E 02-0.17651280E 05    4

ISOPENTANE  API DATA EXTRAPOLATED THROUGH WILHOIT'S POLYNOMIALS. HF298=-153.7 KJ
I-C5H12          I-P10/85C  5.H 12.   0.   0.G   298.150  5000.000  C  72.14980 1
 0.12327787E 02 0.30613087E-01-0.98415785E-05 0.13919776E-08-0.70337345E-13    2
-0.25037492E 05-0.41146667E 02 0.10832882E 01 0.44571076E-01 0.82389934E-05    3
-0.35258047E-07 0.15785762E-10-0.20807535E 05 0.21781982E 02-0.18485976E 05    4

NEOPENTANE C5H12 API DATA EXTRAPOLATED THROUGH WILHOIT'S POLYNOMIALS.
HF298=-167.9 KJ
CH3C(CH3)2CH3      P10/85C  5.H 12.   0.   0.G   298.150  5000.000  C  72.14980 1
 0.10110416E 02 0.35349566E-01-0.11039967E-04 0.14777721E-08-0.68467042E-13    2
-0.25806711E 05-0.33770157E 02 0.72638994E 00 0.48125476E-01 0.15917458E-05    3
-0.26692458E-07 0.12078282E-10-0.22407980E 05 0.18314041E 02-0.20196259E 05    4

C5H12O(L) t-C4H9-O-CH3 Tertiary butyl-methyl ether LIQUID calculated from
thermal measurements.    REF=TRC 1983   HF298=-313.6 kJ
C5H12O tC4H9OCH3  T08/00C  5.H 12.O  1.   0.L   200.000   310.000  A  88.14968 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00 1.81730017E+01-1.70292004E-02 1.27817452E-04    3
-5.81277666E-08-4.62085850E-11-4.33711851E+04-7.15912586E+01-3.77171956E+04    4

C5H12O t-C4H9-O-CH3 Tertiary butyl-methyl ether     SIGMA=1     IA=20.675347
IB=30.958288   IC=30.991722   3x(Ir=0.47   V3=2.4 kcal  ROSYM=3)   Nu=[3089](2),
3006,3003(2),3000,[2986,2945],2940,2935,[2837,2730],1492,1483,[1475],1472,1461,
1459,1457,1443(2),1391,[1372],1365,1249,[1205],1198,1172,1143,[1093,1021],1007,
930,892,[855],831,[724],488,440,394,350,324,275.9,272.7,246.5  REF= NIST 2000,
Webbook, IR in parenthesis and Gaussian 98 B3LYP/6-31G* calc of Jan 1999.
HF298=-283.2 kJ  REF=TRC-83  {HF298=-293.8 kJ REF=NIST 94; HF298=-283.7+/-0.8 kJ
REF=Pedly & Rylance 1977} Max Lst Sq Error Cp @ 1300 K 0.61%
C5H12O  tC4H9OCH3 T08/00C  5.H 12.O  1.   0.G   200.000  6000.000  B  88.14968 1
 1.33868819E+01 3.29283214E-02-1.18027402E-05 1.90207547E-09-1.13712190E-13    2
-4.07919507E+04-4.60060101E+01 4.24395629E+00 3.82110434E-02 2.49992458E-05    3
-5.45089669E-08 2.33555478E-11-3.71488062E+04 6.40373322E+00-3.40609368E+04    4

C6CL6 HEXACHLOROBENZENE DATA FROM STULL WESTRUM & SINKE EXTRAPOLATED USING
WILHOIT'S POLYNOMIALS Max Lst Sq Error Cp @ 1300 K 0.4%  HF298=-8.10 KCAL
C6CL6            T 1/92C   6CL  6    0    0G   298.150  6000.000  B 284.78220 1
 0.25828477E+02 0.83148412E-02-0.33076208E-05 0.57000698E-09-0.35641306E-13    2
-0.13505569E+05-0.99653026E+02 0.46643307E+01 0.79424296E-01-0.98554390E-04    3
 0.61217228E-07-0.15381401E-10-0.82398803E+04 0.66783480E+01-0.40760550E+04    4

C6D5  PHENYL-D5 RAD  IA=33.7696  IB=17.9469  IC=15.8227  SIGMA=2  STATWT=2
NU=2293,943,1037,497,2292,969,827,601,1286,824,662(2),2287,1335(2),814,2265(2),
1552(2),867(2),577(2),795,352(2)  REF=BURCAT,ZELEZNIK & MCBRIDE  MAX LST SQ
ERROR CP @ 1300 K 0.84 % . HF298=306.94 KJ.
C6D5             L12/84C  6.D  5.   0.   0.G   300.000  5000.000  B  82.13651 1
 0.14729492E 02 0.15210535E-01-0.55241635E-05 0.87984575E-09-0.50979217E-13    2
 0.30282629E 05-0.55768127E 02-0.12549782E 01 0.47328766E-01-0.80759883E-05    3
-0.29901972E-07 0.17149060E-10 0.35314063E 05 0.29766983E 02 0.36917128E 05    4
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C6D6  BENZENE-D6  IA=35.8938  IB=IC=17.9469  SIGMA=12  NU=2293,943,1037,497,
2292,969,827,601,1286,824,662(2),2287(2),1335(2),814(2),2265(2),1552(2),867(2),
577(2),795(2),352(2)  REF=SHIMANOUCHI  MAX LST SQ ERROR CP @ 1300 K 0.86 % .
HF298=58.18 KJ REF=BURCAT, ZELEZNIK & MCBRIDE
C6D6              L12/84C  6.D  6.   0.   0.G   300.000  5000.000  B  84.15061 1
 0.15619864E 02 0.17123934E-01-0.62012759E-05 0.98493058E-09-0.56891557E-13    2
-0.14433052E 03-0.63901352E 02-0.20701218E 01 0.52938197E-01-0.96074828E-05    3
-0.32802372E-07 0.19012528E-10 0.54068984E 04 0.30680710E 02 0.69971633E 04    4

C6F6 HEXAFLOROBENZENE   SIGMA=12  IA=IB=79.9862  IC=159.979  NU=1660(2),1534(2),
1498,1327,1156(2),1077,992(2),765,623(2),602,572,546,431(2),389.5(2),304(2),
262.2,256.6(2),218,181,135.7(2) REF=Melius Database Q9X   HF298=-228.64 Kcal
REF=STULL WESTRUM & SINKE  Max Lst Sq Error Cp @ 1300 K 0.48%
C6F6              T03/97C  6.F  6.   0.   0.G   200.000  6000.000  B 186.05642 1
 2.33186087E+01 1.07562779E-02-4.17044638E-06 7.07443606E-10-4.38074922E-14    2
-1.23931487E+05-9.30677826E+01 1.97866627E+00 8.21868402E-02-1.03031945E-04    3
 6.88636763E-08-1.94291617E-11-1.18514980E+05 1.44710988E+01-1.15055458E+05    4

C6F14 PERFLUOROHEXANE (FC-5-1-14)  SIGMA=18  CALCULATED and EXTRAPOLATED USING
NIST 94 AND BOZZELLI & RITTER'S PROGRAM. HF298=-704.87 KCAL Max Lst Sq Error Cp
@ 1000 K 0.07%.
C6F14  FC 51-14   T12/94C   6F  14    0    0G   298.150  5000.000  E 338.04364 1
 0.44067386E+02 0.12770763E-01-0.53399367E-05 0.95791650E-09-0.61923975E-13    2
-0.37074786E+06-0.18473799E+03-0.14298519E+02 0.24055087E+00-0.34353654E-03    3
 0.22553364E-06-0.55889775E-10-0.35851817E+06 0.98855981E+02-0.35470535E+06    4

C6N6O6 BENZOTRIFUROXAN (BTF) SIGMA=3  A=B=0.15716  C=0.07858  NU=86(2),104,164,
183(2),276(2),312,372(2),[420],428(2),509,[570(2)],642(2),649,[651],740(2),
[736(2),810],785,886,931,[935(2),965(2)],1099,[1082(2)],1290,[1304(2),1415(2)],
1487,[1570(2)],1602,1659,[1656(2)] REF=Gong, Xiao & Dong Chineese J. Struct.
Chem. 18,(1999),124-130  NO GASEOUS HEAT OF FORMATION AVAILABLE  HF298(Solid)=
144.9 +/-0.8 kcal REF=Rouse J. Chem. Eng. Data, 21,(1976),16-20.  Max Lst Sq
Error Cp @ 1300 K 0.53 %.
BENZOTRIFUROXAN   T 8/99C  6.N  6.O  6.   0.G   200.000  6000.000  D 252.10284 1
 3.25028258E+01 1.96519737E-02-7.62353333E-06 1.29360949E-09-8.01216134E-14    2
-1.33442030E+04-1.47193860E+02-8.43434844E-01 1.03343605E-01-6.42039528E-05    3
-7.99732470E-09 1.54458617E-11-3.76608113E+03 2.69680087E+01                   4

C6H RAD   T0=0 STATWT=4 IB=60.398 NU=3329,3313,2201,1115,625(3),1570,491(2),
258(2),433(2),105(2) T0=3000. STATWT=2  REF= BAUER & DUFF and BURCAT (unpub).
HF298=248.0 KCAL REF= Kiefer, Sidhu, Kern, Xie, Chen, Harding 1992.   Max Lst Sq
Error Cp @ 6000 K 0.34%
C6H               T 3/92C   6H   1    0    0G   200.000  6000.000  C  73.07394 1
 0.11361786E+02 0.75157820E-02-0.27216114E-05 0.43917513E-09-0.26217995E-13    2
 0.12080112E+06-0.29989833E+02 0.10110111E+01 0.59781961E-01-0.10773934E-03    3
 0.96196601E-07-0.32681317E-10 0.12261638E+06 0.17998104E+02 0.12479773E+06    4

C6H2  HEXATRIYNE  STATWT=1.  SIGMA=2.  IB=63.5805  NU=3313,2201,2019,625,3328,
2125,1115,625(2),491(2),258(2),622(2),433(2),105(2) Ref=Bjarnov, Christiansen &
Nielsen Spectrochim Acta 20A (1974), 1255. HF298=167.5 KCAL REF= Kiefer, Sidhu,
Kern, Xie, Chen, Harding 1992   Max Lst Sq Error @ 1300 K 0.38%
C6H2              T 3/92C   6H   2    0    0G   200.000  6000.000  B  74.08188 1
 0.12532801E+02 0.87766321E-02-0.31329616E-05 0.50371820E-09-0.30071921E-13    2
 0.79784338E+05-0.38858580E+02-0.54109216E+00 0.74532628E-01-0.13578252E-03    3
 0.12226630E-06-0.41825207E-10 0.82115132E+05 0.21882710E+02 0.84288792E+05    4
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C6H3 RAD  STATWT=2.  SIGMA=2.  IA=.278     IB=66.1121  IC=66.3901  NU=3012,629,450,
3102,870,230,1410,1580,530,1090,1100,147,935,1950,490,3305,2100,290,615,107,480
REF=DUFF&BAUER     MAX LST SQ ERROR CP @ 1300K 0.44% HF0=158.3 KCAL HF298=163. KCAL
C6H3              T 2/90C   6H   3    0    0G   200.000  6000.000  C  75.08982 1
 0.12196528E+02 0.11454228E-01-0.41312980E-05 0.66884722E-09-0.40122816E-13    2
 0.77275592E+05-0.35794114E+02 0.17798531E+01 0.50337619E-01-0.65263026E-04    3
 0.47594586E-07-0.14300850E-10 0.79748524E+05 0.15767468E+02 0.82027246E+05    4

C6H3(NO2)3    1,3,5-Tri-Nitro-Benzene   SYMNO = 6  STATWT = 1  IA = 111.42859
IB = 172.18627  IC = 252.862147  Ir(NO2)=5.96  ROSYM = 2  V(2) = 3.11 kcal
NU = 3071,3038,2993,1923,1913,1742,1720,1671,1594,1580,1431,1368,1321,1209,1183,
1121,1113,1018,1000,970,952,939,843,778,751,748,688,680,644,591,568,522,504,448,
393,350,335,323,294,256,251,147,129,87.5,66.  REF =BURCAT, TAE Report # 824 1998
HF298=14.9 kcal    REF = Pedley, Naylor & Kirby 1986    Max Lst Sq Error Cp @
1300 K 0.53%
TRI-NITRO BENZEN  T 5/98C  6.H  3.N  3.O  6.G   200.000  6000.000  C 213.10644 1
 2.87195273E+01 2.08056280E-02-8.03680268E-06 1.35348056E-09-8.32405765E-14    2
-3.92148064E+03-1.15710853E+02 2.18818193E+00 1.02515207E-01-1.05642628E-04    3
 5.50716150E-08-1.13737832E-11 3.11892525E+03 1.95711122E+01 7.49792832E+03    4

C6H4  BENZYNE  SIGMA=2  STATWT=3  IA=13.295  IB=14.247 IC=27.542  NU=1326,985,
1010,991.6,705,1648,848,9(2),671,1110,3046.8(2),1595(2),1480(2),605,6(2),970,
3080(2),405(2)  REF=BAUER & DUFF   HF298=115. KCAL  REF=Pollack & Hehre TETRAHE-
DRON LETT. 21, (1980), 2483. Max Lst Sq Error Cp @ 1300 K 0.56%
C6H4 BENZYNE      T 2/92C   6H   4    0    0G   200.000  6000.000  C  76.09776 1
 0.10582770E+02 0.15914908E-01-0.58202018E-05 0.95108725E-09-0.57425956E-13    2
 0.52834650E+05-0.32571269E+02 0.28042240E+00 0.26170563E-01 0.29996638E-04    3
-0.63979566E-07 0.29103081E-10 0.56470786E+05 0.24784179E+02 0.57869917E+05    4

C6H4  trans-1,5-HEXADIYNE-3ENE  CALCULATED BY STEIN et al., NIST PROGRAM 1991,
VERY ROUGH APPROXIMATE EXTRAPOLATED USING WILHOIT'S POLYNOMIALS HF298=125.8 KCAL
Max Lst Sq Error Cp @ 500 K **2.7%**
C6H4 TRANS        T 2/92C   6H   4    0    0G   298.150  5000.000  F  76.09776 1
 0.17183117E+02 0.66487658E-02-0.12416263E-05 0.14697448E-09-0.91398013E-14    2
 0.56485961E+05-0.64435183E+02 0.19323139E+01 0.39032183E-01-0.69227109E-05    3
-0.27093357E-07 0.15730252E-10 0.61100955E+05 0.16516023E+02 0.63304657E+05    4

C6H4 cis-1,5-HEXADIYNE-3-ENE SAME AS TRANS VALUE EXCEPT FOR HF298=123 KCAL
C6H4 CIS          T 2/92C   6H   4    0    0G   298.150  5000.000  F  76.09776 1
 0.17183117E+02 0.66487658E-02-0.12416263E-05 0.14697448E-09-0.91398013E-14    2
 0.55076954E+05-0.64435183E+02 0.19323139E+01 0.39032183E-01-0.69227109E-05    3
-0.27093357E-07 0.15730252E-10 0.59691948E+05 0.16516023E+02 0.61895650E+05    4

C6H4  H2C=C=C=C=C=CH2  CALCULATED USING BOZZELLI & RITTER'S GROUP COEFFICIENTS
EXTRAPOLATED USING WILHOIT'S POLYNOMIALS. ROUGH ESTIMATES. SIGMA=4
HF298=129.37 KJ  Max Lst Sq Error Cp @ 1000 K 0.33%
C6H4 PENTAENE     T 2/92C   6H   4    0    0G   298.150  5000.000  F  76.09776 1
 0.19093610E+02 0.68060566E-02 0.48521238E-07-0.31308214E-09 0.33682379E-13    2
 0.88787214E+04-0.10402568E+03-0.14635965E+02 0.15912786E+00-0.25869999E-03    3
 0.19718118E-06-0.57216996E-10 0.14773467E+05 0.54503676E+02 0.15559546E+05    4

C6H4  H2C=C=C=CH-CCH  CALCULATED USING BOZZELLI & RITTER'S GROUP COEFFICIENTS
EXTRAPOLATED USING WILHOIT'S POLYNOMIALS. ROUGH ESTIMATES. SIGMA=1
HF298=327.9 KJ  Max Lst Sq Error Cp @ 500 K 1.04%
C6H4 TRIENE-5YNE  T 2/92C   6H   4    0    0G   298.150  5000.000  F  76.09776 1
 0.18201992E+02 0.91911818E-02-0.37060737E-05 0.68444196E-09-0.47362400E-13    2
 0.32259868E+05-0.85556205E+02-0.61605879E+01 0.98677706E-01-0.13382206E-03    3
 0.87972085E-07-0.22435998E-10 0.37906997E+05 0.34807282E+02 0.39437080E+05    4
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C6H4O2 1,4 BENZOQUINONE O=C6H4=O  SIGMA=4  IA=10.07447  IB=20.4035   IC=28.5342
NU*=3339,3278,3073,(2348),1874,1754,1681,1535,1517,1357,1299,(1218,1262,1151),
1077,1055,(962),951,881,(828),763,(714,609,475,430,365,291,187,112,28.5)
REF=IR SPECTRUM NIST WEBBOOK 1997, *(in parenthesis) MOPAC6-AM1  HF298=-122.9 kJ
REF=PEDLEY & NYLOR  Max Lst Sq Error Cp @ 1300 K 0.58%
C6H4O2  O=C6H4=O  T10/97C  6.H  4.O  2.00 0.G   200.000  6000.000  B 108.09656 1
 1.43886174E+01 1.81624210E-02-6.69934678E-06 1.10097880E-09-6.67372266E-14    2
-2.12444054E+04-5.02572901E+01 3.79867882E+00 2.51676569E-02 3.79846917E-05    3
-7.06777516E-08 3.06126573E-11-1.72429606E+04 9.80455363E+00-1.478138819-04    4

HEXA-1,3-DIEN-5-YN-YL RADICAL (C6H5 CHAIN) STATWT=1 SIGMA=1 IA=11.77 IB=35.66
IC=47.43 NU=72,111,252,253,424,415,593,616,677,692,710,760,796,1089,1131,1184,
1352,1584,1720,2311,3275,3421,3440,3640,3795 REF=DEWAR, GARDINER, FRENKLACH &
OREF JACS 109 (1987) 4456. HF298=127 KCAL
C6H5 CHAIN        T09/90C   6H   5    0    0G   200.000  6000.000  B  77.10570 1
 0.13411768E+02 0.14720221E-01-0.50817705E-05 0.79886354E-09-0.46950844E-13    2
 0.58503716E+05-0.41652032E+02 0.77929707E+00 0.54372126E-01-0.47873814E-04    3
 0.16187164E-07 0.33735744E-12 0.61650312E+05 0.22128592E+02 0.63908517E+05    4

C6H5 PHENYL RAD.  SIGMA=2  STATWT=2  IA=13.7884 IB=14.8396  IC=28.628  NU=3062,
992,1326,673,3068,1010,995,703,1310,1150,849(2),3063,1486(2),1038,3047(2),
1596(2),1178(2),606(2),975,410(2)  REF=BURCAT,ZELEZNIK & McBRIDE  MAX LST SQ
ERROR CP @ 1300 K .86 % .  HF298=328.5     KJ
PHENYL RAD        L12/84C  6.H  5.   0.   0.G   300.000  5000.000  B  77.10550 1
 0.11431418E 02 0.17019045E-01-0.58387241E-05 0.88094687E-09-0.48050417E-13    2
 0.33942348E 05-0.38574219E 02-0.23405075E 01 0.42760305E-01-0.25518166E-05    3
-0.30668716E-07 0.16245519E-10 0.38376734E 05 0.35617355E 02 0.39502977E 05    4

C6H5  FULVENYL RADICAL ***VERY ROUGH APPROXIMATION*** FULVENE (5-METHYLENE-1,3
PENTADIENE) - HVIN = FULVENYL RADICAL ON METHYLENE. FULVENE TAKEN FROM MELIUS
DATABASE. SIGMA=2  STATWT=2  HF298=206 kcal
C6H5  FULVENYL R  T05/97C  6.H  5.   0.   0.G   298.150  5000.000  F  77.10570 1
 1.22826190E+01 1.69092440E-02-6.13814391E-06 9.98066903E-10-6.00540634E-14    2
 9.80483438E+04-4.25877305E+01-6.20881786E-01 3.94909636E-02 9.00257390E-06    3
-4.93720771E-08 2.54911533E-11 1.02096373E+05 2.67966630E+01 1.03660511E+05    4

C6H5  FULVENYL RADICAL  METHYLENE-CYCLOPENTA-2,4-DIENE-2-YL  -C(=CH2)C*=CHCH=CH-
SIGMA=1  STATWT=2  IA=9.09378  IB=22.7103  IC=31.8041  NU=3059,3057,3043,3028,
2979,1509,1405,1367,1321,1230,1182,1139,997,952,911,870,853,826,746,734,691,654,
590,580,461,330,200.5  HF298=117.2 +/- 12.3 kcal  REF=C.Melius Database BACMP4
#2538 A72B  Max Lst Sq Error Cp @ 200 K 0.79%
C6H5  FULVENYL M  T05/97C  6.H  5.   0.   0.G   200.000  6000.000  B  77.10570 1
 1.29807636E+01 1.62661044E-02-5.90215593E-06 9.59452737E-10-5.77215384E-14    2
 5.31703711E+04-4.45338857E+01-8.96711182E-01 4.31740526E-02 2.41329970E-06    3
-4.48391263E-08 2.43949284E-11 5.73811680E+04 2.94156683E+01 5.89769932E+04    4

C6H5Br BROMOBENZENE  DATA FROM STULL WESTRUM & SINKE EXTRAPOLATED USING WILHOIT
POLYNOMIALS  Max Lst Sq Error H-H298 @ 300 K 0.76% HF298=25.10 KCAL
C6H5BR            T 1/92C   6H   5BR  1    0G   298.150  6000.000  B 157.00970 1
 0.14996437E+02 0.14432860E-01-0.34629621E-05 0.42896352E-09-0.22127110E-13    2
 0.60318879E+04-0.54089098E+02-0.27725929E+01 0.59329702E-01-0.36394766E-04    3
 0.10605809E-08 0.51502469E-11 0.11137385E+05 0.38720437E+02 0.12630738E+05    4

C6H5Cl CHLOROBENZENE DATA FROM  STULL WESTRUM & SINKE EXTRAPOLATED USING WILHOIT
POLYNOMIALS Max Lst Sq Error Cp @ 1200 K 0.37%  HF298=12.39 KCAL.
C6H5CL            T 1/92C   6H   5CL  1    0G   298.150  6000.000  B 112.55840 1
 0.14388354E+02 0.15909241E-01-0.44684021E-05 0.61870168E-09-0.33950580E-13    2
-0.15529718E+03-0.52147823E+02-0.35215940E+01 0.64559671E-01-0.47928160E-04    3
 0.11765905E-07 0.15381225E-11 0.48148068E+04 0.40540413E+02 0.62348545E+04    4
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C6H5F FLUOROBENZENE DATA FROM  STULL WESTRUM & SINKE EXTRAPOLATED USING WILHOIT
POLYNOMIALS Max Lst Sq Error Cp @ 1200 K 0.48%  HF298=-27.86 KCAL
C6H5F             T 1/92C   6H   5F   1    0G   298.150  6000.000  B  96.10410 1
 0.13603270E+02 0.17680782E-01-0.56138646E-05 0.84146369E-09-0.48322310E-13    2
-0.20280095E+05-0.49526306E+02-0.44173359E+01 0.66471817E-01-0.49219304E-04    3
 0.12039107E-07 0.15890440E-11-0.15246744E+05 0.43825425E+02-0.14019616E+05    4

C6H5NO NITROSO-PHENYL or NITROSO-BENZENE  CALCULATED BY BOZZELLI USING GROUP
ESTIMATES. EXTRAPOLATED TO 6000 K USING WILHOIT'S POLYNOMIALS. HF298=48.0 KCAL
REF=Choo, Golden & Benson, Int. J. Chem Kinet 7,(1975),713. Max Lst Sq Error
Cp @ 1500 K 0.36%.
C6H5NO            T 7/95C   6H   5N   1O   1G   298.150  5000.000  F 107.11184 1
 0.15129273E+02 0.20169394E-01-0.79009702E-05 0.14240839E-08-0.96649392E-13    2
 0.17118219E+05-0.56899184E+02 0.20849489E+01 0.34489960E-01 0.27707248E-04    3
-0.65460444E-07 0.29821820E-10 0.21870293E+05 0.15898367E+02 0.24154400E+05    4

C6H5NO2  Nitro-Benzene   SYMNO = 2   STATWT = 1  IA = 20.6002  IB = 63.9627
IC = 84.5628  Ir(NO2)= 5.96  ROSYM = 2  V(2) = 2.8 kcal/mole    = 3084,2935,
2888,2700,1966,1912,1797,1609,1541,1481,1353,1312,1245,1171,1103,1070,1020,
(1019,1004,999,977),928,(860),854,787,692,(674,665,599,510,436,409,388,254.49,
171.09)     REF =NIST 97 Webbook & Melius Database 1988 R5M   HF298=16.38  kcal
REF = Pedley Naylor & Kirby 1986   Max Lst Sq Error Cp @ 1300 K  61%.
NITRO-BENZENE     T11/97C  6.H  5.N  1.O  2.G   200.000  6000.000  B 123.11124 1
 1.71572651E+01 2.10600071E-02-7.92285643E-06 1.31641516E-09-8.03337816E-14    2
 4.22627769E+02-6.59268666E+01 3.22564706E-01 4.78049433E-02 1.44052454E-05    3
-6.09010999E-08 2.98988437E-11 6.00070276E+03 2.56985144E+01 8.24268899E+03    4

C6H5O  PHENOXY RADICAL   SIGMA=2  STATWT=2  IA=14.8396  IB=30.4574  IC=45.297
NU=3087,3063,3027,1603,1501,1261,1168,1025,999,823,526,958,817,409,973,881,751,
686,503,225,3070,3049,1610,1472,1343,1277,1150,1070,619,403  REF=BURCAT,
ZELEZNIK & MCBRIDE HF298=47.698 KJ  MAX LST SQ ERROR CP @ 1300 K 0.81 % .
PHENOXY RAD       L12/84C  6.H  5.O  1.   0.G   300.000  5000.000  B  93.10490 1
 0.13833984E 02 0.17618403E-01-0.60696257E-05 0.91988173E-09-0.50449181E-13    2
-0.69212549E 03-0.50392990E 02-0.18219433E 01 0.48122510E-01-0.46792302E-05    3
-0.34018594E-07 0.18649637E-10 0.42429180E 04 0.33526199E 02 0.57367379E 04    4

C6H5OO  PEROXYPHENYL  SIGMA=1  STATWT=2   IA=16.0594   IB=51.5184   IC=67.5778
NU=3061,3032,3024,3014,3004,1526,1515,1461,1425,1303,1246,1223,1124,1115,1106,
1032,977,936,924,917,860,788,759,712,629,593,587,457,427,382.5,257.4,216.5,59.5
HF298=39.59 KCAL  REF=C. Melius Database AA3V  Max Lst Sq Error Cp @ 200 K 0.65%
C6H5OO            T03/97C  6.H  5.O  2.   0.G   200.000  6000.000  B 109.10450 1
 1.61783950E+01 1.80959380E-02-6.61459065E-06 1.08059157E-09-6.52339007E-14    2
 1.28261324E+04-5.89741433E+01 1.99359550E-01 4.70697558E-02 8.34324919E-06    3
-5.63540961E-08 2.94168315E-11 1.77945712E+04 2.67267648E+01 1.99223478E+04    4

C6H5OH PHENOL  IA=14.854 IB=32.045 IC=46.8942 NU=3087,3063,3027,1603,1501,
1261,1168,1025,999,823,526,958,817,409,973,881,751,686,503,225,3070,3049,
1610,1472,1343,1277,1150,1070,619,403,3656,1176. HF298= -96.4 KJ.
INTERNAL ROTOR SYMNO=2,V=3468 CAL,IB=1.2236E-40
REF=BURCAT,ZELEZNIK & MCBRIDE  MAX LST SQ ERROR CP/R @ 1300K .75%
C6H5OH            L 4/84C   6H   6O   1    0G   300.000  5000.000  B  94.11280 1
 0.14912073E 02 0.18378135E-01-0.61983128E-05 0.91983221E-09-0.49209565E-13    2
-0.18375199E 05-0.55924103E 02-0.16956539E 01 0.52271299E-01-0.72024050E-05    3
-0.35859603E-07 0.20449073E-10-0.13284121E 05 0.32542160E 02-0.11594207E 05    4

BENZENE Liquid, DATA TAKEN FROM TRC 4/83 TABLES. HF298(L)=49.08 KJ.
C6H6(L)           P10/86C  6.H  6.   0.   0.L   278.680   500.000  C  78.11364 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00 6.36690229E+01-6.00534398E-01 2.66792810E-03    3
-5.06308828E-06 3.63955562E-09-1.67085472E+03-2.43891797E+02 5.90293355E+03    4
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Table 4 (continued)

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C6H6  BENZENE  IA=IB=14.8396  IC=29.6792  SIGMA=12  NU=3062,992,1326,673,3068,
1010,995,703,1310,1150,849(2),3063(2),1486(2),1038(2),3047(2),1596(2),1178(2),
606(2),975(2),410(2)  REF=SHIMANOUCHI  MAX LST SQ ERROR CP @ 1300 K 0.87 % .
HF298=82.8 KJ REF=BURCAT, ZELEZNIK & MCBRIDE
BENZENE            L12/84C  6.H  6.   0.   0.G   300.000  5000.000  B  78.11364 1
 0.11815166E 02 0.19169778E-01-0.65425238E-05 0.98228425E-09-0.53280361E-13    2
 0.40707441E 04-0.43973511E 02-0.32181215E 01 0.47168836E-01-0.21254918E-05    3
-0.34879005E-07 0.18425386E-10 0.89017773E 04 0.36999313E 02 0.99586128E 04    4

C6H6  FULVENE (5-METHYLENE-1,3-CYCLOPENTADIENE)  SIGMA=2  IA=10.1825  IB=21.7319
IC=31.9144  NU=3059,3053,3051,3036,3028,2980,1677,1604,1524,1423,1341,1318,1227,
1081,1078,976,956,946,943,932,863,785,782,770,692,644,606,483,328,199.8
HF298=56.60+/-2.3 KCAL    REF=C.MELIUS DATABASE A70D     Max Lst Sq Error Cp @
200 K 0.95%
C6H6  FULVENE     T03/97C  6.H  6.   0.   0.G   200.000  6000.000  B  78.11364 1
 1.19233607E+01 1.98993861E-02-7.21223888E-06 1.17141499E-09-7.04278845E-14    2
 2.27199368E+04-4.13488172E+01 1.25853571E-01 3.04056534E-02 4.01806332E-05    3
-8.27651456E-08 3.77645005E-11 2.68838408E+04 2.44628931E+01 2.84820633E+04    4

C6H6  1,5-Hexadiyne HCC-CH2CH2-CCH SIGMA=2  IA=3.27754  IB=54.48395  IC=59.74488
NU=76.7,122.6,217,338,376,477,493,710,711,724(2),744,886,931,991,1024,1178,1265,
1282,1366,1450,1458,2156,2157,2157,28832888,2911,2931,3271(2) REF=Melius data
P4A 1988  HF298=99.5+/-4. kcal  REF=NIST 94 Max Lst Sq Error Cp @ 6000 K 0.52%
C6H6   1,5-HEXAD  T12/98C  6.H  6.   0.   0.G   200.000  6000.000  B  78.11364 1
 1.24654128E+01 1.91657440E-02-6.88639447E-06 1.11180288E-09-6.65584946E-14    2
 4.45651230E+04-3.92079382E+01 1.56731808E+00 4.46028542E-02-1.83706506E-05    3
-1.12229558E-08 9.21344087E-12 4.78004378E+04 1.81700373E+01 5.00700582E+04    4

C6H6 2,4 Hexadiyne  CH3-CC-CC-CH3   ESTIMATED USING NIST 94 PROGRAM  SIGMA=18
EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS   HF298=85.9+/-4. kcal
Max Lst Sq Error Cp @ 1500 K 0.23%
C6H6 2,4hexadiyne T12/98C  6.H  6.   0.   0.G   298.150  5000.000  E  78.11364 1
 9.00639501E+00 2.22122051E-02-7.16675669E-06 1.11658702E-09-6.84942130E-14    2
 3.92629088E+04-1.84960261E+01 1.78501070E+00 4.81158811E-02-4.45096787E-05    3
 2.82969725E-08-8.62801909E-12 4.08969044E+04 1.72350672E+01 4.32263116E+04    4

C6H6 1,3-Hexadiyne HCC-CC-CH2CH3   ESTIMATED USING NIST 94 PROGRAM  SIGMA=3
EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS       HF298=90.8+/-5. kcal
Max Lst Sq Error Cp @ 1500 K 0.20%
C6H6 1,3hexadiyne T12/98C  6.H  6.   0.   0.G   298.150  5000.000  E  78.11364 1
 1.15140870E+01 1.92404870E-02-6.35521964E-06 1.01470107E-09-6.34795794E-14    2
 4.07973482E+04-3.17000252E+01-9.46977116E-02 6.33977517E-02-7.75729460E-05    3
 5.81959002E-08-1.86143170E-11 4.34816104E+04 2.55195266E+01 4.56920733E+04    4

C6H6 1,2,3,4-Hexatetraene  H2C=C=CH-CH=C=CH2  SIGMA=2  IA=2.5902727  IB=60.8685
NU=73.7,119.7,230,322,347,479,518,535,661,896,904(2),909,1002,1003,1007,1072,
1126,1240,1370,1434,1476,1974,1979,2963(2),2989,2995,3032(2)  REF=Melius A72A
HF298=94.5+/-3.5 kcal  Max Lst Sq Error Cp @ 6000 K 0.53%
C6H6   1,2,4,5 H  T12/98C  6.H  6.   0.   0.G   200.000  6000.000  E  78.11364 1
 1.26085766E+01 1.91760299E-02-6.92227571E-06 1.12107587E-09-6.72586498E-14    2
 4.19283199E+04-4.01812986E+01 2.52451569E+00 3.59776153E-02 4.93787277E-06    3
-3.58185196E-08 1.82946638E-11 4.52207196E+04 1.44679843E+01 4.75539749E+04    4

C6H6 1,2-Hexadiene-5-yne  H2C=C=C-CH2CH2CCH  SIGMA=1  IA=5.7718   IB=54.03
IC=55.8843  NU=55.9,164,214,332,354,455,533,585,709,724,853,900,904,920,1005(2),
1104,1194,1286,1358,1444,1455,1990,2156,2868,2919,2969,3039,3272  REF= Melius
P13S 1988. HF298=98.6+/-5.6 kcal  Max Lst Sq Error Cp @ 6000 K 0.52%
C6H6   1,2-Hexad  T12/98C  6.H  6.   0.   0.G   200.000  6000.000  B  78.11364 1
 1.25675553E+01 1.91426138E-02-6.89392180E-06 1.11473036E-09-6.68050965E-14    2
 4.40428652E+04-3.88525255E+01 1.93913583E+00 4.09525988E-02-7.95640732E-06    3
-2.25455163E-08 1.34743616E-11 4.73272824E+04 1.77887106E+01 4.96171632E+04    4
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C6H7 1,4-CYCLO-RADICAL STATWT=2 SIGMA=2   IA=15.707  IB=16.0895  IC=31.2965
NU=3017,3002,2998,2984,2983,2799.5,2796,1469.5,1456,1435,1405,1379,1332,1258,
1160,1117,1112,1058.5,953,916,909,898,881.5,876,806,710,657,589.5,552,528,473,
335.5,159  HF298=47.942+/-8.31 KCAL   REF= C. Melius BAC/MP4 Database   Max Lst
Sq Error Cp @ 200 K 0.9%.
C6H7 1,4 CYCLO    T 6/93C   6H   7    0    0G   200.000  6000.000  B  79.12158 1
 0.12801758E+02 0.21924749E-01-0.79713001E-05 0.12972935E-08-0.78100416E-13    2
 0.17889539E+05-0.45804341E+02-0.10303140E+00 0.34393354E-01 0.39788466E-04    3
-0.85116612E-07 0.39012224E-10 0.22425515E+05 0.26022350E+02 0.24125213E+05    4

C6H7 CHAIN RADICAL CALCULATED USING RITTER & BOZZELLI'S ADDITIVITY PROGRAM WITH
EXTRAPOLATION FROM 1,3,5 HEXATRIENE AS PARENT MOLECULE  HF298 =389.15 KJ
C6H7 CHAIN        T12/91C   6H   7    0    0G   298.150  5000.000  F  79.12158 1
 0.15205269E+02 0.18199687E-01-0.66854326E-05 0.11332271E-08-0.72557760E-13    2
 0.40205851E+05-0.52131317E+02-0.94505332E+00 0.61726701E-01-0.45130311E-04    3
-0.10687764E-07 0.14281131E-11 0.44718857E+05 0.31566567E+02 0.46803720E+05    4

C6H5NH2 liquid  ANILINE DATA TAKEN FROM TRC 6/90 HF298=7.529 kcal
C6H5NH2(L) anilin P 6/90C  6.H  7.N  1.   0.L   298.150   552.000  B  93.12832 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00-2.51374023E+02 2.85261227E+00-1.11414497E-02    3
 1.93994205E-05-1.26299216E-08 1.80035120E+04 9.53411670E+02 3.78871828E+03    4

C6H5NH2  ANILINE SIGMA=2 REF=STULL, WESTRUM & SINKE EXTRAPOLATED TO 5000 K USING
BOZZELLI & RITTER'S PROGRAM    HF298=87.03 KJ
C6H7N ANILINE     T 2/92C   6H   7N   1    0G   298.150  5000.000  B  93.12832 1
 0.13217261E+02 0.24501606E-01-0.93690211E-05 0.16310315E-08-0.10639893E-12    2
 0.40229641E+04-0.47212282E+02-0.23879495E+01 0.62140204E-01-0.35907649E-04    3
 0.22025563E-08 0.38067823E-11 0.87295677E+04 0.35046606E+02 0.10468446E+05    4

C6H8 3-METHYL CYCLOPENTADIENE (CH3-C5H5) ESTIMATED USING NIST 94 PROGRAM FROM
2x[CD-(C)(H)]; [CD-(C)(CD)]; [CD-(CD)(H)]; [C-(CD)2(H)2]; [C-(H)3]    ROSYM=3
RING CORRECTION HF=25.1 KJ S=117.2 J  HF298=102.0 KJ  Max Lst Sq Error H-H298 @
500 K 0.68%
C6H8 CY CH3-C5H5  T10/94C   6H   8    0    0G   298.150  5000.000  E  80.12952 1
 0.16399698E+02 0.18988824E-01-0.60996114E-05 0.95861755E-09-0.59364731E-13    2
 0.48834021E+04-0.65341031E+02-0.35829269E+01 0.78077845E-01-0.73143499E-04    3
 0.33645368E-07-0.48086229E-11 0.10447644E+05 0.37418709E+02 0.12267710E+05    4

1,3,5-C6H8  1,3,5 HEXATRIENE EQUILIBRIUM MIXTURE OF THREE ISOMERS TTT, TTC and
CTC REF=PRIVATE COMMUNICATION FROM J.D. VAUGHAN. CFF/PI CALCULATIONS WERE USED
FOR VIBRATIONS AND MMP2 CALCULATIONS WERE USED FOR HF298. HF298=152.58 KJ
VAL FOR TTT NU=3098.3,3091.4,3082.2,3078.8,3063.2(2),2988(2),1664.2,1645.5,
1594.85,1445.4,1419.4,1350,1310,1306,1289,1206.4,1172.9,1082.25,1051,990.43,
952.4,949.25,946.5,858.82,643.67,611.92,589.23,461,393.4,242,214.4,179.7,101.53,
941 IAIBIC=13505.E-117 SIGMA=2 VAL FOR TTC T0=1232.18  NU=3096.3,3084.6,3083.8,
3078.8,3063.2,3062.6,2988(2),1668.6,1640.2,1607.7,1448.22,1437,1341.8,1321.45,
1299.5,1288.5,1200,1089.37,1070,1041.3,1001.34,982.44,953.2,950,940.4,864,649.2,
647,601.84,492.1,383.1,279.23,187.85,171.2,136 IAIBIC=19687.E-117 SIGMA=1
VAL FOR CTC T0=1376.0  NU=3089.7,3084.2,3083.5,3078.82,3062(2),2988.3(2),1669.7,
1645.28,1614.83,1452,1444.36,1345.43,1337.46,1290,1284.7,1142,1042.65,1041,
1018.4,1017.9,955.3,954,950,868.2,658.3,650.2,593.2(2),324.3,257.5,243.73,
221.73,93.59  IAIBIC=17093.E-117 SIGMA=2  Max Lst Sq Error Cp @ 6000 K 0.57%.
C6H8              L 8/89C   6H   8    0    0G   200.000  6000.000  B  80.12952 1
 0.13184588E+02 0.24023820E-01-0.86729021E-05 0.14049681E-08-0.84315805E-13    2
 0.11858656E+05-0.45629943E+02 0.38587790E+01 0.15885821E-01 0.81120967E-04    3
-0.12184205E-06 0.50832636E-10 0.15950538E+05 0.10384627E+02 0.18307022E+05    4
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1,3-CYCLOHEXADIENE C6H8  SIGMA=2  OPT. ISOM=2 STATWT=1  IAIBIC=8.517E-114
NU=3050(4),2939,2838(2),1577,1444,1330,1243,1223,1178(2),1150,1059,994,945,850,
753,559,506,201,2884,1602,1435,1377,1165,1100,1040,1016,927,745,658,468,298
REF=DOROFEEVA GURVICH & JORISH JPCRD 15 (1986) 437  HF298=106.3 KJ  Max Lst Sq
Error Cp @ 6000 K .62%
H8C6 (1,3-CYCLO)  T 2/90H   8C   6    0    0G   200.000  6000.000  B  80.12952 1
 0.11779870E+02 0.25519980E-01-0.92666947E-05 0.15068122E-08-0.90658701E-13    2
 0.65486686E+04-0.41618805E+02 0.17265319E+01 0.14887612E-01 0.94809230E-04    3
-0.14083394E-06 0.58859873E-10 0.11021297E+05 0.19130886E+02 0.12784878E+05    4

1,4-CYCLOHEXADIENE C6H8  SIGMA=4  STATWT=1  IAIBIC=9.26E-114 NU=3032,2822,1680,
1426,1197,854,530,1250,970,370,1240,706,3032,1377,1280,1035,574,2875,1010,985,
403,3042,2840,1439,1405,962,888,2889,962,625,108,3042,1642,1362,1159,887
REF=DOROFEEVA GURVICH & JORISH JPCRD 15 (1986) 437   HF298=109.0 KJ Max Lst Sq
Error Cp @ 6000 K 0.62%.
C6H8 (1,4-CYCLO)  T 2/90C   6H   8    0    0G   200.000  6000.000  B  80.12952 1
 0.11453943E+02 0.25861139E-01-0.94007909E-05 0.15296731E-08-0.92076611E-13    2
 0.69849680E+04-0.40634874E+02 0.19018200E+01 0.14819394E-01 0.91312194E-04    3
-0.13458949E-06 0.55907972E-10 0.11316750E+05 0.17407151E+02 0.13109612E+05    4

C6H9  1,3-HEXADIENE-YL-5 CH2=CHCH=CHCH*CH3 CALCULATED BY Weissman & Benson 1989
EXTRAPOLATED TO 3000 K FOR BETTER FIT.   HF298=44. KCAL   Max Lst Sq Error  Cp @
1200 K 0.56%
C6H9              T 2/92C   6H   9    0    0G   298.150  3000.000  F  81.13746 1
 0.23165919E+02 0.10813608E-01-0.17638168E-05 0.00000000E+00 0.00000000E+00    2
 0.11162402E+05-0.98600332E+02 0.31671271E+00 0.52069818E-01-0.21965057E-04    3
 0.00000000E+00 0.00000000E+00 0.19926824E+05 0.27879902E+02 0.22141533E+05    4

C6H9 1,3-HEXADIENE-YL-6 CH2=CHCH=CHCH2CH2* CALCULATED BY Weissman & Benson 1989
EXTRAPOLATED TO 3000 K FOR BETTER FIT.   HF298=60. KCAL   Max Lst Sq Error  Cp @
1200 K 0.90%
1,3-C6H9          T 2/92C   6H   9    0    0G   298.150  3000.000  F  81.13746 1
 0.21786938E+02 0.11894129E-01-0.21209124E-05 0.00000000E+00 0.00000000E+00    2
 0.20013752E+05-0.89218982E+02 0.20594889E+01 0.46753513E-01-0.18644505E-04    3
 0.00000000E+00 0.00000000E+00 0.27665639E+05 0.20293525E+02 0.30193000E+05    4

C6H9  CYCLOHEXENYL-3    CALCULATED BY Weissman & Benson 1989  EXTRAPOLATED TO
3000 K FOR BETTER FIT.   HF298=30. KCAL   Max Lst Sq Error  Cp @ 1200 K 0.65%
C6H9 CY           T 2/92C   6H   9    0    0G   298.150  3000.000  F  81.13746 1
 0.26295828E+02 0.86828857E-02-0.15770376E-05 0.00000000E+00 0.00000000E+00    2
 0.20863563E+04-0.12573825E+03-0.35714300E+01 0.61696043E-01-0.26928803E-04    3
 0.00000000E+00 0.00000000E+00 0.13657039E+05 0.39986250E+02 0.15096500E+05    4

C6H10  1,3-HEXADIENE    CALCULATED BY Weissman & Benson 1989  EXTRAPOLATED TO
3000 K FOR BETTER FIT.   HF298=13.4 KCAL   Max Lst Sq Error  Cp @ 1200 K 0.65%
C6H10             T 2/92C   6H  10    0    0G   298.150  3000.000  F  82.14540 1
 0.23903966E+02 0.12046216E-01-0.19588306E-05 0.00000000E+00 0.00000000E+00    2
-0.43733937E+04-0.10376594E+03-0.96299362E+00 0.60880377E-01-0.28062414E-04    3
 0.00000000E+00 0.00000000E+00 0.45722054E+04 0.32010145E+02 0.67431033E+04    4

C6H10  CYCLOHEXENE  SIGMA=2 OPT.ISO=2 STATWT=1. IAIBIC=10.71E-114  NU=3040,2940,
2916,2865,2839,1660,1460,1445,1353,1343(2),1240,1222,1140(2),1095,1068,966,905,
812,657,520,392,276,3078,2960,2890,2878,2858,1455,1450,1325,1269,1215,1039,1009,
919,877,719,638,450,165  REF DOROFEEVA GURVICH & JORISH JPCRD 15 (1986) 437.
HF298=-4.6 KJ. Max Lst Sq Error Cp @ 1300 K 0.65%.
C6H10 CY          T 2/90C   6H  10    0    0G   200.000  6000.000  B  82.14540 1
 0.11773904E+02 0.30947360E-01-0.11234330E-04 0.18262494E-08-0.10985119E-12    2
-0.72028376E+04-0.42658688E+02 0.23662378E+01 0.10681712E-01 0.11822112E-03    3
-0.16567854E-06 0.67612802E-10-0.24824973E+04 0.16769357E+02-0.55324968E+03    4
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Table 4 (continued)

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C6H11 RAD trans-HEXENE-3-YL-6 CH3CH2CH=CHCH2CH2* CALCULATED BY Weissman & Benson
1989 EXTRAPOLATED USING WILHOIT'S POLYNOMIALS TO  3000 K FOR BETER FIT.
HF298=34. KCAL    Max Lst Sq Error Cp @ 1200 K 0.6%.
C6H11             T 2/92C   6H  11    0    0G   298.150  3000.000  F  83.15334 1
 0.24938654E+02 0.13258801E-01-0.23302223E-05 0.00000000E+00 0.00000000E+00    2
 0.51145941E+04-0.10690338E+03 0.63802451E+00 0.56209452E-01-0.23047424E-04    3
 0.00000000E+00 0.00000000E+00 0.14624427E+05 0.28133981E+02 0.17109367E+05    4

C6H11  2-METHYLENE-1-PENTEN RADICAL CH2=C(CH2*)C3H7 ESTIMATED TO 1500 K USING
NIST 1994 S&P PROGRAM. EXTRAPOLATED USING WILHOIT'S POLYNOMIALS  HF298=22.3 KCAL
Max Lst Sq Error Cp @ 1500 K 0.32%
C6H11 2M-YL-1ENE  T11/95C   6H  11    0    0G   298.150  5000.000  E  83.15334 1
 0.14315344E+02 0.29968915E-01-0.11190656E-04 0.19538739E-08-0.12975949E-12    2
 0.41879492E+04-0.48649328E+02-0.44578388E+01 0.92957733E-01-0.10459481E-03    3
 0.73429687E-07-0.22511131E-10 0.92087623E+04 0.46514553E+02 0.11221732E+05    4

C6H11  2-METHYL-1-PENTENE-5-YL RADICAL  CH2=C(CH3)C3H6*   ESTIMATED TO 1500 K
USING NIST 1994  S&P PROGRAM. EXTRAPOLATED USING WILHOIT'S POLYNOMIALS
HF298=35.8 KCAL   Max Lst Sq Error Cp @ 500 K 0.38%.
C6H11 2M-1ENE-5YL T11/95C   6H  11    0    0G   298.150  5000.000  E  83.15334 1
 0.14332084E+02 0.29125927E-01-0.10865216E-04 0.19028973E-08-0.12681084E-12    2
 0.11021737E+05-0.46268468E+02 0.28792433E+01 0.40613348E-01 0.24127870E-04    3
-0.61187151E-07 0.27837372E-10 0.15246181E+05 0.17899962E+02 0.18015157E+05    4

C6H11  2-METHYLENE-2-PENTENE RADICAL CH3C(CH2*)=CHC2H5   ESTIMATED TO 1500 K
USING NIST 1994  S&P PROGRAM. EXTRAPOLATED USING WILHOIT'S POLYNOMIALS
HF298=19.4 KCAL    Max Lst Sq Error Cp @ 1500 K 0.35%
C6H11 2M-YL-2ENE  T11/95C   6H  11    0    0G   298.150  5000.000  E  83.15334 1
 0.13721440E+02 0.30578553E-01-0.11448304E-04 0.20028180E-08-0.13320947E-12    2
 0.29302598E+04-0.45729821E+02-0.31609215E+01 0.83898047E-01-0.86350086E-04    3
 0.58303212E-07-0.18068206E-10 0.76320369E+04 0.40737753E+02 0.97624033E+04    4

C6H11  2-METHYL-2-PENTENE-5-YL RADICAL  CH3C(CH3)=CHC2H4*  ESTIMATED TO 1500 K
USING NIST 1994  S&P PROGRAM. EXTRAPOLATED USING WILHOIT'S POLYNOMIALS
HF298=33.9 KCAL   Max Lst Sq Error Cp @ 1500 K 0.36%.
C6H11 2M-2ENE-5YL T11/95C   6H  11    0    0G   298.150  5000.000  E  83.15334 1
 0.12977914E+02 0.30699396E-01-0.11544244E-04 0.20325566E-08-0.13596284E-12    2
 0.10444175E+05-0.39319934E+02 0.50011464E+01 0.18999758E-01 0.79270344E-04    3
-0.11764308E-06 0.48290683E-10 0.14232811E+05 0.98591862E+01 0.17059045E+05    4

C6H11  2-METHYL-2-PENTENE-4-YL RADICAL  (CH3)2C=CHCH*CH3  ESTIMATED TO 1500 K
USING NIST 1994  S&P PROGRAM. EXTRAPOLATED USING WILHOIT'S POLYNOMIALS
SIGMA(Total)=27  HF298=13.9 kcal  Max Lst Sq Error Cp @ 1500 K 0.35%.
C6H11  2M2en4yl   T12/98C  6.H 11.   0.   0.G   298.150  5000.000     83.15334 1
 1.31147352E+01 3.15727540E-02-1.20452883E-05 2.12128274E-09-1.41296360E-13    2
 3.66861307E+02-4.29851318E+01-8.37042333E-02 6.41074536E-02-4.11721524E-05    3
 1.33327906E-08-1.66357198E-12 4.50848380E+03 2.68585899E+01 6.99471165E+03    4

C6H11  2-METHYL-4-PENTENE-3-YL RADICAL  (CH3)2CHCH*CH=CH2  ESTIMATED TO 1500 K
USING NIST 1994  S&P PROGRAM. EXTRAPOLATED USING WILHOIT'S POLYNOMIALS
SIGMA(Total)=9  HF298=18.1 kcal   Max Lst Sq Error Cp @ 1500 0.33%.
C6H11  2M4en3yl   T12/98C  6.H 11.   0.   0.G   298.150  5000.000     83.15334 1
 1.48689689E+01 2.85667539E-02-1.02064984E-05 1.75009081E-09-1.15540896E-13    2
 1.82637290E+03-5.27562387E+01-1.35049158E+00 6.71744272E-02-3.84842989E-05    3
 4.82680598E-09 2.60613922E-12 6.85441542E+03 3.31090604E+01 9.10822165E+03    4
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C6H11  2-METHYL-1-PENTENE-4-YL RADICAL  CH2=C(CH3)CH2CH*CH3  ESTIMATED TO 1500 K
USING NIST 1994  S&P PROGRAM. EXTRAPOLATED USING WILHOIT'S POLYNOMIALS
SIGMA(Total)=9  HF298=32.4 kcal  Max Lst Sq Error Cp @ 300 K **1.7%**
C6H11  2MP1en4yl  T12/98C  6.H 11.   0.   0.G   298.150  2500.000     83.15334 1
 9.64023038E+00 3.59601406E-02-1.33422271E-05 1.91243246E-09-1.01669007E-13    2
 1.12169942E+04-2.58902779E+01-1.77987013E+00 7.10092253E-02-5.11399935E-05    3
 1.75415470E-08-1.56223214E-12 1.40966419E+04 3.20022161E+01 1.63042200E+04    4

C6H11  Cyclohexyl Radical  ESTIMATED USING NIST 94 PROGRAM  SIGMA=2
EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS   HF298=16.3+/-1.7 kcal
Max Lst Sq Error Cp @ 1500 K 0.49%
C6H11  Cyclohexy  T12/98C  6.H 11.   0.   0.G   298.150  5000.000     83.15334 1
 1.28647309E+01 3.52600147E-02-1.39450525E-05 2.51808759E-09-1.70899213E-13    2
 6.15531214E+02-4.88786148E+01-3.76580647E+00 5.88838077E-02 1.22955158E-07    3
-3.30729397E-08 1.42142299E-11 6.76556720E+03 4.36106643E+01 8.20243165E+03    4

C6H12 trans-HEXENE-3 C2H5CH=CHC2H5 CALCULATED BY Weissman & Benson 1989. EXTRA-
POLATED USING WILHOIT'S POLYNOMIAL'S to 3000 K FOR BETER FIT HF298=-12.7 KCAL

Max Lst Sq Error Cp @ 1200 K 0.67%.
C6H12 TRANS-3     T 2/92C   6H  12    0    0G   298.150  3000.000  F  84.16128 1
 0.25377037E+02 0.14838536E-01-0.25998453E-05 0.00000000E+00 0.00000000E+00    2
-0.18845402E+05-0.11235220E+03 0.14726310E+00 0.58607068E-01-0.23303923E-04    3
 0.00000000E+00 0.00000000E+00-0.88337705E+04 0.28264148E+02-0.63908517E+04    4

C6H12  1-HEXENE  API PROJ. 44 DATA EXTRAPOLATED USING WILHOIT'S POLYNOMIALS.
MAX LST SQ ERROR CP @ 1300 K 0.97 % . HF298=-9.96 KCAL
C6H12             T 5/83C   6H  12    0    0G   300.     4000.     C  84.16128 1
 0.18663635E+02 0.20971451E-01-0.31082809E-05-0.68651618E-09 0.16023608E-12    2
-0.13590895E+05-0.70915860E+02 0.19686203E+01 0.47656231E-01 0.66015373E-05    3
-0.37148173E-07 0.16922463E-10-0.77118789E+04 0.20859230E+02-0.50138854E+04    4

C6H12 2-METHYL-1-PENTEN  EXTRAPOLATED FROM STULL WESTRUM & SINKE 1987 CORRECTION
USING WILHOIT'S POLYNOMIALS  HF298=-14.19 KCAL Max Lst Sq Error H @ 300 K 7.2%.
C6H12 2MP-1en     T11/95C   6H  12    0    0G   298.150  5000.000  B  84.16128 1
 0.12620641E+02 0.34649597E-01-0.13383899E-04 0.24131627E-08-0.16477558E-12    2
-0.13612080E+05-0.38598787E+02 0.10315879E+01 0.57920573E-01-0.20275943E-04    3
-0.90784811E-08 0.65369897E-11-0.98286087E+04 0.23785709E+02-0.71406445E+04    4

C6H12 2-METHYL-2-PENTEN  EXTRAPOLATED FROM STULL WESTRUM & SINKE 1987 CORRECTION
USING WILHOIT'S POLYNOMIALS  HF298=-15.98 KCAL Max Lst Sq Error H @ 300 K 7.2%.
C6H12 2MP-2en     T11/95C   6H  12    0    0G   298.150  5000.000  B  84.16128 1
 0.12088676E+02 0.34068725E-01-0.12394277E-04 0.21676186E-08-0.14583479E-12    2
-0.14418698E+05-0.36076756E+02-0.47423428E+00 0.58156280E-01-0.13393809E-04    3
-0.20423535E-07 0.11920207E-10-0.10331807E+05 0.31630843E+02-0.80414023E+04    4

C6H12 4-METHYL-2-PENTEN cis  EXTRAPOLATED FROM STULL WESTRUM & SINKE 1987
CORRECTION USING WILHOIT'S POLYNOMIALS  HF298=-13.73 KCAL Max Lst Sq Error H
@ 300 K 8.6%.
C6H12 4MP-2en     T 5/96C   6H  12    0    0G   298.150  5000.000  B  84.16128 1
 0.13429190E+02 0.33252141E-01-0.12845171E-04 0.23193196E-08-0.15851939E-12    2
-0.13800258E+05-0.44366460E+02 0.39826011E+01 0.33553100E-01 0.43946883E-04    3
-0.79076359E-07 0.33590735E-10-0.98357639E+04 0.10885860E+02-0.69091648E+04    4

C6H12 4-METHYL-2-PENTEN TRANS  EXTRAPOLATED FROM STULL WESTRUM & SINKE 1987
CORRECTION USING WILHOIT'S POLYNOMIALS  HF298=-14.69 KCAL Max Lst Sq Error H
@ 300 K 4.3%.
C6H12  4MP-2en    T11/95C   6H  12    0    0G   298.150  5000.000  B  84.16128 1
 0.12531029E+02 0.34618444E-01-0.13221262E-04 0.23625501E-08-0.16027053E-12    2
-0.13640433E+05-0.39312583E+02 0.13269297E+01 0.63390645E-01-0.39908762E-04    3
 0.12904041E-07-0.15823617E-11-0.10277554E+05 0.19495838E+02-0.73922528E+04    4
```

SIGMA: 12

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C6H12  CYCLOHEXANE  REF=DOROFEEVA GURVICH & JORISH JPCRD 15 (1986) 437   DATA
EXTRAPOLATED THROUGH WILHOIT'S POLYNOMIALS FROM 1600 K. HF298=-123.3 KJ Max Lst
Sq Error Cp @ 1200 K 0.49%.
C6H12 CY          T 2/90C   6H  12    0    0G   200.000  5000.000  B  84.16128 1
 0.10209166E+02 0.41894173E-01-0.17234045E-04 0.32239024E-08-0.22540929E-12    2
-0.21742125E+05-0.38990666E+02 0.40402264E+01-0.61827997E-02 0.17662080E-03    3
-0.22300383E-06 0.86393385E-10-0.16919808E+05 0.85269500E+01-0.14829497E+05    4

N-C6H13  N-HEXYL RADICAL  API-TRC 8/83 DATA TO 3000K EXTRAPOLATED USING
WILHOIT'S POLYNOMIALS TO 5000K. MAX LST SQ ERROR Cp @ 2500 K  0.55 % .
HF298=25.1 KJ
N-C6H13         N-P10/83C   6H  13    0    0G   300.000  5000.000  B  85.16922 1
 0.12759770E 02 0.37134279E-01-0.14256110E-04 0.25052556E-08-0.16459707E-12    2
-0.35693750E 04-0.36999527E 02 0.23062353E 01 0.50200045E-01 0.79387773E-05    3
-0.41260655E-07 0.18794369E-10 0.10269711E 03 0.20896637E 02 0.30188548E 04    4

2-C6H13  2-HEXYL RADICAL ESTIMATED AND ADJUSTED TO N-C6H13 USING NIST 1994 DATA-
BASE FROM 2[C-(H)(H)(H)], 2[C-(C)(C)(H)(H)], 1[C-(C)(C.)(H)(H)], 1[C.-(C)(C)(H)]
ROSYM=9  EXTRAPOLATED USING WILHOIT'S POLYNOMIALS  HF298(ADJUSTED)=5.5 KCAL
S298=98.0 CAL  Max Lst Sq Error Cp @ 1500 K 0.4%.
2C6H13            T12/95C   6H  13    0    0G   298.150  5000.000  F  85.16922 1
 0.13906352E+02 0.34743942E-01-0.12957418E-04 0.22668953E-08-0.15091510E-12    2
-0.44336607E+04-0.43314973E+02 0.54932798E+01 0.24067996E-01 0.74883656E-04    3
-0.11353464E-06 0.46782080E-10-0.39918931E+03 0.84231411E+01 0.27676917E+04    4

C6H13  2-METHYL-PENTANE-1YL RADICAL *CH2CH(CH3)C3H7   ESTIMATED FROM BENSON'S
GROUP VALUES USING NIST 1994 S&P PROGRAM. EXTRAPOLATED TO 5000 K USING WILHOIT'S
POLYNOMIALS   HF298=7.0 KCAL    Max Lst Sq Error Cp @ 1500 K 0.42%
C6H13  2MP-1YL    T11/95C   6H  13    0    0G   298.150  5000.000  E  85.16922 1
 0.14754628E+02 0.33919022E-01-0.12689277E-04 0.22271946E-08-0.14866840E-12    2
-0.39802078E+04-0.49287611E+02 0.47593240E+01 0.25922476E-01 0.79813586E-04    3
-0.12504262E-06 0.52491365E-10 0.46852943E+03 0.10765884E+02 0.35225167E+04    4

C6H13  2-METHYL-PENTANE-5YL RADICAL CH3CH(CH3)C2H4CH2*   ESTIMATED FROM BENSON'S
GROUP VALUES USING NIST 1994 S&P PROGRAM. EXTRAPOLATED TO 5000 K USING WILHOIT'S
POLYNOMIALS   HF298=7.8 KCAL    Max Lst Sq Error Cp @ 1500 K 0.42%
C6H13  2MP-5YL    T11/95C   6H  13    0    0G   298.150  5000.000  E  85.16922 1
 0.14754628E+02 0.33919022E-01-0.12689277E-04 0.22271946E-08-0.14866840E-12    2
-0.35776345E+04-0.49992114E+02 0.47593240E+01 0.25922476E-01 0.79813586E-04    3
-0.12504262E-06 0.52491365E-10 0.87110276E+03 0.10061380E+02 0.39250900E+04    4

C6H13  2-METHYL, 4-PENTYL (SECONDARY)  RADICAL SIGMA=27 ESTIMATED BY NIST 94
EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS  HF298=3.5 KCAL  Max Lst Sq
Error Cp @ 1500 K 0.65%
C6H13-S           T 2/96C   6H  13    0    0G   298.150  5000.000  E  85.16922 1
 0.14511108D+02 0.33358885D-01-0.11999136D-04 0.20518802D-08-0.13465057D-12    2
-0.55776023D+04-0.47880048D+02 0.36434591D+01 0.34219233D-01 0.54975178D-04    3
-0.96175903D-07 0.41130761D-10-0.11610352D+04 0.15269750D+02 0.17612583D+04    4

C6H13  2-METHYL, 2-PENTYL (TERTIARY)  RADICAL SIGMA=27 ESTIMATED BY NIST 94
EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS  HF298=2.2 KCAL  Max Lst Sq
Error Cp @ 1500 K 0.67%
C6H13 2ME 2PENTYL T 1/96C   6H  13    0    0G   298.150  5000.000  E  85.16922 1
 0.14787344E+02 0.33564827E-01-0.12439889E-04 0.21695366E-08-0.14420253E-12    2
-0.63729344E+04-0.49282628E+02 0.17444927E+01 0.53357363E-01-0.14532582E-05    3
-0.30094741E-07 0.14338677E-10-0.17190682E+04 0.22662382E+02 0.11070767E+04    4
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Table 4 (continued)

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C6H14 liquid n-HEXANE DATA TAKEN FROM TRC 4/85  HF298=-47.481 kcal
C6H14(L) n-Hexan  P 4/85C  6.H 14.   0.   0.L   200.000   360.000  C  86.17716 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00-2.48595294E+00 2.71217579E-01-1.10760648E-03    3
 1.64476492E-06 0.00000000E+00-2.86708461E+04 3.61031929E+00-2.38932305E+04    4

C6H14  N-HEXANE   SIGMA=18   TRC 1985 DATA EXTRAPOLATED THROUGH WILHOIT'S POLY-
NOMIALS.  MAX LST SQ ERROR CP @ 1500 K  0.77 % .HF298=-166.92 KJ
C6H14  NORMAL     T12/91C   6H  14    0    0G   298.150  5000.000  C  86.17716 1
 0.12646645E+02 0.40048601E-01-0.15409786E-04 0.27681299E-08-0.18844568E-12    2
-0.26927099E+05-0.39820376E+02 0.33825662E+01 0.39576622E-01 0.42248448E-04    3
-0.76881274E-07 0.31538782E-10-0.23079536E+05 0.14434471E+02-0.20075747E+05    4

C6H14 2-METHYLPENTANE  TRC 1985 DATA EXTRAPOLATED THROUGH WILHOIT'S POLYNOMIALS.
MAX LST SQ ERROR CP @ 1400 K 0.58 %  HF298=-174.55 KJ
H14C6             T12/91H  14C   6    0    0G   298.150  5000.000  C  86.17716 1
 0.13108042E+02 0.39278025E-01-0.14080404E-04 0.24208876E-08-0.16060487E-12    2
-0.28005811E+05-0.43334246E+02-0.18831303E+00 0.62825959E-01-0.96052544E-05    3
-0.26183767E-07 0.13717321E-10-0.23599561E+05 0.28793617E+02-0.20993420E+05    4

C6H14 3-METHYLPENTANE  TRC 1985 DATA EXTRAPOLATED USING WILHOIT'S POLYNOMIALS.
MAX LST SQ ERROR CP @ 1500 K 0.44% HF298=-171.97 KJ
C6H14 3MP         T12/91C   6H  14    0    0G   298.150  5000.000  C  86.17716 1
 0.11469782E+02 0.42180865E-01-0.15849621E-04 0.28068586E-08-0.18972023E-12    2
-0.27169579E+05-0.34201883E+02 0.25431966E+00 0.58351247E-01-0.40723274E-07    3
-0.34483028E-07 0.16336350E-10-0.23291682E+05 0.27495401E+02-0.20683119E+05    4

C6H14 2,2-DIMETHYLBUTANE TRC 1985 DATA EXTRAPOLATED USING WILHOIT'S POLYNOMIALS.
MAX LST SQ ERROR CP @ 1500 0.36%  HF298=-184.68 KJ
C6H14 2,2-DMB     T12/91C   6H  14    0    0G   298.150  5000.000  C  86.17716 1
 0.96971555E+01 0.46148235E-01-0.16623012E-04 0.28333468E-08-0.18611414E-12    2
-0.28192059E+05-0.27863620E+02 0.64064618E+00 0.56146894E-01 0.55680943E-05    3
-0.37647313E-07 0.17161290E-10-0.24881231E+05 0.22759020E+02-0.22211772E+05    4

C6H14 2,3-DIMETHYLBUTANE TRC 1985 DATA EXTRAPOLATED USING WILHOIT'S POLYNOMIALS.
MAX LST SQ ERROR CP @ 1300 K 0.64 % HF298=-176.8 KJ
C6H14 2,3-DMB     T12/91C   6H  14    0    0G   298.150  5000.000  C  86.17716 1
 0.11052547E+02 0.42967887E-01-0.15547966E-04 0.26700033E-08-0.17650517E-12    2
-0.27635374E+05-0.34063265E+02-0.24903827E+01 0.76732667E-01-0.44086761E-04    3
 0.11461954E-07-0.65151136E-12-0.23564889E+05 0.37180699E+02-0.21264031E+05    4

C7F16 PERFLUOROHEPTANE  SIGMA=18  CALCULATED and EXTRAPOLATED USING NIST 93 AND
BOZZELLI & RITTER'S PROGRAM. HF298=-3383.60 KJ REF=DOMALSKI & HEARING JCPRD 22
(1993) p. 1059  Max Lst Sq Error Cp @ 1400 K 0.2%.
C7F16             T12/94C   7F  16    0    0G   298.150  5000.000  D 388.05145 1
 0.49255494E+02 0.15917852E-01-0.66760164E-05 0.12359725E-08-0.84204573E-13    2
-0.42550985E+06-0.20796807E+03-0.31954899E+01 0.18606616E+00-0.21215520E-03    3
 0.11047553E-06-0.21600066E-10-0.41264667E+06 0.55907556E+02-0.40699560E+06    4

PHENYL-CN  (BENZONITRILE) DATA FROM STULL WESTRUM & SINKE EXTRAPOLATED  TO 5000K
USING WILHOIT'S POLYNOMIALS. HF298=52.3 KCAL  Max Lst Sq Error Cp @ 1200 K 0.31%
C7H5N             T 3/93C   7H   5N   1    0G   298.150  5000.000  B 103.12344 1
 0.13986349E+02 0.21028565E-01-0.74936815E-05 0.12924836E-08-0.86479352E-13    2
 0.19941209E+05-0.50121316E+02-0.30769054E+01 0.68729237E-01-0.53234449E-04    3
 0.16528583E-07-0.21922909E-12 0.24618574E+05 0.37871666E+02 0.26318232E+05    4
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Table 4 (continued)

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TNT  C7H5(NO2)3  Tri-Nitro-Toluene Solid  Cp 290-345 REF= Yin,Ziru,Ganghe,
Chengyun 17th Internat. Pyrotech. Seminar 1991 Vol 1, 515-521 S298=32.93 cal
Graphic Integ  HF298(solid)=-15.1+/-1.2 Kcal REF=NIST 98 (Rouse J. Chem. Eng.
Data 21 (1976),16-20)  Max Lst Sq Error Cp @ 340 K **1.7 %**
TNT    Solid Yin  HF298 C  7.H  5.N  3.O  6.S   290.000   353.800  D 227.13332 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00 4.76323267E+03-6.62925737E+01 3.45483562E-01    3
-7.95964538E-04 6.85394484E-07-2.83973511E+05-1.70349206E+04-7.59857165E+03    4

TNT  C7H5(NO2)3  Tri-Nitro-Toluene  SIMNO=2  STATWT=1  IA = 158.50629
IB= 171.65362  IC=314.929913  Ir(NO2)para=5.96  ROSYM=2  V(2)=3.11 kcal
(Ir(NO2)meta=5.96  ROSYM=2  V(2)=7 kcal)x2  Ir(CH3)=0.51666  ROSYM=3  V(3)=3.5
kcal  NU=3080,3050,2989,2942,2875,2828,2747,2700,2450,1945,1915,1858,1817,1790,
1716,1656,1609,1554,1490,1430,1393,1345,1265,1204,1151,1103,1063,1023,942,908,
854,827,780,733,666,651,600,543,524,497,457,371,360,346,320,301,274,264,159,150,
144,106,70  HF298=5.76 kcal  REF=BURCAT  TAE Report # 824 1998. Max Lst Sq Error
Cp @ 1300 K 0.64%
C7H5N3O6  TNT     T 5/98C  7.H  5.N  3.O  6.G   200.000  6000.000  D 227.13332 1
 2.62323485E+01 3.08249282E-02-1.16857989E-05 1.94730669E-09-1.18966543E-13    2
-8.21343086E+03-1.01706192E+02 4.99444797E+00 8.99017655E-02-7.93846083E-05    3
 4.28434430E-08-1.11552302E-11-1.96446053E+03 8.89961538E+00 2.89852800E+03    4

C7H5N5O8 Tetryl Solid N Methyl-N,2,4,6-tetranitroaniline   Cp 290-345 REF= Yin,
Ziru,Ganghe,Chengyun 17th Internat. Pyrotech. Seminar 1991 Vol 1, 515-521
S298=34.29 cal Graphic Integ  HF298(solid)=9.8+/- 1.1 Kcal REF=NIST 98  (Krien,
Licht, Zierath Thermochim Acta 6, (1973), 465-472    Max Lst Sq Error Cp @ 335 K
0.70 %
Tetryl Solid Yin  T 4/99C  7.H  5.N  5.O  8.S   290.000   401.500  D 287.14560 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00-2.53679003E+03 2.97271189E+01-1.28541885E-01    3
 2.45677286E-04-1.74152468E-07 1.72331689E+05 9.49458327E+03 4.93152332E+03    4

BENZALDEHYDE  IA=16.033 IB=53.65 IC=69.661 NU=3084,3063(2),3036,3026,2817,1728,
1614,1603,1491,1460,1387,1314,1276,1202,1168,1160,1074,1026,996,825,649,617,
437,224,1003,996,978,918,852,740,688,450,404,217 ROSYM=2 IR=1.48 INTERNAL ROT
BARRIER V2=1713.8 HF298=-36.8 KJ REF=Ambrose, Connett, Green, Hales, Head, &
Martin J. Chem. Thermo. 7 (1975) 1143. Max Lst Sq Error Cp @ 1200 K 0.39%.
C7H6O             L 3/86C   7H   6O   1    0G   298.150  5000.000  B 106.12404 1
 0.13650737E+02 0.25680419E-01-0.10466729E-04 0.19413430E-08-0.13483792E-12    2
-0.11019744E+05-0.47965796E+02-0.31627334E+01 0.66369245E-01-0.34816353E-04    3
-0.62999377E-08 0.85807101E-11-0.61169349E+04 0.40231735E+02-0.44259974E+04    4

C7H7  BENZYL RAD   STATWT=2.  SIGMA=2.  A0=.189  B0=.0906  C0=.0613  NU=3060(2),
3050,2860,1600,1480,1330,1270,1160(2),1010,980(2),810,520,950,820,360(2),890,
750,640,420,170,3040,3030,2930,1550,1440(2),1350,1300,1070,600,610,(290 TORSION)
REF=Brouwer,Muller-Markgraf & TROE J. Chem. Phys 92 (1988) 4905.    MAX LST SQ
ERROR Cp @ 1300K 0.57%    HF298=210.5 KJ  Ref=Hippler & Troe J. Phys. Chem 94,
(1990), 3803
C7H7              T08/90C   7H   7    0    0G   200.000  6000.000  B  91.13258 1
 0.14043980E+02 0.23493873E-01-0.85375367E-05 0.13890841E-08-0.83614420E-13    2
 0.18564203E+05-0.51665589E+02 0.48111540E+00 0.38512832E-01 0.32861492E-04    3
-0.76972721E-07 0.35423068E-10 0.23307027E+05 0.23548820E+02 0.25317186E+05    4

TOLUENE Liquid DATA TAKEN FROM TRC 10/86 TABLES.  HF298(L)=12.18 KJ.
TOLUENE(L)        P10/86C  7.H  8.   0.   0.L   178.150   500.000  C  92.14052 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00 2.93676022E+01-1.94722686E-01 9.74773096E-04    3
-1.91472689E-06 1.48097019E-09-4.16318442E+03-1.12019966E+02 1.46490894E+03    4
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C7H8  TOLUENE  STATWT=1  SIGMA=1  IA=14.65  IB=47.993  IC=33.341  IR=.5008
POT BARRIER V6=50.    NU=3085,3070,3058,2920,1604,1493,1378,1208,1176,1028,1002,
784,524,973,841,406,2979,1455(3),1040,983,893,734,690,467,217,3037,3028,2950,
1540,1331,1313,1153,1080,1040,620,347  REF=HITCHCOCK & LAPOSA  MAX LST SQ ERROR
CP @ 1300 K 0.9 %. HF298=50. KJ REF=STULL, WESTRUM & SINKE
C7H8              L 6/87C   7H   8    0    0G   200.000  6000.000  B  92.14052 1
 0.12940034E+02 0.26691287E-01-0.96838505E-05 0.15738629E-08-0.94663601E-13    2
-0.69764908E+03-0.46728785E+02 0.16152663E+01 0.21099438E-01 0.85366018E-04    3
-0.13261066E-06 0.55956604E-10 0.40756300E+04 0.20282210E+02 0.60135835E+04    4

C7H8 NORBORNADIENE  2,5-BICYCLOHEPTADIENE  SIGMA=2   IA=19.32836  IB=28.76499
IC=32.96105 REF STRUCT=Boyd et al J. Phys. Chem 75 (1971),1264  NU=3105,3010,
2939,1579,1455,1232,1109,938,877,777,729,417,3073,1287,1240,1111,956,904,741,
475,3075,3005,1319,1267,1157,944,914,871,801,539,3101,2994,1548,1208,1064,1019,
897,656.5,500   REF=Shaw et al J. Chem. Phys 89 (1988),716     HF298=247.6 KJ
REF=STEELE J. Chem Termody. 10,(1978),919 Max Lst Sq Error Cp @ 200 K **1.5%**
C7H8 BICY-DIEN    T 2/95C   7H   8    0    0G   200.000  6000.000  B  92.14052 1
 0.13496865E+02 0.25643891E-01-0.92836633E-05 0.15067572E-08-0.90544980E-13    2
 0.22818374E+05-0.52940311E+02-0.16635648E+01 0.32118722E-01 0.77694587E-04    3
-0.13846610E-06 0.61589660E-10 0.28405811E+05 0.33057840E+02 0.29779265E+05    4

C7H8 1,3,5-CYCLOHEPTATRIENE SIGMA=1 IAIBIC=21.43E+114 NU=3050(6),2950,2850,
1650(3),1450(3),1400(2),1200(3),1100(2),1000(4),950(2),900(2),800,750,700,650,
450(3),350,300,225  REF=DOROFEEVA GURVICH & JORISH  HF298=182.8 kJ  Max Lst Sq
Error Cp @ 200 K 0.86%
C7H8 CYTRIENE     T 2/95C   7H   8    0    0G   200.000  6000.000  C  92.14052 1
 0.13258062E+02 0.26861556E-01-0.97467868E-05 0.15841995E-08-0.95289125E-13    2
 0.15183137E+05-0.49026873E+02 0.85938299E+00 0.28843433E-01 0.66954232E-04    3
-0.11395939E-06 0.49164081E-10 0.20057894E+05 0.22487468E+02 0.21985661E+05    4

C7H8 1,6-HEPTADIYNE  SIGMA=2  HF298=395.8 kJ  REF=NIST 94  DATA EXTRAPOLATED TO
5000 K USING WILHOIT'S POLYNOMIALS  Max Lst Sq Error Cp @ 1500 K 0.6%
C7H8 1,6-DIYNE    T 2/95C   7H   8    0    0G   298.150  5000.000  E  92.14052 1
 0.13001823D+02 0.25607076E-01-0.83584682E-05 0.13207200E-08-0.81972807E-13    2
 0.41975255E+05-0.37320914E+02 0.99595662E+00 0.66544712E-01-0.62569423E-04    3
 0.35335409E-07-0.88673880E-11 0.44836033E+05 0.22638639E+02 0.47603527E+05    4

CRESOL REF=Kudchadker, Kudchadker, Wilhoit & Zwolinski, JPCRD 7 (1978) 417.
ISOMERS WERE COMBINED BY SETTING T0= DELTA E VALUES. BECAUSE OF SLIGHT DIFFERE-
NCES IN CIS AND TRANS M-CRESOL, THEY WERE COMBINED BY SETTING STATWT=2. OTHER
ISOMERS ARE O-CRESOL (CIS AND TRANS) AND P-CRESOL. HF298=-132.298 KJ.
Max Lst Sq Error Cp @ 1300 K 0.6%.
C7H8O CRESOL      L 6/87C   7H   8O   1    0G   200.000  6000.000  B 108.13992 1
 0.15932987E+02 0.27011160E-01-0.99448722E-05 0.16296689E-08-0.98513298E-13    2
-0.23592065E+05-0.59732841E+02 0.42258267E+00 0.45551636E-01 0.32012513E-04    3
-0.81121959E-07 0.37665658E-10-0.18202621E+05 0.26032903E+02-0.15911701E+05    4

BENZYL ALCOHOL FREQUENCIES AND MOMENTS OF INERTIA ESTIMATED FROM BENZALDEHIDE.
SIGMA=2  IA=15.  IB=53.  IC=68. IR=0.14  ROSYM=1 POTENTIAL BARRIER V(1)=800.
NU=3084,3063,3036,3026,2817,1035,1614,1603,1500,1491,1460,1314,1276,1202,1168,
1160,1074,1026,996,825,800,617,437,224,1003,996,978,918,852,740,688,450,404,217,
2800,1250,1150,1050,3680,1345 REF=KAKAR & REINHART J. CHEM. PHYS 52 (1970), 3803
HF298=-100.416 KJOULES. REF=Stein et al., NIST Ref Database #25 (1991)
C7H8O             L 7/87C   7H   8O   1    0G   200.000  6000.000  D 108.13992 1
 0.15281154E+02 0.27208501E-01-0.98584660E-05 0.16012183E-08-0.96278057E-13    2
-0.19700471E+05-0.59418673E+02 0.20642021E+01 0.22775140E-01 0.95972053E-04    3
-0.15085110E-06 0.64175832E-10-0.14285021E+05 0.18148312E+02-0.12077200E+05    4
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C7H10 3,5 DIMETHYL-CYCLO-PENTADIENE   ROSYM=2x3   ESTIMATED BY NIST 94 FROM
2x[C-(H)3]; [CD-(C)2]; [CD-(C)(H)]; [CD-(C)(CD)]; [CD-(CD)(H)]; [C-(CD)2(H)2]
CYCLO CORRECTION FOR HF 25.1 KJ FOR S 117.2 J   HF298=66.7 KJ   Max Lst Sq Error
H-H298 @ 500 K 0.76%
C7H10 CY          T10/94C   7H  10    0    0G   298.150  5000.000  E  94.15640 1
 0.20552365E+02 0.21152399E-01-0.61510211E-05 0.93381729E-09-0.57913697E-13    2
-0.11383855E+04-0.86816803E+02-0.31141443E+01 0.88593226E-01-0.79693884E-04    3
 0.35311116E-07-0.46666666E-11 0.56494240E+04 0.35689345E+02 0.80221204E+04    4

C7H12  NORBORNANE (1,4-BICYCLOHEPTANE)   SIGMA=2  IA=21.71703  IB=32.0313
IC=36.49119  REF=Boyd, Sanwal, Shary-Tehrany & McNally J. PHYS. CHEM. 75, (1971)
,1264  NU=2980,2972,2927,2918,1487,1455(2),1317,1260,1142,993,923,873,818,755,
410,2943,2913(2),1306,1298,1220,1115,968,963,542,172,2971,2949,1453,1315,1279,
1241,1165,1074,975,800,757,342,2967,2960,2926,1463,1302,1214,1109,1025,954,890,
788,451  REF= Shaw, Castro, Dutler, Rauk, Wieser J.Chem Phys 89 (1988),716
HF298=-12.84 +/-1.0 KCAL  REF= Rogers, Choi, Girellini, Holmes J. PHYS. CHEM. 84
,(1980), 1810  Max Lst Sq Error Cp @ 200 K **1.65%**
C7H12  NORBORNANE T 2/95C   7H  12    0    0G   200.000  6000.000  B  96.17228 1
 0.12209671E+02 0.36813654E-01-0.13348120E-04 0.21681847E-08-0.13034960E-12    2
-0.13908324E+05-0.48119383E+02 0.29299287E+01-0.51738445E-02 0.19010706E-03    3
-0.25143626E-06 0.10128615E-09-0.83354164E+04 0.15423398E+02-0.64613020E+04    4

C7H12 CYCLOHEPTENE  SIGMA=2  IAIBIC=32.1E+114  NU=3024,2964,2926,2881,2852(2),
2837,1656,1457,1443,1434,1339,1332,1252,1234,1200,1072,1042,983,875,824,746,691,
479,417,353,190,3062,2963,2924,2854,2842,1447,1439,1391,1357,1323,1270,1234,
1207,1144,1104,1024,985,960,889,832,585,459,312,209    HF298=-9.4 KJ
REF=Dorofeeva, Gurvich & Jorish (1986) Max Lst Sq Error Cp @ 200K 0.99% CALCULA-
TED DATA DO NOT AGREE WELL WITH THE ORIGINAL DATA
C7H12 CY-HEPTENE  T 2/95C   7H  12    0    0G   200.000  6000.000  D  96.17228 1
 0.13885839E+02 0.37228089E-01-0.13526336E-04 0.22001174E-08-0.13239255E-12    2
-0.90383223E+04-0.55685410E+02 0.25521022E+01 0.14373533E-01 0.13613489E-03    3
-0.19136176E-06 0.77956555E-10-0.33917022E+04 0.15627602E+02-0.11305537E+04    4

C7H13 1-HEPTENYL-4/5  Estimated using NIST-94. EXTRAPOLATED from 1600 K
USING WILHOIT'S POLYNOMIALS. MAX LST SQ ERROR CP @ 1500 K 0.38% HF298=129.7 KJ
C7H13 1-heptenyl  T 3/00C  7.H 13.   0.   0.G   298.150  5000.000  D  97.18022 1
 1.60018015E+01 3.54427457E-02-1.32165151E-05 2.31246011E-09-1.53963769E-13    2
 5.72251317E+04-4.44583440E+01 3.79165044E+00 4.06710071E-02 4.73501574E-05    3
-9.16895795E-08 4.01452434E-11 6.20729296E+04 2.56340050E+01 6.52672016E+04    4

C7H14  1-HEPTENE   API DATA EXTRAPOLATED THROUGH WILHOIT'S POLYNOMIALS.
MAX LST SQ ERROR CP @ 1300 K 0.39%. HF298=-14.89 KCAL
C7H14             P12/52C   7H  14    0    0G   298.150  5000.000  C  98.18816 1
 0.13952881E+02 0.41712158E-01-0.16157950E-04 0.29187538E-08-0.19958112E-12    2
-0.14853311E+05-0.43649205E+02 0.19140427E+01 0.58601697E-01 0.16939333E-05    3
-0.38140418E-07 0.18157007E-10-0.10616395E+05 0.22793909E+02-0.74928962E+04    4

C7H14 CYCLOHEPTANE  SIGMA=2  IAIBIC=39.1E+114  NU=2925(7),2860(7),1467,1450,
1446,1440,1430(3),1360,1350,1310(3),1285(2),1230(3),1210,1200(2),1125,1100,1040,
1020,1005(2),950,915,850,830,810,800,735,690,650,513,490,400,335,320,273,186,123
HF298=-118.2 KJ  REF=Dorofeeva, Gurvich & Jorish (1986) Max Lst Sq Error Cp @
200 K **1.1%**  CALCULATED DATA DO NOT AGREE WELL WITH THE ORIGINAL DATA.
C7H14 CY-HEPTANE  T 2/95C   7H  14    0    0G   200.000  6000.000  D  98.18816 1
 0.14662282E+02 0.41924851E-01-0.15223369E-04 0.24749860E-08-0.14888013E-12    2
-0.22745683E+05-0.60364838E+02 0.31165462E+01 0.12618947E-01 0.15692523E-03    3
-0.21682238E-06 0.87851529E-10-0.16705601E+05 0.13720905E+02-0.14216111E+05    4
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Table 4 (continued)

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N-C7H15  N-HEPTYL RADICAL  API-TRC 8/83 DATA TO 3000K EXTRAPOLATED USING
WILHOIT'S POLYNOMIALS.  MAX LST SQ ERROR CP @ 2000 K 0.36% HF298=4.38 KJ.
C7H15              P10/83C   7H  15    0    0G   200.000  5000.000  B  99.19610 1
 0.12660566E+02 0.47893065E-01-0.19735835E-04 0.37298693E-08-0.26299814E-12    2
-0.64258434E+04-0.34510489E+02 0.10280414E+02 0.70155356E-03 0.15955135E-03    3
-0.20959318E-06 0.83344532E-10-0.36030731E+04-0.10315257E+02 0.52799263E+03    4

C7H15  3,3-Di-Methyl-1 Pentyl Radical [C2H5C(CH3)2CH2CH2*]  SIGMA=108 Estimated
Using the Bozzelli-THERM Prog.  Extrapolated Using Wilhoit's Polynomials
1x[C/C4]; 4x[C/C/H3]; 2x[C/C2/H2];H bond =-101.10 kcal HF298=-1.16 kcal  Max
Lst Sq Error Cp @ 1500 K 0.37%
C7H15  NEOHEPTYL  T10/99C  7.H 15.   0.   0.G   298.150  5000.000     99.19610 1
 1.88589786E+01 3.77585789E-02-1.41626975E-05 2.49291206E-09-1.66770014E-13    2
-9.91845317E+03-7.30310151E+01 1.75482995E+00 5.73984184E-02 3.09997695E-05    3
-8.42656048E-08 3.87583179E-11-3.78376835E+03 2.20874184E+01-5.83731332E+02    4

C7H15  3,3-Di-Methyl-2-Pentyl Radical [C2H5C(CH3)2CH*CH3]  SIGMA=162 Estimated
Using the Bozzelli-THERM Prog.  Extrapolated Using Wilhoit's Polynomials
1x[C/C4]; 4x[C/C/H3]; 2x[C/C2/H2];H bond =-98.45 kcal HF298=-3.81 kcal  Max
Lst Sq Error Cp @ 1500 K 0.41%
C7H15 NEOHEPTYL-2 T10/99C  7.H 15.   0.   0.G   298.150  5000.000  E  99.19610 1
 1.81240700E+01 3.84586055E-02-1.45182003E-05 2.56761683E-09-1.72327022E-13    2
-1.11163386E+04-7.02350695E+01 2.09191664E+00 5.73477687E-02 1.54926142E-05    3
-5.34013030E-08 2.27869264E-11-5.13199239E+03 1.95330456E+01-1.91725550E+03    4

C7H15O Neo-HEPTANOL Radical 3,3,-dimethyl-1-pentanoxy radical
C2H5C(CH3)2CH2CH2-O*  Estimated Using Bozzelli's THERM program and extrapolated
to 5000 K using Wilhoit's polynomials. SIGMA=54  HF298=-34.00 kcal   Max Lst Sq
Error Cp @ 1000 K 0.54%.
C7H15O 3,3-dimet  T10/99C  7.H 15.O  1.   0.G   298.150  5000.000  E 115.19550 1
 2.09858953E+01 3.85709050E-02-1.46086654E-05 2.59555359E-09-1.75052645E-13    2
-2.75558714E+04-9.67484012E+01 1.76386765E-01 7.26245771E-02 2.14651033E-07    3
-5.23551849E-08 2.64458952E-11-2.03008094E+04 1.71949368E+01-1.71093666E+04    4

C7H16 liquid n-heptane DATA TAKEN FROM TRC 4/93 HF298=-53.621 kcal
C7H16(L) n-Heptan P 4/93C  7.H 16.   0.   0.L   200.000   380.000  C 100.20404 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00 3.57830581E+01-1.40027125E-01 4.92015800E-04    3
-4.04170872E-07 0.00000000E+00-3.49762365E+04-1.40909575E+02-2.69829808E+04    4

C7H16  N-HEPTANE  API PROJ 44 VALUES EXTRAPOLATED THROUGH WILHOIT'S POLYNOMIALS
MAX LST SQ ERROR CP @ 2100 K 0.31%. HF298=-44.89 KCAL
C7H16              P 4/81C   7H  16    0    0G   300.000  5000.000  C 100.2040  1
 0.17470044E+02 0.42134196E-01-0.16429033E-04 0.29963565E-08-0.20648765E-12    2
-0.31665823E+05-0.64762071E+02 0.11153248E+02-0.94941543E-02 0.19557118E-03    3
-0.24975252E-06 0.98487321E-10-0.26753133E+05-0.15922774E+02-0.22568979E+05    4

C7H16  NEOHEPTANE 3,3 Di-Methyl-Pentane Estimated Using the Bozzelli-THERM Prog
Extrapolated Using Wilhoit's Polynomials 1x[C/C4]; 4x[C/C/H3]; 2x[C/C2/H2];
SIGMA=324 HF298=-50.16 kcal [NIST 94 HF298=-46.89 kcal]  Max Lst Sq Error Cp @
1500 K 0.34%
C7H16  NEOHEPTAN  T10/99C  7.H 16.   0.   0.G   298.150  5000.000  E 100.20404 1
 1.89468643E+01 4.04407738E-02-1.51815251E-05 2.67111667E-09-1.78560754E-13    2
-3.48922658E+04-7.70247830E+01 1.55493237E+00 5.93804185E-02 3.04203450E-05    3
-8.22181963E-08 3.74203901E-11-2.84682415E+04 2.02705469E+01-2.52414153E+04    4
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C7H15OH n-HEPTANOL REF=Stull Westrum & Sinke  Extrapolated Using Wilhoit's Poly-
nomials to 5000 K. HF298=-81.2+/-0.39 kcal   REF=NIST 1998, (Cox & Pilcher) Max
Lst Sq Error Cp @ 1000 K 0.54%.
C7H15OH  Normal   T12/98C  7.H 16.O  1.   0.G   298.150  5000.000  E 116.20344 1
 1.92489075E+01 4.21234021E-02-1.57734301E-05 2.77888406E-09-1.86276082E-13    2
-5.06734146E+04-6.88916894E+01 3.19682451E+00 6.26125522E-02 7.79555247E-06    3
-4.69733504E-08 2.13096626E-11-4.45833633E+04 2.09286236E+01-4.08611933E+04    4

C7H15OH Neo-Heptanol 3,3,-dimethyl-1-pentanol C2H5C(CH3)2CH2CH2-OH
Estimated Using Bozzelli's THERM program and extrapolated to 5000 K using
Wilhoit's polynomials. SIGMA=54  HF298=-85.96 kcal   Max Lst Sq Error Cp @
1000 K 0.54%.
C7H15OH 3,3-dime  T10/99C  7.H 16.O  1.   0.G   298.150  5000.000  E 116.20344 1
 2.15383565E+01 3.99202307E-02-1.50184640E-05 2.65913985E-09-1.78970510E-13    2
-5.39238700E+04-8.57361104E+01 1.09102491E+00 7.20016043E-02 3.94354014E-06    3
-5.62818094E-08 2.79018977E-11-4.67188295E+04 2.65734430E+01-4.32565046E+04    4

C8H RAD  Values calculated using Bozzelli & Ritter's program from C8H2
EXTRAPOLATED USING WILHOIT'S POLYNOMIALS HF298=1162.06 KJ Max Lst Sq Error Cp @
500 K 0.16%
C8H               T 2/92C   8H   1    0    0G   298.150  5000.000  E  97.09594 1
 0.17422244E+02 0.66413688E-02-0.22557166E-05 0.36657347E-09-0.23188722E-13    2
 0.13376514E+06-0.59275082E+02 0.34566807E+01 0.65220393E-01-0.98141367E-04    3
 0.72046762E-07-0.20447036E-10 0.13656779E+06 0.77719815E+01 0.13976290E+06    4

C8H2  OCTATETRAYNE Calculated using Stein's coefficients J.Phys.Chem 89 (1985)
p.3714 BY THE NIST PROGRAM 1991HF298=223.3 KCAL REF=Kiefer, Sidhu, Kern, Xie,
Chen, & Harding  1992. Max Lst Sq Error Cp @ 1200 K 0.25 %
C8H2              T 2/92C   8H   2    0    0G   298.150  5000.000  E  98.10388 1
 0.17007524E+02 0.93656848E-02-0.30485718E-05 0.47653534E-09-0.29169032E-13    2
 0.10628021E+06-0.59224564E+02 0.12470437E+01 0.78392526E-01-0.12416148E-03    3
 0.98381697E-07-0.30063943E-10 0.10942891E+06 0.16048227E+02 0.11236828E+06    4

C8H6  PHENYL-ACETYLENE C6H5CCH SIGMA=2  IA=14.5382  IB=54.405  IC=68.943
NU=3271,3032,3028,3019,3009,3000,2150,1614,1586,1488,1437,1312,1190,1166,1159,
1087,1056,1008,1007,985,973,938,855,767,736,729,696,687,610,549,525,448,404,370,
160.4,142.4  REF=C. MELIUS DATABASE BAC/MP26 #116 P80H  HF298=78.43 KCAL Max Lst
Sq Error Cp @ 200 K 0.68%
C8H6 C6H5CCH      T 9/96C   8H   6    0    0G   200.000  6000.000  B 102.13564 1
 0.15638086E+02 0.22068432E-01-0.80253111E-05 0.13065013E-08-0.78679279E-13    2
 0.32272867E+05-0.59610868E+02-0.87234720E+00 0.51839614E-01 0.66079738E-05    3
-0.55950961E-07 0.29284749E-10 0.37461628E+05 0.29096304E+02 0.39467283E+05    4

C8H6O BENZOFURANE  VERY ROUGH APPROXIMATION BY STEIN & BARTON 298-2500K
EXTRAPOLATED USING WILHOIT'S POLYNOMIALS HF298=6.48 KCAL  REF= STEIN & BARTON
(1981)
C8H6O BENZOFURANE T 1/94C   8H   6O   1    0G   298.150  5000.000  F 118.13504 1
 0.16260779E+02 0.25251982E-01-0.98113297E-05 0.17473791E-08-0.11720720E-12    2
-0.46522585E+04-0.64478655E+02-0.39760390E+01 0.68789961E-01-0.22095246E-04    3
-0.28325945E-07 0.18870094E-10 0.16310801E+04 0.43193929E+02 0.32608440E+04    4

C8H6S BENZOTHIOPHENE SIGMA=1 IAIBIC=1.6013E-112 EXPERIMENTAL DATA OF ENTHALPY
AND ENTROPY 298-700 K EXTRAPOLATED TO 5000 K USING WILHOITS POLYNOMIALS
REF=Chirico, Knipmeyer Neguyen & Steele J. Chem. Thermodynamics 23 (1991), 759
HF298=39.74 KCAL REF= Pedley, Naylor & Kirby 1986
C8H6S             T12/93C   8H   6S   1    0G   298.150  5000.000  D 134.20164 1
 0.22676902D+02 0.21225910D-01-0.92726789D-05 0.17966329D-08-0.12813338D-12    2
 0.89624565D+04-0.10207224D+03 0.21269350D+02-0.94299806D-01 0.35966814D-03    3
-0.39367785D-06 0.14307548D-09 0.15380490D+05-0.65269994D+02 0.19997830D+05    4
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C8H7  STYRENE RADICAL C6H5CH=CH*  REF=Melius Average of data CIS and TRANS equiv
of 50-50% mixture SIGMA=2 STATWT=2   IA 16.14    IB=52.3224  IC=68.4804
I(red)= 1.6096   V2=4.67 kcal    ROSYM=2.      NU=3067,3023,3016,3006,2997,2992,
2941,1501,1487,1451,1426,1369,1292,1245,1188,1146,1124,1114,1028,971,930,918,
899,888,845,797,771,727,701,633,589,578,529,423,418,372,218,205. HF298=93.0 kcal
REF=NIST 94  Max Lst Sq Error Cp @ 200 K 0.75%
STYRENE RADICAL   T 2/99C  8.H  7.   0.   0.G   200.000  6000.000  B 103.14358 1
 1.80458471E+01 2.21498794E-02-8.05082743E-06 1.30961070E-09-7.88615885E-14    2
 3.87090843E+04-7.17917960E+01-8.85283632E-01 5.61565120E-02 1.16600084E-05    3
-6.99146159E-08 3.63590274E-11 4.45850990E+04 2.97497087E+01 4.67991499E+04    4

C8H7N INDOLE (1-BENZAZOLE, 2,3-BENZAPYRROLE) IAIBIC=80998.5  NU=3520,3140,
3083(2),3068(2),1617,1578,1510,1489,1458,1410,1348,1300,1275,1245,1205,1150,
1122,1082,1068,1015,968,930,900,869,860,800,762,761,738,715,625,608,575,544,428,
400(2),240,208  HF298=156.5+/-1.25 KJ  REF=Das, Frenkel, Gadalla, Kudchadker,
Marsh,Rodgers & Wilhoit JPCRD 22 (1993), 658  Max Lst Sq Error Cp @ 200 K 0.88%
C8H7N INDOLE      T03/95C   8H   7N   1    0G   200.000  6000.000  B 117.15032 1
 0.17162122E+02 0.26048457E-01-0.94598392E-05 0.15390002E-08-0.92648224E-13    2
 0.10577803E+05-0.69871764E+02-0.14144508E+01 0.48636966E-01 0.43663151E-04    3
-0.10447498E-06 0.48786402E-10 0.16880142E+05 0.32418878E+02 0.18822516E+05    4

C8H8 CUBANE (Pentacyclo[4.2.0.0.0.0]Octane  SIGMA=24  STATWT=1  IA=AB=IC=24.6449
NU=614.9(2),666.2(3),822.2(3),826.7(3),836.8(3),882.4(2),972,1028,1082.9(3),
1111.4(2),1150.2(3),1170.7(2),1235.6(3),1260.7(3),2927.9,2937.5(3),2946(3),
2963.5 HF298=155.755 Kcal REF=C. Melius Database of BAC/MP4 data. Private Comm.
RK66   Max Lst Sq Error Cp @ 200 K *2.8 %.*
C8H8 CUBANE       T12/94C   8H   8    0    0G   200.000  6000.000  B 104.15152 1
 0.16107210E+02 0.27423168E-01-0.10053212E-04 0.16453491E-08-0.99448320E-13    2
 0.69973199E+05-0.72553695E+02-0.24663483E+01 0.23435851E-01 0.14037784E-03    3
-0.22354648E-06 0.97222204E-10 0.77230359E+05 0.35253221E+02 0.78381028E+05    4

C8H8  STYRENE C6H5CH=CH2  SIGMA=2  CALCULATED USING DATA FROM STULL WESTRUM
& SINKE. EXTRAPOLATED WITH WILHOIT'S POLYNOMIALS.  HF298=35.22 Kcal  Max Lst SQ
Error Cp @ 400 K 1.09% REF=NIST 94, Pedley Naylor & Kirby
C8H8              T12/94C   8H   8    0    0G   298.150  5000.000  B 104.15152 1
 0.16139277E+02 0.24210847E-01-0.72678359E-05 0.11392276E-08-0.72984881E-13    2
 0.10249251E+05-0.61169437E+02-0.10717708E+02 0.12666725E+00-0.17762493E-03    3
 0.14344049E-06-0.47616577E-10 0.16597133E+05 0.71526331E+02 0.17723291E+05    4

C8H9  C6H5CH2CH2 RADICAL  SIGMA=4  IA=17.6933  IB=55.8233  IC=68.9265  NU=3049,
3020,3009,3000,2991,2958,2863,2823,1540,1512,1467,1452,1427,1418,1339,1311,1241,
1159,1149,1134,1113,1048,1033,986,967,943,922,918,868,828,804,727,705,654,595,
535,456,419,383,341,269,152,140,27  HF298=60.32+/-3.43 KCAL     STATWT=2
REF=C. MELIUS DATABASE BAC/MP26 #175 AA1B Max Lst Sq Error Cp @ 200 K 0.7 %.
C8H9 C6H5CH2CH2*  T 9/96C   8H   9    0    0G   200.000  6000.000  C 105.15946 1
 0.17515245E+02 0.28458155E-01-0.10330768E-04 0.16795763E-08-0.10104387E-12    2
 0.22049637E+05-0.68318437E+02 0.13453098E+01 0.44689015E-01 0.46337606E-04    3
-0.10183872E-06 0.46687950E-10 0.27736459E+05 0.21623320E+02 0.30354029E+05    4

C8H10  ETHYL BENZENE C6H5C2H5  SIGMA=6  IA=18.2186  IB=57.2285  IC=68.8635
NU=3022,3010,3001,2988,2986,2924,2915,2891,2866,2858,1618,1594,1493,1477,1465,
1460,1447,1393,1337,1328,1254,1195,1180,1162,1110,1058,1057.5,1017,1010,1002,
980,973,929,919,854,763,761,739,697,609,547,481,407,341,303,212,133,39.8
REF=C.MELIUS DATABASE BAC/MP26 #200 AA0F HF298=7.0 KCAL REF=NIST 94 Max Lst Sq
Error Cp @ 200 K 0.85%.
C8H10 C6H5C2H5    T 9/96C   8H  10    0    0G   200.000  6000.000  C 106.16740 1
 0.15987319E+02 0.32676385E-01-0.11890299E-04 0.19360904E-08-0.11659656E-12    2
-0.47073870E+04-0.63675039E+02 0.24506692E+01 0.26239143E-01 0.99991348E-04    3
-0.15573183E-06 0.65643572E-10 0.10189486E+04 0.16445176E+02 0.35225167E+04    4
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C8H10  1,4-DIMETHYLBENZENE  REF=DRAEGER AND SCOTT  DATA EXTRAPOLATED THROUGH
WILHOIT'S POLYNOMIALS  HF298=18.03 KJ  MAX LST SQ ERROR CP @ 1300 1.12 % .
C8H10              L 2/84C   8H  10    0    0G   300.000  5000.000  B 106.16699 1
 0.15268401E 02 0.34433573E-01-0.13685810E-04 0.21177802E-08-0.11564062E-12    2
-0.61602461E 04-0.59529587E 02-0.16422014E 01 0.58058664E-01 0.55675910E-05    3
-0.45693085E-07 0.21727536E-10 0.10412372E 03 0.34509140E 02 0.21641684E+04    4

C8H15 1-OCTENYL-4 CH2=CHCH2CH*C4H9  Estimated using NIST-94. EXTRAPOLATED from
1600 K USING WILHOIT'S POLYNOMIALS. MAX LST SQ ERROR CP @ 1500 K 0.38%
HF298=109.1 KJ
C8H15 1-octenyl-  T 3/00C  8.H 15.   0.   0.G   298.150  5000.000  D 111.20710 1
 1.86031870E+01 4.07347321E-02-1.52146579E-05 2.66612666E-09-1.77710586E-13    2
 3.77573497E+03-6.42994408E+01 3.96580128E+00 5.00731521E-02 4.58633610E-05    3
-9.55246040E-08 4.20968508E-11 9.47734142E+03 1.90962113E+01 1.31216392E+04    4

C8H16  1-OCTENE   API DATA EXTRAPOLATED THROUGH WILHOIT'S POLYNOMIALS.
MAX LST SQ ERROR CP @ 1300 K 0.94 % . HF298=-19.82 KCAL
1-OCTENE         1-P12/52C  8.H 16.   0.   0.G   300.000  5000.000  C 112.21440 1
 0.20831284E 02 0.38294513E-01-0.12417870E-04 0.17957589E-08-0.93705913E-13    2
-0.20133141E 05-0.79240051E 02 0.26075478E 01 0.64282537E-01 0.92502323E-05    3
-0.51046708E-07 0.23316557E-10-0.13597527E 05 0.21584656E 02-0.99738727E 04    4

N-C8H17  N-OCTYL RADICAL  API-TRC 8/83 DATA TO 3000 K EXTRAPOLATED TO 5000 K
USING WILHOIT'S POLYNOMIALS. MAX LST SQ ERROR CP @ 1200 K .059 % HF298=-16.32 KJ
N-C8H17          N-P10/83C   8H 17    0     0G   300.000  5000.000  B 113.2223  1
 0.17027115E 02 0.49380627E-01-0.19069470E-04 0.33672309E-08-0.22210039E-12    2
-0.10763527E 05-0.56252975E 02 0.26141319E 01 0.67607820E-01 0.11190068E-04    3
-0.56412340E-07 0.25483921E-10-0.57469414E 04 0.23451477E 02-0.19628570E 04    4

n-OCTANE Liquid, DATA TAKEN FROM TRC 10/84  HF298(L)=-59.814 kcal
C8H18(L) n-Octan  P10/84C  8.H 18.   0.   0.L   200.000   372.000  C 114.23092 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00 5.89507891E+01-3.62820096E-01 1.31981734E-03    3
-1.41611726E-06 0.00000000E+00-4.04118242E+04-2.30427236E+02-3.00994016E+04    4

C8H18  NORMAL OCTANE  STUL WESTRUM AND SINKE DATA EXTRAPOLATED THROUGH WILHOIT'S
POLYNOMIALS FROM STULL  MAX LST SQ ERROR .CP @ 1300K 0.86% . HF298=-49.82 KCAL
OCTANE           N-P 4/85C  8.H 18.   0.   0.G   300.000  5000.000  C 114.23020 1
 0.23503891E 02 0.39657507E-01-0.13128325E-04 0.19592787E-08-0.10658157E-12    2
-0.36518059E 05-0.95243149E 02 0.18952761E 01 0.69645584E-01 0.14661359E-04    3
-0.60905563E-07 0.26589383E-10-0.28789637E 05 0.24422028E 02-0.25107010E 05    4

C8H18 liquid ISOOCTANE  DATA TAKEN FROM TRC 10/82 HF298=-61.941 kcal
C8H18(L) isooctan P10/84H 18.C  8.   0.   0.L   200.000   456.000  C 114.23092 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00 2.26508441E+01-4.36695469E-02 2.96290596E-04    3
-2.59700234E-07-4.31948017E-11-3.80663177E+04-8.73625313E+01-3.11697435E+04    4

C8H18 2,2,4 TRIMETHYLPENTANE  API 44 DATA EXTRAPOLATED THROUGH WILHOIT'S
POLYNOMIALS  MAX LST SQ ERROR CP @ 1300K 0.92% . HF298=-53.54 KCAL
ISO-OCTANE       I-P 4/85C  8.H 18.   0.   0.G   298.150  5000.000  C 114.23020 1
 0.19396317E 02 0.48813742E-01-0.15579804E-04 0.21783064E-08-0.10839138E-12    2
-0.37133922E 05-0.78853134E 02 0.42935711E 00 0.76576948E-01 0.84130588E-05    3
-0.58660319E-07 0.27941371E-10-0.30446438E 05 0.25673538E 02-0.26942377E 05    4
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C9H7 INDENYL RADICAL  STATWT=2 SIGMA=1  IA=21.31 IB=51.988  IC=73.298  NU=3053,
3038,3029,3019,3008,2998,2992,1534,1508,1433,1422,1403,1325,1298,1249,1164,1150,
1128,1105,1046,1022,966,937,921,888,852,831,821,804,730,710,691,681,634,562,508,
507,490,383,367,222,184.9  HF298=68.26=/-5.22 KCAL  REF=C. MELIUS DATABASE
BAC/MP26 #205 AA0K  Max Lst Sq Error Cp @ 200 K 0.88 %.
C9H7 INDENYL      T 9/96C   9H   7    0    0G   200.000  6000.000  B 115.15458 1
 0.18554959E+02 0.25035076E-01-0.91457509E-05 0.14934838E-08-0.90133030E-13    2
 0.25721156E+05-0.76300347E+02-0.26698729E+01 0.62177216E-01 0.15067018E-04    3
-0.79645699E-07 0.40918972E-10 0.32386969E+05 0.37861193E+02 0.34349570E+05    4

C9H7N Quinoline BENZO[B]PYRIDINE 1-BEZAZINE   SIGMA=1   IAIBIC=159000.4 E-117
NU=3074,3062,3048,3035,3017,3006,2980,1619,1595,1568,1500,1469,1431,1391,1370,
1312,1253,1216,1189,1140,1117,1093,1032,1012,976,968,952,938,903,864,802,785(2),
759,733,627,611,521,505,476,467,389,377,181,168.     HF298=200.52+/-1.36 kJ
REF= Das et al JPCRD 22 (1993),659   Max Lst Sq Error Cp @ 200 K 0.88%
C9H7N QUINOLINE   T 5/99C  9.H  7.N  1.   0.G   200.000  6000.000  B 129.16132 1
 1.85755750E+01 2.79425650E-02-1.02522932E-05 1.67898241E-09-1.01528223E-13    2
 1.51294620E+04-7.75919222E+01-1.13617529E+00 4.84964316E-02 5.58565955E-05    3
-1.20326645E-07 5.49530942E-11 2.20184652E+04 3.18686011E+01 2.41168752E+04    4

C9H7N ISO-QUINOLINE BENZO[C]PYRIDINE 2-BENZAZINE SIGMA=1 IAIBIC=160900.4 E-117
NU=3089,3060,3055(2),3025,3008,2990,1627,1587,1552,1497,1460,1432,1381,1377,
1315,1273,1255,1179,1140,1118,1095,1034,1013,985,970,959,942,930,831,823,800,
778,765,740,637,610,522,504,479,460,375,354,180,169.   HF298=204.61+/-1.33 kJ
REF= Das et al JPCRD 22 (1993),659     Max Lst Sq Error Cp @ 200 K 0.88%
C9H7N ISOQUINOLI  T 5/99C  9.H  7.N  1.   0.G   200.000  6000.000  B 129.16132 1
 1.85146411E+01 2.79810705E-02-1.02625548E-05 1.68026025E-09-1.01589164E-13    2
 1.56389099E+04-7.71926472E+01-8.22485356E-01 4.62854760E-02 6.07470671E-05    3
-1.24938487E-07 5.65402573E-11 2.24802772E+04 3.06200613E+01 2.46087863E+04    4

C9H8 INDENE  SIGMA=1  IA=21.885  IB=52.67  IC=74.043  NU=3044,3022,3019,3007,
2996,2989,2882,2857,1627,1610,1580,1462,1452,1428,1347,1302,1233,1211,1174,1142,
1135,1100,1095,1054,999,992,974,954,937,910,874,832,802,776,724,706,697,576,544,
516,420,385.5,368.6,205.1,189.9  HF298=39.23 KCAL  REF=C. MELIUS DATABASE
BAC/MP26 #206 AA0J  Max Lst Sq Error Cp @ 200 K 1.01%
C9H8 INDENE       T 9/96C   9H   8    0    0G   200.000  6000.000  B 116.16252 1
 0.17318671E+02 0.28982768E-01-0.10605059E-04 0.17334553E-08-0.10467919E-12    2
 0.11151429E+05-0.71555323E+02-0.68190289E+00 0.41658733E-01 0.70741234E-04    3
-0.13430875E-06 0.59915845E-10 0.17705036E+05 0.29781396E+02 0.19741190E+05    4

C9H10  ALFA-METHYLSTYRENE (BENZENE, 1-METHYLETHENYL-) DATA TO 1000 K FROM STULL
WESTRUM & SINKE & NIST 1994 EXTRAPOLATED USING WILHOIT'S POLYNOMIALS. SIGMA=6
HF298=27.0 KCAL  Max Lst Sq Error Cp @ 400 K **1.0%**  H @ 800 K 0.9%
C9H10             T 1/96C   9H  10    0    0G   298.150  5000.000  C 118.17840 1
 0.18890862E+02 0.31553549E-01-0.12056696E-04 0.21436164E-08-0.14430356E-12    2
 0.43332577E+04-0.75568080E+02 0.58431766E+01 0.17489030E-01 0.12112118E-03    3
-0.17951022E-06 0.75443868E-10 0.10316404E+05 0.36919595E+01 0.13586850E+05    4

C9H12  1-3-5-Tri-Methyl-Benzene, also Mesitylene   DATA 200-1500 K from Dreager
J. Chem. Thermo. 17, (1985), 263-275.  Extrapolated to 5000 K using Wilhoit's
polynomials. HF298=-3.84 kcal  REF=Stull,Westroom & Sinke 1969. Max Lst sq Error
Cp @ 1000 K 0.68%
C9H12  1-3-5-TMB  T 8/00C  9.H 12.   0.   0.G   200.000  5000.000  C 120.19428 1
 1.67073078E+01 3.98877329E-02-1.54373742E-05 2.77050130E-09-1.87953017E-13    2
-1.09906566E+04-6.54478472E+01 3.70645582E+00 3.04050008E-02 9.36818016E-05    3
-1.42836230E-07 5.85223220E-11-4.96186950E+03 1.31400088E+01-1.93235200E+03    4
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Table 4 (continued)

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C9H12  1-2-4-Tri-Methyl-Benzene,   DATA 200-1500 K from Dreager J. Chem. Thermo.
17, (1985), 263-275.  Extrapolated to 5000 K using Wilhoit's polynomials.
HF298=-3.33 kcal  REF=NIST Webbook 2000.   Max Lst sq Error Cp @ 1000 K 0.66%
C9H12  1-2-4-TMB  T 8/00C  9.H 12.   0.   0.G   200.000  5000.000  C 120.19428 1
 1.71329238E+01 3.94083582E-02-1.52208685E-05 2.72757795E-09-1.84838202E-13    2
-1.07469624E+04-6.62588105E+01 5.36104527E+00 2.74614342E-02 9.27107834E-05    3
-1.37606888E-07 5.56796764E-11-5.06812567E+03 5.85157015E+00-1.67571150E+03    4

C9H17 1-NONENENYL-4/5  Estimated using NIST-94. EXTRAPOLATED from 1600 K
USING WILHOIT'S POLYNOMIALS. MAX LST SQ ERROR CP @ 1500 K 0.38% HF298=88.4 KJ
C9H17 1-nonenyl-4 T 3/00C  9.H 17.   0.   0.G   298.150  5000.000  D 125.23398 1
 2.10867922E+01 4.61782938E-02-1.72507130E-05 3.02355150E-09-2.01567606E-13    2
 3.27938951E+01-7.58751351E+01 4.36832491E+00 5.77776115E-02 4.89429265E-05    3
-1.04595584E-07 4.61873643E-11 6.51405343E+03 1.91916207E+01 1.06320156E+04    4

C9H18 1-NONENE  Estimated using NIST-94. EXTRAPOLATED from 1600 K
USING WILHOIT'S POLYNOMIALS. MAX LST SQ ERROR CP @ 1500 K 0.36% HF298=-103.3 KJ
C9H18 1-nonene    T 3/00C  9.H 18.   0.   0.G   298.150  5000.000  D 126.24192 1
 2.18154890E+01 4.80370115E-02-1.79392300E-05 3.14265715E-09-2.09387787E-13    2
-6.30911726E+04-8.29167013E+01 2.62429422E+00 7.18302704E-02 1.92494510E-05    3
-7.29310566E-08 3.39150762E-11-5.59992986E+04 2.40905648E+01-5.19822816E+04    4

N-C9H19  N-NONYL RADICAL  API-TRC 8/83 DATA TO 3000 K EXTRAPOLATED TO 5000 K
USING WILHOIT'S POLYNOMIALS.  MAX LST SQ ERROR CP @ 1200K 0.61 % HF298=-37.03 KJ
N-C9H19          N-P10/83C   9H 19    0     0G   300.000  5000.000  B 127.2491  1
 0.19195267E 02 0.55439249E-01-0.21436601E-04 0.37885144E-08-0.25002987E-12    2
-0.14373711E 05-0.66069458E 02 0.27452002E 01 0.76430142E-01 0.12624764E-04    3
-0.63882226E-07 0.28818781E-10-0.86689141E 04 0.24831818E 02-0.44537129E 04    4

C9H20 liq  Nonane  REF=I.Barin 1987  HF298liq=-275.475 kJ
C9H20(L)          B01/00C  9.H 20.   0.   0.L   298.150   423.430  C 128.25780 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00 3.41721095E+01 2.58204426E-04-6.96987194E-07    3
 6.20423745E-10 0.00000000E+00-4.33267971E+04-1.47402676E+02-3.31318382E+04    4

N-C9H20 N-NONANE  Bureau of Mines Bull 666 1974 DATA TO 1500. K EXTRAPOLATED
USING WILHOIT'S POLYNOMIALS. MAX LST SQ ERROR CP @ 1500 K 0.72 %
HF298=-54.71 kcal
N-C9H20 NONANE    T 5/99C  9.H 20.   0.   0.G   200.000  6000.000  B 128.25780 1
 2.55877522E+01 4.60770651E-02-1.60860633E-05 2.58274408E-09-1.54734690E-13    2
-4.00748448E+04-1.04722466E+02 1.39840225E+01-1.17224978E-02 2.52316467E-04    3
-3.25680364E-07 1.29109135E-10-3.28258409E+04-2.38633750E+01-2.75309838E+04    4

C10D8  NAPHTHALENE-D8  SIGMA=4 IA=32.0228 IB=76.0297 IC=108.0525  NU=2272,2257,
1553,1386,1298,863,835,692,495,785,545,346,875,760,663,410,2302,2275,1604,1330,
1030,929,830,490,800,653,507,177,2286,2258,1545,1258,1050,889,715,328,2289,2258,
1439,1316,1082,880,825,593,791,628,404,163  REF=CHEN, KUDCHADKER AND WILHOIT
MAX LST SQ ERROR CP @ 1300 K 0.85 %. HF298=118.05 KJ
C10D8             T 9/82C  10D   8    0    0G   300.000  5000.000  B 136.22281 1
 0.24693802E+02 0.25579888E-01-0.93010221E-05 0.14824513E-08-0.85934623E-13    2
 0.29915154E+04-0.11214200E+03-0.29223614E+01 0.80820084E-01-0.12762395E-04    3
-0.52788202E-07 0.30022318E-10 0.11687422E+05 0.35703760E+02 0.13205407E+05    4
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Table 4 (continued)

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C10H6 Naphthyne     SYMNO = 1  Ia = 25.100753  Ib = 67.174194   Ic = 92.274938
Nu = 3134,3133,3123,3110,3099,3095,1994,1610,1533,1410,1442,1401,1363,1326,
1286,1212,1203,1154,1127,1089,1082,1020,949,916,890,844,842,780,767,734,701,
677,562,544,499,489,407,398,384,359,196,165.   REF = Curran Et al JPCRD 29,
(2000),     Hf(298)= 119.7 kcal/mole  REF = Wang & Frenklach J. Phys. Chem. 98,
(1994),11465.    Max Lst Sq Error Cp @ 200 K 0.62%
C10H6 Naphtyne    T 7/98C 10.H  6.   0.   0.G   200.000  6000.000  B 126.15764 1
 1.87728941E+01 2.48768793E-02-9.09940935E-06 1.48730676E-09-8.98228135E-14    2
 5.15727443E+04-7.68608875E+01-1.50617131E+00 6.03325879E-02 1.09063952E-05    3
-6.91994009E-08 3.54144371E-11 5.80261788E+04 3.24494940E+01 6.02350349E+04    4

C10H7 Naphtyl radical      STATWT = 2    Ia = 25.3426871    Ib = 68.4922226
Ic = 93.8348672  Nu=3129,3119,3117,3107,3106,3094,3093,2623,1599,1548,1487,
1446,1418,1384,1350,1339,1234,1218,1167,1146,1139,1106,1028,1017,949,925,913,
898,857,830,775,760,753,742,705,609,588,508,490,489,444,386,347,181,166.
REF = Curran Et al JPCRD 29,(2000),          Hf(298)=94.7 kcal/mole
REF = Wang & Frenklach J. Phys. Chem. 98,(1994),11465.   Max Lst Sq Error Cp
@ 200 K 0.81%.
C10H7 Naphtyl rad T 7/98C 10.H  7.   0.   0.G   200.000  6000.000  B 127.16558 1
 1.83535073E+01 2.77474314E-02-1.00885968E-05 1.64229575E-09-9.89002001E-14    2
 3.89261241E+04-7.48978150E+01-1.89559772E+00 5.83077290E-02 2.79388931E-05    3
-9.14375172E-08 4.46422302E-11 4.55409775E+04 3.52453263E+01 4.76546183E+04    4

4-Ethenyl - Phenyl-1-Vinyl Radical  C6H4(C2H)C2H2*    STATWT 2.  Ia=31.301037
Ib=54.020658 Ic=69.949573 Ir(-CH=CH()=2.73405 ROSYM=2 V(3)=4.4 kcal/mole
Nu=3129,3119,3113,3111,3098,3097,3035,1932,1591,1487,1474,1368,1332,1321,
1270,1257,1172,1154,1134,1117,1087,1021,1003,951,915,890,882,816,810,781,761,
704,675,659,585,548,540,504,443,380,336,322,264,206.    REF = Curran et al,
JPCRD 29,(2000),          Hf (298)=147.5 kcal/mole  REF = Colomina et al,
J. Chem. Thermo. 14,(1982),779.   Max Lst Sq Error Cp @ 200 K 0.69%
C6H4(C2H)CH=CH*   T 8/98C 10.H  7.   0.   0.G   200.000  6000.000  B 127.16558 1
 2.00959894E+01 2.63995288E-02-9.54744190E-06 1.54881511E-09-9.30556695E-14    2
 6.51277376E+04-8.23946362E+01-2.07613880E+00 7.07561989E-02-2.27951149E-06    3
-6.32032786E-08 3.52065658E-11 7.18269865E+04 3.55334903E+01 7.42244582E+04    4

C10H7O Naphtoxy radical       STATWT = 2  Ia = 42.113955  Ib = 75.532463
Ic = 117.64642  NU=3134,3132,3124,3114,3110,3099,3098,1598,1555,1545,1511,1479,
1431,1419,1366,1353,1275,1234,1210,1151,1134,1116,1068,1044,1019,964,942,933,
866,865,855,787,767,747,706,701,639,563,524,516,458,453,445,401,279,225,167,120.
REF = Curran et al, 29,(2000),        Hf(298)= 27.6 kcal    REF = NIST 1994
Max Lst Sq Error Cp @ 200 K 0.7%
1-C10H7O* Radical T 7/98C 10.H  7.O  1.   0.G   200.000  6000.000  B 143.16498 1
 2.10591364E+01 2.82563070E-02-1.03328686E-05 1.68867034E-09-1.01974767E-13    2
 4.09143507E+03-8.84963398E+01-1.15176448E+00 6.11354512E-02 3.20151083E-05    3
-9.94285290E-08 4.79990043E-11 1.14058756E+04 3.25584836E+01 1.38887800E+04    4

C10H8  AZULENE     SYGMA=2  IAIBIC=1.88E-112 NU=3070,1690,1634,1621,1577,1535,
1482,1442,1389,1367,1295,1290,1265,1201,1150,1114,1055,1045,1036,1007,978,963,
945,899,855,820,787,766,940,724,708,694,671,653,610,510,475,350,280,200,3070(7),
175  REF=KOVATS , GUNTHARD & PLATTNER  MAX LST SQ ERROR CP @ 1300 K 0.87 %.
HF298=66.9 KCAL REF=STULL WESTRUM & SINKE
H8C10 AZULENE     T 9/82H   8C  10    0    0G   300.000  5000.     B 128.1732  1
 0.19087189E+02 0.28716661E-01-0.98752744E-05 0.14930039E-08-0.81601501E-13    2
 0.24276551E+05-0.81975790E+02-0.48537226E+01 0.73454738E-01-0.38748985E-05    3
-0.53900077E-07 0.28514219E-10 0.31977461E+05 0.47005760E+02 0.33667889E+05    4
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C10H8 Naphthalene SIGMA = 4  Ia = 26.8532  Ib = 67.4189  Ic = 94.2721
Nu= 3092,3090,3065,3060(2),3058,3030,3027,1628,1595,1577,1509,1463,1443,1389,
1380,1361,1265,1242,1209,1168,1145,1144,1125,1025,1008,980,970,958,950,936,
877,876,841,782,778,761,725,617,581,512,506,472,466,386,359,191,176.
REF = REF=CHEN,KUDCHAKER  & WILHOIT  JPCRD 8,(1979),527.     Hf(298)= 35.99 kcal
REF = Colomina et al, J. Chem. Thermo. 14,(1982),779.    Max Lst Sq Error Cp
@ 200 K 0.96%
C10H8 Naphthalene T 7/98C 10.H  8.   0.   0.G   200.000  6000.000  B 128.17352 1
 1.86129884E+01 3.04494175E-02-1.11224825E-05 1.81615474E-09-1.09601281E-13    2
 8.91578988E+03-8.00230396E+01-1.04919475E+00 4.62970781E-02 7.07591636E-05    3
-1.38408111E-07 6.20475407E-11 1.59848987E+04 3.02121626E+01 1.81107678E+04    4

C10H7OH Naphtol     Ia = 43.59471  Ib = 75.763548  Ic = 119.35822   Ir = 0.12236
ROSYM  = 2  V(2) = 3.468 kcal     NU = 3652,(3135),3067,2967,2923,2859,1946,
1905,1847,1828,1820,1718,1682,1634,1591,1520,1462,1404,1359,1277,1239,1189,1152,
1089,1081,1041,1014,(943,925,894),874,(848,819),790,766,(742),715,(704),583,570,
522,479,467,459,(453,411,286,255,220,170). REF = NIST Webbook 1997
Hf(298)= -7.36 kcal     REF =Da Silva et al. J. Chem Thermo. 20,(1988),969
Max Lst Sq Error Cp @ 1300 K 0.63%
NAPHTOL C10H8O I  T 7/98C 10.H  8.O  1.   0.G   200.000  6000.000    144.17292 1
 2.08930252E+01 3.10560066E-02-1.14407562E-05 1.87872866E-09-1.13823881E-13    2
-1.35886443E+04-8.88597101E+01-2.08768263E+00 7.68099506E-02-1.53593023E-05    3
-4.04657632E-08 2.33759779E-11-6.29056385E+03 3.43331051E+01-3.70367466E+03    4

C10H9  2-Hydro-Naphthalene Radical   STATWT = 2   Ia = 27.990458  Ib = 71.911452
Ic = 99.39347  NU= 3126,3110,3106,3095,3093,3090,3082,2851,2843,1636,1575,1528,
1473,1430,1416,1397,1375,1353,1319,1260,1218,1185,1150,1137,1135,1112,1029,1016,
949,928,900,899,891,886,831,764,761,734(2),678,667,594,525,491,484,445,390,344,
256,169,125.  REF =Curran et al, JPCRD 29,(2000),       Hf(298)= 54.86 kcal/mole
REF = Marinov et al, Comb. Sci. Technol. 116-117,(1996), 211.   Max Lst Sq Error
Cp @ 200 K  0.87%
C10H9 2-hydro Rad T 7/98C 10.H  9.   0.   0.G   200.000  6000.000  B 129.18146 1
 1.96879334E+01 3.20520257E-02-1.16715110E-05 1.90182471E-09-1.14603906E-13    2
 1.80099777E+04-8.29833882E+01-1.21356342E+00 5.48913745E-02 5.55281159E-05    3
-1.24860759E-07 5.75105005E-11 2.52575495E+04 3.28077928E+01 2.76064663E+04    4

C10H10 1,2-Dihydro-Naphthalene    SYMNO = 1  Ia = 29.06046  Ib = 72.379179
Ic = 98.883363   Nu = 3123,3108,3106,3092,3087,3082,3007,3000,2930,2915,1644,
1606,1572,1480,1446,1440,1429,1388,1353,1328,1311,1268,1216,1201,1180,1154,1151,
1141,1105,1037,1014,998,945,936,919,902,879,851,795,773,738,732,682,672,574,
540,490,472,408,376,343,258,148,131.  REF = Curran et al JPCRD 29,(2000),
Hf(298)= 28. Kcal  REF = Pedley & Rylance 1977   Max Lst Sq Error Cp @ 6000 K
0.59%
1-2-C10H10        T 7/98C 10.H 10.   0.   0.G   200.000  6000.000  B 130.18940 1
 1.92211178E+01 3.51247274E-02-1.27719042E-05 2.07903232E-09-1.25191968E-13    2
 4.39595221E+03-8.19390283E+01-1.92135165E-01 4.50394780E-02 8.64482370E-05    3
-1.56640588E-07 6.88727900E-11 1.16587583E+04 2.82951960E+01 1.40900666E+04    4

C10H16 JP-10  TETRAHYDRO-DI-CYCLOPENTADIENE also 4,7-Methano-1H-indene,
octahydro   SIGMA=1  HF298=-14.4+/-1. KCAL    VERY ROUGH APPROXIMATION 200-500 K
REF=Boyd, Sanwal, Shary-Tehrany & McNally J. PHYS. CHEM 75, (1971), 1264  EXTRA-
POLATED USING BOZZELLI & RITTER'S POLYNOMIALS
C10H16 JP-10      T12/91C  10H  16    0    0G   298.150  5000.000  F 136.23704 1
 0.21113628E+02 0.54254218E-01-0.21542624E-04 0.38479521E-08-0.25570003E-12    2
-0.20185765E+05-0.10073137E+03-0.11931219E+02 0.11571185E+00-0.45682163E-04    3
-0.69541629E-08 0.62193353E-11-0.84176986E+04 0.80128431E+02-0.72463681E+04    4
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Table 4 (continued)

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C10H19  1,Decenyl-4/5 CH2=CH-CH2-CH*-C5H11 Estimated using NIST-94. EXTRAPOLATED
from 1600 K USING WILHOIT'S POLYNOMIALS.  MAX LST SQ ERROR CP @ 1500 K 0.37%
HF298=67.9 KJ
C10H19  1-deceny  T 3/00C 10.H 19.   0.   0.G   298.150  5000.000  D 139.26086 1
 2.37590285E+01 5.13629059E-02-1.91904058E-05 3.36468639E-09-2.24370651E-13    2
-3.77181269E+03-8.85479830E+01 4.94076996E+00 6.39894278E-02 5.64163880E-05    3
-1.18883384E-07 5.24354590E-11 3.56097203E+03 1.85984224E+01 8.16644637E+03    4

C10H19  1,Decenyl-3 CH2=CH-CH*-C6H11 Estimated using NIST-94. EXTRAPOLATED from
1600 K USING WILHOIT'S POLYNOMIALS. MAX LST SQ ERROR CP @ 1500 K 0.76%
HF298=2.6 KJ
C10H19 1-decenyl  T 3/00C 10.H 19.   0.   0.G   298.150  5000.000  D 139.26086 1
 2.47482587E+01 5.14076858E-02-1.95828774E-05 3.47928330E-09-2.34079322E-13    2
-1.20167044E+04-9.35125879E+01-2.43834540E+01 2.82492767E-01-4.99496066E-04    3
 4.71514086E-07-1.70502072E-10-1.41157149E+03 1.41304170E+02 3.12706341E+02    4

C10H20 1-DECENE  Estimated using NIST-94. EXTRAPOLATED from 1600 K
USING WILHOIT'S POLYNOMIALS. MAX LST SQ ERROR CP @ 1500 K 0.46% HF298=-123.9 KJ
C10H20 1-Decene   T 3/00C 10.H 20.   0.   0.G   298.150  5000.000  D 140.26880 1
 2.43784941E+01 5.33879655E-02-1.99613482E-05 3.50081948E-09-2.33453944E-13    2
-2.72997767E+04-9.49537106E+01 3.47605427E+00 7.65120954E-02 2.93696959E-05    3
-8.88008675E-08 4.03372569E-11-1.94418036E+04 2.22701279E+01-1.49016599E+04    4

C10H20 2-DECENE-trans  Estimated using NIST-94. EXTRAPOLATED from 1600 K
USING WILHOIT'S POLYNOMIALS. MAX LST SQ ERROR CP @ 1500 K 0.35% HF298=-136.2 KJ
C10H20 2-decene-  T 3/00C 10.H 20.   0.   0.G   298.150  5000.000  D 140.26880 1
 2.38184351E+01 5.39053060E-02-2.01372708E-05 3.52862934E-09-2.35146707E-13    2
-2.85920995E+04-9.22267124E+01 3.74608499E+00 7.49426004E-02 2.93412818E-05    3
-8.58775012E-08 3.85491667E-11-2.09365775E+04 2.07575646E+01-1.63810014E+04    4

C10H20 3-DECENE-trans  Estimated using NIST-94. EXTRAPOLATED from 1600 K
USING WILHOIT'S POLYNOMIALS. MAX LST SQ ERROR CP @ 1500 K 0.34% HF298=-135.5 KJ
C10H20 3-decene-  T 3/00C 10.H 20.   0.   0.G   298.150  5000.000  D 140.26880 1
 2.39013980E+01 5.38878964E-02-2.01285612E-05 3.52665091E-09-2.34996859E-13    2
-2.85617759E+04-9.25811186E+01 2.73154321E+00 7.88862849E-02 2.51641756E-05    3
-8.52509662E-08 3.92427894E-11-2.06898473E+04 2.57333929E+01-1.62968112E+04    4

N-C10H21  N-DECYL-1 RADICAL  API-TRC 8/83 DATA TO 3000. K EXTRAPOLATED USING
WILHOIT'S POLYNOMIALS. MAX LST SQ ERROR CP @ 1200 K 0.61 %  HF298=-57.74 KJ
{NIST 94 estimate HF298=-43.8 KJ}
N-C10H21        N-P10/83C  10H  21    0    0G   300.000  5000.000  B 141.2759  1
 0.21322128E 02 0.61573524E-01-0.23849483E-04 0.42209116E-08-0.27889307E-12    2
-0.17967809E 05-0.75656952E 02 0.29391508E 01 0.84870219E-01 0.14858843E-04    3
-0.72042951E-07 0.32363209E-10-0.11598363E 05 0.25938156E 02-0.69445689E 04    4

N-C10H21  N-DECYL-2 RADICAL  Estimated using NIST-94. EXTRAPOLATED from 1600 K
USING WILHOIT'S POLYNOMIALS. MAX LST SQ ERROR CP @ 1500 K 0.34 %  HF298=-58.1 KJ
C10H21 2-decyl    T 3/00C 10.H 21.   0.   0.G   298.150  5000.000  D 141.27674 1
 2.45312418E+01 5.55320406E-02-2.07239376E-05 3.63129156E-09-2.42045771E-13    2
-1.95025142E+04-9.36436619E+01 6.86951665E+00 5.57425508E-02 8.72153686E-05    3
-1.51902528E-07 6.46180282E-11-1.20143727E+04 9.80863792E+00-6.98778401E+03    4

N-C10H21  N-DECYL-3 or 4 RADICAL  Estimated using NIST 94 EXTRAPOLATED from 1600
K USING WILHOIT'S POLYNOMIALS. MAX LST SQ ERROR CP @ 1500 K 0.38% HF298=-58.2 KJ
C10H21 3/4-decyl  T 3/00C 10.H 21.   0.   0.G   298.150  5000.000  D 141.27674 1
 2.44433242E+01 5.56583435E-02-2.07686906E-05 3.63847992E-09-2.42490501E-13    2
-1.94765658E+04-9.31425601E+01 6.86951665E+00 5.57425508E-02 8.72153686E-05    3
-1.51902528E-07 6.46180282E-11-1.20263999E+04 9.80863792E+00-6.99981117E+03    4
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C10H22 liq. Decane REF=I.Barin 1987  HF298liq=-301.038 kJ
C10H22(L)          B01/00C 10.H 22.   0.   0.L   298.150   446.830  C 142.28468 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00 3.77595368E+01 5.43284903E-04-1.44050795E-06    3
 1.25634293E-09 0.00000000E+00-4.74783720E+04-1.64025285E+02-3.62064632E+04    4

N-C10H22  N-DECANE  Bureau of Mines Bull 666 1974 DATA TO 1500. K EXTRAPOLATED
USING WILHOIT'S POLYNOMIALS. MAX LST SQ ERROR CP @ 1300 K 0.70 %
HF298=-59.64 kcal
N-C10H22 DECANE   T 5/99C 10.H 22.   0.   0.G   200.000  6000.000  B 142.28468 1
 2.94782956E+01 4.90518943E-02-1.70317179E-05 2.72919300E-09-1.63370772E-13    2
-4.43022624E+04-1.24062121E+02 1.54328173E+01-1.32979232E-02 2.82480581E-04    3
-3.65923298E-07 1.45372117E-10-3.58632831E+04-2.79454341E+01-3.00118419E+04    4

C10H7C*O Naphthaldehyde radical    STATWT = 2  Ia = 51.315652  Ib = 100.57912
Ic = 151.92712   NU=3128,3126,3118,3114,3107,3099,3097,1809,1622,1584,1562,1507,
1447,1434,1374,1379,1360,1243,1222,1194,1155,1149,1133,1071,1022,994,962,948,
927,905,854,846,791,782,763,727,723,624,612,523,511,494,459,430,392,327,213,178,
170,153,78.3      REF = Curran et al. JPCRD 29,(2000),          Hf(298)= 41.8
kcal   REF = Marinov et al, Comb. Sci. Technol, 116-117,(1996),211.
Max Lst Sq Error Cp @ 1300 K 0.55%
1-C10H7C*O  Radic T 7/98C 11.H  7.O  1.   0.G   200.000  6000.000  B 155.17598 1
 2.27592940E+01 2.95236092E-02-1.08144575E-05 1.76929286E-09-1.06921871E-13    2
 1.06007552E+04-9.54682191E+01 2.47024671E-01 6.23078127E-02 3.25268900E-05    3
-9.98773421E-08 4.79264315E-11 1.80787951E+04 2.74600245E+01 2.10344566E+04    4

C10H7CHO Naphthaldehyde    Ia = 50.406846   Ib = 104.13646  Ic = 154.54331
Ir = 0.148  ROSYM = 2   V(2) = 4.9 kcal/mole   NU=3399,3069,2837,2724,2355,2322,
1945,1811,1775,1713,1631,1588,1579,1517,1460,1411,1404,1373,1347,1252,1221,1218,
1172,1155,1141,1079,1058,1027,971,955,947,921,888,862,806,789,770,758(2),713,
651,616,527,507,492,463,421,389,342,227,206,180,112.    REF =NIST Webbook 1997
Hf(298)=  7.3 kcal   REF = NIST 1994    Max Lst Sq Error Cp @ 1300 K 0.66%
1-C10H7CHO         T 7/98C 11.H  8.O  1.   0.G   200.000  6000.000  B 156.18392 1
 2.42593357E+01 3.16036997E-02-1.18467358E-05 1.96728679E-09-1.20096869E-13    2
-7.83388781E+03-1.07718994E+02-3.75140208E-01 6.11007395E-02 4.92528177E-05    3
-1.17296000E-07 5.31810720E-11 8.41138142E+02 2.88322573E+01 3.67348166E+03    4

C11H9   1-C10H7CH2* 1- Naphtyl Methylene radical   STATWT = 2  Ia = 41.8986174
Ib = 74.3823227  Ic = 116.2722486  Nu=3193,3128,3121,3118,3106,3105,3099,3096,
3094,1610,1559,1537,1500,1486,1439,1433,1395,1362,1347,1282,1230,1214,1168,
1151,1135,1090,1075,1032,943,941,927,907,862,850,834,779,775,753,718,710,701,
619,566,547,493,492,467,436,433,396,303,232,169,95.8    REF = Curran et al,
JPCRD 29,(2000),            Hf (298)= 65.2  kcal   REF = NIST 94 estimate
Max Lst Sq Error Cp @ 200 K 0.71%
1-C10H7-CH2*       T 7/98C 11.H  9.   0.   0.G   200.000  6000.000    141.19246 1
 2.18977539E+01 3.26102636E-02-1.18401218E-05 1.92574628E-09-1.15903442E-13    2
 2.24571098E+04-9.41050741E+01-2.53234304E+00 7.32920338E-02 2.02974707E-05    3
-9.36547823E-08 4.70753594E-11 3.02906705E+04 3.79638513E+01 3.28097266E+04    4

1-C10H7CH3 1-Methyl-Naphthalene  Ia= 43.9442164  Ib= 74.3379622  Ic= 117.7309994
Ir = 0.51387   ROSYM = 3    V(3) = 0.01 kcal/mole   Nu= 3107,3074,3016,2982,
2956,2978,2749,2321,1924,1856,1820,1795,1744,1680,1601,1512,1470,1447,1398,
(1360),1261,(1252),1211,1166,1109,1102,1084,1077,1049,(1026,1022),960,(948,934,
914,874),858,(846,840),787(2),771,711,699,(616),537,532,490,(462),460,(427,404,
269,241,179,161).   REF = NIST Webbook 1997 spectrum    Hf(298)= 27.75 kcal
REF = Speros & Rossini J. Phys. Chem. 64,(1960),1723.    Max Lst Sq Error Cp @
200 K 0.68%
1-C10H7-CH3        T 7/98C 11.H 10.   0.   0.G   200.000  6000.000  B 142.20040 1
 2.17939213E+01 3.60214098E-02-1.33228698E-05 2.19304403E-09-1.33071380E-13    2
 3.16261439E+03-9.48675403E+01-1.03043715E+00 6.03358177E-02 5.45655719E-05    3
-1.22769251E-07 5.54507327E-11 1.13241014E+04 3.22970611E+01 1.39642625E+04    4
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N-C11H24  UNDECANE   REF=TRC11/75 TO 1000 K. EXTRAPOLATED USING WILHOIT'S
POLYNOMIALS.   HF298=-64.60 kcal
N-UNDECANE        T 5/99C 11.H 24.   0.   0.G   200.000  6000.000  C 156.31156 1
 3.41070654E+01 5.07865991E-02-1.73797396E-05 2.76048145E-09-1.64248726E-13    2
-4.88486250E+04-1.47546600E+02 1.67589055E+01-1.35771822E-02 3.08216871E-04    3
-4.00562662E-07 1.59274225E-10-3.89076869E+04-3.15628516E+01-3.25077966E+04    4

O-BIPHENYL RADICAL D9 STATWT=2 SIGMA=1 NU=2287,2280,1571,1412,1188,960,869,835,
688,300,2286,2218,1531,1328,1266,1010,826,790,565,110,832,744,627,540,466,160,
790,652,346,2288,2284,2281,1568,1346,983,846,816,590,2285,2279,1566,1345,1272,
1070,840,835,589,355,775,646,539,500,393,232,660,300  IA=33.21      IB=170.83
IC=194.34 ROSYM=2 IR=8.285 V(2)=1500 REF=BURCAT ZELEZNIK& MCBRIDE HF298=386.5 KJ
O-C12D9          O-L12/84C 12.D  9.   0.   0.G   300.000  5000.000  B 162.25892 1
 0.30123199E 02 0.28328255E-01-0.10366540E-04 0.16593338E-08-0.96527116E-13    2
 0.33207789E 05-0.13520447E 03-0.73299396E 00 0.89836895E-01-0.13731275E-04    3
-0.59427020E-07 0.33702430E-10 0.42943094E 05 0.30028793E 02 0.46486410E 05    4

BIPHENYL D10 REF=BURCAT ZELEZNIK & MCBRIDE HF298=138.41 KJ STATWT=1 SIGMA=4.
NU=SAME AS FOR C12D9 AND ADDITIONAL 2284,952,783  IA=34.79 IB=171.43 IC=196.03
ROSYM=2 IB=8.697 V(2)=1500.
C12D10            L12/84C 12.D 10.   0.   0.G   300.000  5000.000  B 164.27302 1
 0.30905060E 02 0.30349988E-01-0.11095048E-04 0.17755810E-08-0.10332327E-12    2
 0.28834453E 04-0.14245210E 03-0.15793486E 01 0.95059574E-01-0.14532071E-04    3
-0.62645597E-07 0.35530079E-10 0.13137422E 05 0.31516678E 02 0.16647502E 05    4

C12H7   C10H7CC* 1-Ethynyl  Naphthalene Radical    STATWT = 2  Ia = 56.378083
Ib = 87.350853   Ic = 143.58234    NU=3143,3132,3123,3122,3113,3103,3102,1805,
1604,1558,1541,1503,1438,1429,1393,1374,1324,1255,1221,1198,1163,1151,1132,1076,
1030,1015,967,948,934,895,861,848,788,779,755,723,648,628,557,526,523,471,452,
437,411,328,306,184,165,118,92.2  REF = Curran et al. 29,(2000),463
Hf(298)= 166.1 kcal     REF = NIST 1994   Max Lst Sq Error Cp @ 200 K  0.56
1-C10H7-CC* Radi  T 7/98C 12.H  7.   0.   0.G   200.000  6000.000  B 151.18758 1
 2.28546479E+01 2.94181299E-02-1.07719402E-05 1.76194604E-09-1.06462481E-13    2
 7.31301345E+04-9.62295750E+01-1.91438001E-01 6.57353329E-02 2.42664513E-05    3
-9.15358223E-08 4.48817973E-11 8.06649452E+04 2.89829391E+01 8.35842882E+04    4

C12H8  ACENAPHTHYLENE  SIGMA=2  IAIBIC=463 E-114 HF298=259.7 kJ  REF=DOROFEEVA
& Gurvich IVTAN Preprint # 1-263 1989. {HF298=258+/-5.9 kJ REF=NIST Webbook}
Extrapolated to 5000 K using Wilhoit's polynomials. Max Lst Sq Error Cp @ 1300 K
0.47 %
C12H8  ACENAPHTH  T12/00C 12.H  8.   0.   0.G   200.000  5000.000    152.19552 1
 1.93183637E+01 3.90205238E-02-1.63352587E-05 3.10041991E-09-2.19199281E-13    2
 2.15445149E+04-8.32372261E+01-2.81264181E+00 7.04681002E-02 3.15341955E-05    3
-1.05176189E-07 5.08713845E-11 2.88462829E+04 3.75755975E+01 3.12345526E+04    4

C12H8    C10H7CCH 1-Ethynyl  Naphthalene     Ia = 57.461762  Ib =  89.485562
Ic = 146.94732   Ir = 0. NU=3413,3132,3129,3120,3117,3107,3099,3096,2142,1621,
1586,1574,1510,1451,1433,1393,1384,1344,1255,1224,1215,1163,1153,1139,1073,1029,
1013,954,938,922,822,850,848,787,781,762,724,686,635,596,571,565,532,507,479,
462,441,431,359,337,200,171,132,102.   REF = Curran et al. JPCRD 29,(2000),
Hf(298)= 90.6 kcal    REF = Wang & Frenklach J. Phys. Chem 98,(1994),11465.
Max Lst Sq Error Cp @ 1300 K 0.53%
C10H7-CCH         T 7/98C 12.H  8.   0.   0.G   200.000  6000.000  B 152.19552 1
 2.34108373E+01 3.12979308E-02-1.13777419E-05 1.85217551E-09-1.11546889E-13    2
 3.49196941E+04-1.00594596E+02-2.59169367E+00 8.63306190E-02-1.76590976E-05    3
-5.26006488E-08 3.15924760E-11 4.27720678E+04 3.73574503E+01 4.55914299E+04    4
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Table 4 (continued)

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C12H9  1-C10H7CH=CH* 1-Naphtyl-Vinyl radical     STATWT = 2    Ia = 52.035181
Ib = 97.671628   Ic = 148.44918  Ir = 2.73405   ROSYM = 2  V(2)= 4.4 kcal
NU = 3173,3130,3124,3120,3110,3106,3097,3094,3030,1621,1607,1590,1568,1512,1452,
1433,1393,1378,1353,1256,1228,1220,1206,1161,1154,1139,1079,1032,1003,948,934,
915,886,876,863,843,832,782,779,762,719,695,661,610,576,528,506,480,462,427,403,
321,255,193,172,116.   REF = Curran et al. JPCRD 29,(2000),463
Hf(298)= 112.3 kcal    REF = Wang & Frenklach J. Phys. Chem 98,(1994),11465.
Max Lst Sq Error Cp @ 200 K 0.72%
1-C10H7-CH=CH*    T 7/98C 12.H  9.   0.   0.G   200.000  6000.000  B 153.20346 1
 2.44441957E+01 3.26961470E-02-1.18995546E-05 1.93488254E-09-1.16386321E-13    2
 4.52471489E+04-1.05926333E+02-1.42935703E+00 7.39465043E-02 2.97653847E-05    3
-1.09318395E-07 5.40951470E-11 5.35782225E+04 3.42505526E+01 5.65112316E+04    4

C10H7C*=CH2  1,-Vinyl  Naphthalene   STATWT = 2  Ia = 58.410493  Ib = 92.899705
Ic = 150.72887   Ir =3.231365   ROSYM = 2  V(2) = 4.6 kcal   NU = 3132,3126,
3116,3114,3104,3101,3095,3052,2998,1882,1607,1555,1524,1494,1435,1429,1413,1374,
1358,1304,1254,1215,1166,1159,1146,1130,1075,1034,1013,948,947,922,917,852,847,
838,818,776,767,749,706,683,611,578,532,524,483,474,431,419,402,339,257,176,163,
125.  REF = Curran et al. JPCRD 29,(2000),463          Hf(298)= 98.52 kcal
REF = Marinov et al, Comb. Sci. Technol, 116-117,(1996),211.     Max Lst Sq
Error  Cp @ 200 K  0.65 %.
1-C10H7-C*=CH2    T 7/98C 12.H  9.   0.   0.G   200.000  6000.000  B 153.20346 1
 2.45125261E+01 3.26372895E-02-1.18731749E-05 1.93107796E-09-1.16216496E-13    2
 3.83327553E+04-1.05844161E+02-1.43370275E+00 7.71544298E-02 1.83225763E-05    3
-9.54787152E-08 4.85269141E-11 4.65789858E+04 3.40801712E+01 4.95769059E+04    4

C12H9  O-BIPHENYL RAD  SIGMA=1 STATWT=2  IA=28.895  IB=148.3008  IC=178.1957
IR=7.22  SIGMAR=2  V(2)=1000.  NU=3083(2),3031,1583,1497,1275,1157,1025,1019,
996,733,841,399,3052,1603,1448,1357,1185,1145,1032,606,302,904,778,695,543,487,
120,955,775,696,531,470,246,970,834,397,3086(2),3067(2),1608,1440,1397,1182,
1162(2),1077,606,140,3038,1583,1497,1012,993,738   REF=BURCAT ZELEZNIK AND
MCBRIDE   MAX LST SQ ERROR CP @ 1300 K 0.84 % . HF298=427.73 KJ
O-BIPHENYL RAD  O-L12/84C 12.H  9.   0.   0.G   300.000  5000.000  B 153.20310 1
 0.23851303E 02 0.31960227E-01-0.11076719E-04 0.16847825E-08-0.92641173E-13    2
 0.40171297E 05-0.10270549E 03-0.31376228E 01 0.82217276E-01-0.40171444E-05    3
-0.60809782E-07 0.32074482E-10 0.48868754E 05 0.42730362E 02 0.51444448E 05    4

C12H9Cl   CHLOROBIPHENYL  CALCULATED USING BOZZELLI & RITTER'S PROGRAM  AND
EXTRAPOLATED TO 5000 K   SIGMA=2  HF298=148.55 kJ
C12H9CL           T 2/92C  12H   9CL  1    0G   298.150  5000.000  E 188.65616 1
 0.25609923E+02 0.35292178E-01-0.13556100E-04 0.23746797E-08-0.15591758E-12    2
 0.58630132E+04-0.11039461E+03-0.72831130E+01 0.11977430E+00-0.82814312E-04    3
 0.15585591E-07 0.42704031E-11 0.15413066E+05 0.61459201E+02 0.17866357E+05    4

C12H9N  CARBAZOLE, 9-AZAFLUORENE, DIBENZO-PYRROLE  SIGMA=2  IAIBIC=938534.8
NU=3421,3094,3084,3077,3055,3050,3039,3030,2940,1625,1594,1576,1490,1481,1452,
1449,1380,1334,1320,1288,1233,1205,1204,1158,1152,1136,1118,1107,1022,1012,995,
989,939,926,910,893,880,856,835,771,747,741,737,722,691,658,616,566,548,505,467,
445,425,410,310,299,222,220,139,104.   HF298=200.7+/-4.9 kJ    REF= Das et al
JPCRD 22 (1993),659    Max Lst Sq Error Cp @ 200 K 0.79%
C12H9N  CARBAZOLE T 5/99C 12.H  9.N  1.   0.G   200.000  6000.000  B 167.21020 1
 2.55905657E+01 3.50572236E-02-1.28150596E-05 2.09379140E-09-1.26416159E-13    2
 1.21368335E+04-1.15714967E+02-2.39694034E+00 7.70529957E-02 3.99731799E-05    3
-1.26020660E-07 6.11915294E-11 2.12953973E+04 3.66013145E+01 2.41385241E+04    4
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Table 4 (continued)

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C12H10    1-C10H7CH=CH2 Vinyl 1-Naphthalene   Ia = 52.618944  Ib = 100.59202
Ic = 152.02459   Ir = 3.39278   ROSYM = 2   V(2) = 3.06 kcal     Nu = 3168,3130,
3124,3120,3110,3105,3096,3093,3083,3074,1644,1620,1591,1576,1513,1455,1435,1416,
1393,1379,1348,1295,1250,1226,1217,1164,1154,1139,1089,1035,1021,1000,989,948,
935,915,886,883,847,843,788,780,768,722,702,685,587,527,498,482,462,428,397,334,
250,199,175,119.    REF =Curran et al. JPCRD 29,(2000),463    Hf(298)= 51.4 kcal
REF = NIST 1994   Max Lst Sq Error Cp @ 200 K 0.75%
1-C10H7CH=CH2      T11/98C 12.H 10.   0.   0.G   200.000  6000.000  B 154.21140 1
 2.36421335E+01 3.60544766E-02-1.31138294E-05 2.13119639E-09-1.28115416E-13    2
 1.46625473E+04-1.02784235E+02-1.19668570E+00 7.06115758E-02 4.27863652E-05    3
-1.21989834E-07 5.83744402E-11 2.29191651E+04 3.30370914E+01 2.58653366E+04    4

C12H10 BIPHENYL  SIGMA=4  SIGMA BARRIER=2  IA=29.6792  IB=148.4348  IC=178.114
IR=7.4198   V(2)=1000.   NU=3083(2),3052(2),3031,1583(2),1497(2),1275,1151,1025,
1019,996,733,969,841,399,1603,1448,1357,1185,1145,1032,606(2),302,904,778,695,
543,487,120,955,775,696,531,470,246,3086(2),3067(2),1608,1440,1397,1182,1162(2),
1077,140,970,834,397,3038,1046,1012,993,738   REF=KATON AND LIPPINCOTT   MAX LST
SQ ERROR @ 1300 K 0.85 % HF298=182.13 KJ. REF=BURCAT ZELEZNIK & MCBRIDE
C12H10 BIPHENYL   L12/84C 12.H 10.   0.   0.G   300.000  5000.000  B 154.21100 1
 0.24289017E 02 0.34006648E-01-0.11722408E-04 0.17729298E-08-0.96812532E-13    2
 0.10287000E 05-0.10802374E 03-0.40739527E 01 0.86973310E-01-0.42353613E-05    3
-0.64564460E-07 0.34150169E-10 0.19405965E 05 0.44741348E 02 0.21905340E 05    4

1-C10H7CH2CH2*  - Ethyl 1-Naphthalene Radical       STATWT = 2  Ia = 51.627582
Ib = 105.1585   Ic = 155.5285   Ir(-CH2CH2*) = 3.68853  ROSYM = 2  V(3)=3.0 kcal
Ir(-CH2*)=0.276085   ROSYM = 3  V(3) = 3.0 kcal     Nu=3193,3128,3119,3118,3104,
3103,3094,3092,3088,2954,2859,1623,1599,1581,1514,1456,1435,1429,1411,1397,1380,
1362,1289,1246,1220,1217,1180,1159,1154,1139,1083,1075,1031,1022,975,946,936,
913,887,850,836,806,781,778,757,717,692,617,589,527,514,508,472,462,426,400,319,
233,202,170,154.   REF = Curran et al. JPCRD 29,(2000),463    Hf(298)= 70. Kcal
REF = THERM estimate    Max Lst Sq Error Cp @ 200 K  0.64%.
C10H7-CH2CH2*      T 7/98C 12.H 11.   0.   0.G   200.000  6000.000  B 155.21934 1
 2.47911542E+01 3.71007852E-02-1.34341683E-05 2.17751785E-09-1.30703605E-13    2
 2.36520512E+04-1.07491651E+02-1.76566815E+00 8.31852329E-02 1.56729046E-05    3
-9.56306134E-08 4.90427294E-11 3.20816383E+04 3.56277471E+01 3.52251666E+04    4

1-C10H7CH*CH3  - Ethyl 1-Naphthalene Radical      STATWT = 2  Ia=51.627582
Ib=105.1585   Ic=155.5285   Ir(-CH*CH3)= 4.03467   ROSYM = 2   V(3)=2.9 kcal
Ir(-CH3)= 0.417138   ROSYM = 3   V(3)=2.8 kcal    Nu = 3193,3128,3119,3118,
3104,3103,3094,3092,3088,2954,2859,1623,1599,1581,1514,1456,1435,1429,1411,1397,
1380,1362,1289,1246,1220,1217,1180,1159,1154,1139,1083,1075,1031,1022,975,946,
936,913,887,850,836,806,781,778,757,717,692,617,589,527,514,508,472,462,426,400,
319,233,202,170,154.    REF = Curran et al. JPCRD 29,(2000),463
Hf(298)= 52.7 kcal  REF = NIST 94    Max Lst Sq Error Cp @200 K 0.63%
1-C10H7-CH*-CH3   T11/98C 12.H 11.   0.   0.G   200.000  6000.000  B 155.21934 1
 2.45873044E+01 3.73929821E-02-1.36001742E-05 2.21047875E-09-1.32883841E-13    2
 1.49850894E+04-1.05426141E+02-1.14973681E+00 7.78725206E-02 2.87023997E-05    3
-1.08719393E-07 5.37519164E-11 2.33370112E+04 3.42336399E+01 2.65195183E+04    4

C12H12  1-C10H7CH2CH3 1- Ethyl Naphthalene   Ia = 61.540903  Ib = 92.900467
Ic = 147.16558   Ir(C2H5)= 4.472813  ROSYM = 2  V(3) = 2.8 kcal
Ir(CH3)= 0.417138  ROSYM = 3  V(3)=2.8 kcal.    Nu= 3353,3265,3229,3172,3074,
2981,2950,2894,1919,1863,1832,1796,1682,1636,1600,1512,1476,1460,1458,1456,1437,
1399,1382,1369,1366,1326,1259,1246,1226,1216,1172,1154,1140,1087,1069,1048,1031,
1017,960,938,933,914,893,862,838,786,784,768,734,703,641,630,578,553,572,478,
462,429,421,316,289,203,186,171.  REF = NIST Webbook 1997    Hf(298)= 23.16 kcal
REF=Stull, Westroom & Sinke 1969.   Max Lst Sq Error Cp @ 1300 K 0.64%
1-C10H7-C2H5      T 7/98C 12.H 12.   0.   0.G   200.000  6000.000  B 156.22728 1
 2.53697727E+01 4.04594180E-02-1.49784208E-05 2.46402471E-09-1.49382751E-13    2
-8.20299732E+02-1.14459910E+02 1.98405802E-02 6.20844325E-02 7.79624479E-05    3
-1.55438421E-07 6.85371120E-11 8.47514808E+03 2.80182938E+01 1.16544980E+04    4
```

Table 4 (continued)

```
C10H7CH2CH2OH 1-Naphtyl-ethanol  Ia= 65.973401  Ib=130.12903  Ic=178.19701
Ir(-CH2CH2OH)=20.2848     ROSYM = 2   V(3)=2.87 kcal/mole  Ir(-CH2OH)=4.75277
ROSYM=2  V(3)=2.75 kcal  Ir(-OH)=0.139517  ROSYM=1  V(3)=1.03 kcal
Nu=3642,3129,3121,3120,3106,3102,3095,3094,3024,3012,2975,2902,1622,1597,1579,
1515,1469,1455,1448,1435,1396,1383,1380,1368,1347,1303,1248,1226,1221,1183,
1170,1159,1154,1140,1078,1060,1037,1029,984,948,934,916,913,876,858,836,826,
782,779,764,720,686,642,577,548,505,482,463,447,426,407,374,318,249,176,170.
REF = Curran et al. JPCRD 29,(2000),463          Hf(298)= -12.6  kcal
REF = NIST 1994    Max Lst Sq Error  Cp @ 200 K 0.68%
1-C10H7CH2CH2OH   T11/98C 12.H 12.O  1.   0.G   200.000  6000.000  B 172.22668 1
 2.58268752E+01 4.06457048E-02-1.47684231E-05 2.39996250E-09-1.44280394E-13    2
-1.85903264E+04-1.11344593E+02 1.48378862E-01 7.18508197E-02 5.76461168E-05    3
-1.42124444E-07 6.64389673E-11-9.83811550E+03 3.01527814E+01-6.34052999E+03    4

N-C12H26  DODECANE       REF=TRC11/75 TO 1000 K. EXTRAPOLATED USING WILHOIT'S
POLYNOMIALS.   HF298=-69.52 kcal
N-DODECANE        T 5/99C 12.H 26.   0.   0.G   200.000  6000.000  C 170.33844 1
 3.70187925E+01 5.54721488E-02-1.92079548E-05 3.08175574E-09-1.84800617E-13    2
-5.26984458E+04-1.61453501E+02 2.13264480E+01-3.86394002E-02 3.99476113E-04    3
-5.06681097E-07 2.00697878E-10-4.22475053E+04-4.85848300E+01-3.49836226E+04    4

C13H9N  ACRIDINE, 10-AZAANTHRACENE, DIBENZO[b,c]PYRIDINE  SIGMA=2
IAIBIC=1456147.2 E-117  NU=3085(2),3075,3055(2),3037(2),3014(2),1627,1622,1578,
1556,1516,1480,1464,1441,1402,1397,1373,1360,1317,1274,1266,1232,1168,1158,1140,
1121,1109(3),999,974,965,955,934,939,905,901,861,851,814,785,744,735,712,655,
617,600,581,523,477,469,417,401,275,240,217,156,139,106.   HF298=273.9+/-4.1 kJ
REF= Das et al JPCRD 22 (1993),659  Max Lst Sq Error Cp @ 200 K 0.89%
C13H9N  ACRIDINE  T 5/99C 13.H  9.N  1.   0.G   200.000  6000.000  B 179.22120 1
 2.58635113E+01 3.78898227E-02-1.39284598E-05 2.28395317E-09-1.38235768E-13    2
 2.04600506E+04-1.17880104E+02-8.48162121E-01 6.17087256E-02 8.87124926E-05    3
-1.77383638E-07 7.97811734E-11 2.99816376E+04 3.14075642E+01 3.29424103E+04    4

C13H9N PHENANTHRIDINE,  9-AZAPHENANTHRENE, 3,4-BENZOQUINOLINE  SIGMA=2
IAIBIC=1612079.0 E-117  NU=3082,3072,3064,3037,3047,3037,3034,3019,3002,1615,
1600,1587,1575,1525,1485,1455,1445,1425,1405,1390,1345,1290,1245,1227,1190,1173,
1163,1135,1110,1094,1046,1035,1001,970,943,895,876,874,832,819,791,775,750,725,
713,712,711,620,576,548,536,505,494,460,435,415,408,395,279,240,234,170,108.
HF298=240.5+/-4.2 kJ  REF= Das et al JPCRD 22 (1993),659   Max Lst Sq Error Cp
@ 1300 K 0.60%
C13H9N PHENANTHRI T 5/99C 13.H  9.N  1.   0.G   200.000  6000.000  B 179.22120 1
 2.65281408E+01 3.72382530E-02-1.36796636E-05 2.24215437E-09-1.35664146E-13    2
 1.63827924E+04-1.21651719E+02-3.42969371E+00 8.74937697E-02 2.13315768E-05    3
-1.06800353E-07 5.35979203E-11 2.60563650E+04 4.04426399E+01 2.89253366E+04    4

C14H10 ANTHRACENE SIGMA=4  IA=39.0139  IB=185.153  IC=224.165  NU=390,624,753,
1007,1159,1260,1402,1478,1559,3028,3050,3081,139,488,760,860,980,236,473,739,
948,234,652,907,1146,1271,1316,1447,1625,3023,3056,3083,288,526,775,886,915,970,
599,809,999,1063,1166,1344,1398,1455,1538,3050,3092,390,523,901,1102,1180,1223,
1334,1490,1633,3055,3071,105,166,468,727,876,952  HF298= 230.1 KJ REF=KUDCHADKER
KUDCHADKER & ZWOLINSKI J. Chem. Thermodynamics 11, (1979), 1051  MAX LST SQ
ERROR @ 200 K 0.87%.
C14H10 ANTHRACENE T 1/94C  14H  10    0    0G   200.000  6000.000  B 178.23340 1
 0.26567127E+02 0.39790904E-01-0.14577610E-04 0.23850396E-08-0.14413090E-12    2
 0.14850923E+05-0.12283160E+03-0.15665980E+01 0.69536302E-01 0.78609880E-04    3
-0.17056214E-06 0.78003880E-10 0.24656643E+05 0.33282196E+02 0.27674511E+05    4
```

Table 4 (continued)

```
C14H10 PHENANTRENE  SIGMA=2  IA=51.7329  IB=147.737  IC=199.470  NU=247,408,548,
711,832,1038,1094,1144,1163,1203,1247,1304,1352,1431,1443,1526,1602,1626,3002,
3037,3057,3072,3082,123,279,395,513,594,726,763,791,880,946,969,108,234,426,441,
494,713,735,819,874,951,441,536,619,712,876,1001,1040,1095,1173,1227,1282,1340,
1430,1458,1502,1572,1616,3019,3034,3047,3064,3094  HF298=207.1 KJ REF=KUDCHADKER
KUDCHADKER & ZWOLINSKI J.Chem. Thermodynamics 11, (1979), 1051. MAX LST SQ ERROR
@ 200 K 0.73%.
C14H10 PHENANTHRE T 1/94C  14H  10    0    0G   200.000  6000.000  B 178.23340 1
 0.26602474E+02 0.39769744E-01-0.14572026E-04 0.23843296E-08-0.14409548E-12    2
 0.12132838E+05-0.12266672E+03-0.33646717E+01 0.85073271E-01 0.37531110E-04    3
-0.12664499E-06 0.61445705E-10 0.22019878E+05 0.40596218E+02 0.24908263E+05    4

C14H14 BIBENZYL C6H5C2H4C6H5  CALCULATED USING BENSON'S GROUP ADDITIVITY
METHOD. EXTRAPOLATED AND ESTIMATED BY B.M. COLKET (UNPUBLISHED).
HF298=143.51 KJ
C14H14            A 6/83C  14H  14    0    0G   300.     3000.     E 182.2646  1
 0.72920350E 01 0.92502000E-01-0.51686410E-04 0.13627090E-07-0.13811480E-11    2
 0.10316730E 05-0.11327380E 02-0.13889580E 02 0.17209840E 00-0.17006600E-03    3
 0.96018880E-07-0.23732530E-10 0.15032340E 05 0.92707360E 02 0.17216410E+05    4

C16H10    PYRENE  SIGMA=2   IA=82.22  IB=149.195  IC=231.42   NU=3020,3019,3014,
3013,3003,3002,2996,2994,2993,2992,1654,1621,1604,1603,1566,1499,1493,1432,1427,
1425,1394,1384,1296,1281,1230,1220,1217,1203,1183,1164,1151,1134,1074,1071,1049,
1028,999,992,988,982,975,922,916,911,850,822,807,800,778,777,756,715,704,671(2),
569,564,524,523,504,485,483(2),440,392,391,341,255,245,210,149.5,95.1
REF=C.MELIUS DATABASE BAC/MP22 #255 AA70  HF298=225.7 KJ   REF=Smith et. al,
J. Chem. Thermody 12,(1980),919   Max Lst Sq Error Cp @ 200 K 0.8%.
C16H10  PYRENE    T10/96C  16H  10    0    0G   200.000  6000.000  B 202.25540 1
 0.29910014E+02 0.42668069E-01-0.15733834E-04 0.25851725E-08-0.15667980E-12    2
 0.12786491E+05-0.14186953E+03-0.40420321E+01 0.91549657E-01 0.51443344E-04    3
-0.15276576E-06 0.73087530E-10 0.24094241E+05 0.43665312E+02 0.27145316E+05    4

C18H12 Naphthacene (bi-naphthalene) SIGMA=4 IAIBIC=8764. E-114 REF=Dorofeeva &
Gurvich Preprint IVTAN 1-238 1988 CALCULATED BY GROUP APPROXIMATIONS. EXTRAPO-
LATED from 1600 to 5000 K using Wilhoit's POLYNOMIALS. HF298=290. kJ Max Lst Sq
Error Cp @ 200 K 0.87%
C18H12            T 2/00C 18.H 12.   0.   0.G   200.000  5000.000  D 228.29328 1
 2.95586152E+01 5.85686068E-02-2.41993527E-05 4.54440129E-09-3.18688238E-13    2
 2.00626643E+04-1.40019146E+02-3.28166681E+00 9.79369796E-02 7.11673376E-05    3
-1.83222246E-07 8.55531781E-11 3.11971518E+04 4.09026837E+01 3.48787842E+04    4

C18H12 TRIPHENYLENE  SIGMA=6 IAIBIC=8620. E-114  REF= Dorofeeva & Gurvich 1988
Preprint IVTAN 1-238 1988   CALCULATED BY GROUP APPROXIMATIONS. EXTRAPOLATED
from 1600 to 5000 K using Wilhoit's POLYNOMIALS. HF298=274.2 kJ Max Lst Sq
Error Cp @ 200 K 0.73%
C18H12            T 2/00C 18.H 12.   0.   0.G   200.000  5000.000  D 228.29328 1
 2.96559160E+01 5.84891457E-02-2.41670003E-05 4.53859641E-09-3.18308300E-13    2
 1.82004887E+04-1.40400680E+02-2.34768051E+00 9.51418980E-02 7.53347608E-05    3
-1.86896616E-07 8.69659877E-11 2.91123994E+04 3.62593629E+01 3.29784918E+04    4

C22H14 PENTACENE (5 benzene rings in a row)  SIGMA=4  IAIBIC=33150 E-114
REF= Dorofeeva & Gurvich 1988  Preprint IVTAN 1-238 1988   CALCULATED BY GROUP
APPROXIMATIONS. EXTRAPOLATED from 1600 to 5000 K using Wilhoit's POLYNOMIALS.
HF298=355 kJ   Max Lst Sq Error Cp @ 200 K 0.73%
C22H14 PENTACENE  T 2/00C 22.H 14.   0.   0.G   200.000  5000.000  D 278.35316 1
 3.58785167E+01 7.04948125E-02-2.91706302E-05 5.48297466E-09-3.84747182E-13    2
 2.47407667E+04-1.74816699E+02-3.96027507E+00 1.17841522E-01 8.87303666E-05    3
-2.25804141E-07 1.05493453E-10 3.82520100E+04 4.47088716E+01 4.26964427E+04    4
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Table 4 (continued)

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C22H14 Pentafene  SIGMA=2 IAIBIC=39980 E-114  REF= Dorofeeva & Gurvich 1988
Preprint IVTAN 1-238 1988   CALCULATED BY GROUP APPROXIMATIONS. EXTRAPOLATED
from 1600 to 5000 K using Wilhoit's POLYNOMIALS.  HF298=355 kJ   Max Lst Sq
Error Cp @ 200 K 0.74%
C22H14 Pentafene  T 2/00C 22.H 14.   0.   0.G   200.000  5000.000    278.35316 1
 3.61985500E+01 7.00125090E-02-2.89502373E-05 5.43945174E-09-3.81596217E-13    2
 2.34318128E+04-1.75725046E+02-3.89059592E+00 1.18588915E-01 8.58495971E-05    3
-2.22381690E-07 1.04152452E-10 3.70146204E+04 4.50315090E+01 4.14937260E+04    4

C24H17    TRIPHENYLBENZENE RADICAL  (Outer Phenyl Radical in Para Position)
CALCULATED FROM PARENT MOLECULE C24H18 - USING THE NIST 1994 APPROXIMATION.
PROGRAM EXTRAPOLATED USING WILHOIT'S POLYNOMIALS   SIGMA=8   STATWT=2
HF298=623.2 KJ
C24H17            T 5/94C  24H  17    0    0G   298.150  5000.000  E 305.39898 1
 0.49910305E+02 0.60606660E-01-0.21521091E-04 0.37044273E-08-0.24654232E-12    2
 0.51609915E+05-0.23666063E+03-0.16409043E+02 0.22672428E+00-0.14001458E-03    3
-0.27875115E-08 0.24713123E-10 0.70999336E+05 0.11051039E+03 0.74953305E+05    4

C24H18 TRIPHENYLBENZENE CALCULATED USING BENSON'S GROUP ADDITIVITY THROUGH
BOZZELLI & RITTER'S PROGRAM EXTRAPOLATED USING WILHOIT'S POLYNOMIALS   SIGMA=48
HF298=373.05 KJ  REF=NIST 1994
C24H18            T 2/92C  24H  18    0    0G   298.150  5000.000  E 306.40692 1
 0.51756648E+02 0.59862451E-01-0.20502137E-04 0.34944485E-08-0.23287566E-12    2
 0.20652114E+05-0.25140500E+03-0.14447245E+02 0.21329283E+00-0.99995340E-04    3
-0.44814755E-07 0.40108023E-10 0.40647672E+05 0.98249347E+02 0.44867346E+05    4

C60 BUCKMINSTERFULLERENE - FOOTBALLENE  SYMNO=180. IA=IB=IC=994.2 REF=Froimowitz
J. Comp. Chem. 12 (1991),1129  NU=1469,497,1429(3),1183(3),577(3),528(3),273(5),
437(5),711(5),773(5),1100(5),1255(5),1427(5),1575(5),943,397(4),461(4),585(4),
1021(4),1383(4),1536(4),325(4),611(4),658(4),834(4),1410(4),1535(4),309(5),
428(5),503(5),610(5),1122(5),1373(5),1592(5),493(3),705(3),806(5),1274(3),
1449(3),457(3),632(3),545(3),315(3),887(3),1139(3),1496(3)  REF= Wu et al, Chem.
Phys. Let. 137, (1987), 291  HF298=618+/-25  KCAL REF=Beckhaus et al., Angew.
Chem Int. Ed. 31 (1992) 63  Max Lst Sq Error Cp @ 1300 K 0.65%
C60               T 6/93C  60    0    0    0G   200.000  6000.000  C 720.66000 1
 0.99843418E+02 0.78857558E-01-0.30608799E-04 0.51957690E-08-0.32188408E-12    2
 0.26670488E+06-0.54587488E+03-0.33579084E+02 0.42844440E+00-0.31712321E-03    3
 0.47546257E-07 0.27677699E-10 0.30465122E+06 0.14832875E+03 0.31098790E+06    4

C70 (Elipsoid) SYMNO=40. IA=1220.5 IB=IC=1429.5  NU=1568,1465,1383,1232,1185,
1062,732,682,571,474,404,260,1532,1452,1298,1146,859,828,653,568,484,1640(2),
1568(2),1499(2),1424(2),1383(2),1369(2),1245(2),1200(2),1118(2),961(2),931(2),
819(2),748(2),711(2),650(2),585(2),560(2),498(2),412(2),361(2),327(2),1645(2),
1583(2),1513(2),1463(2),1433(2),1332(2),1265(2),1212(2),1064(2),966(2),868(2),
822(2),781(2),773(2),756(2),722(2),667(2),570(2),501(2),425(2),305(2),216(2),
1658,1454,1342,1041,899,774,722,544,335,1565,1389,1270,1217,1168,895,684,592,
485,326,1647(2),1592(2),1461(2),1440(2),1360(2),1317(2),1232(2),1186(2),1069(2),
909(2),806(2),766(2),753(2),699(2),559(2),538(2),489(2),419(2),243(2),1642(2),
1551(2),1531(2),1460(2),1418(2),1358(2),1245(2),1141(2),1107(2),939(2),867(2),
819(2),739(2),710(2),682(2),610(2),515(2),405(2),391(2),314(2) REF=BURCAT TAE #
680, 1992 HF298=692 KCAL  Max Lst Sq Error Cp @ 200 K 0.82%
C70               T 6/93C  70    0    0    0G   200.000  6000.000  E 840.77000 1
 0.10677602E+03 0.10200334E+00-0.39562455E-04 0.67122022E-08-0.41568097E-12    2
 0.29769320E+06-0.59941734E+03-0.31366983E+02 0.33484410E+00 0.98587783E-04    3
-0.44663983E-06 0.22008836E-09 0.34260294E+06 0.14891614E+03 0.34822593E+06    4
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Table 4 (continued)

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JET-A Fuel, Liquid, HF298(L)= -303.5 kJ  REF=Gracia-Salcedo,Brabbs & McBride
NASA TM 101475 1988. HF298(L)= -265.09 kJ  REF=M. Rachner ISRN DLR Mitt-98-01 1998
JET-A(L)          L 6/88C  12H  23    0    0L   220.000   550.000  C 167.31370 1
     0.00000000     0.00000000    0.00000000     0.00000000     0.00000000     2
     0.00000000     0.00000000 0.19049613E 02-0.16918532E-01 0.63022035E-03     3
-0.13336577E-05 0.94335638E-09-0.44803964E 05-0.67690200E 02-0.36498744E 05     4

JET-A REF=Gracia-Salcedo,Brabbs & McBride NASA TM 101475 1988. and M.Rachner
ISRN DLR Mitt-98-01 1998   HF298=-211.47 kJ  REF=M. Rachner ISRN DLR
Mitt-98-01 1998
JET-A(G)          L 6/88C  12H  23    0    0G   273.150  5000.000  C 167.31370 1
 0.24880201E 02 0.78250048E-01-0.31550973E-04 0.57878900E-08-0.39827968E-12     2
-0.38508837E 05-0.95568240E 02 0.20869217E 01 0.13314965E 00-0.81157452E-04     3
 0.29409286E-07-0.65195213E-11-0.31310966E 05 0.25442305E 02-0.25432647E 05     4

Cl   HF298=121.302+/-0.008 kJ  REF=JANAF
CL                J 6/82CL 1.   0.   0.   0.G   200.000  6000.000  B  35.45270 1
 2.94658358E+00-3.85985408E-04 1.36139388E-07-2.17032923E-11 1.28751025E-15     2
 1.36970327E+04 3.11330136E+00 2.26062480E+00 1.54154399E-03-6.80283622E-07     3
-1.59972975E-09 1.15416636E-12 1.38552986E+04 6.57020799E+00 1.45891941E+04     4

DCl DEUTEROCHLORIC ACID  T0=0 STATWT=1 Be=5.444  WE=2144  WEXE=26.9 ALFAE=0.1121
T0=75160   STATWT=2    Be=5.1793   WE=2199   WEXE=26.9  ALFAE=0.1121
T0=76520   STATWT=1    Be=1.555    WE=684.6  WEXE=26.9  ALFAE=0.1121
T0=77525   STATWT=2    Be=4.9605   WE=2114.1 WEXE=26.9  ALFAE=0.1121
HF298=-93.345+/-0.21 kJ   REF=JANAF
DCL               J 6/77D  1.CL 1.   0.   0.G   300.000  5000.000  B  37.46680 1
 2.95720340E+00 1.59181600E-03-6.33202720E-07 1.17556580E-10-8.15999110E-15     2
-1.21735150E+04 5.89879666E+00 3.82692130E+00-2.50133260E-03 6.04661240E-06     3
-4.48375190E-09 1.13676410E-12-1.23019210E+04 1.89177776E+00-1.12270035E+04     4

DOCl   SIGMA=1  T0(STATWT)=0(1),22000(3)  IAIBIC=9.0222E-117  NU=2666,911,728
HF298=-78.24+/-2.1 kJ  REF=JANAF
DOCL              J 3/79D  1.O  1.CL 1.   0.G   300.000  5000.000  B  53.46620 1
 4.43507610E+00 2.53223870E-03-1.03123310E-06 1.90054540E-10-1.26823840E-14     2
-1.09194020E+04 2.72715963E+00 2.47904180E+00 1.08458960E-02-1.52283050E-05     3
 1.14373140E-08-3.42049250E-12-1.05180920E+04 1.21267106E+01-9.41045332E+03     4

ClF   T0=0  STATWT=1  Be=0.51409  WE=784.49  WEXE=6.201  ALFAE=0.004329
T0=18721    STATWT=6  Be=0.37026  WE=312.74  WEXE=2.207  ALFAE=0.0139
HF298=-50.292+/-0.42 kJ  REF=JANAF
CLF               J 6/77CL 1.F  1.   0.   0.G   300.000  5000.000  B  54.45110 1
 2.84862330E+00 3.17332790E-03-2.05233870E-06 5.21627330E-10-3.74722620E-14     2
-6.92788240E+03 9.31699651E+00 2.64455690E+00 6.24812560E-03-9.03543510E-06     3
 6.34005750E-09-1.74353720E-12-7.04691060E+03 9.63042791E+00-6.04884780E+03     4

ClF3  SIGMA=2  STATWT=1  IA=6.1123  IB=18.1568  IC=24.2691  NU=752,703,528,434,
326,364  HF298=-158.67+/-2.9 kJ   REF=JANAF
CLF3              J 9/65CL 1.F  3.   0.   0.G   300.000  5000.000  B  92.44791 1
 8.95359670E+00 1.17221630E-03-5.08961880E-07 9.75634890E-11-6.88587310E-15     2
-2.20759680E+04-1.80815549E+01 2.89491190E+00 2.47185500E-02-3.51393230E-05     3
 2.25595910E-08-5.32619780E-12-2.07986400E+04 1.13816921E+01-1.91052460E+04     4

ClO  T0=0  STATWT=4  Be=0.6433  De=2.2  WE=866 WEXE=7.5  ALFAE=0.0069
HF298=101.22+/-2.1 kJ  REF=JANAF
CLO               J 6/61CL 1.O  1.   0.   0.G   300.000  5000.000  B  51.45210 1
 4.09126190E+00 5.00031260E-04-1.87782060E-07 3.50976710E-11-2.42050380E-15     2
 1.08532230E+04 3.61889244E+00 2.81793640E+00 4.45313330E-03-4.41248930E-06     3
 1.59209420E-09-1.44862420E-14 1.11713970E+04 1.00579823E+01 1.21736480E+04     4
```

```
ClO2  O-Cl-O  SIGMA=2  A000=1.6006  B000=0.33283  C000=0.27553  NU=1109,945,447
STATWT=2  x11=-4.4  x22=0  x33=-2.0  x12=-3.0  x23=-13  x31=-14.4  g22=0
HF298=104.6+/-6.3 kJ  REF=JANAF
CLO2  (OClO)        J 3/61CL 1.O  2.   0.   0.G   300.000  5000.000  A  67.45150 1
 5.72497580E+00 1.46452300E-03-5.99843510E-07 1.13887500E-10-7.97947760E-15    2
 1.06062640E+04-2.57902748E+00 2.88781660E+00 9.28760080E-03-7.08240400E-06    3
 6.34533760E-10 9.68016050E-13 1.13673770E+04 1.20200293E+01 1.25803228E+04    4

CLOO RADICAL  STATWT=2   IA=1.0968  IB=10.2167  IC=11.3135  NU=1000,300,900
HF298=23 KCAL  MAX LST SQ ERROR CP @ 1300 0.2%   REF=Estimated
CLOO                L 4/84CL  1O   2    0    0G   300.000  5000.000  E  67.45180 1
 0.60288639E 01 0.10057015E-02-0.40009184E-06 0.69837636E-10-0.44704535E-14    2
 0.95408711E 04-0.32185535E 01 0.34938974E 01 0.71383193E-02-0.28676532E-05    3
-0.37120573E-08 0.26473615E-11 0.10247160E 05 0.99912157E 01 0.11574121E 05    4


ClO3F  Perchloryl Fluoride REF=JANAF 3/61 HF298=-5.688 kcal   Max Lst Sq Error
Cp @ 2500 K 0.26%.
CLO3F               L 5/95CL 1.O  3.F  1.   0.G   200.000  6000.000  B 102.44930 1
 9.84020286E+00 3.25550966E-03-1.28321227E-06 2.19710639E-10-1.36348643E-14    2
-6.48553280E+03-2.47267180E+01 6.05661163E-01 3.52831180E-02-4.51135948E-05    3
 2.82788050E-08-7.03541332E-12-4.26508565E+03 2.13532322E+01-2.86229640E+03    4

CL2  REF ELEMENT   P  89CL 2.   0.   0.   0.G   200.000  6000.000  B  70.90540 1
 4.74727508E+00-4.88581710E-04 2.68444871E-07-2.43476083E-11-1.03683148E-15    2
-1.51101862E+03-3.44551305E-01 2.73638114E+00 7.83525700E-03-1.45104963E-05    3
 1.25730834E-08-4.13247145E-12-1.05880114E+03 9.44555879E+00 0.00000000E+00    4

Cl2O  SIGMA=2  STATWT=1  IA=2.0224  IB=23.0829  IC=25.1033  NU=686,640,300
HF298=87.86+/-6.7 kJ  REF=JANAF
CL2O                J12/65CL 2.O  1.   0.   0.G   300.000  5000.000  B  86.90480 1
 6.43400620E+00 6.27288090E-04-2.69332520E-07 5.10763940E-11-3.56915450E-15    2
 8.48605300E+03-4.93672407E+00 3.25452380E+00 1.27994490E-02-1.78824600E-05    3
 1.12643830E-08-2.59642520E-12 9.16574230E+03 1.05712106E+01 1.05680184E+04    4


Cl2O2  (Cl-O-O-Cl) SIGMA=2  IA=5.538 IB=35.2672 IC=38.6944  IR=2.26835  ROSYM=2
POTENTIAL BARRIER V(3)=2581. cm-1 REF= BAC/MP4 CALCULATIONS BY MELIUS (private
communication). NU=752,650,648,437,328  HF0=34.2 KCAL HF298=33.216 KCAL
REF=Lee, Rohlfing & Rice J. Chem Phys.97 (1992), 6593. Max Lst Sq Error Cp @
1200 K 0.30%
CL2O2               T 2/94CL  2O   2    0    0G   200.000  6000.000  B 102.90420 1
 0.97241408E+01 0.29991597E-03-0.22394766E-06 0.48423798E-10-0.34559904E-14    2
 0.13444436E+05-0.20745767E+02 0.18634070E+01 0.33285997E-01-0.57276349E-04    3
 0.46928825E-07-0.14956803E-10 0.15100165E+05 0.17205914E+02 0.16714845E+05    4

Cr REFERENCE ELEMENT  REF=JANAF HF298=0.0 kJ
Cr(cr)REF ELEMENT J 6/73CR 1.   0.   0.   0.S   200.000   311.500  B  51.99610 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00 7.84826024E+00-1.16276020E-01 8.12369251E-04    3
-2.30807086E-06 2.35328142E-09-8.98013946E+02-2.75733139E+01 0.00000000E+00    4
Cr(cr)              J 6/73CR 1.   0.   0.   0.S   311.500  2130.000  B  51.99610 1
 4.59782637E+00-4.81791132E-03 5.84129754E-06-2.07036847E-09 2.82102268E-13    2
-1.31489668E+03-2.24454748E+01 1.82863471E+00 4.19562267E-03-2.82735082E-06    3
-9.15990578E-10 1.55203040E-12-7.05502663E+02-8.69806103E+00 0.00000000E+00    4
Cr(L)               J 6/73CR 1.   0.   0.   0.L  2130.000  2952.000  B  51.99610 1
 4.73028477E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 5.75359221E+02-2.45318309E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    4
```

Table 4 (continued)

```
Cr Gaseous form REF=JANAF HF298=397.48 +/- 4.2 kJ  Transition from Liquid to Gas
at 2952 K
Cr                J 6/79CR 1.   0.   0.   0.G   200.000  6000.000  B  51.99610 1
 3.08497752E+00-1.44703683E-03 1.08492194E-06-2.35643635E-10 1.86355816E-14    2
 4.68928202E+04 3.65913914E+00 2.50259371E+00-2.76560170E-05 1.03974095E-07    3
-1.61996406E-10 8.89391985E-14 4.70600237E+04 6.71107210E+00 4.78055833E+04    4

CrN  Chromium Nitride CONDENSED HF298(S)=-117.15 +/- 8.4 kJ  REF=JANAF
CrN(s)            J12/73CR 1.N  1.   0.   0.S   300.000  2500.000  B  66.00284 1
 5.69445390E+00 5.30116900E-04 2.27058290E-07-8.14832540E-11 1.08037960E-14    2
-1.58360020E+04-2.81317040E+01 9.71529040E+00-2.37753720E-02 5.25610150E-05    3
-4.83907470E-08 1.62707570E-11-1.63234220E+04-4.57300500E+01-1.41071233E+04    4

CrN  Chromium Nitride  T0=0.0  WE=[1000] WEXE=[5.] BE=[0.56115]  ALFAE=[0.00375]
RE=[1.65] STATWT=4  T0=[15000] STATWT=8  T0=[20000]  STATWT=4   REF=JANAF
HF298=501.01 +/- 20.9 kJ
CrN               J12/73CR 1.N  1.   0.   0.G   300.000  5000.000  C  66.00284 1
 3.86496020E+00 8.51604560E-04-4.40707580E-07 1.06676010E-10-8.37314220E-15    2
 5.94774370E+04 5.29506757E+00 2.93046360E+00 3.03770420E-03-1.27139640E-06    3
-1.17812490E-09 8.55513490E-13 5.97442030E+04 1.01918812E+01 6.07397802E+04    4

CrO  Chromium Oxide  T0=0  WE=898.8  WEXE=6.50   Be=0.5286 ALFAE=0.0050 RE=1.627
STATWT=10   T0=16584.5  STATWT=10   REF=JANAF  HF298=188.28 +/- 41.8 kJ
CrO               J12/73CR 1.O  1.   0.   0.G   300.000  5000.000  B  67.99550 1
 4.01398180E+00 6.27002450E-04-2.79567940E-07 6.00031000E-11-4.40579160E-15    2
 2.13466930E+04 5.55171510E+00 2.84149960E+00 4.09533580E-03-3.57764630E-06    3
 8.17104390E-10 2.40720090E-13 2.16460670E+04 1.15179922E+01 2.26454051E+04    4

CrO2   SIGMA=2  STATWT=3  IAIBIC=332.6337 E-117   NU=998,[300],1008  REF=JANAF
HF298=-75.312 +/- 41.8 kJ
CrO2              J12/73CR 1.O  2.   0.   0.G   300.000  5000.000  B  83.99490 1
 5.84999980E+00 1.27251010E-03-5.49205480E-07 1.04974910E-10-7.39954860E-15    2
-1.10421830E+04-1.74497632E+00 3.30126450E+00 8.16258570E-03-5.89076800E-06    3
 1.61708560E-11 1.08162670E-12-1.03535690E+04 1.13991138E+01-9.05799743E+03    4

CrO3   SIGMA=6  STATWT=1  IA=IB=10.5494  IC=21.0987  NU=[875],[500],969(2),
[425](2)  REF=JANAF  HF298=-292.88 +/- 41.8 kJ
CrO3              J12/73CR 1.O  3.   0.   0.G   300.000  5000.000  B  99.99430 1
 8.16289460E+00 2.04508390E-03-8.85941310E-07 1.69762820E-10-1.19877650E-14    2
-3.80925570E+04-1.58958945E+01 1.90728580E+00 2.30496080E-02-2.65012940E-05    3
 1.28624130E-08-1.83819910E-12-3.66086800E+04 1.53451415E+01-3.52251261E+04    4

Cr2N  Chromium Nitride Crystal  HF298(S)=-125.52 +/- 12.6 kJ  REF=JANAF
Cr2N(s)           J12/73CR 2.N  1.   0.   0.C   300.000  2500.000  B 117.99894 1
 8.09841850E+00 1.85336110E-03 1.42273060E-06-5.58963900E-10 6.93071100E-14    2
-1.76848010E+04-3.91474720E+01 2.03033880E+00 3.40064410E-02-6.15249460E-05    3
 5.31425480E-08-1.67695210E-11-1.67683130E+04-1.16006980E+01-1.50979548E+04    4

Cr2O3 Chromium Oxide  CONDENSED HF298(S)=-1134.70 +/- 8.4 kJ  REF=JANAF
Cr2O3(s)          J12/73CR 2.O  3.   0.   0.S   300.000  2603.000  B 151.99040 1
 1.40122350E+01 1.38239780E-03-2.37792260E-07 1.69950850E-10-3.77058570E-14    2
-1.40982170E+05-7.11015690E+01 2.93327730E+01-1.02073850E-01 2.36011030E-04    3
-2.25780190E-07 7.77992890E-11-1.42404060E+05-1.35742810E+02-1.36519668E+05    4
Cr2O3(L)          J12/73CR 2.O  3.   0.   0.L  2603.000  5000.000  B 151.99040 1
 1.88711050E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-1.33694980E+05-9.99614700E+01 1.88711050E+01 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-1.33694980E+05-9.99614700E+01 0.00000000E+00    4
```

Table 4 (continued)

```
Cr2FeO4 Dichromium Ferrum Tetraoxide.   Data taken from I.Barin 1989.
HF298(S)=-1458.124 kJ
Cr2FeO4            B  /89CR 2.FE 1.O  4.   0.S   298.150  2123.000  C 223.83480 1
 1.55564505E+01 1.09205438E-02-6.78459948E-06 2.55612113E-09-3.64830765E-13    2
-1.80620170E+05-7.50507389E+01-1.86852265E+00 1.04789892E-01-1.95035400E-04    3
 1.68861646E-07-5.48639301E-11-1.78056165E+05 3.76236322E+00-1.75371008E+05    4

Cr3C2  3-Chromium 2-Carbide Solid.  Data taken from I.Barin 1989
HF298(S)=-85.354 kJ
Cr3C2(S)           B  /89C  2.CR 3.   0.   0.S   298.150  2168.000  C 180.01030 1
 1.43803845E+01 2.40334724E-03 9.15436967E-07-2.48561026E-10 2.79849340E-14    2
-1.50902114E+04-7.34861883E+01-1.68140483E+00 7.44936012E-02-1.22150468E-04    3
 9.39505934E-08-2.71337291E-11-1.21690265E+04 2.29813080E+00-1.02656681E+04    4

Cr7C3  7-Chromium 3-Carbide Solid.  Data taken from I. Barin 1989.
HF298(S)=-160.666 kJ.
Cr7C3(S)           B  /89C  3.CR 7.   0.   0.S   298.150  2053.000  C 400.00570 1
 2.69325544E+01 8.13786676E-03 1.71106267E-07 2.14298486E-10-5.73918629E-14    2
-2.81724038E+04-1.32914128E+02 1.26480339E+00 1.35085980E-01-2.36886549E-04    3
 1.97374948E-07-6.14407486E-11-2.39729821E+04-1.44012483E+01-1.93235681E+04    4

Cr23C6  23-Chromium 6-Carbide Solid.  Data taken from I. Barin 1989.
HF298(S)=-328.444 kJ.
C6Cr23             B  /89C  6.CR23.   0.   0.S   298.150  1793.000  C1267.97630 1
 9.01158896E+01-3.96673567E-03 2.71679400E-05-9.85562288E-09 1.44623799E-12    2
-6.83766452E+04-4.44799405E+02 1.38920966E+01 3.31573484E-01-5.26586194E-04    3
 3.94794929E-07-1.08766607E-10-5.44583198E+04-8.42575556E+01-3.95025083E+04    4

D  DEUTERIUM  HF298=221.720+/-0.004 kJ  REF=JANAF
D                  J 3/82D  1.   0.   0.   0.G   200.000  6000.000  A   2.01410 1
 2.50000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 2.59212596E+04 5.91714338E-01 2.50000000E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 2.59212596E+04 5.91714338E-01 2.66666346E+04    4

DF DEUTEROFLUORIC ACID  T0=0  STATWT=1  Be=11.000 cm-1  WE=2998.19  WEXE=45.76
ALPHAE=0.2907   T0=83755   STATWT=1   Be=2.121 cm-1  WE=839.4  WEXE=8.9
ALPHAE=0.00712   HF298=-275.51+/- 0.8 kJ   REF=JANAF
DF                 J 6/77D  1.F  1.   0.   0.G   300.000  5000.000  B  21.01251 1
 2.72646200E+00 1.50912930E-03-5.17049380E-07 8.54853710E-11-5.41960240E-15    2
-3.39369400E+04 5.82982015E+00 3.49813860E+00 2.21767930E-04-1.33202400E-06    3
 2.56194930E-09-1.15122410E-12-3.41832320E+04 1.65507895E+00-3.31376542E+04    4

HD PROTODEUTERIUM  FROM ORIGINAL TABLES REF=Gurvich 89 HF0=332. JOULES  Max  Lst
Sq Error Cp @ 1200 K 0.29%
HD                 RUS 89H   1D   1    0    0G   200.000  6000.000  A   3.02204 1
 0.28013292E+01 0.11551332E-02-0.30563875E-06 0.45079706E-10-0.26239290E-14    2
-0.74612859E+03 0.12240059E+01 0.34824186E+01 0.27847427E-03-0.96849954E-06    3
 0.13687843E-08-0.46789813E-12-0.10058062E+04-0.25976195E+01 0.38781531E+02    4

DHO  STATWT=1  SIGMA=1  A0=23.4105  B0=9.0975  C0=6.4137  NU=2725,1402,3707
X11=-41.51  X22=-11.9  X33=-82.34  X12=-16.98  X23=-20.08  X13=-12.91  W0=14.5
ALFAA1=0.253   ALFAA2=-1.798   ALFAA3=1.087   ALFAB1=0.199   ALFAB2=-0.147
ALFAB3=0.125   ALFAC1=0.1098   ALFAC2=0.071   ALFAC3=0.0881  TAAA=-0.056322
TBBB=-0.0024192  TCCC=-0.00047276  TAAB=0.005895   TBBC=-0.00075778
TAAC=0.00083015  TABA=-0.0074348  REF=Gurvich 1989  HF298=-245.276 KJ  Max Lst
Sq Error Cp @ 6000 K 0.22%
HDO                L 5/95H   1D   1O   1    0G   200.000  6000.000  A  19.02144 1
 0.27939505E+01 0.33086588E-02-0.10334334E-05 0.15472460E-09-0.87503559E-14    2
-0.30407527E+05 0.72889151E+01 0.42115416E+01-0.23855882E-02 0.82921720E-05    3
-0.71895657E-08 0.22865905E-11-0.30709525E+05 0.40224847E+00-0.29499754E+05    4
```

Table 4 (continued)

```
DHO2  STATWT=1  SIGMA=1   A0=7.48  B0=.832  C0=.792  BROT1=30.573  BROT2=.551
BROT3=.0662  V(1)=-2044 cm-1  V(2)=-1292. cm-1  V(3)=-94. cm-1   NU=3620,1332,
871,2659,984  X11=-90.  X12=-10.  X13=-10.  X15=-122.  X16=-2.  X22=-9.  X23=-7.
X25=-8.  X26=-3.  X33=-10.  X35=-8.  X36=-2.  X55=-48.  X56=-2.  X66=-2.
ALFAA1=-.23  ALFAA2=.09  ALFAA3=.03  ALFAA5=-.09  ALFAA6=.08  ALFAB1=-.003
ALFAB2=-.003   ALFAB3=-.006   ALFAB5=-.001   ALFAB6=-.001   ALFAC1=.001
ALFAC2=-.003   ALFAC3=-.012   ALFAC5=.0005   ALFAC6=-.003   DJ=3E-6  DK=.0005
DJK=-.000015  REF=Gurvich 1989  HF0=-134.358 KJ  Max Lst Sq Error Cp @ 6000 K
0.32 %.
HDO2              L 5/95H   1D   1O   2    0G   200.000  6000.000  A  35.02084 1
 0.48569842E+01 0.41449474E-02-0.14036401E-05 0.22259619E-09-0.13165755E-13    2
-0.18651434E+05 0.74277419E-01 0.41089805E+01 0.13881673E-02 0.13185181E-04    3
-0.18475659E-07 0.76010528E-11-0.18236260E+05 0.50328708E+01-0.16865900E+05    4

OD DEUTERYL RADICAL FROM ORIGINAL DATA HF0=36.852 KJ REF=GURVICH 89 Max Lst Sq
Error Cp @ 6000 K 0.2%
OD                RUS 89O   1D   1    0    0G   200.000  6000.000  A  18.01350 1
 0.28342371E+01 0.14734180E-02-0.50643349E-06 0.84794290E-10-0.53143844E-14    2
 0.36312839E+04 0.63935773E+01 0.40708924E+01-0.28210086E-02 0.50328224E-05    3
-0.30857249E-08 0.68372023E-12 0.33502462E+04 0.26044498E+00 0.44772871E+04    4

OD- DEUTERYL ION FROM ORIGINAL DATA   HF0=-139.198 KJ REF=GURVICH 89 Max Lst Sq
Error Cp @ 2500 K 0.11%
OD-               RUS 89O   1D   1E   1    0G   298.150  6000.000  A  18.01405 1
 0.27763885E+01 0.15258004E-02-0.52291732E-06 0.84887426E-10-0.48226449E-14    2
-0.18319323E+05 0.53434282E+01 0.35593270E+01-0.24042233E-03-0.23249148E-06    3
 0.17198317E-08-0.94690846E-12-0.18536277E+05 0.12466308E+01-0.17484852E+05    4

DO2 REF=TSIV 1978 RESTORED FROM TABLES. HF298=3.0 KCAL ESTIMATED TO BE
IN ACORDANCE WITH HF298=3.8 KCAL FOR HO2 REF=FISHER & ARMENTRAOUT
J. CHEM PHYS 94 (1990) 4396.  Max Lst Sq Error Cp @ 2000 K 0.36%
DO2               T 8/90D   1O   2    0    0G   200.000  6000.000  B  34.01290 1
 0.44354892E+01 0.21024087E-02-0.58614106E-06 0.76176322E-10-0.39154549E-14    2
-0.72881937E+02 0.17367047E+01 0.40300583E+01-0.27943088E-02 0.18446677E-04    3
-0.22459242E-07 0.88008330E-11 0.30953985E+03 0.52282493E+01 0.15096500E+04    4

D2  REF ELEMENT    P  89D  2.   0.   0.   0.G   200.000  6000.000  B   4.02820 1
 2.73068929E+00 1.48004781E-03-4.79314848E-07 7.89496274E-11-4.88380823E-15    2
-7.95267504E+02 1.64266094E+00 3.49546974E+00 2.58348159E-04-1.31762502E-06    3
 2.42912018E-09-1.05982498E-12-1.04631580E+03-2.51905534E+00 0.00000000E+00    4

D2O  DEUTERATED WATER  SIGMA=2  IAIBIC=0.039948E-117  NU=2788.02,2671.69,1178.33
HF298=-249.203+/-0.067 kJ  REF=JANAF
D2O               J 6/77D  2.O  1.   0.   0.G   300.000  5000.000  B  20.02760 1
 2.72645950E+00 3.98451730E-03-1.49326260E-06 2.63497720E-10-1.76495570E-14    2
-3.09026380E+04 7.31820104E+00 3.85411310E+00 1.47122880E-04 3.00690060E-06    3
-1.77476280E-09 2.30188620E-13-3.11516510E+04 1.73341954E+00-2.99728411E+04    4

D2O2  DEUTERIUM PEROXIDE   A0=4.92  B0=0.788  C0=0.733 NU=2667,1028,869,2661,
947  POT. BARRIER V(1)=1029 V(2)=651  V(3)=51 1/CM  X11=-48  X12=-6  X13=-8
X15=-88  X16=-2  X22=-5  X23=-5  X25=-6  X26=-2  X33=-10  X35=-8  X36=-1
X55=-47  X56=-2  X66=-2  ALFA1A=-0.09  ALFA2A=.04  ALFA3A=.03  ALFA5A=-.09
ALFA6A=.07  ALFA1B=-0.001  ALFA2B=-.002  ALFA3B=-.006  ALFA5B=-0.001  ALFA6B=
-0.001 ALFA1C=.0005  ALFA2C=-.002  ALFA3C=-.001  ALFA5C=.0005      ALFA6C=-0.003
REF = TSIV 1978  HF298=-144.3 KJ
D2O2              R  78 D   2O   2    0    0G   300.000  5000.000  A  36.0270  1
 0.53462811E+01 0.38918597E-02-0.13136314E-05 0.20201987E-09-0.11233771E-13    2
-0.19302543E+05-0.29733829E+01 0.34752569E+01 0.72003081E-02-0.12431274E-05    3
-0.23989009E-08 0.10817658E-11-0.18677613E+05 0.72012196E+01-0.17336680E+05    4
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Table 4 (continued)

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D2S  DEUTERATED SULFIDE  SIGMA=2  IAIBIC=0.3445e-117  NU=1999,1896.38,855.45
HF298=-23.891+/- 0.8 kJ  REF=JANAF
D2S                J 6/77D  2.S  1.   0.   0.G   300.000  5000.000  B  36.09420 1
 3.66629010E+00 3.49922640E-03-1.42072840E-06 2.66856390E-10-1.86847390E-14    2
-4.21473080E+03 3.79969952E+00 3.80708240E+00 3.75963110E-04 5.75307990E-06    3
-5.34857400E-09 1.40540830E-12-4.06612190E+03 3.87928732E+00-2.87340817E+03    4

ELECTRON GAS  HF298=0.0 KJ  REF=TSIV
ELECTRON GAS       L 6/88E   1    0    0    0G   200.000  6000.000      0.00055 1
 0.25000000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-0.74537500E+03-0.11720813E+02 0.25000000E+01 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-0.74537500E+03-0.11720813E+02 0.00000000E+00    4

F   HF298=79.39+/-0.3 kJ  REF=JANAF
F                  J 6/82F   1    0    0    0G   200.000  6000.000  A  18.99840 1
 0.26716339E+01-0.17461853E-03 0.69066504E-07-0.11953478E-10 0.75236739E-15    2
 0.87874123E+04 0.39842568E+01 0.24196743E+01 0.29392909E-02-0.89212228E-05    3
 0.99118537E-08-0.37947152E-11 0.87573220E+04 0.47468987E+01 0.95483679E+04    4

FO    T0=0  STATWT=2  BE=1.05870547  DE=4.28739E-6  WE=1052.99376  WEXE=9.90030
WEYE=-0.068456  WEZE=-0.0010881  WX4=-5.945E05   ALPHAE=-0.0138015    T0=193.80
STATWT=2    BE=1.05870547    DE=4.28739E-6    WE=1052.99376    WEXE=9.90030
WEYE=-0.068456  WEZE=-0.0010881  WX4=-5.945E05  ALPHAE=-0.0138015
HF298=109. +/-10 KJ REF=M.W.Chase JPCRD 25 (1996),551   Max Lst Sq Error Cp @
400 K 0.34%
FO                 T02/97F  1.O  1.   0.   0.G   200.000  6000.000  B  34.99780 1
 4.04358718E+00 4.70079704E-04-1.77422596E-07 3.07337664E-11-1.89555657E-15    2
 1.18043072E+04 2.67152065E+00 4.36059545E+00-5.48738471E-03 1.79802594E-05    3
-2.02488481E-08 7.76046052E-12 1.19308947E+04 2.17960016E+00 1.31096120E+04    4

FO2   O-F-O SIGMA=2  STATWT=2  IA=2.9573  IB=4.9779  IC=7.9351  [T0=1049.3
STATWT=2]   NU=1050,600,1200  HF298=378.6+/-20 kJ  REF=Chase JPCRD 25 (1996),551
Max Lst Sq Error Cp @ 400 K 0.31%.
FO2  O-F-O         T02/97F  1.O  2.   0.   0.G   200.000  6000.000  C  50.99720 1
 6.49648829E+00 6.38829325E-04-2.77513327E-07 5.02595013E-11-3.24465492E-15    2
 4.32341942E+04-7.76168669E+00 3.29857287E+00 2.70051715E-03 1.70484353E-05    3
-2.93209657E-08 1.31782595E-11 4.43324550E+04 1.00991006E+01 4.55348541E+04    4

FO2  F-O-O  SIGMA=1  STATWT=2  IA=1.0714  IB=8.3532  IC=9.4246  [T0=8630
STATWT=2]  NU=1487,376,579.3  HF298=25.4 +/-2. kJ  REF=Chase JPCRD 25 (1966),551
Max Lst Sq Error Cp @ 1200 K 0.27%.
FO2    F-O-O       T02/97F  1.O  2.   0.   0.G   200.000  6000.000  B  50.99720 1
 6.04302238E+00 6.92267660E-04-1.41442202E-07 1.67666488E-11-1.02129739E-15    2
 1.03557297E+03-3.85061644E+00 3.13625166E+00 1.16477108E-02-1.82583930E-05    3
 1.50964178E-08-5.01239416E-12 1.73596746E+03 1.05579694E+01 3.05490041E+03    4

F2  REF ELEMENT   P   89F  2.   0.   0.   0.G   200.000  6000.000  A  37.99681 1
 3.86166219E+00 7.88367679E-04-1.81982940E-07-9.17436560E-12 2.65193472E-15    2
-1.23238655E+03 2.04119869E+00 3.20832415E+00 1.25919179E-03 3.89747979E-06    3
-7.22184984E-09 3.31837862E-12-1.03425794E+03 5.61903603E+00 0.00000000E+00    4

F2O  F-O-F  SIGMA=2  STATWT=1  IA=1.4392  IB=7.7225  IC=9.1617  NU=928,461,831
HF298=24.5 +/-2. kJ  REF+Chase JPCRD 25 (1996),551   Max Lst Sq Error Cp@ 400 K
0.23 %.
F2O    F-O-F       T02/97F  2.O  1.   0.   0.G   200.000  6000.000  B  53.99621 1
 6.09441350E+00 9.35752176E-04-3.68365373E-07 6.30915232E-11-3.93240210E-15    2
 8.81010873E+02-5.71955641E+00 2.70544144E+00 1.13932938E-02-1.10416725E-05    3
 3.12878548E-09 5.35111181E-13 1.72474894E+03 1.14130862E+01 2.94665591E+03    4
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Table 4 (continued)

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F2O2  F-O-O-F  SIGMA=1 STATWT=1  IA=4.1409 IB=16.747 IC=19.247  NU=1210,630.360,
202,614,466  HF298=19.2+/-2. kJ REF=Chase JPCRD 25 (1996),551  Max Lst Sq Error
Cp @ 1200 K 0.24%.
F2O2   F-O-O-F    T02/97F  2.O  2.   0.   0.G   200.000  6000.000  B  69.99561 1
 8.65313841E+00 1.38744460E-03-5.45255838E-07 9.32973782E-11-5.81148645E-15    2
-6.00315684E+02-1.69990476E+01 2.14499092E+00 2.93661262E-02-4.95837066E-05    3
 4.05447634E-08-1.28893609E-11 7.28484617E+02 1.42352517E+01 2.30921606E+03    4

Fe REFERENCE ELEMENT HF298=0.0 kJ  REF=JANAF
Fe(a)             J 3/78FE 1.   0.   0.   0.S   200.000  1042.000  B  55.84700 1
 4.69080173E+03-9.90659991E+00 2.69427446E-03 5.54445321E-06-3.01659823E-09    2
-1.41547586E+06-2.49294387E+04 2.41337476E+00-1.57780744E-03 2.14701339E-05    3
-3.80171438E-08 2.20426984E-11-7.74380998E+02-1.06560296E+01 0.00000000E+00    4
Fe(b)             J 3/78FE 1.   0.   0.   0.S  1042.000  1184.000  B  55.84700 1
 6.59678809E+02-1.14058217E+00 4.96306997E-04 0.00000000E+00 0.00000000E+00    2
-2.52106802E+05-3.65665236E+03 0.00000000E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    4
Fe(c)             J 3/78FE 1.   0.   0.   0.S  1184.000  1665.000  B  55.84700 1
 6.10109990E+01-1.60945061E-01 1.68369493E-04-7.74563702E-08 1.33091290E-11    2
-1.65335454E+04-3.13710668E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    4
Fe(d)             J 3/78FE 1.   0.   0.   0.S  1665.000  1809.000  B  55.84700 1
-4.35904698E+02 7.68489448E-01-4.46898892E-04 8.67070913E-08 0.00000000E+00    2
 1.87925534E+05 2.45057619E+03 0.00000000E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    4
Fe(L)             J 3/78FE 1.   0.   0.   0.L  1809.000  6000.000  B  55.84700 1
 5.53538332E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-1.27428941E+03-2.94772271E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    4

Fe HF298=415.5 +/- 1.3 kJ  REF=JANAF
Fe                J 3/78FE 1.   0.   0.   0.G   200.000  6000.000  B  55.84700 1
 3.26197970E+00-1.05582533E-03 5.92906998E-07-1.07189455E-10 7.48064402E-15    2
 4.90969873E+04 3.52443894E+00 1.70744428E+00 1.06339224E-02-2.76118171E-05    3
 2.80917854E-08-1.01219824E-11 4.91843725E+04 9.80811099E+00 4.99728787E+04    4

Fe+ ion  HF298=[1181.144] kJ  REF=JANAF
Fe+               J 6/84FE 1.E -1.   0.   0.G   298.150  6000.000  C  55.84645 1
 3.33602399E+00-2.72549262E-04 8.05440344E-09 1.51229089E-11-1.43376595E-15    2
 1.41036455E+05 2.86476968E+00 2.76418106E+00 2.86948238E-03-7.61235651E-06    3
 8.18183334E-09-3.11792199E-12 1.41159039E+05 5.53997981E+00 1.42058161E+05    4

Fe- ion  HF298=[393.338] kJ  REF=JANAF
Fe-               J 6/84FE 1.E  1.   0.   0.G   298.150  6000.000  C  55.84755 1
 3.36310586E+00-8.29375042E-04 3.12426241E-07-5.20068355E-11 3.17875241E-15    2
 4.63564307E+04 2.76802421E+00 1.52174510E+00 9.79673193E-03-2.11078670E-05    3
 1.84820903E-08-5.89537134E-12 4.65710215E+04 1.08683385E+01 4.73074180E+04    4

FeCl  Ferrous Chloride  T0=0  STATWT=6  WE=404.92  WEXE=1.19  BE=[0.17795]
ALFAE=[0.00075] T0=200 STATWT=8  T0=1000 STATWT=8  T0=4000  STATWT=8 REF=JANAF
HF298=251.0 +/- 84 kJ
FeCL              J 6/65FE 1.CL 1.   0.   0.G   300.000  5000.000  A  91.29970 1
 4.69406690E+00 1.16040780E-04-2.08401750E-08-1.76265560E-12 5.23138140E-16    2
 2.87903440E+04 4.19355506E+00 3.78858260E+00 4.36780110E-03-6.69223280E-06    3
 4.17074540E-09-8.46867730E-13 2.89200970E+04 8.35336756E+00 3.01925149E+04    4

FeCl2 Ferric Chloride CONDENSED  REF=JANAF  HF298(S)=-341.833 +/- 0.42 kJ
FeCL2(s)          J12/70FE 1.CL 2.   0.   0.S   300.000   950.000  C 126.75240 1
 7.11222710E+00 1.10869530E-02-1.70727420E-05 1.35158170E-08-4.13650360E-12    2
-4.36009850E+04-2.89940550E+01 7.11222710E+00 1.10869530E-02-1.70727420E-05    3
 1.35158170E-08-4.13650360E-12-4.36009850E+04-2.89940550E+01-4.11137739E+04    4
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Table 4 (continued)

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FeCL2(L)          J12/70FE 1.CL 2.   0.   0.L   950.000  5000.000  C 126.75240 1
 1.22888630E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-4.11098210E+04-5.31930570E+01 1.22888630E+01 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-4.11098210E+04-5.31930570E+01 0.00000000E+00    4

FeCl2  Ferric Chloride T0=0 STATWT=10  B0=0.050489  NU=327,88(2),492 SIGMA=2
T0=4800  STATWT=10  T0=7140  STATWT=5  HF298=-141.+/-2.1 kJ  REF=JANAF
FeCL2             J12/70FE 1.CL 2.   0.   0.G   300.000  5000.000  B 126.75240 1
 6.94926010E+00 5.33716410E-04 7.02212070E-08-6.14754900E-11 6.79331430E-15    2
-1.90458320E+04-3.75951441E+00 5.45575050E+00 7.96329270E-03-1.25939640E-05    3
 8.99767340E-09-2.32423630E-12-1.88442970E+04 3.02284219E+00-1.69583047E+04    4

FeCl3  Ferrun Chloride  CONDENSED  HF298(S)=-399.405+/-0.84 kJ  REF=JANAF
FeCL3(s)          J 6/65FE 1.CL 3.   0.   0.S   200.000   577.000  C 162.20510 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00-7.39556855E+00 2.02608434E-01-8.44505923E-04    3
 1.59286602E-06-1.07989321E-09-5.00144664E+04 2.44450935E+01-4.80371062E+04    4
FeCL3(L)          J 6/65FE 1.CL 3.   0.   0.L   577.000  6000.000  C 162.20510 1
 1.61031270E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-4.84135278E+04-6.75758990E+01 1.61031270E+01 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-4.84135278E+04-6.75758990E+01-4.80371062E+04    4

FeCl3  SIGMA=6 STATWT=6  IA=IB=41.5834  IC=83.1667  nu=130(2),160,310(2),350
HF298=-253.13 +/- 5.0 kJ  REF=JANAF
FeCL3             J 6/65FE 1.CL 3.   0.   0.G   300.000  5000.000  C 162.20510 1
 9.77711060E+00 2.44213620E-04-1.03139940E-07 1.92074260E-11-1.31792990E-15    2
-3.34395700E+04-1.45491463E+01 7.56148730E+00 9.73382490E-03-1.55433050E-05    3
 1.11863680E-08-3.00229980E-12-3.30136240E+04-3.98583203E+00-3.04431637E+04    4

FeO  Ferric Oxide  REF=JANAF  HF298(S)=-272.044 kJ
FeO(s)            J 6/65FE 1.O  1.   0.   0.S   300.000  1650.000  C  71.84640 1
 5.83164890E+00 1.42751560E-03-9.32081430E-08-6.59977630E-12-2.25121430E-14    2
-3.45669020E+04-2.64469900E+01 5.31954750E+00 2.20965910E-03 1.07217750E-06    3
-2.79297290E-09 1.33207330E-12-3.44071650E+04-2.36860340E+01-3.27183475E+04    4
FeO(L)            J 6/65FE 1.O  1.   0.   0.L  1650.000  5000.000  C  71.84640 1
 8.20224820E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-3.38486150E+04-4.00791290E+01 8.20224820E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-3.38486150E+04-4.00791290E+01 0.00000000E+00    4

FeO Ferrum Oxide  T0=0  STATWT=10 WE=880.0  WEXE=5.0  BE=[0.4184] ALFAE=0.00293
T0=10000 STATWT=10  T0=16000  STATWT=5  HF298=251.04 +/- 20.9 kJ
FeO               J 9/66FE 1.O  1.   0.   0.G   300.000  5000.000  B  71.84640 1
 4.20498170E+00 2.68384520E-04-8.94267360E-08 3.18559110E-11-3.39225430E-15    2
 2.88291700E+04 4.83043159E+00 2.82452560E+00 4.30492070E-03-4.10847810E-06    3
 1.32011890E-09 7.13162170E-14 2.91940350E+04 1.18911760E+01 3.01938519E+04    4

Fe(OH)2 Ferric Hydroxide  HF298(S)=-574.04 +/- 2.9 kJ   REF=JANAF
Fe(OH)2(s)        J 6/66FE 1.O  2.H  2.   0.C   300.000  1500.000  B  89.86168 1
 7.40318080E+00 1.19817420E-02-1.49576110E-06-5.05263590E-09 2.00371110E-12    2
-7.15922660E+04-3.46732670E+01 1.00912180E+01 4.45231410E-03 4.06668550E-06    3
-4.00945250E-09 2.39471640E-13-7.22776880E+04-4.84000340E+01-6.90429813E+04    4

Fe(OH)2  Ferrum Hydroxide  T0=0  STATWT=5  IA=0.2814  IB=18.6208  IC=18.9022
NU=2300,450,800,750,320,700,400,2600,570  SIGMA=2  HF298=-330.54 +/- 2.1 kJ
Fe(OH)2           J12/66FE 1.O  2.H  2.   0.G   200.000  6000.000  C  89.86168 1
 8.96262012E+00 4.20137342E-03-1.61017443E-06 2.68347076E-10-1.63497305E-14    2
-4.27994358E+04-1.86912367E+01-1.67667734E+00 6.16931464E-02-1.20738995E-04    3
 1.09814026E-07-3.72856831E-11-4.11289708E+04 2.96771710E+01-3.97541166E+04    4
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Table 4 (continued)

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Fe(OH)3  Ferrum Hydroxide HF298(S)=-832.62 +/-12.6 kJ   REF=JANAF
Fe(OH)3(s)          J 6/66FE 1.O  3.H  3.   0.C   300.000  1500.000  B 106.86902 1
 8.02239260E+00 1.64201350E-02-1.23693780E-07-6.81928380E-09 2.32769070E-12    2
-1.03213360E+05-3.79340200E+01 4.41168360E+00 3.26824620E-02-2.23938150E-05    3
 2.86467920E-09 2.26223210E-12-1.02718340E+05-2.13310140E+01-1.00141482E+05    4

FeS Ferrum Monosulfide CONDENSED  REF=JANAF  HF298(S)=-101.67 +/- 0.8 kJ
FeS(a)              J 9/77FE 1.S  1.   0.   0.S   300.000   411.000  B  87.91300 1
 1.89776270E+01-1.09542820E-01 2.21860160E-04 0.00000000E+00 0.00000000E+00    2
-1.49952420E+04-7.81254350E+01 1.89776270E+01-1.09542820E-01 2.21860160E-04    3
 0.00000000E+00 0.00000000E+00-1.49952420E+04-7.81254350E+01-1.22458515E+04    4
FeS(b)              J 9/77FE 1.S  1.   0.   0.S   411.000   598.000  B  87.91300 1
 8.70285050E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-1.46897380E+04-4.20821020E+01 8.70285050E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-1.46897380E+04-4.20821020E+01 0.00000000E+00    4
FeS(c)              J 9/77FE 1.S  1.   0.   0.S   598.000  1463.000  B  87.91300 1
-2.68304830E+00 3.67651040E-02-5.21822740E-05 3.16071700E-08-6.41260410E-12    2
-1.14986840E+04 1.62391240E+01 9.37241760E+00 9.41620590E-04-1.58298640E-05    3
 1.83808810E-08-5.77070670E-12-1.45816850E+04-4.51415160E+01 0.00000000E+00    4
FeS(L)              J 9/77FE 1.S  1.   0.   0.L  1463.000  5000.000  B  87.91300 1
 7.52328060E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-1.01642370E+04-3.19709300E+01 7.52328060E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-1.01642370E+04-3.19709300E+01 0.00000000E+00    4

FeS  Ferrum Monosulfide   HF298=370.767 kJ   Data from I. Barrin Database 1989.
FeS(G)              B  /89FE 1.S  1.   0.   0.G   298.150  3000.000  C  87.91100 1
 4.14494627E+00 7.05834738E-04-5.16986528E-07 1.86466769E-10-2.22683845E-14    2
 4.33002296E+04 6.46991922E+00 2.90286012E+00 6.65546290E-03-1.14989921E-05    3
 9.33240931E-09-2.89374741E-12 4.35159803E+04 1.22605433E+01 4.45927661E+04    4

FeSO4  Ferrous Soulfate  REF=JANAF  HF298(S)=-928.85 +/-8.4 kJ
FeSO4(s)            J 6/66FE 1.S  1.O  4.   0.S   300.000  2000.000  C 151.91060 1
 1.16089290E+01 1.38046970E-02-9.81263800E-06 3.60878110E-09-5.09762790E-13    2
-1.16191860E+05-5.64778170E+01 3.50576840E+00 3.70297010E-02-2.90335310E-05    3
 4.57785890E-09 2.62020870E-12-1.14162500E+05-1.52232410E+01-1.11717626E+05    4

FeS2 Pyrite  REF=JANAF  HF298(S)=-171.54 +/-2.1 kJ
FeS2(s)             J 9/77FE 1.S  2.   0.   0.C   300.000  1400.000  C 119.97900 1
-8.85153200E+01 3.27489310E-01-4.10574390E-04 2.29281460E-07-4.77644150E-11    2
-4.65124760E+02 4.41730450E+02 4.03456630E-01 4.26746840E-02-8.40306260E-05    3
 7.63014410E-08-2.54323160E-11-2.20459270E+04-5.54563930E+00-2.06325071E+04    4

Fe2Cl4  (FeCl2)2  T0=0 STATWT=10  IA=31.1433  IB=218.7538  IC=IA + IB
NU=[30,50,80,90,110,125,150,180,200,249,325,438] T0=4600  STATWT=10  T0=7140
STATWT=5  REF=JANAF  HF298=-431.37 +/- 4.2 kJ
Fe2CL4              J12/70FE 2.CL 4.   0.   0.G   300.000  5000.000  B 253.50480 1
 1.53575000E+01 6.42078610E-04 2.08177300E-08-5.15805590E-11 6.06734950E-15    2
-5.65100370E+04-3.18965871E+01 1.27382420E+01 1.32355580E-02-2.16418730E-05    3
 1.59936670E-08-4.35070970E-12-5.61065790E+04-1.98247491E+01-5.18820452E+04    4

Fe2Cl6  (FeCl3)2  SIGMA=4  IA=116.3664  IB=194.7424  IC=311.1088  NU=350,310,
300,260,250,230,200,120,110(3),100,95,90,85,70,35,18  HF298=-654.38 +/- 8.4 kJ
REF = JANAF
Fe2CL6              J 6/65FE 2.CL 6.   0.   0.G   200.000  6000.000  B 324.41020 1
 2.15645031E+01 4.62349015E-04-1.84952078E-07 3.20143043E-11-2.01002737E-15    2
-8.52432375E+04-5.86538185E+01 1.42211808E+01 4.35485968E-02-9.60390188E-05    3
 9.37463081E-08-3.36051626E-11-8.41996265E+04-2.59244694E+01-7.87030865E+04    4
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Table 4 (continued)

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Fe2O3 HEMATITE  HF298(S)=-824.248 kJ  Data from I. Barin Database  1989
Fe2O3(S) Solid-A  B  /89FE 2.O  3.   0.   0.S   298.150   960.000  C 159.68820 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00 1.52218166E-01 6.70757040E-02-1.12860954E-04    3
 9.93356662E-08-3.27580975E-11-1.01344092E+05-6.15024507E+00-9.91336832E+04    4
Fe2O3(S) Solid-B  B  /89FE 2.O  3.   0.   0.S   960.000  1700.000  C 159.68820 1
 3.53051527E+02-9.72758065E-01 1.04598367E-03-4.95511272E-07 8.73647747E-11    2
-1.95976954E+05-1.81528607E+03 8.01447907E+01-6.20141606E-02 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-1.36185811E+05-4.61194426E+02-9.91336832E+04    4

Fe3C  Triferrumcarbide   HF298(S)=25.104 kJ  Data from I. Barin database 1989.
Fe3C (S) Solid-A  B  /89C  1.FE 3.   0.   0.S   298.150   485.000  C 179.54600 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00 9.68770665E+00 1.04155445E-02-9.03325722E-07    3
 7.59127519E-10 0.00000000E+00-3.25545652E+02-4.56881802E+01 3.01929999E+03    4
Fe3C (S) Solid-B  B  /89C  1.FE 3.   0.   0.S   485.000  1500.000  C 179.54600 1
 1.29117933E+01 1.45677470E-03 5.11471347E-08-2.03130285E-11 2.64589235E-15    2
-1.62949142E+01-5.96219813E+01 1.28970825E+01 1.48707284E-03 3.83705751E-08    3
-2.70661902E-11 6.58822517E-15-1.15745541E+01-5.95430074E+01 3.01929999E+03    4
Fe3C (L) Liquid   B  /89C  1.FE 3.   0.   0.L  1500.000  2000.000  C 179.54600 1
 1.46661913E+01-1.66080339E-04 1.41368457E-07-5.33048944E-11 7.51357777E-15    2
 5.30022441E+03-6.59621815E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 3.01929999E+03    4

Fe3O4  MAGNETITE  HF298(s)=-1118.383 kJ  Data from I. Barin database 1989
Fe3O4(S) Solid-A  B  /89FE 3.O  4.   0.   0.S   298.150   850.000  C 231.53260 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00 4.84450959E+00 4.39051578E-02 5.24676763E-05    3
-2.20801809E-07 1.74856371E-10-1.38015344E+05-2.38418082E+01-1.34509791E+05    4
Fe3O4(S) Solid-B  B  /89FE 3.O  4.   0.   0.S   850.000  1870.000  C 231.53260 1
 8.84307558E+01-1.48964861E-01 1.25760044E-04-4.70060974E-08 6.78732076E-12    2
-1.62143803E+05-4.63815254E+02 7.97181560E+01-9.83508037E-02 4.36398095E-05    3
 0.00000000E+00 0.00000000E+00-1.61758880E+05-4.27156556E+02-1.34509791E+05    4
Fe3O4(L) Liquid   B  /89FE 3.O  4.   0.   0.L  1870.000  2000.000  C 231.53260 1
 2.45827554E+01 1.11718119E-03-2.88207928E-07 0.00000000E+00 0.00000000E+00    2
-1.26461365E+05-1.15899474E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00-1.34509791E+05    4

H  HF0=211.801 KJ  REF=C.E. Moore "Selected Tables of Atomic Spectra" NSRDS-NBS
Sec 6 1972 p. A1 I.
H                 L 6/94H   1    0    0    0G   200.000  6000.000  A   1.00794 1
 0.25000000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.25473660E+05-0.44668285E+00 0.25000000E+01 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 0.25473660E+05-0.44668285E+00 0.26219035E+05    4

H+  HF0=1530.048 KJ REF=Moore NSRDS-NBS 3, SEC6, 1972.
H+                L 7/88H   1E  -1    0    0G   200.000  6000.000  B   1.00739 1
 0.25000000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.18402143E+06-0.11406466E+01 0.25000000E+01 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 0.18402143E+06-0.11406466E+01 0.18476680E+06    4

H-  HF0=132.834 KJ  REF=JANAF 1982
H-                L/7/88H   1E   1    0    0G   298.150  6000.000  B   1.00849 1
 0.25000000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.15976167E+05-0.11390139E+01 0.25000000E+01 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 0.15976167E+05-0.11390139E+01 0.16721542E+05    4
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Table 4 (continued)

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HBr HYDROBROMIC ACID CALCULATED FROM ORIGINAL TABLES   REF=Gurvich 1989
HF298=-36.29 KJ Max Lst Sq Error Cp @ 6000 K 0.32%
HBR                 RUS 89H   1BR  1    0    0G   200.000  5000.000  B  80.91194 1
 0.28330819E+01 0.14872632E-02-0.51463345E-06 0.87853840E-10-0.57591453E-14    2
-0.52289003E+04 0.74405672E+01 0.34894141E+01 0.27295667E-03-0.15997163E-05    3
 0.33659948E-08-0.16408428E-11-0.54089034E+04 0.39796907E+01-0.43646589E+04    4


HCl HYDROCHLORIC ACID CALCULATED FROM ORIGINAL TABLES  REF=Gurvich 1989
HF298=-92.31 KJ Max Lst Sq Error Cp @ 6000 K 0.17%
HCL                 RUS 89H   1CL  1    0    0G   200.000  6000.000  B  36.46064 1
 0.27575767E+01 0.14538737E-02-0.47964697E-06 0.77790943E-10-0.47957377E-14    2
-0.11913766E+05 0.65219722E+01 0.34637647E+01 0.47648423E-03-0.20030122E-05    3
 0.33171437E-08-0.14495818E-11-0.12144352E+05 0.26642828E+01-0.11102278E+05    4

HOCl  SIGMA=1   STATWT=1  IAIBIC=4.357   NU=3609.2,1240,725   HF0=-72.8 KJ
REF=Gurvich 89   Max Lst Sq Error Cp @ 400 K 0.25%
HOCL                RUS 89H   1O   1CL  1    0G   200.000  6000.000  B  52.46004 1
 0.43664934E+01 0.20513656E-02-0.67087650E-06 0.10131893E-09-0.57791828E-14    2
-0.10576070E+05 0.28049555E+01 0.35465037E+01 0.23321738E-02 0.52331522E-05    3
-0.97366010E-08 0.44672936E-11-0.10299629E+05 0.73974601E+01-0.91094784E+04    4

HF HYDROFLUORIC ACID CALCULATED FROM ORIGINAL TABLES  REF=Gurvich 1989
HF298=-273.3 KJ Max Lst Sq Error Cp @ 1200 K 0.35%
HF                  RUS 89H   1F   1    0    0G   200.000  6000.000  B  20.00634 1
 0.29204304E+01 0.85796097E-03-0.16306811E-06 0.13780358E-10-0.29021238E-15    2
-0.33685882E+05 0.42144066E+01 0.34811480E+01 0.21334107E-03-0.68985280E-06    3
 0.85966803E-09-0.23549086E-12-0.33913127E+05 0.10259567E+01-0.32870247E+05    4

HOF    SIGMA=1    STATWT=1    IAIBIC=1.464    NU=3537,1359,886    HF0=-94 KJ
REF=Gurvich 89  Max Lst Sq Error Cp @ 400 K 0.29%
HOF                 RUS 89H   1O   1F   1    0G   200.000  6000.000  B  36.00574 1
 0.41252846E+01 0.23151964E-02-0.77666557E-06 0.11954885E-09-0.69172673E-14    2
-0.13072651E+05 0.28986184E+01 0.39203542E+01-0.13992801E-02 0.13911528E-04    3
-0.17901805E-07 0.72456494E-11-0.12851722E+05 0.48785828E+01-0.11654111E+05    4

HI  HYDROIODIC ACID  SIGMA=2  Be=6.512  WE=2309.06  WEXE=39.73  ALFAE=0.1715
HF298=26.359+/-0.21 kJ  REF=JANAF
HI                  J 9/61H  1.I  1.   0.   0.G   300.000  5000.000  B 127.91241 1
 2.91040080E+00 1.56881880E-03-5.92276320E-07 1.05370940E-10-7.03751160E-15    2
 2.25086590E+03 7.86447051E+00 3.69637220E+00-1.42247550E-03 3.01311880E-06    3
-1.26664030E-09-3.50987650E-14 2.10735810E+03 4.08812111E+00 3.17030779E+03    4

HNO NITROGEN OXIDE-HYDRIDE  STATWT=1  SIGMA=1  A0=18.476  B0=1.411  C0=1.306
NU=2684,1501,1565  DJ=.4050E-5  DJK=.98E-4  DK=.4485E-2      T0=6280  STATWT=3
A0=22.156  B0=1.325  C0=1.242  NU=2850,992,1468    T0=13154.4  STATWT=1
A0=22.156  B0=1.325  C0=1.242  NU=2854,981,1421   REF=Jacox (1988)  HF0=105. KJ
REF=Gurvich 1989  Max Lst Sq Error Cp @ 6000 K 0.91%
HNO                 L12/89H   1N   1O   1    0G   200.000  3500.000  A  31.01408 1
 0.31655229E+01 0.30000862E-02-0.39436619E-06-0.38575815E-10 0.70807189E-14    2
 0.11194426E+05 0.76477833E+01 0.45352475E+01-0.56853972E-02 0.18519850E-04    3
-0.17188273E-07 0.55583207E-11 0.11039881E+05 0.17431919E+01 0.12271645E+05    4

HNO2 NITROUS ACID  STATWT=1 SIGMA=1  A0=3.0783  B0=.41663  C0=.36698  NU=3588,
1699,1265,791,593,540   T0=140.   STATWT=1  SIGMA=1   A0=2.7899   B0=.43796
C0=.37856  NU=3424,1640,1261,853,608,638  REF=Gurvich 1989  HF0=-72.8 KJ  Max
Lst Sq Error Cp @ 6000 K 0.32 %.
HNO2                RUS 89H   1N   1O   2    0G   200.000  6000.000  B  47.01348 1
 0.57919018E+01 0.36515212E-02-0.12928936E-05 0.20688716E-09-0.12315254E-13    2
-0.11565589E+05-0.40558233E+01 0.32141709E+01 0.81276869E-02 0.16602559E-05    3
-0.95285182E-08 0.48715058E-11-0.10753237E+05 0.98219504E+01-0.94355439E+04    4
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HNO3 NITRIC ACID   STATWT=1   SIGMA=1   A0=.434005   B0=.403610   C0=.208831
BROT=.135 v(2)=2730 cm-1  ROSYM=2 NEL=100    NU=3550,1708,1331,1325,879,647,579,
762  REF=Gurvich 1989  HF0=-124.2 KJ  Max Lst Sq Error Cp @ 1300 K 0.49 %
HNO3                L 4/90H   1N   1O   3    0G   200.000  6000.000     63.01288 1
 0.80037397E+01 0.44984461E-02-0.17365219E-05 0.29369198E-09-0.18148285E-13    2
-0.19256280E+05-0.16098258E+02 0.17449337E+01 0.18804057E-01-0.81595875E-05    3
-0.57859036E-08 0.44377077E-11-0.17380530E+05 0.16954532E+02-0.16105924E+05    4

OH  HYDROXIL RADICAL FROM ORIGINAL DATA  HF298= 39.34 KJ REF= TSIV
OH                  RUS 78O   1H   1    0    0G   200.000  6000.000  A  17.00734 1
 2.83864607E+00 1.10725586E-03-2.93914978E-07 4.20524247E-11-2.42169092E-15    2
 3.94395852E+03 5.84452662E+00 3.99201543E+00-2.40131752E-03 4.61793841E-06    3
-3.88113333E-09 1.36411470E-12 3.61508056E+03-1.03925458E-01 4.73234213E+03    4

OH+  HYDROXIL POSITIVE ION FROM ORIGINAL DATA HF298=1290.204 KJ  REF=TSIV 78
OH+                 RUS 78O  1.H  1.E -1.   0.G   298.150  6000.000  A  17.00679 1
 2.68358997E+00 1.57006432E-03-5.39972805E-07 9.37643859E-11-5.70068055E-15    2
 1.54395744E+05 6.44375888E+00 3.50502572E+00 2.41313749E-04-1.42200949E-06    3
 2.64780232E-09-1.17038711E-12 1.54127124E+05 1.97907627E+00 1.55174989E+05    4

OH-  HYDROXIL  ION  FROM ORIGINAL DATA  HF0=-150.805 KJ  REF=TSIV 78
OH-                 L 3/93O  1.H  1.E  1.   0.G   298.150  6000.000  A  17.00789 1
 2.83405701E+00 1.07058023E-03-2.62459398E-07 3.08376435E-11-1.31383862E-15    2
-1.80186974E+04 4.49464762E+00 3.43279956E+00 6.19656310E-04-1.89930992E-06    3
 2.37365946E-09-8.55103755E-13-1.82613086E+04 1.06053670E+00-1.72227709E+04    4

HO2 RADICAL  GROUND STATE STATWT=2  A0=20.356 B0=1.118 C0=1.056 NU=3436.2,
1391.75,1097.63 EXCITED STATE T0=7029.684 A0=20.486  B0=1.021 C0=0.968
NU=3268.5,1285,929.068 STATWT=2 REF=JACOX JPCRD 17, (1988) P.269
HF298=12.55 KJ     REF=Hills & Howard J. CHEM. PHYS 81 (1984), 4458
HO2                 L 5/89H   1O   2    0    0G   200.000  6000.000  B  33.00674 1
 0.41722659E+01 0.18812098E-02-0.34629297E-06 0.19468516E-10 0.17609153E-15    2
 0.61818851E+02 0.29577974E+01 0.43017880E+01-0.47490201E-02 0.21157953E-04    3
-0.24275961E-07 0.92920670E-11 0.29480876E+03 0.37167010E+01 0.15096500E+04    4

HPO  PHOSPHORUS OXYHYDRIDE  SIGMA=1  STATWT=1  IAIBIC=5.437  NU=2330,1188,985
T0=19032.8  STATWT=1  SIGMA=1  HF0=-53. KJ  REF=Gurvich 1989  Max Lst Sq Error
Cp @ 6000 K 0.38%
HPO                 RUS 89H   1P   1O   1    0G   200.000  6000.000  B  47.98110 1
 0.42999621E+01 0.26002099E-02-0.99411489E-06 0.16916642E-09-0.10420412E-13    2
-0.84075730E+04 0.27172028E+01 0.40742366E+01-0.31019711E-02 0.18964972E-04    3
-0.22506453E-07 0.86340185E-11-0.80437690E+04 0.53965266E+01-0.68397546E+04    4

SH  T0(STATWT)=0(2),377.01(2) Be=9.601  WE=2689.6  WEXE=45.5  ALFAE=0.285
    T0=30663(2)  Be=8.521  WE=1979.8  WEXE=97.65  ALFAE=0.464
    T0=59622(2)  Be=8.785  WE=2670.6  WEXE=56.8   ALFAE=0.259
T0=63900(4),71195(4),71318(2),76708(4) Be=9.601 WE=2689.6  WEXE=45.5 ALFAE=0.285
T0=79343(4),80848(4)   HF298=139.33+/-5.0 kJ  REF=JANAF
SH                  J 6/77S  1.H  1.   0.   0.G   300.000  5000.000  A  33.07394 1
 3.00145370E+00 1.33949570E-03-4.67896630E-07 7.88040150E-11-5.02804530E-15    2
 1.59053200E+04 6.28462715E+00 4.44203220E+00-2.43591970E-03 1.90645760E-06    3
 9.91666300E-10-9.57407620E-13 1.55232580E+04-1.14449035E+00 1.67577318E+04    4

S-OH RADICAL  STATWT=2  SIGMA=1  IA=0.1222028  IB=5.0098556  IC=5.132059
NU=3638,1184,826  HF298=-4.994+/-10. KCAL  REF=C. Melius BAC/MP4 DATABASE,
Private Communication  Max Lst Sq Error Cp @ 400 K 0.35%
SOH                 T 4/93S   1O   1H   1    0G   200.000  6000.000  B  49.07334 1
 0.43544347E+01 0.20549939E-02-0.67083934E-06 0.10119158E-09-0.57672355E-14    2
-0.39895568E+04 0.32303081E+01 0.36922437E+01 0.44545692E-03 0.10785948E-04    3
-0.15975515E-07 0.68858806E-11-0.37006791E+04 0.73216957E+01-0.25130640E+04    4
```

Table 4 (continued)

```
HS=O RADICAL   STATWT=2  SIGMA=1  IA=0.272571  IB=4.331163   IC=4.603734
NU=751,1060.5,2543  HF298=-1.143 KCAL estimated. REF=C. MELIUS  BAC/MP4 Database
Private Communication  Max Lst Sq Error Cp @ 6000 K 0.32%
HSO               T 4/93H   1S   1O   1    0G   200.000  6000.000  B  49.07334 1
 0.45416010E+01 0.22648458E-02-0.83152058E-06 0.13614796E-09-0.82290966E-14    2
-0.21608556E+04 0.23357633E+01 0.34130925E+01 0.32105128E-02 0.38960721E-05    3
-0.81958128E-08 0.37789804E-11-0.17554966E+04 0.86522782E+01-0.57517665E+03    4

HSO2 HOSO RADICAL STATWT=2 SIGMA=1 IA=2.397408  IB=8.7861523  IC=11.010938
IR=0.11955  NU=403.6,788,1011,1111,3608  ROSYM=2  POT BARRIER V(3)=409.2 cm-1
HF298=-61.158 KCAL  REF=C. MELIUS BAC/MP4 Database, Private communication
Max Lst Sq Error Cp @ 6000 K 0.19%
HO2S              T11/96H   1O   2S   1    0G   200.000  6000.000  B  65.07274 1
 6.45143466E+00 2.48602888E-03-8.43212436E-07 1.30962437E-10-7.63196759E-15    2
-3.29875786E+04-4.61876333E+00 3.69601366E+00 9.53437650E-03-3.92988151E-06    3
-4.41313434E-09 3.33020726E-12-3.22589853E+04 9.59023664E+00-3.07751148E+04    4

HSO3 HOSO2 RADICAL STATWT=2  SIGMA=1 IA=9.4168978  IB=9.7757253  IC=16.401348
IR=0.125875  NU=323.6,433,444,675,818,1110,1196,3562  ROSYM=2  POT BARRIER
V(3)=954.8 cm-1  REF=C. MELIUS BAC/MP4 Database, Private communication
HF298=-92.1 KCAL REF=Margitan J.J. JPC 88 (1984), 3314    Max Lst Sq Error
Cp @ 6000 K 0.18%.
HSO3              T 3/93H   1S   1O   3    0G   200.000  6000.000  B  81.07214 1
 0.91911575E+01 0.27980912E-02-0.97493219E-06 0.15441946E-09-0.91299297E-14    2
-0.49457258E+05-0.18510636E+02 0.90501684E+00 0.38941616E-01-0.63379448E-04    3
 0.49872276E-07-0.15179855E-10-0.47836694E+05 0.21006792E+02-0.46304593E+05    4

HS2 RADICAL VERY VERY ROUGH GRAPHICAL ESTIMATION OF Cp ACCORDING TO HO2 AND H2O2
S ESTIMATED BY BENSON 1976 HF298=27.0 KJ REF=Luke & McLean (1985) J. Phys. Chem.
89, p.4592
HS2               T 3/94H   1S   2    0    0G   298.150  5000.000  F  65.13994 1
 0.46552282E+01 0.29202531E-02-0.11010941E-05 0.18878697E-09-0.12318000E-13    2
 0.16492900E+04 0.27987542E+01 0.40214995E+01 0.31961918E-02 0.21507270E-05    3
-0.48650943E-08 0.21391804E-11 0.18942796E+04 0.64213003E+01 0.32457475E+04    4

H2   HF298= 0.0  REF=TSIV
H2  REF ELEMENT   RUS 78H   2    0    0    0G   200.000  6000.000  A   2.01588 1
 0.29328305E+01 0.82659802E-03-0.14640057E-06 0.15409851E-10-0.68879615E-15    2
-0.81305582E+03-0.10243164E+01 0.23443029E+01 0.79804248E-02-0.19477917E-04    3
 0.20156967E-07-0.73760289E-11-0.91792413E+03 0.68300218E+00 0.00000000E+00    4

H2F2   SIGMA=1  IAIBIC=20.   NU=4038,4081,171,588,519,226    HF0=-566.5 KJ
REF=Gurvich 89  Max Lst Sq Error Cp @ 1300 K  0.18%
H2F2              RUS 89H   2F   2    0    0G   200.000  6000.000  B  40.01269 1
 0.65095969E+01 0.19848359E-02-0.46422746E-06 0.49022863E-10-0.18846028E-14    2
-0.70500916E+05-0.61547561E+01 0.33553129E+01 0.22103635E-01-0.43986009E-04    3
 0.40099889E-07-0.13495484E-10-0.70212768E+05 0.72994688E+01-0.68545684E+05    4

H2O Water CONDENSED  REF=NASA Unpublished
H2O(s)            L 8/89H  2.O  1.   0.   0.S   200.000   273.150     18.01528 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00 5.29677970E+00-6.75749247E-02 5.16942109E-04    3
-1.43853360E-06 1.52564794E-09-3.62266557E+04-1.79220428E+01-3.59742186E+04    4
H2O(L)            L 8/89H  2.O  1.   0.   0.L   273.150   600.000  C  18.01528 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00 7.25575005E+01-6.62445402E-01 2.56198746E-03    3
-4.36591923E-06 2.78178981E-09-4.18865499E+04-2.88280137E+02-3.43772513E+04    4
```

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H2O REF=Wooley J. RES. NBS 92 (1987), 35. HF298=-241.826 KJ based on HF298(L)
from Cox, Wagman & Medvedev CODATA KEY VAL. for THERMO, Hemisphere 1989 p.21
and heat of vap. from Haar, Gallagher & Kell NBS/NRC Tables, Hemisphere 1984.
H2O                 L 5/89H   2O   1    0    0G   200.000  6000.000  A  18.01528 1
 0.26770389E+01 0.29731816E-02-0.77376889E-06 0.94433514E-10-0.42689991E-14    2
-0.29885894E+05 0.68825500E+01 0.41986352E+01-0.20364017E-02 0.65203416E-05    3
-0.54879269E-08 0.17719680E-11-0.30293726E+05-0.84900901E+00-0.29084817E+05    4

H2O2 liquid Hydrogen Peroxide REF=Gurvich 1989  HF298=-44.880 kcal   Max Lst Sq
Error Cp @ 2000 K 0.0017%
H2O2(L)             RUS/89H  2.O  2.   0.   0.L   272.740  6000.000     34.01468 1
 1.07426738E+01 1.64789013E-06-7.92451706E-10 1.53610575E-13-1.04359108E-17    2
-2.57871325E+04-4.80251356E+01 1.07394015E+01 2.99630938E-05-7.13210384E-08    3
 7.09751854E-11-2.53463009E-14-2.57871465E+04-4.80128553E+01-2.25843640E+04    4

H2O2  HF298= -135.88 KJ  REF=TSIV
H2O2                L 2/93H  2.O  2.   0.   0.G   200.000  6000.000  B  34.01468 1
 4.57333537E+00 4.04984070E-03-1.29479479E-06 1.97281710E-10-1.13402846E-14    2
-1.80548121E+04 7.04278488E-01 4.27611269E+00-5.42822417E-04 1.67335701E-05    3
-2.15770813E-08 8.62454363E-12-1.77542989E+04 3.43505074E+00-1.63942313E+04    4

H2S  CALCULATED FROM ORIGINAL VALUES REF=Gurvich 1989      HF298=-20.60 KJ
Max Lst Sq Error Cp @ 6000 K 0.38%
H2S                 RUS 89H   2S   1    0    0G   200.000  6000.000  B  34.08188 1
 0.29770813E+01 0.36005325E-02-0.12328487E-05 0.19692654E-09-0.11677327E-13    2
-0.35155970E+04 0.67868340E+01 0.41194112E+01-0.18771599E-02 0.82066045E-05    3
-0.70594243E-08 0.21405829E-11-0.36819294E+04 0.15345832E+01-0.24775964E+04    4

H2SO4(L)            J 9/77H  2.S  1.O  4.   0.L   300.000  1000.000  C  98.07948 1
 9.94215250E+00 2.17863690E-02 3.49744580E-06-3.35488570E-09 1.16995860E-12    2
-1.01859790E+05-4.43986950E+01 9.94215250E+00 2.17863690E-02 3.49744580E-06    3
-3.35488570E-09 1.16995860E-12-1.01859790E+05-4.43986950E+01-9.79023828E+04    4

H2SO4  SULFURIC ACID  SIGMA=2  STATWT=1  IAIBIC=4060  NU=3610,1140,1223,833,550,
270,310,360,3610,1160,883,380,1453,310,569   HF0=-719. KJ  REF=Gurvich  89
Max Lst Sq Error Cp @ 6000 K 0.29%.
H2SO4               RUS 89H   2S   1O   4    0G   200.000  6000.000  B  98.07948 1
 0.11407764E+02 0.64745016E-02-0.22684185E-05 0.36060760E-09-0.21373380E-13    2
-0.92351192E+05-0.32141307E+02 0.15878661E+01 0.40882366E-01-0.48845763E-04    3
 0.29014503E-07-0.66858915E-11-0.90040015E+05 0.16687780E+02-0.88126868E+05    4

H2S2 HS-SH VERY ROUGH ESTIMATION FROM BENSON (1976) (Cp300) COMPARED WITH H2O2
HF298=4.0 KCAL  REF=Benson Chem. Rev. 1978
H2S2                T 3/94H   2S   2    0    0G   298.150  5000.000  F  66.14788 1
 0.65731735E+01 0.25619139E-02-0.69109315E-06 0.94286242E-10-0.52907210E-14    2
-0.24677791E+03-0.72991840E+01 0.21128554E+01 0.21398828E-01-0.33893856E-04    3
 0.28468801E-07-0.95576325E-11 0.67951055E+03 0.14205983E+02 0.20128667E+04    4

H3F3  SYGMA=3  IAIBIC=2000.  NU=3200(3),275(3),1000(3),550.(3)  HF0=-873. KJ
Max Lst Sq Error Cp @ 6000 K 0.27%
H3F3                RUS 89H   3F   3    0    0G   200.000  6000.000  C  60.01903 1
 0.87390503E+01 0.59975373E-02-0.20456662E-05 0.31840506E-09-0.18565610E-13    2
-0.10935328E+06-0.18233375E+02 0.15442408E+01 0.38576820E-01-0.59195549E-04    3
 0.45635939E-07-0.13570689E-10-0.10801711E+06 0.15744454E+02-0.10628128E+06    4

H3O+ HYDRONIUM ION  SIGMA=3  STATWT=1  IAIBIC=.0287  NU=3490,960,3610(2),1590(2)
HF298=598. KJ   REF=Gurvich 1989   Max Lst Sq Error Cp @ 6000 K 0.29%
H3O+                RUS 89H   3O   1E  -1    0G   298.150  6000.000  B  19.02267 1
 0.24964777E+01 0.57284481E-02-0.18395322E-05 0.27357729E-09-0.15409386E-13    2
 0.70972911E+05 0.74585048E+01 0.37929561E+01-0.91087830E-03 0.11636414E-04    3
-0.12136548E-07 0.42616180E-11 0.70751240E+05 0.14715543E+01 0.71922458E+05    4
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H4F4   SIGMA=4    IAIBIC=17000.    NU=3200(4),275(4),1000(4),550(4),40,20
HF0=-1174. KJ   REF=Gurvich 89    Max Lst Sq Error Cp @ 6000 K 0.26%
H4F4              RUS 89H   4F   4    0    0G   200.000  6000.000  C  80.02537 1
 0.12317199E+02 0.79983433E-02-0.27282048E-05 0.42465241E-09-0.24761183E-13    2
-0.14704897E+06-0.31058240E+02 0.26932762E+01 0.51626337E-01-0.79360527E-04    3
 0.61278889E-07-0.18250746E-10-0.14526330E+06 0.14381384E+02-0.14275433E+06    4

H5F5    SIGMA=5   IAIBIC=100000.  NU=3200(5),275(5),1000(5),550(5),40(2),20(2)
HF0=-1475.  REF=Gurvich 89  KJ Max Lst Sq Error Cp @ 6000 K 0.26%
H5F5              RUS 89H   5F   5    0    0G   200.000  6000.000  C 100.03172 1
 0.15895341E+02 0.99991630E-02-0.34107496E-05 0.53090070E-09-0.30956799E-13    2
-0.18474466E+06-0.44099390E+02 0.38423046E+01 0.64675877E-01-0.99525494E-04    3
 0.76921762E-07-0.22930752E-10-0.18250949E+06 0.12802019E+02-0.17922738E+06    4

H6F6  SIGMA=6  STATWT=1  IAIBIC=495000.  NU=3065,1029,203,537,26,551(2),3322(2),
991(2),327(2),33(2),550,3403,979,356,53,3153(2),1017(2),252(2),545(2),15(2)
HF0=-1788. KJ  Max Lst Sq Error Cp @ 6000 K 0.25%.
H6F6              RUS 89H   6F   6    0    0G   200.000  6000.000  B 120.03806 1
 0.19464060E+02 0.11926891E-01-0.40493043E-05 0.62823170E-09-0.36546130E-13    2
-0.22389232E+06-0.56827093E+02 0.47664477E+01 0.78603132E-01-0.12115664E-03    3
 0.93614852E-07-0.27894457E-10-0.22117213E+06 0.12546784E+02-0.21715593E+06    4

H7F7  SIGMA=7  IAIBIC=1800000.  NU=3200(7),275(7),1000(7),550(7),40(4),20(4)
REF=Gurvich 89  HF0=-2080. KJ  Max Lst Sq Error Cp @ 6000 K 0.25%
H7F7              RUS 89H   7F   7    0    0G   200.000  6000.000  C 140.04440 1
 0.23051635E+02 0.14000785E-01-0.47758323E-05 0.74339634E-09-0.43347992E-13    2
-0.26049687E+06-0.70563434E+02 0.61403336E+01 0.90775247E-01-0.13985636E-03    3
 0.10820867E-06-0.32291248E-10-0.25736269E+06 0.92617199E+01-0.25253430E+06    4

He  HF298=0.0 KJ  REF=McBride, Heimel, Ehlers & Gordon "Thermodynamic Properties
to 6000K ..." NASA SP-3001 1963.
He REF ELEMENT    L10/90HE 1.   0.   0.   0.G   200.000  6000.000  B   4.00260 1
 2.50000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-7.45375000E+02 9.28723974E-01 2.50000000E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-7.45375000E+02 9.28723974E-01 0.00000000E+00    4

He+  HF298=2378.68 KJ  REF=C.E. Moore U.S. Nat. Bur. Stand. NSRDS-NBS 34 1970.
He+               L10/92HE 1.E -1.   0.   0.G   298.150  6000.000  B   4.00205 1
 2.50000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 2.85315086E+05 1.62166556E+00 2.50000000E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 2.85315086E+05 1.62166556E+00 2.86060462E+05    4

I  HF298=106.76+/-0.04 kJ  REF=JANAF
I                 J 6/82I  1.   0.   0.   0.G   200.000  6000.000  A 126.90447 1
 2.61667712E+00-2.66010320E-04 1.86060150E-07-3.81927472E-11 2.52036053E-15    2
 1.20582790E+04 6.87896653E+00 2.50041683E+00-4.48046831E-06 1.69962536E-08    3
-2.67708030E-11 1.48927452E-14 1.20947990E+04 7.49816581E+00 1.28402035E+04    4

INO2 NITRO-IODINE  SIGMA=2  IAIBIC=9.848 E-114  NU=1500,1250,500,400,320(2)
HF298=14.4+/-1 kcal REF=estimated by Van den Berg & Troe J. Chem. Phys. 64,
(1976),736 Max Lst Sq Error Cp @ 400 K 0.34%
INO2 NITRO-IODIN  T05/99I  1.N  1.O  2.   0.G   200.000  6000.000  C 172.91001 1
 7.95621858E+00 2.06254528E-03-8.00706693E-07 1.35937003E-10-8.42239842E-15    2
 4.51430115E+03-1.11369097E+01 3.03369023E+00 2.20635097E-02-3.60079637E-05    3
 3.05880596E-08-1.03317241E-11 5.62372932E+03 1.28994935E+01 7.24631999E+03    4
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IO  T=0  STATWT=2 BE=0.340206 DE=3.6E-6 WE=681.6004 WEXE=4.3699 ALPHAE=0.0026296
T0=2091  STATWT=2 BE=0.340206 DE=3.6E-6 WE=681.6004 WEXE=4.3699 ALPHAE=0.0026296
T0=21577.81  STATWT=2 BE=0.27635 DE=3.2E-6 WE=514.57 WEXE=5.52 ALPHAE=0.00273
T0=24698   STATWT=2 BE=0.27635 DE=3.2E-6 WE=514.57 WEXE=5.52 ALPHAE=0.00273
HF298=126 +/- 18 kJ  REF=C.W.Chase JPCRD 25 (1966),1297      Max Lst Sq Error
Cp @ 1300 K 0.66%.
IO                T02/97I  1.O  1.   0.   0.G   200.000  6000.000  A 142.90387 1
 4.43373036E+00 8.12520620E-04-3.07327741E-07 6.49186840E-11-1.64640359E-15    2
 1.36225573E+04 2.96744910E+00 2.90243248E+00 5.16413407E-03-6.69836698E-06    3
 5.78794148E-09-2.15394553E-12 1.41080990E+04 1.10195868E+01 1.51542304E+04    4

IO2  I-O-O   SIGMA=1  STATWT=2  IA=1.1391  IB=33.4021  IC=34.5412  NU=1500,150,
275  HF298=116.5+/- 40 kJ  REF= C.W.Chase JPCRD 25 (1966),1297  Max Lst Sq Error
Cp @ 1300 K 0.22%
IO2   O-O-I       T02/97I  1.O  2.   0.   0.G   200.000  6000.000  C 158.90327 1
 5.98554951E+00 1.00992962E-03-3.88836232E-07 6.56594736E-11-4.05315145E-15    2
 1.20886501E+04 1.04056474E+00 5.01488370E+00 4.03669659E-03-5.27430680E-06    3
 4.73349091E-09-1.84251518E-12 1.23751572E+04 6.06532665E+00 1.40116495E+04    4

IO2  O-I-O   SIGMA=2  STATWT=2  IA=3.4373  IB=12.1991  IC=16.3491  NU=765,192,
800  HF298=159.3+/- 25 kJ  REF= C.W.Chase JPCRD 25 (1966),1297  Max Lst Sq Error
Cp @ 2300 K 0.13%.
IO2   O-I-O       T02/97I  1.O  2.   0.   0.G   200.000  6000.000  C 158.90327 1
 6.34102047E+00 6.83348986E-04-2.69576480E-07 4.62346615E-11-2.88443810E-15    2
 1.70776899E+04-2.88252557E+00 3.42630811E+00 1.04246908E-02-1.18836503E-05    3
 5.37825233E-09-5.47457748E-13 1.77689996E+04 1.16760933E+01 1.91592770E+04    4

IO3   SIGMA=3  STATWT=2  IA=IB=14.7650  IC=16.7280  NU=780,357,809.(2),326.(2)
HF298=241.9+/- 50 kJ  REF= C.W.Chase JPCRD 25 (1966),1297  Max Lst Sq Error
Cp @ 1200 K 0.20%
IO3               T02/97I  1.O  3.   0.   0.G   200.000  6000.000  C 174.90267 1
 8.79038934E+00 1.25737248E-03-4.96749925E-07 8.52803184E-11-5.32401360E-15    2
 2.61270594E+04-1.59036984E+01 1.87546093E+00 2.97337732E-02-4.73077645E-05    3
 3.59378000E-08-1.06083014E-11 2.75649245E+04 1.74919459E+01 2.90937169E+04    4

I2 IS NOT A REFERENCE ELEMENT. HF298=62.421 kJ and HF=0 ABOVE 457.7 K. REF=JANAF
I2                J 9/61I   2   0    0     0G   300.000  5000.000  B 253.8089  1
 0.44710820E+01 0.10020430E-03-0.14380573E-07 0.27741939E-11-0.19669640E-15    2
 0.61639529E+04 0.58150347E+01 0.41670013E+01 0.14456721E-02-0.22818415E-05    3
 0.17076469E-08-0.47899533E-12 0.62206616E+04 0.72552216E+01 0.75073722E+04    4

I2O I-I-O   SIGMA=1  STATWT=3  IA=5.1010  IB=112.5438  IC=117.6448  NU=750,100,
170  HF298=106.7+/- 40 kJ  REF= C.W.Chase JPCRD 25 (1966)1297  Max Lst Sq Error
Cp @ 1200 K 0.07%.
I2O  I-I-O        T02/97I  2.O  1.   0.   0.G   200.000  6000.000  C 269.80834 1
 6.67743067E+00 3.35545667E-04-1.32620068E-07 2.27738344E-11-1.42202132E-15    2
 1.07480142E+04 1.43598484E+00 4.83414789E+00 7.77521188E-03-1.20331147E-05    3
 8.84990542E-09-2.52444240E-12 1.11361166E+04 1.03678902E+01 1.28329872E+04    4

I2O I-O-I   SIGMA=2  STATWT=1  IA=2.8860  IB=119.9153  IC=122.8013  NU=475,100,
525  HF298=119.5+/- 25 kJ  REF= C.W.Chase JPCRD 25 (1966)1297  Max Lst Sq Error
Cp @  700 K 0.17%
I2O   I-O-I       T02/97I  2.O  1.   0.   0.G   200.000  6000.000  C 269.80834 1
 6.69553230E+00 3.20537584E-04-1.27603300E-07 2.20163162E-11-1.37922928E-15    2
 1.22845166E+04-1.37479980E+00 3.43863289E+00 1.69797854E-02-3.36137723E-05    3
 3.04801550E-08-1.03756973E-11 1.28341774E+04 1.36477676E+01 1.43724645E+04    4
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Kr  HF298=0.0 KJ  REF=C.E. Moore U.S. Nat. Bur. Stand. NSRDS-NBS 34/35 1970.
Kr  REF ELEMENT   L10/90KR 1.   0.   0.   0.G   200.000  6000.000  B  83.80000 1
 2.50000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-7.45375000E+02 5.49095651E+00 2.50000000E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-7.45375000E+02 5.49095651E+00 0.00000000E+00    4

Kr+               L10/92KR 1.E -1.   0.   0.G   298.150  6000.000  B  83.79945 1
 2.18968725E+00 4.63775689E-04-1.29507482E-07 1.31158688E-11-3.84977987E-16    2
 1.62583110E+05 8.62427685E+00 2.48153546E+00 1.49864676E-04-4.15576590E-07    3
 4.40237547E-10-1.19374746E-13 1.62460592E+05 6.95257995E+00 1.63204264E+05    4

MnO Manganese Oxide Data from Barin Database 1989  HF298(S)=-385.221 kJ
MnO (S)           B  /89MN 1.O  1.   0.   0.S   298.150  2115.000  C  70.93745 1
 1.35627103E+01-2.23122322E-02 2.45011706E-05-1.09793320E-08 1.74986515E-12    2
-5.02522690E+04-6.60188273E+01 2.56643455E+00 1.55785511E-02-2.79738618E-05    3
 2.42198962E-08-7.86883817E-12-4.75857738E+04-1.10409128E+01-4.63311729E+04    4
MnO (L)           B  /89MN 1.O  1.   0.   0.L  2115.000  2500.000  C  70.93745 1
-2.63748329E+01 5.81346781E-02-3.75984688E-05 1.07961809E-08-1.16134596E-12    2
-2.88800210E+04 1.56912584E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00-4.63311729E+04    4

MnO2 Manganese Dioxide  Data from Barin Database 1989  HF298(S)=-520.029 kJ
MnO2(S)           B  /89MN 1.O  2.   0.   0.S   298.150   800.000  C  86.93685 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00-4.79951256E+00 7.20358836E-02-1.55128177E-04    3
 1.55651945E-07-5.93342269E-11-6.32245896E+04 1.78855218E+01-6.25447561E+04    4

Mn2O3  Dimanganese Trioxide  Data from Barin Database 1989.  HF298(S)=-959.0 kJ
Mn2O3 (S)         B  /89MN 2.O  3.   0.   0.S   298.150  1400.000  C 157.87430 1
 4.13175143E+00 2.94925699E-02-2.97408107E-05 1.57530821E-08-3.14027515E-12    2
-1.17345192E+05-1.71563396E+01 3.73625576E+00 4.53603719E-02-7.84795848E-05    3
 6.79682080E-08-2.20889333E-11-1.17901390E+05-1.85906447E+01-1.15340772E+05    4

Mn3O4  Trimanganese Tetraoxide  Data from Barin 1989. HF298(S)=-1434.191 kJ
Mn3O4  Solid-A    B  /89MN 3.O  4.   0.   0.S   298.150  1445.000  C 228.81175 1
 9.24690980E+00 3.03097632E-02-2.77876351E-05 1.42175100E-08-2.74343370E-12    2
-1.70540047E+05-4.13240828E+01 5.30992963E+00 6.45031044E-02-1.12103682E-04    3
 9.70819405E-08-3.15481785E-11-1.70549547E+05-2.65839957E+01-1.66912903E+05    4
Mn3O4  Solid-B    B  /89MN 3.O  4.   0.   0.S  1445.000  1835.000  C 228.81175 1
 2.18396178E+01 8.24501377E-03-7.43602439E-06 2.97586871E-09-4.45964303E-13    2
-1.74631781E+05-1.12000838E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00-1.66912903E+05    4

Mn5N2  Pentamanganese Dinitride  Data from Barin 1989  HF298(S)=-204.2 kJ
Mn5N2(S)          B  /89MN 5.N  2.   0.   0.S   298.150   800.000  C 302.70373 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00 1.53753139E+01 1.93066443E-02 5.09039170E-08    3
-6.55123649E-11 3.04082415E-14-3.00020762E+04-7.08162751E+01-2.45594749E+04    4

MnS  Manganese Monosulfide (Green) Data from Barin  HF298(S)=-214.414 kJ
MnS   Solid       B  /89MN 1.S  1.   0.   0.S   298.150  1803.000  C  87.00405 1
 5.73936431E+00 9.01938576E-04 3.02740651E-11 1.69143122E-12-5.47133193E-16    2
-2.75139333E+04-2.35653794E+01 5.73590949E+00 9.12003512E-04-1.77463767E-08    3
 2.06928531E-11-8.38201915E-15-2.75127688E+04-2.35470661E+01-2.57621916E+04    4
MnS   Liquid      B  /89MN 1.S  1.   0.   0.L  1803.000  2200.000  C  87.00405 1
 7.36336543E+00 1.36969500E-03-1.02073380E-06 3.37546304E-10-4.17948179E-14    2
-2.67980686E+04-3.37306895E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00-2.57621916E+04    4
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MnS2  Manganese Disulfide  Data fron Barin Database  HF298(S)=-223.844  kJ
MnS2 (S)            B  /89MN 1.S  2.   0.   0.S   298.150   700.000  C 119.07005 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00 4.48568512E+00 2.44442175E-02-5.26856546E-05    3
 5.76754423E-08-2.41568621E-11-2.89830667E+04-1.89489535E+01-2.69220916E+04    4

Mo Molibden REFERENCE ELEMENT HF298(S)=0.0  REF=JANAF
Mo(cr)              J 3/78MO 1.   0.   0.   0.S   200.000  2896.000  B  95.94000 1
 5.38432823E+00-6.01622180E-03 6.01482526E-06-2.32962338E-09 3.52007808E-13    2
-1.62657220E+03-2.62488891E+01 1.32884141E+00 9.82553689E-03-2.10929825E-05    3
 2.09509528E-08-7.60703244E-12-6.84364789E+02-6.29286538E+00 0.00000000E+00    4

Mo(L)               J 3/78MO 1.   0.   0.   0.L  2896.000  6000.000  B  95.94000 1
 4.52894999E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 2.02140667E+03-2.28074752E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    4

MoC  Molibdenum Monocarbide Gamma  Data from Barin 1989  HF298(S)=-28.451 kJ
MoC  Solid-C        B  /89C  1.MO 1.   0.   0.S   298.150  1400.000  C 107.95100 1
 1.95688580E+00 7.45582204E-03-4.92462131E-06 1.16731721E-09 5.69099576E-14    2
-4.30569462E+03-8.78043176E+00 1.75407212E+00 8.17609975E-03-5.89254003E-06    3
 1.74969447E-09-7.50126171E-14-4.25959002E+03-7.77690797E+00-3.42184927E+03    4

MoO2  Molibdenum Dioxide Solid Data from Barin 1989 HF298(S)=-588.94 kJ
MoO2  Solid         B  /89MO 1.O  2.   0.   0.S   298.150  2000.000  C 127.93880 1
 5.57003335E+00 7.01737124E-03-4.11649672E-06 1.48282458E-09-1.41613677E-13    2
-7.28178014E+04-2.82261435E+01 6.56226971E-01 3.36489565E-02-5.76641545E-05    3
 4.88255458E-08-1.56544560E-11-7.21036803E+04-6.04322444E+00-7.08327971E+04    4

MoO2  Molibdenum Dioxide Gas Data from Barin Database 1989  HF298=-8.314 kJ
MoO2                B  /89MO 1.O  2.   0.   0.G   298.150  3000.000  C 127.93880 1
 4.14494627E+00 7.05834738E-04-5.16986528E-07 1.86466769E-10-2.22683845E-14    2
-2.29247521E+03 6.46991922E+00 2.90286012E+00 6.65546290E-03-1.14989921E-05    3
 9.33240931E-09-2.89374741E-12-2.07672445E+03 1.22605433E+01-9.99938661E+02    4

Mo2C  DiMolibdenum Carbide  Data from Barin Database 1989 HF298(S)=-53.137 kJ
Mo2C(S)             B  /89MO 2.C  1.   0.   0.S   298.150  1400.000  C 203.89100 1
 2.63292301E+00 1.91409016E-02-1.95825211E-05 8.67987123E-09-1.10539752E-12    2
-7.76509118E+03-1.17561621E+01 2.42024100E+00 2.50702462E-02-3.73749151E-05    3
 2.75982039E-08-7.94799883E-12-7.94734639E+03-1.19156150E+01-6.39087571E+03    4

N    REF=C.E. Moore "Selected Tables of Atomic Spectra" NSRDS-NBS Sec 5 1975
p. A7 I. HF298=472.68 KJ  REF=CODATA Key Values 1989 p.22.
N                   L 6/88N   1    0    0    0G   200.000  6000.000  A  14.00674 1
 0.24159429E+01 0.17489065E-03-0.11902369E-06 0.30226244E-10-0.20360983E-14    2
 0.56133775E+05 0.46496095E+01 0.25000000E+01 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 0.56104638E+05 0.41939088E+01 0.56850013E+05    4

ND  T0=0  STATWT=3  Be=8.993  WE=2422   WEXE=50.6  ALFAE=0.252
HF298=375.305+/-20.9 kJ  REF=JANAF
ND                  J 6/77N  1.D  1.   0.   0.G   298.150  5000.000  B  16.02080 1
 2.82970340E+00 1.65841750E-03-6.32873330E-07 1.14776850E-10-7.83185840E-15    2
 4.42559510E+04 5.99346190E+00 3.72064880E+00-1.53418480E-03 3.18774260E-06    3
-1.50914010E-09 9.71261140E-14 4.40727560E+04 1.63638980E+00 4.51390710E+04    4

NDH  REF=Burcat  Obtained from (NH2 + ND2)/2   HF298=187.862+/-2.0 kJ. Max Lst
Sq Error Cp @ 2000 K  0.46%
NHD    Radical      T04/97N  1.H  1.D  1.   0.G   200.000  5000.000  D  17.02878 1
 3.05621369E+00 3.29951143E-03-1.17319396E-06 2.23377976E-10-1.67307373E-14    2
 2.15414279E+04 5.65331410E+00 4.16883275E+00-2.22264864E-03 8.52003690E-06    3
-7.23221826E-09 2.15517566E-12 2.13883297E+04 5.85380736E-01 2.25944764E+04    4
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ND2  SIGMA=2  STATWT=1  IA=0.5832  IB=2.178  IC=2.7612  NU=2400,2300,1490,1150,
1058,750   HF298=185.353+/-8.4 kJ   REF=JANAF
ND2                 J 6/77N  1.D  2.   0.   0.G   298.150  5000.000  C  18.03490 1
 3.35153910E+00 3.37631620E-03-1.32134570E-06 2.68006790E-10-2.08101740E-14    2
 2.10777490E+04 4.36071310E+00 4.02697800E+00-1.40851280E-03 7.77658150E-06    3
-6.49675750E-09 1.75541700E-12 2.10980280E+04 1.74167630E+00 2.22927630E+04    4

ND2H   REF=BURCAT   ND2 + NH3 - NH2  HF298=-50.919 kJ  Max Lst Sq Error H-H298
**6.0%** @ 600 K  Cp **2.1%** @ 600 K  S **3.1%** @ 900 K
ND2H                T04/97N  1.D  2.H  1.   0.G   200.000  5000.000  D  19.04288 1
 2.36500514E+00 7.36877446E-03-2.88232186E-06 5.18352154E-10-3.54808494E-14    2
-7.20071934E+03 8.67575769E+00 4.04335565E+00-2.22717358E-03 1.52167970E-05    3
-1.42569646E-08 4.55831451E-12-7.33906535E+03 1.40516840E+00-6.12411315E+03    4

ND3  DEUTERATED AMONIA  SIGMA=3  STATWT=1  IAIBIC=0.25775E-117  NU=2652(2),2495,
1225(2),793  HF298=-58.576+/-0.4 kJ  REF=JANAF
ND3                 J 6/77N  1.D  3.   0.   0.G   298.150  5000.000  B  20.04901 1
 3.19615660E+00 6.73117580E-03-2.64234000E-06 4.76308680E-10-3.28048280E-14    2
-8.39665270E+03 4.14974150E+00 2.94278390E+00 5.10352910E-03 2.73928210E-06    3
-4.68476620E-09 1.62766740E-12-8.16515630E+03 6.14205470E+00-7.04511980E+03    4

NF  CALCULATED FROM ORIGINAL DATA REF=Gurvich 1989  HF0=233. KJ
NF                  RUS 89N  1.F  1.   0.   0.G   200.000  6000.000  B  33.00514 1
 4.06042292E+00 3.50654850E-04-6.95721815E-08 1.45925454E-11-1.56372401E-15    2
 2.66711982E+04 2.08774805E+00 3.59927999E+00-2.18190788E-03 1.14106853E-05    3
-1.40068494E-08 5.53332638E-12 2.69702525E+04 5.35573603E+00 2.80221438E+04    4

NF2 RADICAL  SIGMA=2  STATWT=2  A0=2.35149  B0=.396015  C0=.338116  NU=1074,573,
931  TAAA=-.000259  TBBB=-2.7E-6   TAAB=9.9E-6  TABA=-4.2E-6  TCCC=-1.3E-6
TAAC=1.9E-6   TBBC=-1.8E-6  HF0=37 KJ  REF=Gurvich 1989  Max Lst Sq Error Cp @
400 K 0.33%
NF2                 L 5/95N   1F   2    0    0G   200.000  6000.000  B  52.00355 1
 0.58364792E+01 0.12115300E-02-0.46827522E-06 0.79997253E-10-0.49773112E-14    2
 0.21075383E+04-0.41367038E+01 0.30383609E+01 0.66254958E-02 0.16160965E-05    3
-0.98870122E-08 0.52618129E-11 0.29422774E+04 0.10741500E+02 0.41398711E+04    4

NF3  SIGMA=3  STATWT=1 A0=0.1948  B0=C0=0.35628    NU=1032,647,908(2),493(2)
X11=-2.8  X12=-3.5  X13=-9.9  X14=-2.3  X22=-2.5  X23=-6.5  X24=-2.4  X33=-3.5
X34=-1.5  X44=-0.6  ALFAA1=9.8E-4 ALFAA2=.000573  ALFAA3=9.22E-4  ALFAA4=6.51E-4
ALFAB1=-.001438  ALFAB2=.001288  ALFAB3=.0002629  ALFAB4=.0001493
ALFAC1=-.001438  ALFAC2=.001288  ALFAC3=.0002629  ALFAC4=.0001493
DJ=4.85E-7  DK=3.27E-7   DJK=-7.475E-7   REF=Gurvich 89   HF298=-131.7  KJ
Max Lst Sq Error Cp @ 400 K 0.3%
NF3                 L 5/95N   1F   3    0    0G   200.000  6000.000  A  71.00195 1
 0.80969263E+01 0.22248772E-02-0.73845724E-06 0.13242062E-09-0.82140433E-14    2
-0.18767390E+05-0.16378386E+02 0.13184910E+01 0.23460985E-01-0.23520025E-04    3
 0.82591366E-08 0.18896563E-12-0.17084267E+05 0.17841863E+02-0.15839779E+05    4

NH    REF=TSIV 78 (Error found in H-H0 of Gurvich 1989). HF298=357. KJ
REF=Anderson J.Phys. Chem. 93 (1989), 530  Max Lst Sq Error Cp @ 6000 K 0.28%
NH                  L11/89N   1H   1    0    0G   200.000  6000.000  A  15.01468 1
 0.27836929E+01 0.13298429E-02-0.42478047E-06 0.78348504E-10-0.55044470E-14    2
 0.42134514E+05 0.57407798E+01 0.34929084E+01 0.31179197E-03-0.14890484E-05    3
 0.24816442E-08-0.10356967E-11 0.41894294E+05 0.18483277E+01 0.42940822E+05    4

NH+  GENERETED FROM ORIGINAL VALUES  HF0=1656.3 KJ  REF= Gurvich 1989
NH+                 L 2/89N  1.H  1.E -1.   0.G   298.150  6000.000  B  15.01413 1
 2.95918980E+00 1.34991719E-03-4.61487782E-07 8.26977666E-11-5.55758913E-15    2
 1.99524505E+05 5.59978021E+00 4.61611136E+00-3.13435677E-03 2.91705130E-06    3
 2.57384848E-10-7.31431347E-13 1.99085043E+05-2.92758460E+00 2.00347960E+05    4
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NHF RADICAL STATWT=2  SIGMA=1  IAIBIC=1.221  NU=3200,1000,1432  T0=20141.26
STATWT=2  SIGMA=1  HF298=112. KJ  REF=Gurvich 1989  Max Lst Sq Error Cp @ 6000 K
0.29%
NHF               RUS 89N   1H   1F   1    0G   200.000  6000.000  B  34.01308 1
 0.38957856E+01 0.26972954E-02-0.96413416E-06 0.15656481E-09-0.93275479E-14    2
 0.12097631E+05 0.45781245E+01 0.41481642E+01-0.33379936E-02 0.17632209E-04    3
-0.20570502E-07 0.79043064E-11 0.12263155E+05 0.45024858E+01 0.13470427E+05    4

NHF2  SIGMA=1  IAIBIC=109.9  NU=3193,1424,1307,970,888,500  REF=Gurvich 1989
HF298=-103 KJ Max Lst Sq Error Cp @ 6000 K 0.38%
NHF2              RUS 89N   1H   1F   2    0G   200.000  6000.000  B  53.01149 1
 0.56498758E+01 0.39393919E-02-0.14331458E-05 0.23343765E-09-0.14065134E-13    2
-0.14562287E+05-0.36451783E+01 0.33212629E+01 0.35048001E-02 0.16269284E-04    3
-0.25711192E-07 0.10991340E-10-0.13632111E+05 0.99205457E+01-0.12387982E+05    4

NH2 AMIDOGEN RADICAL SIGMA=2 STATWT=2  A=23.692  B=12.939  C=8.181  NU=3219,
1497,3301 TAAA=-.0744 TBBB=-.6E-2  TCCCC=-.92E-2  TAAB=0.0156  TAAC=-).26E-2
TBBC=-0.022  TABA=-.35E-2  T0=10250. SIGMA=2  STATWT=2  IAIBIC=0.00287E-117
NU=3225,633,3500   REF=M. Jacox JPCRD 17 (1988), 282 and TSIV 78  HF0=192.0 KJ
REF=Anderson J.Phys.Chem 93 (1989), 530  Max Lst Sq Error Cp @ 6000 K 0.28%
NH2               L12/89N   1H   2    0    0G   200.000  6000.000  A  16.02262 1
 0.28476611E+01 0.31428453E-02-0.89866557E-06 0.13032357E-09-0.74885356E-14    2
 0.21823916E+05 0.64718133E+01 0.42055601E+01-0.21355282E-02 0.72682021E-05    3
-0.59302799E-08 0.18067218E-11 0.21535223E+05-0.14663231E+00 0.22747541E+05    4

NH2D   REF=BURCAT  NH2 + ND3 - ND2  HF298=-44.081 kJ  Max Lst Sq Error H-H298 @
600 K **4.6%**
NH2D              T04/97N  1.H  2.D  1.   0.G   200.000  5000.000  D  18.03672 1
 2.63913593E+00 6.56150529E-03-2.37234899E-06 4.00847337E-10-2.63129116E-14    2
-6.35155863E+03 6.50813546E+00 3.85166967E+00-1.06064928E-03 1.55181750E-05    3
-1.78471387E-08 6.74076997E-12-6.50794315E+03 1.20003299E+00-5.30169547E+03    4

NH2F   SIGMA=1  IAIBIC=3.06  NU=3260,3210,1620,1500,1280,910  HF298=-75. KJ
REF=Gurvich 1989  Max Lst Sq Error Cp @ 6000 K 0.47%.
NH2F              RUS 89N   1H   2F   1    0G   200.000  6000.000  B  35.02102 1
 0.34379333E+01 0.56345867E-02-0.19763269E-05 0.31384602E-09-0.18569992E-13    2
-0.10454484E+05 0.60423912E+01 0.44307579E+01-0.70044845E-02 0.32429410E-04    3
-0.35524163E-07 0.13059948E-10-0.10252553E+05 0.32967779E+01-0.90203752E+04    4

NH3  AMONIA  GENERATED FROM ORIGINAL VALUES  HF298=-45.94 KJ  REF=Gurvich 1989
NH3  AMONIA       RUS 89N  1.H  3.   0.   0.G   200.000  6000.000  A  17.03056 1
 2.71709692E+00 5.56856338E-03-1.76886396E-06 2.67417260E-10-1.52731419E-14    2
-6.58451989E+03 6.09289837E+00 4.30177808E+00-4.77127330E-03 2.19341619E-05    3
-2.29856489E-08 8.28992268E-12-6.74806394E+03-6.90644393E-01-5.52528050E+03    4

NH2OH  HYDROXYLAMINE  STATWT=1  SIGMA=1  A0=6.370312  B0=.841238  C0=.839105
NU=3620,3297,1605,1357,1115,895,3350,765,386  T0=3800. STATWT=1 HF298= -50.0 KJ
REF=TSIV+Gurvich 89
NH2OH             RUS 78N   1H   3O   1    0G   200.000  6000.000  B  33.02996 1
 0.38808544E+01 0.81574618E-02-0.28263348E-05 0.43796511E-09-0.25274751E-13    2
-0.75876998E+04 0.37931250E+01 0.32101336E+01 0.61970334E-02 0.11058271E-04    3
-0.19665010E-07 0.88242437E-11-0.73091267E+04 0.79330377E+01-0.60135835E+04    4


NH4+  AMONIUM ION  SIGMA=12  STATWT=1  IAIBIC=.106E-117    NU=3250,1700(2),
3350(3),1430(3)   HF298=644.9 KJ  REF=TSIV
NH4+              RUS 78N   1H   4E  -1    0G   298.150  6000.000  C  18.03795 1
 0.13156479E+01 0.96493541E-02-0.32905419E-05 0.51205492E-09-0.29850594E-13    2
 0.76727757E+05 0.12093408E+02 0.50221425E+01-0.11710230E-01 0.39760767E-04    3
-0.36942723E-07 0.12026708E-10 0.76303001E+05-0.42054342E+01 0.77563825E+05    4
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NH4ClO4(I) and (II) Amonium Perchlorate crystal  REF=JANAF HF298=-70.69 kcal
NH4CLO4(I)        J12/62N  1.H  4.CL 1.O  4.S   200.000   513.150  C 117.48880 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00 6.35703886E+00 4.13638533E-02-5.92805489E-05    3
 8.96504531E-08-4.96854073E-11-3.89362027E+04-2.44599186E+01-3.55723861E+04    4
NH4CLO4(II)       J12/62N  1.H  4.CL 1.O  4.S   513.150  1500.000  C 117.48880 1
 1.55208289E+02-1.85584191E-01 7.02879745E-05 0.00000000E+00 0.00000000E+00    2
-1.10827457E+05-8.51152444E+02 2.57678288E+03-1.79847751E+01 4.36807324E-02    3
-4.44267613E-05 1.61939332E-08-3.01717712E+05-1.08243913E+04-3.55723861E+04    4

NO  GENERATED FROM ORIGINAL VALUES  HFO=82.09 KJ REF=Gurvich 1989
NO                RUS 89N  1.O  1.   0.   0.G   200.000  6000.000  A  30.00614 1
 3.26071234E+00 1.19101135E-03-4.29122646E-07 6.94481463E-11-4.03295681E-15    2
 9.92143132E+03 6.36900518E+00 4.21859896E+00-4.63988124E-03 1.10443049E-05    3
-9.34055507E-09 2.80554874E-12 9.84509964E+03 2.28061001E+00 1.09770882E+04    4

NO+  GENERATED FROM ORIGINAL VALUES  HF0=982.137 KJ  REF=Gurvich 1989
NO+               RUS 89N  1.O  1.E -1.   0.G   298.150  6000.000  A  30.00559 1
 2.94587702E+00 1.40325260E-03-4.95503196E-07 7.95948973E-11-4.72076668E-15    2
 1.18244340E+05 6.70644634E+00 3.69301231E+00-1.34229158E-03 2.67343395E-06    3
-1.02609308E-09-6.95610492E-14 1.18103055E+05 3.09126691E+00 1.19166025E+05    4

NOCl  SIGMA=1  STATWT=1  A0=2.9145  B0=.19139  C0=.17933    NU=1800,596,332
X11=-17.8  X12=0. X13=-.6  X22=-2.6  X23=-4.3  X33=-1.    ALFAA1=.04016
ALFAA2=-.03888  ALFAA3=-.01061  ALFAB1=-.00033  ALFAB2=.00053  ALFAB3=-.0016
ALFAC1=-.00013  ALFAC2=.00069  ALFAC3=.00153  TAAA=-.00057778   TBBB=-9.75E-7
TAAB=8.5222E-6  TABA=-3.6732E-6   TCCC=-.7.032E-7     TAAC=5.2943E-6
TBBC=-8.2374E-7    T0=10000.  STATWT=3 SIGMA=1   T0=16000.  STATWT=1 SIGMA=1
REF=Gurvich 1989   HF0=54.6 KJ  Max Lst Sq Error Cp @ 1300 0.66%.
NOCL              L 5/95N   1O   1CL  1    0G   200.000  6000.000  A  65.45884 1
 0.61799190E+01 0.28500775E-03 0.17276529E-06-0.30166754E-10 0.90192767E-15    2
 0.56327606E+04-0.43234813E+01 0.32325533E+01 0.11886435E-01-0.21070873E-04    3
 0.19552938E-07-0.69926270E-11 0.63635546E+04 0.10277271E+02 0.77048343E+04    4

NOF  SIGMA=1  A0=3.175188  B0=.395080  C0=.350519  NU=1844,756,520   X11=-17.5
X12=1.5  X13=2.  X22=-4.7  X23=-2.  X33=-1.5  ALFAA1=.0345  ALFAA2=-.01912
ALFAA3=-.01354  ALFAB1=-.00014  ALFAB2=.00166  ALFAB3=.00484  ALFAC1=.00024
ALFAC2=.00184  ALFAC3=.0047  TAAA=-.00052  TBBB=-3.32E-6  TAAB=.000014
TABA=-9.66E-6  TCCC=-1.89E-6  TAAC=4.68E-6  TBBC=-2.46E-6  T0=15000.  SIGMA=1
STATWT=3  HF298=-65. KJ  REF=Gurvich 1989  mAX lST sQ eRROR Cp @ 6000 K 0.4%.
NOF               L 5/95N   1O   1F   1    0G   200.000  6000.000  A  49.00454 1
 0.52530781E+01 0.19000792E-02-0.75667187E-06 0.15514137E-09-0.10897571E-13    2
-0.96262527E+04-0.98536249E+00 0.28886971E+01 0.10359580E-01-0.13880734E-04    3
 0.10416535E-07-0.32433490E-11-0.90357928E+04 0.10837381E+02-0.78176585E+04    4

NOF3  SIGMA=3 IAIBIC=3250.  NU=1689,740,542,884(2),528(2),398(2)  HF298=-187. KJ
REF=Gurvich 1989  Max Lst Sq Error Cp @ 1200 K 0.34%
NOF3              RUS 89N   1O   1F   3    0G   200.000  6000.000  B  87.00135 1
 0.10122162E+02 0.29210198E-02-0.11381315E-05 0.19369199E-09-0.12021234E-13    2
-0.26123657E+05-0.26256953E+02-0.15692449E+00 0.44229130E-01-0.68789152E-04    3
 0.52715545E-07-0.15911878E-10-0.23898778E+05 0.23733541E+02-0.22490802E+05    4
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NO2  STATWT=2  SIGMA=2  A0=8.002509  B0=.4336646  C0=.4104926  NU=1320,750,1616
X11=-8.1  X12=-9.7  X13=-29.8  X22=-.5  X23=-2.7  X33=-15.6  ALFAA1=-.0753
ALFAA2=-.364  ALFAA3=.2208  TAAA=-.11367E-1  TBBB=-.14180E-5  TCCC=-.89140E-6
TAAB=.6906E-4  TAAC=.31970E-4  TBBC=-.10890E-5  TABA=-.8215E-5  ALFAB1=.002354
ALFAB3=.002718  ALFAC1=.00282  ALFAC2=-.00095  ALFAC3=.00264     TO=11956.
STATWT=2.  T0=14744.  STATWT=2  T0=26000.  STATWT=4  T0=27000.  STATWT=4
T0=31000.  STATWT=2  T0=40125  STATWT=2  HF0=37.0 KJ REF= Gurvich 1989.
NO2                L 7/88N   1O   2    0    0G   200.000  6000.000  A  46.00554 1
 0.48847540E+01 0.21723955E-02-0.82806909E-06 0.15747510E-09-0.10510895E-13    2
 0.23164982E+04-0.11741695E+00 0.39440312E+01-0.15854290E-02 0.16657812E-04    3
-0.20475426E-07 0.78350564E-11 0.28966180E+04 0.63119919E+01 0.41124701E+04    4

NO2-    STATWT=1  SIGMA=2  IA=.649  IB=5.907  IC=6.556  NU=1330,810,1245
HF298=-200.035 KJ REF= Gurvich 1989. Max Lst Sq Error Cp @ 1300 K 0.34%
NO2-               RUS 89N   1O   2E   1    0G   298.150  6000.000  B  46.00609 1
 0.50533023E+01 0.20755476E-02-0.87000155E-06 0.16107454E-09-0.10344873E-13    2
-0.25904369E+05-0.15407134E+01 0.30978573E+01 0.37047376E-02 0.59296511E-05    3
-0.10949983E-07 0.46273153E-11-0.25179837E+05 0.94822771E+01-0.24058613E+05    4

NO2Cl  SIGMA=2  STATWT=1  A0=.44334  B0=.172637  C0=.1240691  NU=1286,793,370,
1685,408,652  TAAA=-2.04E-6    TBBB=-.59E-6   TAAB=.28E-6   TABA=-.86E-6
TCCC=-.15E-6    TAAC=-.17E-7   TBBC=-.284E-6  REF=Gurvich 1989  HF298=12.5 KJ
Max Lst Sq Error Cp @ 1300 K 0.38 %
NO2CL              L 5/95N   1O   2CL  1    0G   200.000  6000.000  A  81.45824 1
 0.73973930E+01 0.26288293E-02-0.10108361E-05 0.17126196E-09-0.10596506E-13    2
-0.11593163E+04-0.10963487E+02 0.23950579E+01 0.19208111E-01-0.23484888E-04    3
 0.15177254E-07-0.41194825E-11 0.11500810E+03 0.14274389E+02 0.15033959E+04    4

NO2F  SIGMA=2  STATWT=1  A0=.440348  B0=.3818057  C0=.2041075  NU=1310,822,568,
1792,560,742   TAAA=-1.328E-6  TBBB=-2.623E-6  TCCC=-.224E-6  TAAB=.415E-6
TABA=-1.63E-6  TAAC=-.167E-6  TBBC=-.66E-6  HF298=-109. KJ  REF=Gurvich 1989
Max Lst Sq Error Cp @ 1300 K 0.4%.
NO2F               L 5/95N   1O   2F   1    0G   200.000  6000.000  A  65.00394 1
 0.70399495E+01 0.29695800E-02-0.11442077E-05 0.19364501E-09-0.11972566E-13    2
-0.15731594E+05-0.10688099E+02 0.18781432E+01 0.17625040E-01-0.15399750E-04    3
 0.47606145E-08 0.18294737E-12-0.14326397E+05 0.15869654E+02-0.13109612E+05    4

NO3  SIGMA=6  STATWT=2  IA=IB=6.4277  IC=12.8555  NU=1158(2),940,704(2),765
HF298=71.13 KJ  REF=JANAF
NO3                J12/64N  1.O  3.   0.   0.G   200.000  6000.000  C  62.00494 1
 7.48347734E+00 2.57772041E-03-1.00945831E-06 1.72314072E-10-1.07154015E-14    2
 5.70919428E+03-1.41618155E+01 2.17359310E+00 1.04902697E-02 1.10472650E-05    3
-2.81561854E-08 1.36583958E-11 7.39219877E+03 1.46022098E+01 8.55492386E+03    4

NO3- ION   STATWT=1  SIGMA=6   IAIBIC=480.E-117   NU=1055,830,1370(2),720(2)
HF0=-298.0 KJ  REF= Gurvich 1989
NO3-               RUS 89N  1.O  3.E  1.   0.G   298.150  6000.000  B  62.00549 1
 6.88404739E+00 3.16062982E-03-1.23048782E-06 2.09257989E-10-1.29795471E-14    2
-4.00548152E+04-1.17087097E+01 1.21258521E+00 1.71545193E-02-1.05270457E-05    3
-1.16074097E-09 2.33114998E-12-3.84077713E+04 1.79933865E+01-3.73779731E+04    4

NO3F  SIGMA=1  IAIBIC=3300.  IR=1.709  ROSYM=2. POT. BARRIER V(2)=3510. cm-1
NU=1759,1301,928,804,663,455,303,709  HF298=15. KJ  REF=Gurvich 1989  Max Lst
Sq Error Cp @ 1300 K 0.52%
NO3F               RUS 89N   1O   3F   1    0G   200.000  5000.000  B  81.00334 1
 0.98118818E+01 0.35639389E-02-0.15419861E-05 0.27634191E-09-0.17658973E-13    2
-0.18356434E+04-0.22945174E+02 0.23251747E+01 0.26601706E-01-0.29142030E-04    3
 0.15590927E-07-0.32832597E-11 0.15666889E+03 0.15244961E+02 0.18040750E+04    4
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N2  HF298= 0.0 KJ  REF=TSIV
N2  REF ELEMENT   RUS 78N   2    0    0    0G   200.000  6000.000  A  28.01348 1
 0.29525407E+01 0.13968838E-02-0.49262577E-06 0.78600091E-10-0.46074978E-14    2
-0.92393753E+03 0.58718221E+01 0.35309628E+01-0.12365950E-03-0.50299339E-06    3
 0.24352768E-08-0.14087954E-11-0.10469637E+04 0.29674391E+01 0.00000000E+00    4

N2D2-cis  STATWT=1  SIGMA=2  IA=.5832  IB=2.1780  IC=2.7612  NU=2300,1490,1058,
2400,1150,750  HF298=207.11 KJ  REF=JANAF
N2D2   Cis        J 6/77N  2.D  2.   0.   0.G   298.150  5000.000  C  32.04160 1
 4.01190860E+00 6.16993650E-03-2.57108910E-06 4.83639280E-10-3.38931910E-14    2
 2.32104290E+04 1.83805160E+00 2.97738700E+00 4.11130230E-03 8.78870250E-06    3
-1.23688270E-08 4.55193770E-12 2.37836210E+04 8.50070960E+00 2.49095210E+04    4

N2F2 ISOMERS CIS AND TRANS WERE MIXED BY INCLUDING THEM AS EXCITED STATES. 1 IS
CIS AND 2 IS TRANS  SIGMA=2  IAIBIC=668.2  NU=1525,896,341,300,952,737  T0=470.
SIGMA=2   IAIBIC=390.  NU=1523,1018,603,362,990,422  HF0=67. KJ  REF=Gurvich 89
Max Lst Sq Error Cp @ 1300 K 0.30%.
N2F2              RUS 89N   2F   2    0    0G   200.000  6000.000  B  66.01029 1
 0.79266250E+01 0.21002389E-02-0.81722252E-06 0.13894835E-09-0.86178747E-14    2
 0.47212571E+04-0.14265182E+02 0.26944269E+01 0.19996317E-01-0.25239401E-04    3
 0.15967248E-07-0.40786186E-11 0.60030677E+04 0.11933973E+02 0.75018251E+04    4

N2F4   EQUILIBRIUM MIXTURE OF TRANS AND GAUCHE ISOMERS.   SIGMA=2   STATWT=1
IAIBIC=13800.  NU=1039,719,601,354,962,252,131,873,999,542,494,467    T0=100.
SIGMA=2  STATWT=1  IAIBIC=11800.  NU=1027,946,733,587,423,298,115,1012,931,515,
288,242  HF298=-22. KJ  REF=Gurvich 1989  Max Lst Sq Error Cp @ 1300 0.27%
N2F4              RUS 89N   2F   4    0    0G   200.000  6000.000  B 104.00709 1
 0.13251312E+02 0.28400333E-02-0.11179520E-05 0.19147494E-09-0.11934318E-13    2
-0.73226616E+04-0.39550630E+02 0.13352845E+01 0.47397540E-01-0.66795981E-04    3
 0.45073083E-07-0.11856992E-10-0.46441011E+04 0.19044610E+02-0.26459767E+04    4

N2H  (NNH) STATWT=2  IA=0.131  IB=1.789419  IC=1.92025  NU=1129,1484,2926
REF=C.Melius BAC/MP4 Calculations, Private Communication  HF298=*59.636+/-3.24*
KCAL    Max Lst Sq Error Cp @ 6000 K 0.38%
N2H               T07/93N   2H   1    0    0G   200.000  6000.000  B  29.02142 1
 0.37667545E+01 0.28915081E-02-0.10416620E-05 0.16842594E-09-0.10091896E-13    2
 0.28650697E+05 0.44705068E+01 0.43446927E+01-0.48497072E-02 0.20059459E-04    3
-0.21726464E-07 0.79469538E-11 0.28791973E+05 0.29779411E+01 0.30009829E+05    4

N2H2 SIGMA=2 STATWT=1 A0=10.00021  B0=1.304194  C0=1.149861  NU=1286,
1529,1583,3120.3,3131,1600    T0=3000.  STATWT=1   SIGMA=2   IAIBIC=1.46E-117
NU=1390,1470,1670,3040,3090,1100  T0=6000. STATWT=3  IAIBIC=1.58E-117  NU=1360,
1485,1580,3330,3380,1200  T0=6700.  STATWT=1   T0=14000.   STATWT=3   T0=20700.
STATWT=3  T0=17400.  STATWT=1  HF298=211.86 KJ REF= Gurvich 1989.
N2H2              L 5/90N   2H   2    0    0G   200.000  6000.000  A  30.02936 1
 0.13111509E+01 0.90018727E-02-0.31491187E-05 0.48144969E-09-0.27189798E-13    2
 0.24786417E+05 0.16409109E+02 0.49106602E+01-0.10779187E-01 0.38651644E-04    3
-0.38650163E-07 0.13485210E-10 0.24224273E+05 0.91027970E-01 0.25480756E+05    4

NH2NO2  NITRAMIDE  IAIBIC=637.10E-117  NU=3359,1558,1350,951,798,693,629,3478,
1613,1227,485,402   HF298= -3.0 KJ  REF= Dorofeeva & Tolmach. Thermochim. Acta
240,(1994),47-66. Max Lst Sq Error Cp @ 1300 0.52 %.
NH2NO2 NITRAMIDE  T10/99H  2.N  2.O  2.   0.G   200.000  6000.000  B  62.02816 1
 7.73743619E+00 7.14052586E-03-2.51282392E-06 3.99637625E-10-2.36573378E-14    2
-3.51433007E+03-1.49368357E+01 1.65916283E+00 2.08441985E-02-7.27880677E-06    3
-8.06033366E-09 5.57689747E-12-1.70435024E+03 1.71495596E+01-3.60815009E+02    4
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N2H3 Hydrazine Radical STATWT=2 SIGMA=1 IA=0.40875  IB=2.7303  IC=3.05753
IR=0.09528  POTENTIAL BARRIER V(2)=3609.5 cm-1 ROSYM=2  NU=3455,3339,3283,1650,
1449.5,1159,1129,742   REF=C. Melius BAC/MP4 Calculations Private Communication
HF298=***53.79+/-17.0 KCAL***  Max Lst Sq Error Cp @ 6000 K 0.58%
H3N2              T 7/93H   3N   2    0    0G   200.000  6000.000  B  31.03730 1
 0.43414654E+01 0.75280979E-02-0.27478351E-05 0.44688178E-09-0.26846990E-13    2
 0.25176779E+05 0.98835045E+00 0.33151120E+01 0.21514763E-02 0.21849694E-04    3
-0.29813376E-07 0.12038856E-10 0.25844190E+05 0.82263324E+01 0.27068024E+05    4

N2H4 liquid Hydrazine REF=JANAF HF298=12.042  REF=Gurvich 1989       Max Lst Sq
Error H-H0 @ 300 K 0.60%
N2H4(L) Hydrazin  J12/65N  2.H  4.   0.   0.L   200.000   800.000     32.04524 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00 1.20310475E+01-1.58854987E-02 7.53502039E-05    3
-9.15945394E-08 4.07674892E-11 2.67428635E+03-5.18137624E+01 6.05923187E+03    4

N2H4 HYDRAZINE  STATWT=1  SIGMA=1 IAIBIC=7.0E-117  IR=0.146   ROSYM=2
ROTATION BARRIER  V(2)=1700. cm-1   NU=3280,3325,1587,1275,1098,780,3314,3350,
1628,1275,937.2   HF298= 95.18+/-4.2 KJ   REF=Gurvich 1989.
N2H4 HYDRAZINE    L 5/90N  2.H  4.   0.   0.G   200.000  6000.000  B  32.04524 1
 4.93957357E+00 8.75017187E-03-2.99399058E-06 4.67278418E-10-2.73068599E-14    2
 9.28265548E+03-2.69439772E+00 3.83472149E+00-6.49129555E-04 3.76848463E-05    3
-5.00709182E-08 2.03362064E-11 1.00893925E+04 5.75272030E+00 1.14474575E+04    4

N2O  STATWT=1  B0=.4190113  NU=1277,589,2224  X11=-3.842  X12=.182  X13=-27.352
X22=-.271 X23=-14.672  X33=-15.155  G22=.366  Y111=-.021  Y112=-.152  Y122=-.030
Y222=-.007  Y113=-.338  Y133=.124  Y123=.390  Y223=.059  Y233=.029  Y333=-.002
W0=29.55  ALFAB1=.001917  ALFAB2=-.000577  ALFAB3=.003481  D0=17.59E-8
HF298= 81.6 KJ REF= Gurvich 1989.
N2O             L 7/88N   2O    1    0    0G     200.000  6000.000  A  44.01288 1
 0.48230729E+01 0.26270251E-02-0.95850872E-06 0.16000712E-09-0.97752302E-14    2
 0.80734047E+04-0.22017208E+01 0.22571502E+01 0.11304728E-01-0.13671319E-04    3
 0.96819803E-08-0.29307182E-11 0.87417746E+04 0.10757992E+02 0.98141682E+04    4

N2O+ ION  STATWT=2 B0=.411407  NU=1737,461(2),1126  T0=132.4 STATWT=2  T0=28229.
STATWT=2  HF=1333.399+/-0.63 KJ  REF=JANAF
N2O+              J12/70N   2O   1E  -1    0G   298.150  6000.000  B  44.01233 1
 0.55285660E+01 0.19596138E-02-0.75377712E-06 0.12704886E-09-0.78022397E-14    2
 0.15842390E+06-0.44187923E+01 0.32869103E+01 0.74022215E-02-0.48666444E-05    3
 0.73292750E-09 0.29823434E-12 0.15910253E+06 0.74013737E+01 0.16037012E+06    4

N2O3  STATWT=1  SIGMA=1  IAIBIC=3562E-117  IR=1.124 ROT. BARRIER V(2)=490. cm-1
ROSYM=2    NU=1832,1630,1305,773,414,260,160,337    T0=14100.  STATWT=1
HF0=91.2 KJ REF= Gurvich 1989.
N2O3              L 4/90N  2.O  3.   0.   0.G   200.000  6000.000  B  76.01168 1
 9.08583845E+00 3.37756330E-03-1.31583890E-06 2.30762329E-10-1.47151267E-14    2
 7.27160146E+03-1.55361904E+01 5.81083964E+00 1.43330962E-02-1.96208597E-05    3
 1.73060735E-08-6.46553954E-12 8.19184453E+03 1.20461321E+00 1.04192062E+04    4

N2O4  STATW=1  SIGMA=4  IAIBIC=10500.E-117  IR=3.22  ROSYM=2  POTENTIAL BARRIER
V(2)=1600.cm-1  ROT LEVELS=187   NU=1373,812,260,751,1710,480,430,675,1758,270,
1264  HF0=20.4 KJ   REF= Gurvich 1989.
N2O4              RUS 89N   2O   4    0    0G   200.000  6000.000  B  92.01108 1
 1.15752899E+01 4.01616086E-03-1.57178323E-06 2.68274309E-10-1.66922019E-14    2
-2.92191226E+03-3.19488439E+01 3.02002308E+00 2.95904321E-02-3.01342458E-05    3
 1.42360407E-08-2.44100049E-12-6.40040162E+02 1.18059606E+01 1.33632866E+03    4
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N2O5  STATWT=1  SIGMA=2  IAIBIC=29700.E-117  IR=4.8  POT. BARRIER V(2)=660. cm-1
ROSYM=2 ROT. LEVELS=187 (TWO EQUIVALENT ROTORS) NU= 1728,353(2),1338,1247,860,
743(2),85,645,614,577,1728,353   HF298= 13.3 KJ  REF= Gurvich 1989.
N2O5              L 4/90N  2.O  5.   0.   0.G   200.000  6000.000  B 108.01048 1
 1.31108082E+01 4.87435791E-03-1.87548389E-06 3.16374121E-10-1.95926845E-14    2
-3.11634700E+03-3.46877692E+01 3.68767444E+00 3.92120798E-02-5.53770029E-05    3
 4.20097833E-08-1.31260710E-11-8.30291184E+02 1.21967866E+01 1.59961321E+03    4

N3 AZIDE  SIGMA=2 STATWT=2  B0=.43113  NU=1400,737(2),2150  T0=71.9  STATWT=2
HF298=436.0 KJ REF=Gurvich 1989.
N3                L 7/88N   3    0    0    0G   200.000  6000.000  B  42.02022 1
 0.46410423E+01 0.27697073E-02-0.10492244E-05 0.17534989E-09-0.10748867E-13    2
 0.50698450E+05-0.93977465E+00 0.28606338E+01 0.42487681E-02 0.51459781E-05    3
-0.10148208E-07 0.44189545E-11 0.51369210E+05 0.91159496E+01 0.52438448E+05    4

N3H  SIGMA=1 STATWT=1  A0=20.380639  B0=.4014156  C0=.3929878  NU=3340,2140,
1264,1150.5,534,607  DJ=1.64E-7 DJK=2.63E-5  DK=7.67E-3  HF298=294.0 KJ
REF= Gurvich 1989.
N3H               L 7/88N   3H   1    0    0G   200.000  6000.000  A  43.02816 1
 0.51470168E+01 0.43055846E-02-0.15270346E-05 0.24629401E-09-0.14714317E-13    2
 0.33428392E+05-0.22553714E+01 0.28851146E+01 0.94434034E-02-0.38791657E-05    3
-0.18940565E-08 0.16018507E-11 0.34117203E+05 0.97168511E+01 0.35359871E+05    4

Ne    HF298= 0.0 KJ REF=McBride, Heimel, Ehlers & Gordon "Thermodynamic Proper-
ties to 6000 K..." NASA SP-3001  1963.
NE REF ELEMENT    L10/90NE  100  000  000  0G   200.000  6000.000  B  20.1797  1
 0.25000000E 01 0.             0.             0.             0.                2
-0.74537500E 03 0.33553227E 01 0.25000000E 01 0.             0.                3
 0.             0.            -0.74537498E 03 0.33553227E 01 0.00000000E+00    4

Ne+  HF298=2087. KJ  REF+C.E. Moore U.S. Nat. Bur. Stand. NSRDS-NBS 34 1970
Ne+               L10/92NE 1.E -1.   0.   0.G   298.150  6000.000  B  20.17915 1
 2.90399557E+00-3.63794635E-04 1.31873359E-07-2.14209210E-11 1.28778499E-15    2
 2.50143726E+05 2.56310321E+00 1.94106917E+00 4.40016552E-03-8.57047417E-06    3
 6.99691689E-09-2.11573625E-12 2.50294275E+05 6.99178683E+00 2.51005687E+05    4

Ni REFERENCE ELEMENT  Condensed Phase HF298(S)=0.0 kJ  REF=JANAF
Ni(cr)            J12/76NI 1.   0.   0.   0.S   200.000   631.000  B  58.69340 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00 3.92097614E+00-2.34184719E-02 1.34230145E-04    3
-2.75971639E-07 1.98530861E-10-8.62387206E+02-1.56856186E+01 0.00000000E+00    4
Ni(cr)            J12/76NI 1.   0.   0.   0.S   631.000  1728.000  B  58.69340 1
 9.58208572E+00-1.78945122E-02 1.97185112E-05-9.11957952E-09 1.58728609E-12    2
-2.61782185E+03-4.74612393E+01 4.85484877E+02-2.30395380E+00 4.10622634E-03    3
-3.23350101E-06 9.49617381E-10-8.11709085E+04-2.25428960E+03 0.00000000E+00    4
Ni(L)             J12/76NI 1.   0.   0.   0.L  1728.000  6000.000  B  58.69340 1
 4.67989094E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-3.22238346E+02-2.33517797E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    4

NiO  Nickel Oxide  Data from Barin Database 1989  HF298(S)=-239.70 kJ
NiO  Solid-A      B  /89NI 1.O  1.   0.   0.S   298.150   525.000  C  74.689   1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00-1.57324752E+01 1.79860646E-01-5.57051845E-04    3
 7.23393852E-07-2.80704261E-10-6.79031544E+02 5.95039043E+01-9.99938661E+02    4
NiO  Solid-B      B  /89NI 1.O  1.   0.   0.S   525.000   565.000  C  74.689   1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00-4.05614678E+00 2.02539491E-02 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-1.82561755E+02 2.29564525E+01-9.99938661E+02    4
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NiO  Solid-C       B  /89NI 1.O  1.   0.   0.S   565.000  2228.000  C  74.689   1
 8.54519666E+00-6.01462324E-03 5.06266530E-06-1.02231132E-09-5.77542484E-14    2
-3.39816451E+03-4.28164283E+01 5.32267831E+00 7.63070044E-03-1.69937025E-05    3
 1.50561208E-08-4.50262391E-12-2.77681950E+03-2.74214599E+01-9.99938661E+02    4
NiO  Liquid        B  /89NI 1.O  1.   0.   0.L  2228.000  2500.000  C  74.689   1
 6.50276297E+00 4.91821956E-05-2.06203183E-08 2.87842575E-12 0.00000000E+00    2
 4.43423749E+03-2.91641267E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00-9.99938661E+02    4

NiS  Nickel Sulfide Condensed phase  REF=JANAF  HF298(S)=-87.86+/-6.3 kJ
NiS(b) Crystal     J12/76NI 1.S  1.   0.   0.S   300.000   652.000  B  90.75940 1
 2.51505130E+00 1.98108790E-02-4.47517130E-05 5.35527360E-08-2.47391510E-11    2
-1.18972750E+04-1.22988050E+01 2.51505130E+00 1.98108790E-02-4.47517130E-05    3
 5.35527360E-08-2.47391510E-11-1.18972750E+04-1.22988050E+01-1.05681072E+04    4
NiS(a) Crystal     J12/76NI 1.S  1.   0.   0.S   652.000  1249.000  B  90.75940 1
-2.16882770E+00 2.04672610E-02-1.52390680E-05 4.52420390E-09 0.00000000E+00    2
-9.25397310E+03 1.60189760E+01 1.59778550E+00 1.62791590E-02-2.39592640E-05    3
 1.96652470E-08-5.99935920E-12-1.06051920E+04-4.99884140E+00 0.00000000E+00    4
NiS(L)  Liquid     J12/76NI 1.S  1.   0.   0.L  1249.000  5000.000  B  90.75940 1
 9.23426080E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-1.10536520E+04-4.57697360E+01 9.23426080E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-1.10536520E+04-4.57697360E+01 0.00000000E+00    4

NiS2 Condensed Phase REF=JANAF  HF298(S)=-131.376 +/- 16.7 kJ
NiS2(s)            J 3/77NI 1.S  2.   0.   0.C   300.000  1280.000  C 122.82540 1
 5.27426400E+00 9.08709310E-03-5.82010990E-06 1.70500810E-09 0.00000000E+00    2
-1.75287250E+04-2.33922190E+01 7.74493490E+00 2.53517140E-03-9.97675870E-08    3
 1.07829500E-10-4.19129410E-14-1.82225390E+04-3.62243880E+01-1.58013948E+04    4
NiS2(L)            J 3/77NI 1.S  2.   0.   0.C  1280.000  5000.000  C 122.82540 1
 1.09452410E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-1.23449250E+04-4.97206240E+01 1.09452410E+01 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-1.23449250E+04-4.97206240E+01 0.00000000E+00    4

Ni3S2 Condensed phase  REF=JANAF   HF298(S)=-216.31 +/- 5. kJ
Ni3S2(I)           J12/76NI 3.S  2.   0.   0.S   300.000   829.000  C 240.21220 1
 6.92383000E+00 4.04466800E-02-7.30739570E-05 7.10070760E-08-2.62218590E-11    2
-2.93621960E+04-3.27350520E+01 6.92383000E+00 4.04466800E-02-7.30739570E-05    3
 7.10070760E-08-2.62218590E-11-2.93621960E+04-3.27350520E+01-2.60177884E+04    4
Ni3S2(II)          J12/76NI 3.S  2.   0.   0.S   829.000  1062.000  C 240.21220 1
 2.26855850E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-2.93134790E+04-1.11689780E+02 2.26855850E+01 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-2.93134790E+04-1.11689780E+02 0.00000000E+00    4
Ni3S2(L)           J12/76NI 3.S  2.   0.   0.L  1062.000  5000.000  C 240.21220 1
 2.30680390E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-2.73444020E+04-1.12118110E+02 2.30680390E+01 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-2.73444020E+04-1.12118110E+02 0.00000000E+00    4

Ni3S4  Solid  REF=JANAF  HF298(S)=-301.11 +/- 25.1 kJ
Ni3S4(s)           J 3/77NI 3.S  4.   0.   0.C   300.000  1100.000  C 304.34420 1
 1.46738180E+01 1.72757180E-02 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-4.13600010E+04-6.63291620E+01 1.46711930E+01 1.72771640E-02-2.75692840E-09    3
 1.02338580E-11-6.29839560E-15-4.13584790E+04-6.63129390E+01-3.62163568E+04    4

O  HF298=249.17 KJ  REF=C.E. Moore "Selected Tables of Atomic Spectra" NSRDS-NBS
Sec 7 1976 p. A8 I
O                  L 1/90O  1.   0.   0.   0.G   200.000  6000.000  A  15.99940 1
 2.54363697E+00-2.73162486E-05-4.19029520E-09 4.95481845E-12-4.79553694E-16    2
 2.92260120E+04 4.92229457E+00 3.16826710E+00-3.27931884E-03 6.64306396E-06    3
-6.12806624E-09 2.11265971E-12 2.91222592E+04 2.05193346E+00 2.99687009E+04    4
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O- OXYGEN ION  HF0=95.093 KJ  REF=Gurvich 89
O-                RUS 89O  1.E  1.   0.   0.G   298.150  6000.000  B  15.99995 1
 2.54474868E+00-4.66695419E-05 1.84912310E-08-3.18159131E-12 1.98962894E-16    2
 1.14822713E+04 4.52131018E+00 2.90805921E+00-1.69804907E-03 2.98069956E-06    3
-2.43835127E-09 7.61229313E-13 1.14138341E+04 2.80339097E+00 1.22272740E+04    4

O2  CALCULATED FROM ORIGINAL VALUES  HF298=0 KJ  REF=Gurvich 1989.
O2 REF ELEMENT    RUS 89O   2   0     0    0G   200.000  6000.000  A  31.99880 1
 3.66096083E+00 6.56365523E-04-1.41149485E-07 2.05797658E-11-1.29913248E-15    2
-1.21597725E+03 3.41536184E+00 3.78245636E+00-2.99673415E-03 9.84730200E-06    3
-9.68129508E-09 3.24372836E-12-1.06394356E+03 3.65767573E+00 0.00000000E+00    4

O2+  CALCULATED FROM ORIGINAL VALUES HF0=1165.0 KJ  REF=Gurvich 1989.
O2+               RUS 89O  2.E -1.   0.   0.G   298.150  6000.000  A  31.99825 1
 3.31675922E+00 1.11522244E-03-3.83492556E-07 5.72784687E-11-2.77648381E-15    2
 1.39876823E+05 5.44726469E+00 4.61017167E+00-6.35951952E-03 1.42425624E-05    3
-1.20997923E-08 3.70956878E-12 1.39742229E+05-2.01326941E-01 1.40937762E+05    4

O2-  CALCULATED FROM ORIGINAL VALUES HF0=-42.5 KJ  REF=Gurvich 1989.
O2-               L 4/89O  2.E  1.   0.   0.G   298.150  6000.000  A  31.99935 1
 3.95666294E+00 5.98141823E-04-2.12133905E-07 3.63267581E-11-2.24989228E-15    2
-7.06287229E+03 2.27871017E+00 3.66442522E+00-9.28741138E-04 6.45477082E-06    3
-7.74703380E-09 2.93332662E-12-6.87076983E+03 4.35140681E+00-5.77639825E+03    4

O3  OZONE  SIGMA=2  STATWT=1   A0=3.553664  B0=.4452762  C0=.394758   NU=1103,
701,1042   X11=-4.9   X12=-9.1   X13=-34.8    X22=-1.0    X23=-17.   X33=-10.6
ALFAA1=-.002981  ALFAA2=-.053415  ALFAA3=.053118  ALFAB1=.002554  ALFAB2=.001269
ALFAB3=.003992   ALFAC1=.002319   ALFAC2=.002307  ALFAC3=.003613  W=-27.05
TAAA=-8.1429E-6  TBBB=-2.3864E-6  TCCC=-1.2694E-6 TAAB=16.947E-6  TAAC=3.2717E-6
TBBC=-1.6665E-6  TABA=-9.2093E-6  T0=10000.  STATWT=3  SIGMA=2   IAIBIC=48.
NU=600(2),350  T0=12500.  STATWT=3  SIGMA=2  IAIBIC=51.  NU=600(2),350
T0=13000.  STATWT=1 SIGMA=6  IAIBIC=32.  NU=850,500(2)  T0=13500.  STATWT=3
SIGMA=2  IAIBIC=48.  NU=600(2),350  HF298=141.8 KJ  REF= Gurvich 1989.
O3                L 5/90O   3    0    0    0G   200.000  6000.000  A  47.99820 1
 1.23302914E+01-1.19324783E-02 7.98741278E-06-1.77194552E-09 1.26075824E-13    2
 1.26755831E+04-4.08823374E+01 3.40738221E+00 2.05379063E-03 1.38486052E-05    3
-2.23311542E-08 9.76073226E-12 1.58644979E+04 8.28247580E+00 1.70545228E+04    4

P   HF298=-316.39+/-1.0 kJ   REF=JANAF
P                J12/82P  1.   0.   0.   0.G   200.000  6000.000  B  30.97376 1
 2.80721555E+00-5.30841988E-04 2.44543046E-07-2.05708252E-11-2.94546619E-16    2
 3.71892748E+04 3.67764723E+00 2.50004278E+00-4.38968637E-07 1.58131741E-09    3
-2.33900457E-12 1.20510940E-15 3.73073754E+04 5.38414719E+00 3.80527536E+04    4

PCl3   SIGMA=3  STATWT=1  IA=IB=32.3918  IC=57.6799  NU=510,507(2),259,187(2)
HF298=-288.70+/-5.4 kJ   REF=JANAF
PCL3              J 6/70P  1.CL 3.   0.   0.G   300.000  5000.000  B 137.33186 1
 9.45661160E+00 6.02784010E-04-2.58468780E-07 4.89042800E-11-3.40832850E-15    2
-3.77045574E+04-1.69296498E+01 5.25905370E+00 1.78805660E-02-2.73175850E-05    3
 1.88982400E-08-4.87384960E-12-3.68644304E+04 3.25232968E+00-3.47080119E+04    4
```

Table 4 (continued)

```
PF  SIGMA=1 T0(STATWT)=0(3)  BE=0.5665  WE=846.75  WEXE=4.489  ALFAE=0.00456
      T0(STATWT)=7090.41(2)  BE=0.5699  WE=858.79  WEXE=4.438  ALFAE=0.00467
     T0(STATWT)=13353.91(1)  BE=0.5725  WE=866.14  WEXE=4.51   ALFAE=0.0045
     T0(STATWT)=29338.69(2)  BE=0.4632  WE=436     WEXE=1.5    ALFAE=0.004
     T0(STATWT)=29481.80(2)  BE=0.4663  WE=436     WEXE=1.5    ALFAE=0.0038
     T0(STATWT)=29623.06(2)  BE=0.4693  WE=436     WEXE=1.5    ALFAE=0.0037
     T0(STATWT)=35812.29(2)  BE=0.4848  WE=413     WEXE=1.5    ALFAE=0.0062
HF298=-52.25+/-20.9 kJ  REF=JANAF
PF                J 6/77P  1.F  1.   0.   0.G   300.000  5000.000  A  49.97217 1
 4.28444030E+00 4.65131920E-05 1.29231550E-07-3.54596860E-11 2.93086420E-15    2
-7.67566495E+03 2.40196395E+00 2.67608630E+00 5.57221620E-03-7.28377960E-06    3
 4.58194390E-09-1.11881060E-12-7.28916135E+03 1.04341832E+01-6.29944377E+03    4

PF2   SIGMA=2   T0(STATWT)=0(2),25000(2),28000(2),30000(2)  IA=2.9836  IB=9.1077
IC=12.0913  NU=852,831,353  HF298=-488.256+/-20.9 kJ   REF=JANAF
PF2               J 6/77P  1.F  2.   0.   0.G   300.000  5000.000  C  68.97057 1
 6.09265880E+00 1.03133240E-03-4.53710200E-07 8.70455830E-11-5.97140520E-15    2
-6.07553254E+04-3.78513004E+00 2.44285260E+00 1.51863310E-02-2.21969240E-05    3
 1.56489320E-08-4.32983720E-12-5.99609804E+04 1.40371170E+01-5.87248863E+04    4

PF3  SIGMA=3  STATWT=1  IA=IB=10.8265  IC=17.6633  NU=892,860(2),487,344(2)
HF298=-958.441+/-3.8 kJ   REF=JANAF
PF3               J12/69P  1.F  3.   0.   0.G   300.000  5000.000  B  87.96897 1
 8.43477330E+00 1.73939200E-03-7.51198080E-07 1.43442470E-10-1.00939790E-14    2
-1.18180783E+05-1.64636020E+01 2.36218780E+00 2.28200450E-02-2.76566420E-05    3
 1.44909620E-08-2.46023600E-12-1.16776903E+05 1.36864320E+01-1.15275206E+05    4

PF5  SIGMA=6  STATWT=1  IA=2.23  IB=IC=269    NU=1025(2),947(5),817,640,575,
532(2),514(2),179(2)   HF298=-1594.409+/-2.9 kJ   REF=JANAF
PF5               J12/69P  1.F  5.   0.   0.G   300.000  5000.000  B 125.96578 1
 1.28461840E+01 3.51044850E-03-1.51986040E-06 2.91019040E-10-2.05347080E-14    2
-1.96362263E+05-3.94755420E+01 1.05232490E+00 4.44540040E-02-5.39014290E-05    3
 2.84166860E-08-4.91432680E-12-1.93632313E+05 1.90890100E+01-1.91765100E+05    4

PH  SIGMA=1  T0(STATWT)=0(3),7650(2),15150(1),29560(6),38110(2),57490(1)
BE=8.412  WE=2380  WEXE=55   ALFAE=0.28  HF298=236.097+/-33.5 kJ    REF=Lewis
(JANAF's HF298=253.55 is erroneous)
PH                J 6/67P  1.H  1.   0.   0.G   300.000  5000.000  C  31.98170 1
 3.07454420E+00 1.16989470E-03-3.03816540E-07 4.44363140E-11-2.70009750E-15    2
 2.74268316E+04 5.76804846E+00 3.68034330E+00-1.27560180E-03 2.59324420E-06    3
-8.43541070E-10-1.72086090E-13 2.73339656E+04 2.91864116E+00 2.83957262E+04    4

PH3  PHOSPHINE  SIGMA=3  STATWT=1  IA=IB=0.6264  IC=0.7201  NU=2328(2),2323,
1122(2),992   HF298=5.424+/-1.7 kJ   REF=Lewis  (JANAF's HF298=22.89 kJ is
erroneous)
PH3               J 6/62P  1.H  3.   0.   0.G   300.000  5000.000  B  33.99758 1
 3.34487940E+00 6.57709410E-03-2.63367550E-06 4.77446600E-10-3.23543900E-14    2
-8.16176752E+02 3.95479617E+00 3.15819350E+00 2.49414920E-03 9.02552530E-06    3
-1.02279040E-08 3.28342500E-12-4.61237252E+02 6.23722477E+00 6.52312908E+02    4

PN  PHOSPHORUS NITRIDE  SIGMA=1   STATWT=1   BE=0.7862   WE=1337.24   WEXE=6.983
ALFAE=0.00557   HF298=104.78+/-5.0 kJ  REF=JANAF
PN                J 9/62P  1.N  1.   0.   0.G   300.000  5000.000  B  44.98050 1
 3.64192260E+00 9.44606720E-04-3.89234800E-07 7.32158260E-11-5.09616320E-15    2
 1.13936880E+04 4.19044189E+00 3.37552390E+00-4.10093860E-04 5.12651510E-06    3
-5.94788980E-09 2.12135820E-12 1.15788400E+04 6.10290619E+00 1.26017849E+04    4
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PO  SIGMA=1 T0(STATWT)=0(2),224(2),30696(2),32884(4),38055(4),40485(2),43629(2),
47251(2),48580(4)  BE=0.7337  WE=1233.3  WEXE=6.56  ALFAE=0.0056
HF298=-29.597+/-4.2  kJ  REF=Lewis  (JANAF'S HF298=23.55 kJ is erroneous).
PO                  J 6/71P  1.O  1.   0.   0.G   300.000  5000.000  B  46.97316 1
 3.84279220E+00 7.23644560E-04-2.89341990E-07 5.30135540E-11-3.54953730E-15    2
-4.79945495E+03 4.55237735E+00 3.96130800E+00-2.12353990E-03 7.52012190E-06    3
-7.59509120E-09 2.56375910E-12-4.69896895E+03 4.58369215E+00-3.55964877E+03    4

PO2  SIGMA=2  STATWT=2  IA=0.8775  IB=9.9337  IC=10.8112  NU=1044,980,515
HF298=-314.524 kJ  REF=JANAF
PO2                 J 9/62P  1.O  2.   0.   0.G   300.000  5000.000  C  62.97256 1
 5.69132780E+00 1.48068660E-03-6.54256920E-07 1.27932310E-10-9.20992770E-15    2
-3.97947254E+04-2.81972206E+00 2.33452730E+00 1.25021000E-02-1.43361950E-05    3
 7.67621660E-09-1.54016940E-12-3.89688654E+04 1.40544350E+01-3.78293636E+04    4

P2   SIGMA=2   STATWT=1   BE=0.30327   WE=780.43   WEXE=2.804   ALFAE=0.00142
HF298=143.65+/-2.1 kJ  REF=JANAF
P2                  J 6/61P  2.   0.   0.   0.G   300.000  5000.000  B  61.94752 1
 4.16117330E+00 3.96208000E-04-1.55803390E-07 2.90934740E-11-2.00424580E-15    2
 1.59468693E+04 2.24109239E+00 2.83911070E+00 4.82661930E-03-5.49474880E-06    3
 2.58005070E-09-3.22364530E-13 1.62597073E+04 8.84241009E+00 1.72771170E+04    4

P4    SIGMA=12    STATWT=1    IA=IB=IC=25.1209    NU=606,464.5(3),363
HF298=58.9+/-2.1 kJ  REF=JANAF
P4                  J 6/61P  4.   0.   0.   0.G   300.000  5000.000  B 123.89505 1
 9.22627890E+00 8.68941280E-04-3.77583380E-07 7.23796660E-11-5.10661090E-15    2
 4.09054959E+03-1.96417049E+01 3.53533000E+00 2.41252920E-02-3.64627590E-05    3
 2.49169060E-08-6.32985630E-12 5.23553359E+03 7.75589569E+00 7.08599199E+03    4

P4O6  (P2O3)2  SIGMA=12  STATWT=1  IAIBIC=483801.7E-117  NU=1029(2),919(2),
643(3),636(3),613(2),465(2),407(3),370(3),302(3)  HF298=-2144.519+/-33.5 kJ
REF=Lewis  (JANAF's HF298=-2214.31 is erroneous).
P4O6                J12/62P  4.O  6.   0.   0.G   300.000  5000.000  B 219.89145 1
 2.23829590E+01 6.41271290E-03-2.84877920E-06 5.58964390E-10-4.03341410E-14    2
-2.65985440E+05-9.04488339E+01-5.41216630E+00 1.22358190E-01-1.95002050E-04    3
 1.48292330E-07-4.37707920E-11-2.60299220E+05 4.33724011E+01-2.66312810E+05    4

P4O10  (P2O5)2  SIGMA=12  STATWT=1  IA=IB=IC=143.243  NU=1417,1390(3),1015(3),
952(2),764(3),750(3),721,650(2),573(3),470(3),424,329(3),278(2),257(3),170(3)
HF298=-2904.08+/-8.9 kJ  REF=JANAF
P4O10               J12/65P  4.O 10.   0.   0.G   300.000  5000.000  B 283.88905 1
 2.89396590E+01 1.24520960E-02-5.48543200E-06 1.07047430E-09-7.69568570E-14    2
-3.60148633E+05-1.23859447E+02-4.41428830E+00 1.37590810E-01-1.92685980E-04    3
 1.32720680E-07-3.63113780E-11-3.52629523E+05 4.01782260E+01-3.49287392E+05    4

P4O10(s)            J12/65P  4.O 10.   0.   0.S   300.000  1500.000  C 283.88905 1
-4.33006250E+01 2.15673760E-01-1.76863440E-04 6.76428520E-08-9.91087100E-12    2
-3.53461393E+05 2.26054720E+02 3.95560990E-01 1.13338170E-01-1.24099820E-04    3
 9.77156010E-08-3.41078390E-11-3.66256443E+05-3.80906970E+00-3.62020394E+05    4

S(S) REF ELEMENT  J 9/77S   10   00   00   0S   300.000   388.360  A  32.0660  1
 0.              0.              0.              0.              0.              2
 0.              0.              0.18018871E+01 0.31543881E-02 0.              3
 0.              0.             -0.68614468E+03-0.72259874E+01 0.0       E+00   4

S(L) REF ELEMENT  J 9/77S   10   00   00   0L   388.360  5000.000  A  32.0660  1
 0.33906200E+01 0.71182514E-03-0.39087832E-06 0.87327456E-10-0.68755181E-14    2
-0.63358440E+03-0.14788307E+02-0.38449885E+02 0.25707392E+00-0.55555365E-03    3
 0.51325813E-06-0.17253650E-09 0.42933552E+04 0.16753043E+03 0.0       E+00    4
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Table 4 (continued)

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S   HF298=276.98+/-0.25 kJ   REF=JANAF
S                 J 9/82S  1.   0.   0.   0.G   200.000  6000.000  B  32.06600 1
 2.87936498E+00-5.11050388E-04 2.53806719E-07-4.45455458E-11 2.66717362E-15    2
 3.25013791E+04 3.98140647E+00 2.31725616E+00 4.78018342E-03-1.42082674E-05    3
 1.56569538E-08-5.96588299E-12 3.25068976E+04 6.06242434E+00 3.33128471E+04    4

SC1  SIGMA=1  T0(STATWT)=0(2),400(2),25000(4)  BE=0.2406   WE=536  WEXE=2.08
ALFAE=0.00126  HF298=156.46+/-16.7 kJ   REF=JANAF
SCL               J 6/78S  1.CL 1.   0.   0.G   300.000  5000.000  C  67.51870 1
 4.59472600E+00-5.97717860E-05 4.52264950E-08-9.37184350E-12 8.07357270E-16    2
 1.74524260E+04 2.37985153E+00 3.70558800E+00 5.27186230E-03-1.13718200E-05    3
 1.04978270E-08-3.53184080E-12 1.75611590E+04 6.27945123E+00 1.88189067E+04    4

SC12  SIGMA=2   T0(STATWT)=0(1),25810(1),29762(1)    IA=5.8026   IB=29.1706
IC=34.9733   NU=528,525,205   HF298=-17.57+/-3.3 kJ   REF=JANAF
SCL2              J 6/78S  1.CL 2.   0.   0.G   300.000  5000.000  B 102.97140 1
 6.62714620E+00 4.27470190E-04-1.88168810E-07 3.57611550E-11-2.38494000E-15    2
-4.20002190E+03-4.23237025E+00 3.59663710E+00 1.43271930E-02-2.51991970E-05    3
 2.05728820E-08-6.39769080E-12-3.63758370E+03 1.00605557E+01-2.11344531E+03    4

SD  SIGMA=1  T0(STATWT)=0(2)  BE=4.949 WE=1930.4  WEXE=23.44  ALFAE=0.101
T0(STATWT)=376.8(2),30769(2)  BE=4.392 WE=1417    WEXE=48.85  ALFAE=0.105
T0(STATWT)=59566(2)           BE=4.532 WE=1917.7  WEXE=29.3   ALFAE=0.105
T0(STATWT)=63872(4),71205(4),71328(2)   BE=4.949  WE=1930.4  WEXE=23.44
ALFAE=0.101  T0(STATWT)=76717(4),79320(4),80858(4)   HF298=138.49+/- 5.0 kJ
REF=JANAF
SD                J 6/77S  1.D  1.   0.   0.G   300.000  5000.000  A  34.08010 1
 3.34719880E+00 1.21296460E-03-4.77301380E-07 8.83236690E-11-6.07405910E-15    2
 1.56271470E+04 4.87764189E+00 4.72855970E+00-5.09398810E-03 9.91346050E-06    3
-7.32908130E-09 1.94616080E-12 1.53995790E+04-1.56847961E+00 1.66570071E+04    4

SF  SIGMA=1  T0(STATWT)=0(2),398(2),24991(2),25601(2)  BE=0.55427  WE=830
WEXE=4.7  ALFAE=0.0042  HF298=12.97+/-6.3 kJ  REF=JANAF
SF                J 6/76S  1.F  1.   0.   0.G   300.000  5000.000  C  51.06440 1
 4.36908850E+00 1.92044240E-04-6.66303650E-08 1.24485900E-11-7.65374940E-16    2
 2.20185260E+02 2.07596854E+00 3.42081750E+00 4.55111980E-03-7.93725640E-06    3
 6.50047110E-09-2.02896650E-12 3.96095030E+02 6.54700574E+00 1.56005789E+03    4

SF2  SIGMA=2  STATWT=1  IA=3.1377  IB=9.1367  IC=12.2744  NU=840,809,357
HF298=-296.646+/-16.7 kJ  REF=JANAF
SF2               J 6/76S  1.F  2.   0.   0.G   300.000  5000.000  C  70.06281 1
 6.11941960E+00 1.00514240E-03-4.46533130E-07 8.76240100E-11-6.32365120E-15    2
-3.77142410E+04-4.55717403E+00 2.41030560E+00 1.55901210E-02-2.31780180E-05    3
 1.65834970E-08-4.64657610E-12-3.69163730E+04 1.35066804E+01-3.56790061E+04    4

SF3   SIGMA=2  T0(STATWT)=0(2),25000(2)  IA=5.8076  IB=17.0895  IC=22.8971
NU=850,725,550,450,350,300   HF298=-503.03+/-33.5 kJ  REF=JANAF
SF3               J 6/77S  1.F  3.   0.   0.G   300.000  5000.000  C  89.06121 1
 8.80768970E+00 1.36716760E-03-6.08083330E-07 1.18830220E-10-8.44709150E-15    2
-6.34404940E+04-1.67648869E+01 1.87777280E+00 3.12340350E-02-5.15713790E-05    3
 4.02473220E-08-1.21105940E-11-6.20679390E+04 1.63694361E+01-6.05016370E+04    4

SF4  SIGMA=2  STATWT=1  IA=12.5525  IB=20.5464  IC=26.0707  NU=891.5,867,728,
558.4,532.5,475,353,233,228   HF298=-763.162+/-20.9 kJ   REF=JANAF
SF4               J 6/76S  1.F  4.   0.   0.G   300.000  5000.000  B 108.05961 1
 1.11243830E+01 2.14579940E-03-9.54524440E-07 1.87461110E-10-1.35359530E-14    2
-9.55816690E+04-2.88756477E+01 1.28196450E+00 4.35698990E-02-7.01251680E-05    3
 5.36772440E-08-1.59143560E-11-9.35867010E+04 1.84198703E+01-9.17889260E+04    4
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SF5  PENTAFLUOROSULFUR  SIGMA=4  T0(STATWT)=0(2),10000(2),20000(2),25000(2),
30000(2)  IA=30.7102  IB=IC=21.4728  NU=812(2),800,600,552(2),550(2),450,400,
350(2)   HF298=-908.447+/-15.1 kJ   REF=JANAF
SF5                 J12/77S  1.F  5.   0.   0.G   300.000  5000.000  C 127.05802 1
 1.36105630E+01 2.65231300E-03-1.16914630E-06 2.42451320E-10-1.83147180E-14    2
-1.14002930E+05-4.30151012E+01-1.71476620E+00 6.87160080E-02-1.14079330E-04    3
 8.93363790E-08-2.69404290E-11-1.10961780E+05 3.02724678E+01-1.09262883E+05    4

SF5Br  SIGMA=4  STATWT=1  IA=32.145  IB=IC=71.9835  NU=892(2),848,694,621,597,
580(2),502,423(2),325,279,225(2)  HF298=-972.8+/-59 kJ  REF=JANAF
SF5BR               J12/77S   1F   5BR  1    0G   200.000  6000.000  C 206.96202 1
 0.16222709E+02 0.28929217E-02-0.11443577E-05 0.19662531E-09-0.12282470E-13    2
-0.12263690E+06-0.54750256E+02-0.19908752E+01 0.82938683E-01-0.14215649E-03    3
 0.11560301E-06-0.36238714E-10-0.11904847E+06 0.32112843E+02-0.11700028E+06    4

SF5Cl  SIGMA=4  STATWT=1  IA=30.9468  IB=IC=46.3888  NU=909(2),855,707,625,602,
579(2),505,441(2),402,332,287(2)  HF298=-1038.9+/-10.5 kJ   REF=JANAF
SF5CL               J12/77S   1F   5CL  1    0G   200.000  6000.000  B 162.51072 1
 0.16068448E+02 0.30531997E-02-0.12076664E-05 0.20749336E-09-0.12960964E-13    2
-0.13058312E+06-0.55651991E+02-0.31561325E+01 0.87699695E-01-0.15063852E-03    3
 0.12275611E-06-0.38552637E-10-0.12680072E+06 0.36001021E+02-0.12495024E+06    4

SF6  HEXAFLUOROSULFUR  SIGMA=24  STATWT=1  IA=IB=IC=30.8679  NU=947.5(3),773.1,
641.7(2),615.3(3),525(3),347(3)  HF298=-1220.473 +/-0.8 kJ  REF=JANAF
SF6                 J 6/76S  1.F  6.   0.   0.G   300.000  5000.000  B 146.05642 1
 1.51629500E+01 4.38423180E-03-1.94863370E-06 3.82471960E-10-2.76050500E-14    2
-1.52268010E+05-5.44157194E+01-3.83880880E+00 8.32217210E-02-1.31816890E-04    3
 9.96361540E-08-2.92487670E-11-1.48364770E+05 3.71611426E+01-1.46791868E+05    4

SN  SIGMA=1 T0(STATWT)=0(2),223(2)  BE=0.7762  WE=1220  WEXE=7.75  ALFAE=0.0064
HF298=263.6+/-105 kJ  REF=JANAF
SN                  J 6/61S  1.N  1.   0.   0.G   300.000  5000.000  C  46.07274 1
 3.84939760E+00 7.27567880E-04-2.93702030E-07 5.50136280E-11-3.81235510E-15    2
 3.04599620E+04 4.43127355E+00 3.94229710E+00-2.00355150E-03 7.35346440E-06    3
-7.51685600E-09 2.55910980E-12 3.05639490E+04 4.58030805E+00 3.17016142E+04    4

SO  T0(STATWT)=0(3)         BE=0.72082  WE=1148.19  WEXE=6.12  ALFAE=0.00574
T0(STATWT)=6350(2)          BE=0.7119   WE=1148.19  WEXE=6.12  ALFAE=0.00574
T0(STATWT)=10510(1)         BE=0.70261  WE=1067.66  WEXE=7.8   ALFAE=0.00635
T0(STATWT)=38292(2)         BE=0.6067   WE=415.2    WEXE=1.6   ALFAE=0.0194
T0(STATWT)=38455(2)         BE=0.6107   WE=413.3    WEXE=1.6   ALFAE=0.0194
T0(STATWT)=38616(2)         BE=0.6164   WE=412.7    WEXE=1.7   ALFAE=0.0204
T0(STATWT)=41629(3)         BE=0.502    WE=630.4    WEXE=4.8   ALFAE=0.0062
T0(STATWT)=42200(6)         BE=0.5      WE=170      WEXE=0     ALFAE=0
HF298=5.01+/-1.3 kJ   REF=JANAF
SO                  J 6/77S  1.O  1.   0.   0.G   300.000  5000.000  A  48.06540 1
 4.01428730E+00 2.70228170E-04 8.28966670E-08-3.43237410E-11 3.11214440E-15    2
-7.10519560E+02 3.49973505E+00 3.14902330E+00 1.18393470E-03 2.57406860E-06    3
-4.44434190E-09 1.87351590E-12-4.04075710E+02 8.31987915E+00 6.02271219E+02    4

SOF2  THYONYL FLUORIDE  SIGMA=1  STATWT=1  IA=9.7369  IB=10.0399  IC=16.9332
NU=1330,808.2,747,530.4,392.5,377.8   HF298=-543.92+/-105 kJ   REF=JANAF
SOF2                J 6/72S  1.O  1.F  2.   0.G   300.000  5000.000  B  86.06221 1
 8.08742120E+00 2.10957160E-03-9.08669120E-07 1.73448340E-10-1.22141580E-14    2
-6.82381590E+04-1.38555915E+01 2.47490660E+00 2.09524260E-02-2.41642770E-05    3
 1.21203770E-08-1.93387310E-12-6.68976020E+04 1.41973405E+01-6.54188894E+04    4
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SO2     O-S-O     SIGMA=2  STATWT=1   IA=1.38   IB=8.131   IC=9.534
NU=1361.76,1151.38,517.69   HF298=-296.842+/-0.21 kJ   REF=JANAF
SO2                J 6/61S  1.O  2.   0.   0.G   300.000  5000.000  B  64.06480 1
 5.24513640E+00 1.97042040E-03-8.03757690E-07 1.51499690E-10-1.05580040E-14    2
-3.75582270E+04-1.07404892E+00 3.26653380E+00 5.32379020E-03 6.84375520E-07    3
-5.28100470E-09 2.55904540E-12-3.69081480E+04 9.66465108E+00-3.57007867E+04    4

SO2C1F  SULFURYL CHLORIDE FLUORIDE  SIGMA=1  STATWT=1  IA=16.4743   IB=29.0842
IC=29.3031  NU=1467,1228,824,629,510,474,423,308,300  HF298=-556.5+/-21 kJ
REF=JANAF
SO2CLF             J 6/71S  1.O  2.CL 1.F  1.G   300.000  5000.000  B 118.51590 1
 1.01182860E+01 3.14889940E-03-1.34715140E-06 2.55803100E-10-1.79382560E-14    2
-7.05092910E+04-2.31278508E+01 2.98175280E+00 2.64491670E-02-2.92001820E-05    3
 1.39576110E-08-2.03044870E-12-6.87614970E+04 1.27316812E+01-6.69282620E+04    4

SO2C12  SULFURYL CHLORIDE  SIGMA=2   STATWT=1  IA=24.052  IB=36.0706  IC=43.8672
NU=1434,1205,586,577,406,388,363,209,208   HF298=-354.80+/-2.1 kJ   REF=JANAF
SO2CL2             J 6/71S  1.O  2.CL 2.   0.G   300.000  5000.000  B 134.97020 1
 1.05509370E+01 2.67343010E-03-1.14282300E-06 2.16862000E-10-1.51991510E-14    2
-4.62950560E+04-2.43078570E+01 4.38516770E+00 2.32121570E-02-2.65321120E-05    3
 1.34999230E-08-2.28192810E-12-4.48029740E+04 6.57867880E+00-4.26726368E+04    4

SO2F2  SULFURYL FLUORIDE  SIGMA=2   STATWT=1  IA=16.3467  IB=16.5727  IC=16.5756
NU=1502,1269,885,848,553,544,539,388,384    HF298=-758.559+/-8.4 kJ   REF=JANAF
SO2F2              J 6/71S  1.O  2.F  2.   0.G   300.000  5000.000  B 102.06161 1
 9.60788850E+00 3.71110260E-03-1.58991140E-06 3.02324640E-10-2.12285770E-14    2
-9.47547680E+04-2.28489419E+01 1.73246800E+00 2.85017600E-02-2.94537980E-05    3
 1.24013000E-08-1.17155330E-12-9.27813930E+04 1.69484101E+01-9.12343116E+04    4

SO3  SIGMA=6   STATWT=1   IA=IB=8.1493  IC=16.2987     NU=1391,1068,529,495
HF298=-395.765+/-0.71 kJ   REF=JANAF
SO3                J 9/65S  1.O  3.   0.   0.G   300.000  5000.000  B  80.06420 1
 7.07573760E+00 3.17633870E-03-1.35357600E-06 2.56309120E-10-1.79360440E-14    2
-5.02113760E+04-1.11875176E+01 2.57803850E+00 1.45563350E-02-9.17641730E-06    3
-7.92030220E-10 1.97094730E-12-4.89317530E+04 1.22651384E+01-4.75978348E+04    4

S2 T0(STATWT)=0(3)  BE=0.2946 WE=724.67  WEXE=2.836  ALFAE=0.00157   DE=2.134E-7
T0(STATWT)=4700(2)  BE=0.2923 WE=702.35  WEXE=3.09   ALFAE=0.0017    DE=2.04E-7
T0(STATWT)=8500(1)  BE=0.29   WE=700.87  WEXE=3.47   ALFAE=0.0016    DE=2.0E-7
T0(STATWT)=21855(6) BE=0.2284 WE=488.6   WEXE=2.63   ALFAE=0.0014    DE=1.996E-7
HF298=128.60+/-0.3 kJ  REF=JANAF
S2                 J 9/77S  2.   0.   0.   0.G   300.000  5000.000  A  64.13200 1
 3.98860690E+00 5.57750510E-04-5.01892780E-08-1.54703190E-11 2.66617710E-15    2
 1.41980150E+04 4.49119159E+00 2.85857540E+00 5.17583550E-03-6.54934340E-06    3
 3.39986430E-09-4.01567660E-13 1.44124020E+04 9.89127849E+00 1.54434020E+04    4

S2Cl   (S-S-Cl)  SIGMA=1  T0(STATWT)=0(2),23000(2),26000(2),30000(2)  IA=5.0613
IB=26.8624  IC=31.9237  NU=550,500,200   HF298=78.6+/-8.4 kJ   REF=JANAF
S2CL               J 6/78S  2.CL 1.   0.   0.G   300.000  5000.000  C  99.58470 1
 6.62294250E+00 4.37477870E-04-1.94304060E-07 3.66970150E-11-2.30912150E-15    2
 7.36474510E+03-2.94188157E+00 3.62917020E+00 1.41777000E-02-2.49191780E-05    3
 2.03331190E-08-6.32030790E-12 7.91952490E+03 1.11746042E+01 9.44875520E+03    4

S2Cl2   (Cl-S-S-Cl)  SIGMA=2  IA=68.8282  IB=60.6645  IC=15.2331  IR=5.487
ROTATION BARRIER  V0=8387.  V2=-3917.  V3=-490. cm-1  HF298=-4.0 kcal  REF=JANAF
S2CL2              L 4/93S  2.CL 2.   0.   0.G   200.000  6000.000  B 135.03740 1
 9.46841020E+00 1.12186352E-03-6.92784280E-07 1.38654463E-10-9.29397839E-15    2
-5.05019524E+03-1.52950441E+01 3.47905708E+00 3.25370028E-02-6.63904620E-05    3
 6.21124845E-08-2.17112325E-11-4.02225567E+03 1.22791824E+01-2.01286666E+03    4
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S2F2   THIOTHIONYL FLUORIDE  S-S-F2  SIGMA=1       T0(STATWT)=0(1),34000(1)
IA=10.2965   IB=21.0146   IC=27.5332   NU=760.5,718.5,692.3,411.2,330,274
HF298=-401.413+/-41.8 kJ  REF=JANAF
S2F2 (SSF2)        J 6/76S  2.F  2.   0.   0.G   300.000  5000.000  B 102.11681 1
 8.82958920E+00 1.34072340E-03-5.96153210E-07 1.16854000E-10-8.40610860E-15    2
-5.12234920E+04-1.60942430E+01 1.92539690E+00 3.10520790E-02-5.11986690E-05    3
 3.98812160E-08-1.19774150E-11-4.98547610E+04 1.69255960E+01-4.82791800E+04    4

S2F2  FLUORODISULFANE   FS-SF  IA=7.3579  IB=30.4921  IC=32.6808  NU=717,680.8,
614.6,319.8,301,182.5  HF298=-336.435+/-41.6 kJ   REF=JANAF
FS2F               J 6/76F  2.S  2.   0.   0.G   300.000  5000.000  B 102.11681 1
 9.03087760E+00 1.11307760E-03-4.96295140E-07 9.76154130E-11-7.05574520E-15    2
-4.34215640E+04-1.69373960E+01 2.84494960E+00 2.82028400E-02-4.73576220E-05    3
 3.73947520E-08-1.13467000E-11-4.22164310E+04 1.25369140E+01-4.04641320E+04    4

S2F10  SIGMA=8  STATWT=1  IA=61.4204  IB=IC=119.3402  IR=15.354  INT ROT BARRIER
V=8.0 kcal  NU=938,913,860(2),826(2),728(2),690,684,642,634(2),624(2),571,
544(2),509(2),425(2),410(2),247,188(2),150(2)  HF298=-2064.386+/-29.3 kJ
REF=JANAF
S2F10              J12/77S   2F  10    0    0G   200.000  6000.000  B 254.11603 1
 0.28671327E+02 0.57615941E-02-0.24727206E-05 0.44061086E-09-0.28058011E-13    2
-0.25862467E+06-0.12091379E+03-0.67788927E+01 0.15100498E+00-0.24103120E-03    3
 0.18355215E-06-0.54374282E-10-0.25118529E+06 0.50552882E+02-0.24828715E+06    4

S2O  S-S-O    SIGMA=1  STATWT=1  IA=2.0209   IB=16.6326   IC=18.6536  NU=1165,
679,388   HF298=-56.48+/-33.5 kJ   REF=JANAF
S2O                J 9/65S  2.O  1.   0.   0.G   300.000  5000.000  B  80.13140 1
 5.90375240E+00 1.23699750E-03-5.45707900E-07 1.06598420E-10-7.66882430E-15    2
-8.77520900E+03-2.26999836E+00 2.84142570E+00 1.21884100E-02-1.60002410E-05    3
 1.03092890E-08-2.64491200E-12-8.06030150E+03 1.29180736E+01-6.79363039E+03    4

S8  SIGMA=8  STATWT=1  IA=IB=1.28594  IC=2.36042  NU=475(3),471(2),437(2),411,
248(2),243,218,191(2),152(2),56(2)  HF298=100.42+/-0.63 kJ  REF=JANAF
S8                 J 9/77S  8.   0.   0.   0.G   200.000  6000.000  B 256.52800 1
 2.07249521E+01 1.34686111E-03-5.37225946E-07 9.28122853E-11-5.81951340E-15    2
 5.53344324E+03-6.74805287E+01 4.19700496E+00 9.15503597E-02-1.91263611E-04    3
 1.80177196E-07-6.30393695E-11 8.12071691E+03 7.58043917E+00 1.20776811E+04    4

Si  Silicon  REFERENCE ELEMENT  HF298=0. kJ  REF=Gurvich 1991
Si(cr)             RUS 91SI 1.   0.   0.   0.S   200.000  1690.000  B  28.08550 1
 1.75547382E+00 3.17285497E-03-2.78236402E-06 1.26458065E-09-2.17128464E-13    2
-6.28657363E+02-8.55341177E+00-1.29176912E-01 1.47203139E-02-2.76510160E-05    3
 2.41878251E-08-7.93452912E-12-4.15516417E+02-3.59570008E-01 0.00000000E+00    4
Si(L)              RUS 91SI 1.   0.   0.   0.L  1690.000  6000.000  B  28.08550 1
 3.27138941E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 4.88286795E+03-1.32665477E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    4

SiC  Silicon Carbide  REF=JANAF
SiC(b)             J 3/67SI 1.C  1.   0.   0.S   300.000  4000.000  B  40.09650 1
 3.79748090E+00 3.18728860E-03-1.45023340E-06 3.15497440E-10-2.61589910E-14    2
-1.02919370E+04-2.10677910E+01-2.47159070E+00 3.06937830E-02-4.92630850E-05    3
 3.86263890E-08-1.17616210E-11-9.06912600E+03 8.80092140E+00-8.80624423E+03    4

SiO2 Quarz  REF=JANAF  HF298(S)=-910.857 +/- 1.7 kJ
SiO2(Lqz)          J 6/67SI 1.O  2.   0.   0.S   200.000   847.000  B  60.08430 1
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.00000000E+00 0.00000000E+00-7.58511380E-01 3.05773989E-02-4.00861855E-05    3
 2.16194849E-08-6.17249042E-13-1.10371483E+05 1.78384529E+00-1.09550292E+05    4
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SiO2(hqz)          J 6/67SI 1.O  2.   0.   0.S   847.000  1696.000  B  60.08430 1
 7.23537106E+00 7.61842227E-04 4.89502294E-07-2.35754591E-10 4.20839131E-14    2
-1.11823834E+05-3.69642796E+01 7.11787621E+00 1.13819527E-03 3.69734234E-08    3
 0.00000000E+00 0.00000000E+00-1.11794194E+05-3.63708064E+01-1.09550292E+05    4
SiO2(L)            J 6/67SI 1.O  2.   0.   0.L  1696.000  6000.000  B  60.08430 1
 1.03160657E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-1.14600563E+05-5.76266603E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00-1.09550292E+05    4

Si2N2O  Silicon Oxynitride REF=Fegley Comm. Am. Ceram. Soc. 1981 C124-C126
HF298(S)=-947.71 kJ
Si2N2O(s)          L 1/84SI 2.N  2.O  1.   0.S   298.150  2500.000  B 100.18388 1
 1.18490230E+01 2.42446810E-03 3.65292350E-07-4.25788290E-10 8.62759300E-14    2
-1.18214940E+05-6.42500920E+01-4.12268540E+00 5.41728140E-02-4.23929300E-05    3
-1.07245950E-08 1.73668580E-11-1.14746000E+05 1.48221580E+01-1.13982840E+05    4

Si3N4  Silicon Nitride  REF=JANAF  HF298(S)=-744.752 +/- 29.3 kJ
Si3N4(a)           J 3/67SI 3.N  4.   0.   0.S   300.000  3000.000  B 140.28346 1
 2.79817450E+00 2.79750180E-02-1.50205780E-05 3.58722880E-09-3.17769690E-13    2
-9.10172410E+04-8.92688190E+00 7.16356800E+00 1.90071110E-02-1.14693330E-05    3
 7.06659150E-09-2.74586400E-12-9.24666510E+04-3.24424310E+01-8.95746895E+04    4

SiS2  Silicon Disulfide  Data from Barin Database 1989  HF298(S)=-213.384 kJ.
SiS2  Solid        B  /89SI 1.S  2.   0.   0.S   298.150  1363.000  C  92.21750 1
 8.40271418E+00 3.13408157E-03-2.30381538E-06 1.32114291E-09-2.82789755E-13    2
-2.82649031E+04-3.89938340E+01 8.91436638E+00 1.35634414E-03 2.22767520E-09    3
-3.02264623E-12 1.41797358E-15-2.83821677E+04-4.15331497E+01-2.56640500E+04    4
SiS2  Liquid       B  /89SI 1.S  2.   0.   0.L  1363.000  1500.000  C  92.21750 1
 1.20789350E+01-2.42499074E-06 8.45243131E-10 0.00000000E+00 0.00000000E+00    2
-3.04270857E+04-6.17829516E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00-2.56640500E+04    4

Xe  HF298=0.0 REF=C.E. Moore "Atomic Energy Levels" NSRDS-NBS 34 and NSRDS-
NBS 35 1970.
Xe REF ELEMENT     L12/91XE 1.   0.   0.   0.G   200.000  6000.000  B 131.29000 1
 2.50005322E+00-1.05136544E-07 6.75326897E-11-1.70944909E-14 1.47681049E-18    2
-7.45394186E+02 6.16412898E+00 2.50000000E+00-8.99141330E-14 2.52196860E-16    3
-2.92186662E-19 1.18949218E-22-7.45375000E+02 6.16441993E+00 0.00000000E+00    4

Xe+  HF298=1176.552 kJ  REF=JANAF 1985
Xe+                L10/92XE 1.E -1.   0.   0.G   298.150  6000.000  B 131.28945 1
 2.58350579E+00-1.53488750E-04 8.09594639E-08-1.14289234E-11 4.82081406E-16    2
 1.40730117E+05 7.09057067E+00 2.50007477E+00-6.25614186E-07 1.86430963E-09    3
-2.35599457E-12 1.07219368E-15 1.40761095E+05 7.55040436E+00 1.41506477E+05    4
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Table 5. Enthalpy of formation, Heat content and Entropy at 298 K calculated from the polynomials in Table I

Compound	Mol. Wgt.	$\Delta_f H_{298}$	± kJ/mol	C_{p298} J/mol	S_{298} J/mol	
Air (standard mixture)	28.96518	-0.126		29.104	198.824	#
AL(cr) REFERENCE ELEMENT	26.98154	0		24.2	28.3	*
AL	26.98154	329.7	±4.2	21.391	164.555	#
ALH	27.98948	259.4	±20	29.348	187.857	*
ALO	42.98094	66.944	±8	30.874	218.385	*
ALOH	43.98888	-179.92	±13	31.877	216.419	*
ALO2	58.98034	-86.192	±32	49.893	251.834	*
ALO2H	59.98828	-460.247	±63	50.197	254.389	*
AL2O	69.96248	-145.186	±17	52.035	252.336	*
AL2O2	85.96188	-394.554	±32	67.192	280.996	*
AL2O3(S)	101.96128	-1675.709		79.075	50.972	*
AR REFERENCE ELEMENT	39.948	0		20.786	154.847	*
Ar+	39.94745	1526.778		20.984	166.406	#
B	10.811	560	±12	20.797	153.438	#
B(S) REFERENCE ELEMENT	10.81	0.001		11.521	5.899	*
BCL	46.2637	141.417		31.675	213.246	*
BCLF	65.2621	-313.792	±29	42.557	264.655	*
BCL2	81.7164	-79.493	±12.6	47.438	272.691	*
BCL3	117.1691	-402.945	±2.1	62.476	290.188	*
BF	29.8094	-115.896	±13.8	29.567	200.473	*
BF2	48.80781	-589.959	±13	40.558	247.161	*
BF3	67.80621	-1135.646	±1.7	50.492	254.367	*
BH	11.81894	442.657	±8.4	29.178	171.849	*
BHF2	49.81575	-733.858	±3.3	42.341	244.025	*
BH2	12.82688	200.83	±63	34.062	180.211	*
BH3	13.83482	106.689	±10	36.211	187.886	*
BO	26.8104	-0.001	±8	29.179	203.472	*
BOCL	62.2631	-316.298	±29	45.102	237.435	*
BOF	45.8088	-602	±13	40.996	224.806	#
BOF2	64.80721	-836.817	±15	50.253	267.853	*
BO2	42.8098	-284.518	±8	43.293	229.817	*
B2	21.622	829.687	±33.5	31.595	202.076	#
B2O	37.6214	96.234	±105	38.402	227.747	*
B2O2	53.6208	-456.037	±8.4	57.4	242.629	*
B2O3(L)	69.6182	-1253.249		61.795	78.83	*
B2O3	69.6202	-835.975	±4.2	66.969	283.799	*
B3O3CL3	186.7893	-1631.706	±8	131.737	382.418	*
B3O3F3	137.42641	-2365.152	±4.2	115.13	342.475	*
B3O3H3 BOROXIN	83.45502	-1217.544	±42	87.833	291.912	#
H3B3O6 BORIC ACID	131.45322	-2271.833	±13	137.613	347.631	*
Br	79.904	111.86	±0.06	20.789	175.017	#
BRO	95.9034	125.8	±2.4	34.17	232.921	#
BrO2 Br-O-O	111.9028	108	±40	48.873	288.83	#
BrO2 O-Br-O	111.9028	152	±25	45.364	271.112	#
BrO3	127.9022	221	±50	59.995	284.507	#
Br2 REFERENCE ELEMENT	159.808	0		36.048	245.394	*
Br2O BrBr-O	175.8074	168	±20	51.385	312.704	#
Br2O Br-O-Br	175.8074	107.6	±3.5	50.168	290.823	#
C(GR) REFERENCE ELEMENT	12.011	0		8.528	5.734	*
C	12.011	716.67	±0.45	20.839	158.102	#
C+	12.01045	1809.434		20.974	154.664	#
CBrClF2	165.36451	-435	±15	74.65	318.725	#

Table 5 (Continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$	± kJ/mol	C_{p298} J/mol	S_{298} J/mol	
CBrF3 Freon 1301	148.91021	-648.8		69.27	297.698	#
CBr2F2	209.81581	-380	±15	77	325.413	#
CCL	47.4637	502.093	±20	32.255	224.516	*
CCLF	66.4621	25.876		40.018	257.95	#
COCLF	82.4615	-426.779	±33	52.402	277.019	*
CCLF2	85.46051	-275		55.172	287.353	#
CCLF3 FC-13	104.45891	-707.93	±3.3	66.888	285.357	#
CLCN	61.47044	137.952		45.333	236.344	*
COCL	63.4631	-62.756	±42	45.103	265.974	*
CCL2	82.9164	238.5	±21	46.327	265.364	*
CCL2F	101.9148	-105		59.119	298.916	#
CCL2F2 FREON-12	120.91321	-493.294		72.429	300.988	#
COCL2 PHOSGEN	98.9158	-219.5		57.761	283.752	#
CCL3	118.3691	79.506	±8	63.752	296.858	*
CCL3F FC-11	137.3684	-284.934		78.267	310.045	#
CCL4	153.823	-95.815		83.618	309.995	#
CD	14.0251	593.303		29.174	189.049	*
CDH3	17.0489	-78.469		36.395	200.027	*
CDO	30.0245	40.644		35.842	229.314	#
CD2	16.0392	382.601		36.282	204.302	*
CD2O	32.0386	-114.903		38.048	225.057	*
CD3	18.0533	137.537		41.845	207.031	*
CD3NO2	64.05885	-61.789		63.166	291.669	#
CD4 RRHO	20.0674	-89.022		40.479	198.995	*
CD4 * ANHARMONIC	20.0674	-89.022		40.519	199.003	*
CF	31.0094	255.229	±8	30.034	213.028	*
FCN	45.01614	35.987	±16.7	42.359	225.416	*
COF	47.0088	-171.539	±63	38.943	248.48	*
CF2	50.00781	-182.008	±6.3	38.95	240.832	*
COF2	66.00721	-640		47.365	258.971	#
CF3	69.00621	-470.29	±4.2	49.843	265.089	*
CF3I	195.91068	-589.11	±3.3	70.941	307.633	#
CF3OO RADICAL	101.00501	-627.349		79.392	315.015	#
CF4 FC-14	88.00461	-933		61.73	261.845	#
CH	13.01894	597.36	±17.5	29.175	183.037	#
CHBrF2 HBFC-22B1	130.91975	-422		58.767	295.23	#
CHCL	48.47189	308.285		36.75	234.778	*
CHCLF	67.4703	-83.681		50.466	280.878	#
CHCLF2 HCFC-22	86.46845	-475	±15	55.854	280.921	#
CHCL2	83.92487	73.908		52.782	277.75	*
CHCL2F FC-21	102.9233	-284.934		61.077	293.204	#
CHCL3 CHLOROFORM	119.3779	-102.928		65.5	295.666	#
CHD2NO2	63.05268	-57.716		60.806	289.264	#
CHD3	19.0612	-85.305		38.893	208.581	*
CHF RADICAL	32.01734	163.176		34.585	228.715	#
CHF2	51.01575	-254		45.279	258.506	#
CHF3 FLUOROFORM	70.01415	-693.289		51.139	268.509	#
HCN	27.02568	135	±4	35.857	201.825	#
HNC	27.02568	194.378	±9	40.271	205.511	#
HNCO	43.02508	-116.734		45.038	238.227	#
CHN2	41.03242	319.796	±23.4	48.059	248.503	#
CH(NO2)3	151.03556	-13.389		134.09	435.569	#
HCO	29.01834	42	±0.8	34.591	224.336	#
CHO+	29.0178	833.059		36.015	203.32	*
COOH	45.01774	-213		43.61	251.736	#

Table 5 (Continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$	± kJ/mol	C_{p298} J/mol	S_{298} J/mol	
HCOO* Radical	45.01774	-150.624		39.748	239.743	#
HCS	45.08494	300.47		37.059	236.148	#
CH2 TRIPLET	14.02688	390.417		33.763	194.899	#
CH2 SINGLET	14.02688	424.732		33.775	188.716	*
CH2BrCL HALON101	129.38358	-45	±15	52.726	287.29	#
CH2CL	49.47979	116.875		43.201	243.375	*
CH2CLF GC-31	68.4782	-264.432		47.038	264.307	#
CH2CL2	84.9328	-95.396		50.939	270.333	#
CH2DNO2	62.04652	-52.532		58.983	286.942	#
CH2D2	18.0551	-81.769		37.51	207.911	*
CH2F	33.02528	-32		40.292	236.529	#
CH2F2 FC-32	52.02369	-452.709		42.869	246.347	#
H2CN RADICAL	28.03362	240.162		37.768	224.304	#
HCNH trans	28.03362	298.738		38.072	229.017	#
HCNH cis	28.03362	319.658		38.892	229.493	#
H2NCO	44.03302	-23.305	±9.9	52.926	256.458	#
CH2NO CH2=N-O*	44.03302	173.427	±21	49.153	249.913	#
H2CNO H2C*N=O	44.03302	223.928	±8.4	42.388	244.644	#
NITRO-METHYL RAD	60.03242	152.465		58.862	288.218	#
Methyl Nitrate Radical	76.03182	98.952		76.78	312.169	#
CH2N2 CYANAMIDE	42.04036	135.888	±20	51.505	247.641	#
H2CN2 HN=C=NH	42.04036	149.005	±15	50.223	247.113	#
CH2N2 H2C=N=N	42.04036	286.382	±25	51.144	240.982	#
H2CN2 CY DIAZIRENE	42.04036	320.143	±20	41.383	236.962	#
CH2(NO2)2	106.03796	-61.505		86.352	358.098	#
CH2O FORMALDEHYDE	30.02628	-108.58		35.388	218.764	#
HCOOH FORMIC ACID	46.02568	-378.57		41.305	247.148	#
H2CS	46.09288	114.683		38.196	236.949	#
CH3	15.03482	146.858	±1	38.412	193.965	#
CH3BR	94.93882	-37.656		42.426	245.81	#
CH3CL	50.4877	-81.966		40.707	234.182	#
CH3F FC-41	34.03322	-237.66		37.501	231.578	#
CH3I	141.93929	210.874		74.935	355.64	#
CH3N (H2C=NH)	29.04156	84.015		38.084	221.567	#
CH3NO NITROSOMETHYL	45.04096	79.002	±7.3	50.77	260.833	#
OCHNH2 FORMAMIDE	45.04096	-195.263	±10.5	48.473	253.646	#
CH2NOH	45.04096	29.288		53.359	248.547	#
NCH3O FORMIMIDIC ACID	45.04096	-148.436	±10.9	43.477	254.079	#
H3CNO CH2-NH=O	45.04096	59.032	±11.5	44.542	250.67	#
CH3NO2 NITRO-METHANE	61.04036	-80.751		55.528	282.863	#
CH3NO3 METHYL-NITRATE	77.03976	-122.005		76.597	305.793	#
CH3N2 CH3N=N*	43.0483	247.651	±12	53.694	257.186	#
CH3O	31.03422	16.318		43.512	229.39	#
CH2OH	31.03422	-17.8	±1.3	48.369	243.919	#
CH3O2 Peroxymethyl Radical	47.034	28.087		54.527	262.622	*
CH3S	47.10082	124.6		53.205	245.982	#
CH4 RRHO	16.0428	-74.89	±0.5	35.446	186.167	*
CH4 ANHARMONIC	16.04276	-74.6		35.691	186.371	#
CH4N CH3NH*	30.0495	187.569	±4.8	47.372	235.967	#
(NH2)2C=O Urea	60.05564	-235.5		79.088	282.953	#
CH4N4O2 Nitroguanidine, Picrite	104.06852	1.	±20	114.92	352	#
CH3OH(L)	32.04216	-238.911		81.082	127.269	#
CH3OH	32.04216	-200.94		44.039	239.81	#
CH4O2 CH3OOH	48.04156	-139.746	±5	60.229	255.787	#
CH4S CH3SH	48.10876	-22.525		50.415	258.382	#

Table 5 (Continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$	± kJ/mol	C_{p298} J/mol	S_{298} J/mol	
CH5N CH3-NH2	31.0574	-23.025		50.505	240.75	*
CH5N2 CH3N*NH2	45.06418	215.183	±5.5	63.575	260.107	#
CH5N4 GUANIDINE	59.07092	-15.	±10.	80.489	278.706	#
CH6N2	46.07212	94.558		66.915	268.989	#
CN	26.01774	437.102	±6.3	29.156	202.643	#
CNO	42.01714	131.796		40.096	232.287	#
CNN	40.02448	400.651		42.282	232.092	#
NCN (NCN)	40.02448	500.795		43.144	227.851	#
C(NO2)4	196.03316	82.383		176.119	503.723	#
CO	28.0104	-110.53	±0.17	29.141	197.657	#
COS	60.0764	-138.399	±1	41.556	231.475	*
CO2	44.0098	-393.51	±0.13	37.135	213.787	#
CP	42.98476	72.464		29.955	216.273	#
CS	44.077	280.334	±25	29.789	210.444	*
CS2	76.143	116.947	±0.84	45.674	237.879	*
C2	24.022	830.856		43.208	199.416	#
C2Br2F4 HALON 2402	259.82361	-790.776	±4.2	120.019	252.529	#
C2CL	59.4747	494.09		45.046	241.948	#
C2CL2	94.9274	209.631	±42	65.668	271.942	*
C2CL2F4 FC-114	170.92101	-900.4		116.6	364.2	#
C2CL3	130.3801	190.28		76.033	328.166	#
CCl2F-CCLF2	187.37531	-705.8		121	386.9	#
C2CL3F3 FC-113A	187.37531	-740.6		120.3	369.3	#
C2CL4	165.834	-12.13		94.92	340.925	#
C2CL5	201.2855	39		118.832	397.906	#
C2CL6	236.74	-138.91		136.545	398.545	#
C2D2	28.0502	222.194		49.556	208.92	*
C2D2O	44.0496	39.932		55.669	249.614	*
C2D4	32.0784	30.279		52.064	230.672	*
C2OD4	48.0778	-180.582		64.697	275.315	*
C2D6	36.1066	-110.676		64.743	244.479	*
C2D6N2	64.12001	119.248		92.1	312.346	*
C2D6O	52.10601	-209.49		77.528	283.259	*
C2F	43.0204	353.855		42.6	231.036	#
C2F2	62.01881	20.926	±21	56.997	244.077	*
C2F3	81.01721	-228.175		66.178	297.643	#
C2F4 FC-1114	100.01561	-658.569	±2.9	80.568	300.042	*
C2F5	119.01402	-891.192		94.111	341.49	#
C2F6 FC-116	138.01242	-1343.9	±5	106.427	332.158	#
CF3-O-O-CF3	170.01122	-1507.077		137.807	433.17	#
C2H ETHYNYL	25.02994	568.522	±3	41.999	213.304	#
C2HCL	60.48264	213.8	±42	54.32	241.999	#
C2HCLF2-1,1 FC-1122	98.47945	-334		72.063	302.885	#
C2HCLF2 cis	98.47945	-323.569		75.394	305.096	#
C2HCLF2 trans	98.47945	-323.103		75.149	304.318	#
CF2H-CCLF2 FC-124A	136.47625	-903.3		100.4	351.1	#
CF3-CHCLF HCFC124	136.47625	-924.7		99.06	349.6	#
CF3-CHCL2 HCFC123	152.93055	-743.9		102.6	352.6	#
CF2CL-CHFCL FC123A	152.93055	-710		104.5	368.1	#
CFCL2-CHF2	152.93055	-702.1		104.5	361.7	#
C2HCL3	131.38804	-4.1		80.016	324.941	#
C2HCL4	166.84074	45		99.253	365.817	#
C2HF	44.0283	125.532	±63	52.426	231.637	*
C2HF5 FC-125	120.02196	-1104.576		95.679	333.816	#
HCCN	39.03668	610.431	±100	54.238	240.596	#

Table 5 (Continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$	± kJ/mol	C_{p298} J/mol	S_{298} J/mol	
HCCO	41.02934	177.402	±8.8	48.417	245.287	#
H2C2 VINYLIDENE	26.03788	414.788		42.614	221.021	#
C2H2 ACETYLENE	26.03788	227.4		44	200.917	#
C2H2F2 FC-1132A	64.03469	336.4		60.123	266.041	#
H2C2F2	64.03469	313.192		58.349	268.723	#
F2C2H2 FC-1132	64.03469	310.038		60.074	267.847	#
C2F3H2	83.03309	-517.142		79.499	303.093	#
1,2-C2H2(NO2)2	118.04896	59.413		110.488	359.186	#
CH2CO	42.03728	-47.698	±1.7	51.744	241.896	#
HCCOH ETHYNOL	42.03728	93.186	±18.3	57.403	249.142	#
C2H2O2 TRANS GLYOXAL	58.03668	-212		59.535	272.295	#
C2H2O2 CIS GLYOXAL	58.03668	-212		59.941	271.112	#
C2H3 VINYL RADICAL	27.04582	299.74	±5	43.64	233.953	#
C2H3CL	62.49852	23		53.681	264.024	#
C2H3F2	65.04263	-302.503		67.256	288.291	#
C2H3F3 FC-143A	84.04103	-745.589		78.45	287.273	#
C2H3N CH3CN Methylcyanide	41.0526	87.863		52.194	243.414	*
C2H3NO2 Nitroethylene	73.05136	33.284		73.68	300.503	#
C2H3O (CH3CO) RADICAL	43.04522	-10		50.784	267.449	#
OH3C2 (*CH2CHO) RADICAL	43.04522	25.102		54.974	267.919	*
C2H3O OXYRANE RADICAL	43.04522	139.83		41.649	361.49	#
C2H4 ETHYLENE	28.0536	52.294		42.799	219.18	*
C2H4F RADICAL	47.05216	-72.216		58.857	273.845	#
C2H4CL RADICAL	63.50646	90.12		58.635	281.459	#
C2H4O VINYL-ALCOHOL	44.05316	-124.683		61	289.996	#
C2H4O OXYRANE	44.05316	-52.635	±0.63	47.624	242.87	#
CH3CHO ACETALDEHYDE	44.05316	-166.19		55.319	263.952	#
CH3COOH ACETIC ACID	60.0524	-432.253		63.472	283.363	*
C2H4O2CL2	130.95796	-231.375		109.993	362.046	#
(HCOOH)2 Formic Acid dimer	92.0512	-820.951		96.177	332.671	*
C2H5 ETHYL RADICAL	29.0617	118.658	±2	50.483	247.119	#
C2H5Br BROMOETHANE	108.9657	-64.015		64.643	287.483	#
C2H5CL CHLOROETHANE	64.5144	-111.713		62.718	275.851	#
C2H5F FLUOROETHANE	48.0601	-261.5		58.152	264.224	#
C2H5I IODOETHANE	155.96617	-8.368		65.94	296.311	#
C2H5NO2 NITROETHANE	75.06724	-103.784		79.018	320.512	#
C2H5ONO2 ETHYLNITRATE	91.06664	-154.975		95.103	328.863	#
OC2H5 ETHOXY RADICAL	45.0609	-16.744		56.615	268.589	*
H5C2O RADICAL	45.0609	-20.915		60.753	277.278	*
C2OH5 RADICAL	45.0609	-20.93		62.37	280.88	*
C2H5O RADICAL	45.0609	-8.379		64.884	281.942	*
C2H5O2CL Chloroperoxyethane	96.5132	-212.966		92.223	336.239	#
C2H6 ETHANE	30.0694	-83.863		52.397	229.08	*
C2H6N (CH3)2N Dimethylazide	44.07638	159.1		67.126	273.3	#
C2H6N2 AZOMETHANE	58.0828	148.684		77.872	289.777	*
(CH3)2N-NO2	90.08192	-4.8		103.204	328.138	#
C2H5OH(L) ETHANOL LIQUID	46.06904	-277.508		112.248	160.101	#
C2H5OH ETHANOL	46.06904	-234.95		65.309	280.593	#
CH3OCH3 DIMETHYLETHER	46.06904	-184.054		65.823	267.381	#
C2H6O2 PEROXYETHANE	62.06844	-173.636		82.969	314.534	#
C2H6S C2H5SH Ethanethiol	62.13564	-46.108		72.676	296.102	#
C2H6S (CH3SCH3)Methylsulfide	62.13564	-37.53		74.099	285.851	#
C2H6S2 CH3-SS-CH3	94.20164	-24.142		94.307	336.645	#
C2H7N2 (CH3)2N-NH*	59.09106	168.197	±8.4	83.605	271.96	#
C2H8N2 SYM Dimethylhydrazine	60.099	94.491	±7.5	82.347	287.346	#

Table 5 (Continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$	± kJ/mol	C_{p298} J/mol	S_{298} J/mol	
C2H8N2 UNSYM	60.099	53.22		91.524	302.186	#
CCN	38.02874	604.799		44.578	239.034	#
CNC	38.02874	654.917		45.05	233.823	#
C2N2	52.03548	309.1		57.084	242.092	#
C2(NO2)6 Hexanitroethane	300.05524	179		273.376	667.098	#
C2O	40.0214	291.036		43.093	233.613	#
C3	36.033	839.949		42.202	237.61	#
C3D4	44.0894	262.675		64.125	254.286	*
C3D6	48.1176	32.885		72.411	251.394	*
C3F6 Hexafluoropropene	150.02342	-1125.078		113.246	354.412	#
C3F7 RADICAL	169.02182	-1347.122		135.964	416.386	#
C3F8 FC-218	188.02023	-1760.121		147.248	406.145	#
C3H	37.04094	684.084		38.101	226.742	#
C3HF7 FC-227EA	170.02976	-1564.816		136.690	399.058	#
C3HN	51.04768	353.966		64.768	236.563	#
C3H2(1) CyPropenylidene	38.04888	476.976		44.222	236.204	#
C3H2(3) H2CCC**	38.04888	651.030		54.719	254.549	#
C3H2(3) *HC=C=CH*	38.04888	517.142		67.953	260.782	#
C3H2(1) *HC=C=CH*	38.04888	579.902		58.770	245.928	#
C3H2N HC*=CH-CN	52.05562	405.848		66.526	270.705	#
C3H3 PROPARGYL RADICAL	39.05682	346—349	±4	64.891	256.659	#
CLC3H3 1-Chloropropine	74.50952	147.277		71.659	284.052	#
C3H3Cl CH2Cl-CCH	74.50952	162.729		73.747	296.899	#
3-C3H3Cl CY	74.50952	218.333		66.257	281.203	#
C3H3Cl CHCl=C=CH2	74.50952	160.851		70.089	290.465	#
C3H3N CH2=CHCN	53.06356	183.678		63.764	273.926	#
C3H3O CH2=CHC*=O	55.05622	72.383		62.548	269.534	#
H4C3 PROPYNE	40.06476	185.431		60.731	248.298	#
C3H4 ALLENE	40.06476	190.92		58.88	243.431	#
C3H4 CYCLOPROPENE	40.0648	276.991		52.996	243.616	*
C3H4CL *CH=CH-CH2CL	75.51746	235.559		73.638	311.29	#
CLC3H4 CH2-C*H-CHCL	75.51746	107.11		74.224	312.545	#
C3H4N CH3-CH*-CN	54.0715	195		63.6	285.5	#
C3H4N2 1,3-DIAZOLE	68.07824	140.959	±28	65.701	273.426	#
1,3,3 TRI-NITRO-AZETIDINE	192.08812	128.449		134.987	357.315	#
C3H4O ACROLEIN	56.06416	-74.475		66.991	269.879	#
C3H5 Symmetric Allyl Radical	41.0727	163.594		63.387	258.886	#
T-C3H5 CH3C*=CH2 " "	41.0727	237.651		61.663	266.064	#
S-C3H5 CH3CH=CH* " "	41.0727	262.755		61.166	271.207	#
C3H5CL Chloropropene	76.5254	-26.778		75.73	306.687	#
C3H5N PROPIONITRILE	55.07944	50.626		73.053	286.604	#
CH3CH=CHNO2	87.07824	9.987		93.59	330.004	#
NITRO-CYCLO-PROPANE	87.07824	17.573		90.787	317.042	#
C3H5N3O9 NITROGLYCERINE	227.08752	-279.073		234.24	545.865	#
C2H5CO	57.0721	-36.02		76.197	308.03	#
CH2COCH3	57.0721	-14.058		68.193	301.769	#
C3H5O Propylene Oxide Radical	57.0721	110.332		69.059	293.968	#
C3H6 PROPYLENE	42.0806	20.413		64.388	266.538	*
C3H6 CYCLOPROPANE	42.0806	53.303		55.633	237.446	*
N-NITRO-AZETIDIN	102.09292	114.123		100.656	328.954	#
RDX Solid	222.11748	79.078		284.884	146.189	#
RDX 135 Triazine	222.11748	192		230.174	482.441	#
C2H5CHO Propionaldehyde	58.08004	-192.046		80.73	304.51	#
CH3COCH3 ACETONE	58.08004	-217.15		74.205	295.661	#
C3H6O PROPYLENE OXIDE	58.0798	-92.762		72.688	281.362	*

Table 5 (Continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$	± kJ/mol	C_{p298} J/mol	S_{298} J/mol	
C3H6O CY OXETANE	58.08004	-80.542	±8.4	59.315	273.885	#
C3H6O Vinylmethylether	58.08004	-108.002		76.874	307.691	#
C3H6O Cyclopropanol	58.08004	-114.3		70.618	288.8	#
C3H6S THIETHANE	74.14664	60.584		70.418	278.343	#
N-C3H7 PROPYL RADICAL	43.0883	100.5	±2	71.23	289.465	*
I-C3H7 ISOPROPYL RADICAL	43.0883	93.286	±2	66.155	289.341	*
1-C3H7I Iodopropane	169.99305	-31.999	±2	85.883	332.737	#
2-C3H7I "	169.99305	-40.865	±2	91.193	334.082	#
C3H5NH2 CY-PROPYLAMINE	57.09499	77.389		89.045	285.464	*
C3H7N AZETIDINE	57.09532	98.198		67.14	267.274	#
C3H7NO2 Nitropropane	89.09412	-124.265		104.085	350.046	#
C3H7NO3 NPN Propylnitrate	105.09352	-174.054		123.239	362.601	#
C3H7O N-PROPOXY RAD.	59.08798	-37.656		81.634	309.616	#
C3H8 PROPANE	44.0962	-103.854	±0.6	73.563	270.182	*
C3H7OH PROPANOL	60.09592	-255.2		85.56	322.58	#
(CH3)2CHOH	60.09592	-272.7		89.594	309.221	#
C3O2	68.0318	-93.64		67.37	276.816	#
C4	48.044	1033.904		57.272	252.862	#
C4F6 Perfluoro 1,3-Butadiene	162.0343	-1004.122		137.272	388.442	*
F6C4 Perfluorocyclobutene	162.03439	-1210.843		131.589	379.256	*
C4F8 Perfluorocyclobutane	200.03123	-1513.6		145.483	405.3	#
C4F10 FC-3110 Perfluorobutane	238.02803	-2137.417		189.038	480.624	#
C4H	49.05194	803.328		66.759	265.569	#
C4H2 Butadiyne	50.05988	440.492		73.647	255.977	#
C4H3	51.06782	483.751		70.011	289.709	#
C4H4 1-Butene 3-yne	52.07576	308.446		72.951	278.926	#
C4H4 Cyclobutadiene	52.07576	385		60.969	251.442	#
C4H4N2 PYRAZINE	80.08924	195.811	±1.3	73.945	280.378	#
C4H4N2 PYRIMIDINE	80.08924	196.648	±0.84	73.69	280.677	#
C4H4O FURAN	68.07516	-34.685		65.407	267.251	#
C4H4O VINYL-KETENE	68.07516	7.615		89.301	301.081	#
C4H4O2 1,4-DIOXIN	84.07456	-140		81.278	290.435	#
C4H4S Thiophene	84.14176	114.9		72.818	278.778	#
N-C4H5	53.0835	345.157	±6	77.472	288.649	*
I-C4H5	53.0835	330.844		78.929	283.108	*
T-C4H5	53.0835	302.184		77.016	289.322	*
C4H5N PYRROLE	67.09044	108.18	±0.81	71.6	270.722	#
C4H5N Cyclopropanecarbonitrile	67.09044	184.096	±0.84	78.659	295.809	#
C4H6 2-Butayn	54.091	146.306		78.374	285.349	*
1,3-C4H6 Butadiene	54.0914	108.983		79.531	278.301	*
1,2-C4H6 Butadiene	54.0914	164.593		80.384	291.728	*
C4H6 Cyclobutene	54.09164	156.7		64.414	262.076	#
C4H6CL2 1,4-Dichlorobutene	124.99704	-58.158		112.131	380.744	#
CL2C4H6 3,4-Dichlorobutene	124.99704	-69.036		113.637	380.744	#
C4H6O 2,5 Di-Hydro FURAN	70.09104	-108.78		75.6	284.25	#
2,5 C4H6S Dihydrothiophene	86.15764	86.9		83.306	297.089	#
N-C4H7 3-Butene 1-yl Radical	55.09958	192.464		82.372	320.076	#
I-C4H7 (CH2=CHCH*CH3)	55.0993	126.509		83.331	295.977	*
T-C4H7 (*CH2CH=CHCH3)	55.0993	128.309		82.743	300.124	*
C4H7 2-Methyl-Allyl Radical	55.09958	121.336		86.566	292.043	#
C4H7 Cyclobutyl Radical	55.09958	214.221		67.713	292.462	#
C4H7O 2-Butanone Radical	71.09898	-20.585		94.546	346.561	#
C4H7O CH2=C(CH3)CH2O*	71.09898	51.714		97.234	332.251	#
C4H8 CH2=CH-CH2-CH3	56.107	-0.544		85.362	307.923	*
H8C4 CH2=C(CH3)2	56.107	-17.161		87.976	296.668	*

Table 5 (Continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$	± kJ/mol	C_{p298} J/mol	S_{298} J/mol	
C4H8 2-Butene trans	56.107	-10.975		81.112	300.751	*
C4H8 2-Butene cis	56.107	-7.426		85.227	295.879	*
C4H8 CYCLOBUTENE	56.10752	28.4		70.564	264.396	
beta HMX solid	296.15664	74.894		307.302	145.101	#
C4H8N8O8 HMX	296.15664	187.862		275.455	568.833	#
C4H8O 2-Methyl-Allyl Alcohol	72.10692	-165.686		102.907	343.088	#
C4H8O 2-BUTANONE	72.10692	-238.362		102.432	339.991	#
H8C4O 2,3-Dimethyloxyrane	72.10692	-129.704		97.077	307.524	#
OC4H8 ETHYL-OXYRANE	72.10692	-117.152		95.099	322.168	#
C4H8O Tetrahydrofuran, Oxolan	72.10692	-184.18		76.25	302.41	#
C4H8O2 1,4 DIOXANE	88.10632	-314.428	±7	92.568	294.582	#
(CH3COOH)2 Acetic Acid dimer	120.1048	-929.029		137.27	414.263	*
C4H8O4 Tetraoxocan	120.10512	-620.2		116.255	340.343	#
C4H8S Tetrahydrothiophen	88.17352	-34.1		92.55	309.627	#
1,4-C4H8S2 Dithiane	120.23952	0		109.655	326.252	*
1,3-C4H8S2 Dithiane	120.23952	-10		110.434	333.542	#
C4H9,n-Butyl Radical	57.11546	66.53		97.67	328.519	#
C4H9, I-Butyl Radical	57.11546	57.32		95.53	318.649	#
S-C4H9 sec Butyl Radical	57.11546	70		91.434	325.424	#
C4H9,t-Butyl Radical	57.11546	51.7		78.225	319.719	#
C4H9N PYROLIDINE	71.1222	-3.59	±0.8	82.112	309.206	#
C4H9NO2 Nitrobutane	103.121	-143.93		115.119	369.874	#
C4H9O n-BUTOXY RAD	73.11486	-58.158		104.655	349.364	#
C4H9O I-BUTOXY RAD	73.11486	-67.781		103.379	338.067	#
C4H9O S-BUTOXY RAD	73.11486	-73.22		106.684	343.088	#
C4H9O T-BUTOXY RAD	73.11486	-92.048		107.334	313.8	#
C4H10 n-Butane	58.123	-125.78	±0.67	98.613	309.739	*
I-C4H10 ISOBUTANE	58.123	-134.648	±0.63	96.645	295.358	*
C4H10FO2P SARIN	140.09437	-963.157	±40	161.667	412.013	#
C4H10O-N 1-BUTANOL	74.1228	-274.68		108.168	361.616	#
C4H10O-S 2-BUTANOL	74.1228	-292.629		111.134	363.877	#
C4H10O-T 2-Methylpropanol	74.1228	-312.628		113.481	329.72	#
C4N2 Carbon Subnitrid	76.0574	533.477	±0.8	85.93	290.022	*
C5	60.055	1050.924		75.507	271.678	#
C5F12 FC 4-1-12	288.03584	-2543.311		229.036	555.108	#
C5H	61.0629	778.276		65.158	260.415	*
C5H2	62.0709	691.412		82.981	266.639	*
C5H3 1,3-Pentadiyne-5-yl Rad.	63.07882	602.58		87.499	295.196	#
C5H3 HCCCH*CCH)	63.07882	564.61	±43	93.241	306.147	#
C5H3 Cyclopentatriene-yl	63.07882	697.77	±75	70.898	281.721	#
C5H3N HCC-CH=CH-CN	77.08556	416.308		94.266	321.833	#
C5H4 1,3-Pentadiyne	64.08676	399.572		90.418	296.646	#
C5H4 1,4-Pentadiyne	64.08676	464.771	±18	87.227	296.685	#
C5H4 Penta-Tetraene	64.08676	481.578		91.262	294.135	#
H4C5 1,2-Pentadiene-4-yne	64.08676	443.952	±25	86.759	301.388	#
C5H4 Cyclo-Pentatriene.	64.08676	551.485		73.235	279.6	#
C5H4N *CH=CH-CH=CH-CN	78.0935	476.976	±12.5	98.742	330.536	#
C5H4N meta-Pyridyl Radical	78.0935	383.254		75.73	292.88	#
C5H4O Cyclopentadiene-1-one	80.08616	55.229		80.941	289.977	#
C5H4O2 3 ketene	96.08556	-129.788		117.919	352	#
C5H5 3en1-yne5-yl	65.0947	406.3	±8.4	91.333	307.1	#
C5H5 CY	65.0947	266.102		76.605	279.485	#
C5H5N PYRIDINE	79.10144	140.37	±0.54	77.746	282.759	#
C5H4OH CYCLO RAD	81.0941	66.526		95.625	310.007	#
1,3C5H5O CY RADICAL	81.0941	59.8		90.023	307.695	#

Table 5 (Continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$	± kJ/mol	C_{p298} J/mol	S_{298} J/mol	
1,4C5H5O CY RADICAL	81.0941	103.3		90.479	307.805	#
2,4-c-C5H5O CY RADICAL	81.0941	221.758		83.1	302.922	*
C5H5O2 2-pentenedialdehyde R	97.0935	-83.638		110.293	391.33	#
C5H5O2 2-pentenedialdehyde R	97.0935	-72.76		113.89	387.94	#
C5H6 1-ene-2-yne	66.10264	249.366		89.238	320.076	#
C5H6 3-enE-1-yne	66.10264	256.479		94.424	314.637	#
CYCLOPENTADIENE	66.10264	134.3		75.368	274.154	#
C5H6N2 2-AMINOPYRIDINE	94.11612	118.616	±0.84	103.84	309.401	#
2,4-C5H5OH	82.10204	7.9		91.437	304.61	#
1,3-C5H5OH	82.10204	-24.3		94.957	304.343	#
1,4 C5H5OH	82.10204	-27.2		95.023	304.565	#
C5H7	67.11058	221.752		97.487	312.126	#
C5H7 CY	67.11058	166.88		79.892	308.24	#
C5H7CL	102.56328	71.128		110.541	373.213	#
C5H7CL2	138.01598	61.505		123.595	303.758	#
C5H7NO	97.11672	-108.7		120.7	387.6	#
C5H8 Pentadiene	68.11852	76.149		100.834	320.076	#
C5H8 ISOPRENE	68.11852	75.73		104.6	315.641	#
C5H8 Cyclopentene	68.11852	32.7		81.275	291.267	#
C5H8CL	103.57122	79.078		118.156	375.723	#
PETN Solid	316.13828	-538.481		353.757	101.964	#
C5H8N4O12 PETN	316.13828	-387.02		294.758	614.706	#
C5H9 CY	69.12646	115.06		78.68	300.83	#
C5H9 2-PENTEN-5-YL	69.12646	158.992		106.274	358.569	#
H9C5 2-PENTEN-1-YL	69.12646	112.968		104.6	347.272	#
C5H9 3M1BUTEN3YL	69.12646	80.751		106.512	316.729	#
C5H9 3M1BUTEN1YL	69.12646	212.129		117.555	337.9	#
C5H9 3M1BUTEN4YL	69.12646	176.983		114.868	344.092	#
C5H9N	83.1332	75.312	±8.4	99.27	274.978	#
C5H10 1-PENTENE	70.134	-21.273		109.588	345.789	*
C5H10 2-PENTENE	70.1344	-31.757		108.449	340.41	#
C5H10 2MB-1ene	70.1344	-36.317		109.956	339.532	#
C5H10 2MB-2ene	70.1344	-42.551		105.018	338.569	#
C5H10 2MB-3ene	70.1344	-28.953		118.616	333.465	#
C5H10 Cyclopentane	70.1344	-78.4		82.759	292.86	#
C5H10O TetraHydroPYRAN	86.1338	-223.844	±0.84	124.343	309.616	#
N-C5H11 n-pentyl	71.14234	55.605		118.049	371.707	#
S-C5H11 1methyl-butyl	71.14234	45.564		119.653	369.949	#
T-C5H11	71.1419	32.6		98.855	366.37	#
C5H11 neopentyl	71.14234	34.392		118.84	333.423	#
C5H11NO2 Nitropentane	117.14788	-164.431		137.1	390.905	#
C5H12 PENTANE	72.1498	-146.762		119.95	349.379	#
I-C5H12 Isopentane	72.1498	-153.702		118.854	343.629	#
CH3C(CH3)2CH3 Neopentane	72.1498	-167.922		121.429	304.811	#
C6CL6 Hexachlorobenzene	284.7822	-33.89		175.31	441.203	#
C6D5 Deuterated phenyl radical	82.13651	306.981		95.461	300.474	*
C6D6 Deuterated Benzene	84.15061	58.217		100.94	282.612	*
C6F6 Hexafluorobenzene	186.05642	-956.63		157.938	384.457	#
C6F14 FC 51-14Perfluorohexane	338.04364	-2949.201		269.551	629.592	#
C6N6O6 BENZOTRIFUROXAN	252.10284	N/A		200.972	416.395	#
C6H	73.07394	1037.632		96.024	312.451	#
C6H2	74.08188	700.82		104.103	299.19	#
C6H3	75.08982	682.016		100.896	319.344	#
C6H3(NO2)3 Trinitrobenzene	213.10644	62.342		205.633	485.335	#
C6H4 BENZYNE	76.09776	481.16		77.192	291.093	#

Table 5 (Continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$	± kJ/mol	C_{p298} J/mol	S_{298} J/mol	
C6H4 TRANS	76.09776	526.347		102.772	321.331	#
C6H4 CIS	76.09776	514.632		102.772	321.331	#
C6H4 PENTAENE	76.09776	129.37		121.268	72.24	#
C6H4 TRIENE-5YNE	76.09776	327.9		112.4	198.82	#
C6H4O2 O=C6H4=O	108.09656	-122.9		108.485	333.212	#
C6H5 CHAIN	77.1057	531.368		109.472	339.195	#
C6H5 PHENYL RAD	77.1055	328.456		78.964	288.337	*
C6H5 FULVENYL RAD	77.1057	861.886		90.183	291.404	#
C6H5 FULVENYL Rad. Melius	77.1057	490.365	±52	93.077	307.123	#
C6H5Br	157.0097	105.018		97.696	324.386	#
C6H5CL	112.5584	51.84		98.031	313.465	#
C6H5F	96.1041	-116.566		94.433	302.629	#
C6H5NO NITROSOBENZENE	107.11184	200.832		110.848	322.377	#
C6H5NO2 NITRO-BENZENE	123.11124	68.534		120.38	348.8	#
C6H5O PHENOXY RAD	93.1049	47.716		94.416	307.816	*
C6H5OO PEROXYPHENYL	109.1045	165.645		114.023	347.776	#
C6H5OH PHENOL	94.1128	-96.375		103.599	314.864	*
C6H6(L)	78.11364	49.08		135.95	173.44	#
C6H6 BENZENE	78.11364	82.811		82.127	269.065	*
C6H6 FULVENE	78.11364	236.814	±10	90.362	294.123	#
C6H6 1,5-hexadiyine	78.11364	416.308	±16.7	108.155	328.43	#
C6H6 2,4hexadiyne	78.11364	359.406	±16.7	106.891	332.628	#
C6H6 1,3hexadiyne	78.11364	379.907	±20.9	110.641	340.159	#
C6H6 1,2,4,5 Hexatetraene	78.11364	395.388		107.136	328.569	#
C6H6 1,2-Hexadiene-5-yne	78.11364	412.542		107.68	336.912	#
C6H7 1,4 CYCLO Radical	79.12158	200.589	±35	97.618	305.835	#
C6H7 CHAIN	79.12158	389.15		109.544	353.27	#
C6H5NH2(L) aniline	93.12832	31.501		191.92	190.598	#
C6H7N ANILINE	93.12832	87.04		108.385	319.27	#
C6H8 CY CH3-C5H5	80.12952	102		116.8	310.3	#
C6H8 1,3,5-HEXATRIENE	80.12952	152.214		107.911	330.388	#
H8C6 (1,3-CYCLO)	80.12952	106.3		94.168	303.419	#
C6H8 (1,4-CYCLO)	80.12952	109		94.053	296.34	#
C6H9 1,3 hexadiene 5-yl Rad.	81.13746	184.096		115.478	367.774	#
1,3-C6H9 hexadiene 6-yl Rad.	81.13746	251.04		119.244	375.305	#
C6H9 Cyclohexenyl-3	81.13746	125.52		103.345	306.269	#
C6H10 1,3-HEXADIENE	82.1454	56.066		122.173	361.079	#
C6H10 Cyclohexene	82.1454	-4.6		101.464	310.633	#
C6H11 trans 3-hexene-6-yl Rad	83.15334	142.256		127.612	394.97	#
C6H11 CH2=C(CH2*)C3H7	83.15334	93.303		130.77	372.376	#
C6H11 CH2=C(CH3)C3H6*	83.15334	149.787		130.797	390.786	#
C6H11 CH3C(CH2*)=CHC2H5	83.15334	81.17		129.538	369.029	#
C6H11 CH3C(CH3)=CHC2H4*	83.15334	141.838		124.52	387.438	#
C6H11 (CH3)2C=CHCH*CH3	83.15334	58.158		130.623	364.008	#
C6H11 (CH3)CHCH*CH=CH2	83.15334	75.73		128.086	364.008	#
C6H11 2-Methyl-1-pentene-4-yl	83.15334	135.562		127.196	340.159	#
C6H11 Cyclohexy Radical	83.15334	68.199		108.397	328.026	#
C6H12 TRANS-3-HEXENE	84.16128	-53.137		129.286	378.652	#
C6H12 1-HEXENE	84.16128	-41.688		132.311	384.82	*
C6H12 2MP-1ene	84.16128	-59.371		135.603	382.167	#
C6H12 2MP-2ene	84.16128	-66.86		126.608	378.443	#
C6H12 4MP-2ene CIS	84.16128	-57.446		133.553	373.338	#
C6H12 4MP-2ene TRANS	84.16128	-61.463		141.419	368.276	#
C6H12 CYCLOHEXANE	84.16128	-123.3		105.341	297.276	#
N-C6H13 n - HEXYL RAD.	85.16922	25.102		141.63	407.654	*

Table 5 (Continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$	± kJ/mol	C_{p298} J/mol	S_{298} J/mol	
2-C6H13 2-HEXYL RAD.	85.16922	23.012		138.739	410.032	#
C6H13 2MP-1YL	85.16922	29.288		138.717	400.409	#
C6H13 2MP-5YL	85.16922	32.635		138.717	394.551	#
C6H13-S 2ME - 4PENTYL	85.16922	14.644		137.263	398.317	#
C6H13-T 2ME 2PENTYL	85.16922	9.205		140.012	400.827	#
C6H14(L) n-Hexan	86.17716	-198.661		195.481	296.089	#
C6H14 n-Hexane	86.17716	-166.92		142.59	388.85	#
H14C6 2-METHYLPENTANE	86.17716	-174.55		142.21	380.98	#
C6H14 3MP	86.17716	-171.97		140.21	383.03	#
C6H14 2,2-DMBUTANE	86.17716	-184.68		141.46	358.34	#
C6H14 2,3-DMBUTANE	86.17716	-176.8		139.41	365.92	#
C7F16 Perfluoroheptane	388.05145	-3383.969		300.804	704.075	#
C7H5N C6H5-CN Benzonitrile	103.12344	218.823		109.077	321.038	#
TNT Solid	227.13332	-63.178		244.68	137.779	#
C7H5N3O6 TNT	227.13332	24.1		214.425	507.087	#
C7H5N5O8 Tetryl Solid	287.1456	41.003		290.913	143.469	#
C7H6O BENZALDEHYDE	106.12404	-36.8		111.673	336.019	#
C7H7 BENZYL RADICAL	91.13258	210.5		109.126	321.133	#
TOLUENE(L)	92.14052	12.18		157.29	221.03	#
C7H8 TOLUENE	92.14052	50		103.283	320.187	#
C7H8 Norbornadiene	92.14052	247.6		96.748	295.226	#
C7H8 1,3,5-Cycloheptatriene	92.14052	182.8		106.251	316.365	#
C7H8 1,6-Heptadiyne	92.14052	395.8		134.202	379.7	#
C7H8O CRESOL	108.13992	-132.298		124.694	355.881	#
C7H8O BENZYL-ALCOHOL	108.13992	-100.416		115.529	330.58	#
C7H10 3,5-dimethyl-CPD	94.1564	66.7		142.3	341.9	#
C7H12 NORBORNANE	96.17228	-53.723	±4.2	103.291	307.66	#
C7H12 CY-HEPTENE	96.17228	-9.4		120.422	324.001	#
C7H14 n-HEPTENE	98.18816	-62.3		155.226	423.588	#
C7H14 CY-HEPTANE	98.18816	-118.2		131.171	336.512	#
C7H15 n-HEPTYL RAD.	99.1961	4.39		164.43	447.92	#
C7H15 NEOHEPTYL	99.1961	-4.853		163.769	414.969	#
C7H15 NEOHEPTYL-2	99.1961	-15.941		160.737	405.848	#
C7H15O 3,3dimethyl1-pentanoxy	115.1955	-142.256		171.86	328.026	#
C7H16(L) n-Heptan	100.20404	-224.35		224.982	328.561	#
C7H16 n-HEPTANE	100.204	-187.65		165.18	427.98	*
C7H16 NEOHEPTAN	100.20404	-209.87		166.955	395.221	#
C7H15OH n-Heptanol	116.20344	-339.741		178.605	480.449	#
C7H15OH Neoheptanol	116.20344	-359.657		179.907	448.901	#
C8H	97.09594	1162.06		132.416	358.74	#
C8H2	98.10388	934.287		132.638	347.69	#
C8H6 C6H5CCH	102.13564	328.151		115.734	327.918	#
C8H6O BENZOFURANE	118.13504	27.112		116.137	331.373	#
C8H6S	134.20164	166.272		131.558	337.481	#
STYRENE RADICAL	103.14358	389.112		127.45	344.397	#
C8H7N INDOLE	117.15032	156.5	±1.25	121.264	332.373	#
C8H8 CUBANE	104.15152	651.7	±30	98.47	271.426	#
C8H8 STYRENE	104.15152	147.36		122.089	345.096	#
C8H9 C6H5CH2CH2*	105.15946	252.379	±15	136.843	364.712	#
C8H10 C6H5C2H5	106.1674	29.288		129.321	344.466	#
C8H10 Di METHYLBENZENE	106.16699	17.994		125.745	352.115	*
1-C8H16 1-OCTENE	112.2144	-82.905		178.155	462.399	*
N-C8H17 N-OCTYL RAD	113.2223	-16.323		186.847	486.834	*
C8H18(L) n-Octan	114.23092	-250.262		254.149	361.071	#
C8H18 OCTANE	114.2302	-208.755		187.57	466.872	*

Table 5 (Continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$	± kJ/mol	C_{p298} J/mol	S_{298} J/mol	
C8H18(L) isooctan	114.23092	-259.161		238.998	328.109	#
C8H18 ISO-OCTANE	114.2302	-224.013		188.529	422.894	#
C9H7 INDENYL	115.15458	285.6	±22	128.21	342.843	#
C9H7N QUINOLINE	129.16132	200.52		129.153	344.075	#
C9H7N ISOQUINOLINE	129.16132	204.61		128.983	344.568	#
C9H8 INDENE	116.16252	164.138	±1	124.226	335.846	#
C9H10 METHYLSTYRENE	118.1784	112.968		146.858	383.673	#
C9H12 1,3,5-Trimethylbenzene	120.19428	-16.067		147.800	385.300	#
C9H12 1,2,4-Trimethylbenzene	120.19428	-13.933		154.508	395.765	#
C9H17 1-Nonenyl Radical	125.23398	88.400		195.709	520.900	#
C9H18 1-Nonene	126.24192	-432.207		200.269	505.000	#
N-C9H19 n-NONYL RAD	127.2491	-37.037		209.44	526.427	*
N-C9H20 liq. NONANE	128.2578	-275.475		284.386	393.673	#
N-C9H20 NONANE	128.2578	-228.907		210.413	506.431	#
C10D8 NAPHTHALENE-D	136.22281	118.111		156.96	350.669	*
C10H6 Naphtyne	126.15764	500.825		132.178	347.542	#
C10H7 Naphtyl Radical	127.16558	396.225		132.841	352.133	#
C6H4(C2H)CH=CH*	127.16558	617.140		144.841	367.587	#
C10H7O* Naphthol Radical	143.15498	115.478		146.882	373.015	#
H8C10 AZULENE	128.1732	279.932		128.868	338.065	*
C10H8 NAPHTHALENE	128.1732	150.606	±1.5	132.317	333.299	*
C10H8O Naphtol	144.17292	-30.794		154.318	368.709	#
C10H9 2-HydroNaphthalen Rad	129.18146	229.534		143.289	363.659	#
C10H10 1,2-DihydroNapthalene	130.1894	117.152		143.955	359.383	#
C10H16 JP-10	136.23704	-60.25	±4.2	152.756	370.57	#
C10H19 1-Decenyl 4/5 Radical	139.26086	67.900		218.653	560.300	#
C10H19 1-Decenyl 3 Radical	139.26086	2.600		221.077	567.300	#
C10H20 1-Decene	140.26880	-123.900		223.362	544.500	#
C10H20 2-Decene-trans	140.26880	-136.200		222.222	541.000	#
C10H20 3-Decene-trans	140.26880	-135.500		220.659	542.600	#
N-C10H21 n-DECYL 1-Radical	141.27674	-57.75		232.061	566.02	*
C10H21 n-Decyl – 2-Radical	141.27674	-58.100		230.534	567.300	#
C10H21 n-Decyl-3/4 Radical	141.27674	-58.200		230.534	567.300	#
N-C10H22 liq DECANE	142.28468	-301.039		314.511	425.889	#
N-C10H22 gas-DECANE	142.28468	-249.534		233.049	545.677	#
1-C10H7C*O Naphtaldehyde Rd.	155.17598	174.891		161.693	399.949	#
1-C10H7CHO Naphtaldehyde	156.18392	30.543		162.397	383.881	#
1-C10H7-CH2* Methyl-Naphthyl	141.19246	272.797		158.090	378.770	#
1-C10H7-CH3 MethylNaphthalen	142.20040	116.106		157.922	381.348	#
C11H24 N-UNDECANE	156.31156	-270.286		255.684	584.923	#
O-C12D9 O-BIOPHENYL R	162.25892	386.58		195.578	428.768	*
C12D10 BIPHENYL – D	164.27302	138.488		200.307	413.489	*
1-C10H7-C≡C* EthynylNaphthyl	151.18758	694.962		162.077	397.847	#
C12H8 Acenaphthylene	152.19552	259.7		154.775	358.632	#
C10H7-C≡CH EthynylNaphthalen	152.19552	379.070		169.895	391.974	#
1-C10H7-CH=CH* Vinyl-Naphthy	153.20346	469.863		172.891	404.234	#
1-C10H7-C*=CH2	153.20346	412.208		175.034	407.260	#
O-C12H9 O-BIPHENYL RAD	153.2031	427.757		163.464	405.034	*
C12H9CL	188.65616	148.55		178.868	433.51	#
C12H9N CARBAZOLE	167.2102	200.7		176.877	388.305	#
1-C10H7-CH=CH2	154.21140	215.058		173.671	400.851	#
C12H10 BIPHENYL	154.21140	182.155		166.617	388.866	*
1-C10H7-CH2CH2*	155.21934	292.88		185.266	418.370	#
1-C10H7-CH*-CH3	155.21934	220.497		184.272	426.717	#
1-C10H7-C2H5 EthylNaphthalen	156.22728	96.901		181.943	406.323	#

Table 5 (Continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$	± kJ/mol	C_{p298} J/mol	S_{298} J/mol	
1-C10H7CH2CH2OH	172.22668	-52.718		195.002	447.806	#
C12H26 N-DODECANE	170.33844	-290.872		278.32	624.253	#
C13H9N ACRIDINE	179.2212	273.9		177.643	394.998	#
C13H9N PHENANTHRIDINE	179.2212	240.5		184.131	391.6	#
C14H10 ANTHRACENE	178.2334	230.1		184.993	392.693	#
C14H10 PHENANTHRENE	178.2334	207.1		186.787	394.614	#
C14H14 BIBENZYL	182.2646	143.146		205.045	483.271	*
C16H10 PYRENE	202.2554	225.7		202.501	407.513	#
C18H12 Naphthacene	228.29327	290.000		233.343	441.654	#
C18H12 Triphenylene	228.29327	274.2		236.543	441.657	#
C22H14 Pentacene	278.35315	355.000		281.951	494.186	#
C22H14 Pentafene	278.35315	345.000		282.920	501.187	#
C24H17 Triphenylbenzene Rad.	305.39898	623.2		323.134	652.000	#
C24H18 Triphenylbenzene	306.40692	373.05		327.478	621.65	#
C60	720.66	2585.712	±105	560.816	591.403	#
C70	840.77	2895.328		558.171	589.535	#
JET-A(L)	167.3137	-303.469		350.336	448.112	#
JET-A(G)	167.3137	-211.46		293.494	612.539	#
CL	35.4527	121.302	±0.008	21.838	165.192	#
DCL	37.4668	-93.347	±0.21	29.174	192.744	*
DOCL	53.4662	-78.243	±2.1	38.539	240.31	*
CLF	54.4511	-50.293	±0.42	32.082	217.939	*
CLF3	92.44791	-158.851	±2.9	63.996	281.633	*
CLO	51.4521	101.218	±2.1	31.558	226.646	*
CLO2 (OClO)	67.4515	104.599	±6.3	42.003	257.213	*
CLOO	67.4518	96.238		43.982	264.994	*
CLO3F	102.4493	-23.799		64.927	278.989	#
CL2 REFERENCE ELEMENT	70.9054	0		33.949	223.082	*
CL2O	86.9048	87.868	±6.7	47.884	267.976	*
CL2O2	102.9042	138.976		65.034	295.883	#
Cr(cr) REFERENCE ELEMENT	51.9961	0		23.434	23.618	*
Cr	51.9961	397.48		20.786	174.313	#
CrN(s)	66.00284	-117.294	±8.4	51.093	37.215	*
CrN	66.00284	505.022	±20.9	30.753	230.553	*
CrO	67.9955	188.285		31.33	239.27	*
CrO2	83.9949	-75.313		43.404	269.245	*
CrO3	99.9943	-292.88		56.124	266.201	*
Cr2N(s)	117.99894	-125.532		66.318	64.921	*
Cr2O3(s)	151.9904	-1135.094		120.644	79.812	*
Cr2FeO4	223.8348	-1458.124		133.69	141.963	#
Cr3C2(S)	180.0103	-85.354		99.326	85.437	#
Cr7C3(S)	400.0057	-160.666		209.764	200.999	#
C6Cr23	1267.9763	-328.444		628.117	612.119	#
D	2.0141	221.72	±0.004	20.786	123.352	#
DF	21.01251	-275.523	±0.8	29.139	179.704	*
HD	3.02204	0.322		29.2	143.799	#
HDO	19.02144	-245.276		33.798	199.517	#
HDO2	35.02084	-140.232		43.779	243.581	#
OD	18.01350	37.226		29.939	189.666	#
OD-	18.01405	-145.378		29.143	178.409	#
DO2	34.0129	12.552		35.844	232.77	#
D2 REFERENCE ELEMENT	4.0282	0		29.195	144.96	*
D2O	20.0276	-249.209	±0.067	34.256	198.342	*
D2O2	36.027	-144.146		45.368	241.739	*
D2S	36.0942	-23.891	±0.8	35.752	215.295	*

Table 5 (Continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$	± kJ/mol	C_{p298} J/mol	S_{298} J/mol	
ELECTRON GAS	0.00055	0		20.786	20.979	*
F	18.9984	79.39	±0.3	22.746	158.75	#
FO	34.9978	109	±10	31.99	216.377	#
FO2 O-F-O	50.9972	378.6	±20	41.126	251.289	#
FO2 F-O-O	50.9972	25.4	±2	44.453	259.511	#
F2 REFERENCE ELEMENT	37.99681	0		31.304	202.792	*
F2O F-O-F	53.99621	24.5	±2	43.302	247.46	#
F2O2 F-O-O-F	69.99561	19.2	±2	62.073	277.214	#
Fe(a) REFERENCE ELEMENT	55.847	0		25.094	27.321	*
Fe	55.847	415.5		25.675	180.49	#
Fe+	55.84645	1181.144		26.068	181.859	#
Fe-	55.84755	393.338		25.023	180.2	#
FeCL	91.2997	251.036		38.245	257.577	*
FeCL2(s)	126.7524	-341.841		76.707	117.954	*
FeCL2	126.7524	-141		57.624	299.297	*
FeCL3(s)	162.2051	-399.405		96.651	142.338	#
FeCL3	162.2051	-253.12		77.78	344.226	*
FeO(s)	71.8464	-272.037		49.972	60.754	*
FeO	71.8464	251.047		31.415	241.926	*
Fe(OH)2(s)	89.86168	-574.059		97.079	87.875	*
Fe(OH)2	89.86168	-330.536		71.505	283.092	#
Fe(OH)3(s)	106.86902	-832.627		101.928	104.627	*
FeS(a)	87.913	-101.818		50.214	59.883	*
FeS(G)	87.911	370.767		34.002	252.344	#
FeSO4(s)	151.9106	-928.877		100.666	120.949	*
FeS2(s)	119.979	-171.549		62.18	52.926	*
Fe2CL4	253.5048	-431.374		125.966	464.528	*
Fe2CL6	324.4102	-654.378		173.665	536.945	#
Fe2O3(S) Solid-A	159.6882	-824.248		103.866	87.404	#
Fe3C (S) Solid-A	179.546	25.104		105.868	104.6	#
Fe3O4(S) Solid-A	231.5326	-1118.383		150.73	146.147	#
H	1.00794	217.998	±0.006	20.786	114.718	#
H+	1.00739	1536.245		20.786	108.948	#
H-	1.00849	139.031		20.786	108.961	#
HBr	80.91194	-36.29		29.141	198.698	#
HCL	36.46064	-92.31		29.136	186.901	#
HOCL	52.46004	-75.741		37.285	236.587	#
HF	20.00634	-273.3		29.137	173.775	#
HOF	36.00574	-96.898		35.94	226.757	#
HI	127.91241	26.36	±0.21	29.153	206.592	*
HNO	31.01408	102.033	±10.5	33.88	220.92	#
HNO2	47.01348	-78.452		46.32	254.071	#
HNO3	63.01288	-133.913		54.109	266.878	#
OH	17.00734	39.347		29.886	183.74	#
OH+	17.00679	1290.204		29.196	182.746	#
OH-	17.00789	-143.199		29.141	172.433	#
HPO	47.9811	-56.869		35.81	235.685	#
SH	33.07394	139.332	±5	32.459	195.638	*
SOH	49.07334	-20.895	±42	36.707	239.818	#
HSO	49.07334	-4.782	±7.3	37.659	242.486	#
HO2	33.00674	12.552		34.893	229.106	#
HO2S	65.07274	-255.88	±6	50.708	276.742	#
HSO3	81.07214	-385		67.209	294.061	#
HS2	65.13994	26.987		42.018	252.295	#
H2 REFERENCE ELEMENT	2.01588	0		28.836	130.679	*

Table 5 (Continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$	± kJ/mol	C_{p298} J/mol	S_{298} J/mol	
H2F2	40.01269	-569.924		58.132	260.905	#
H2O(L)	18.01528	-285.83		75.351	69.939	#
H2O	18.01528	-241.826	±0.04	33.588	188.829	#
H2O2(L)	34.01468	-187.778		89.328	109.604	#
H2O2	34.01468	-136.31		42.388	234.527	#
H2S	34.08188	-20.6		34.248	205.803	#
H2SO4(L)	98.07948	-814.01		138.594	156.907	*
H2SO4	98.07948	-732.732		84.401	299.289	#
H2S2	66.14788	16.736		51.209	260.663	#
H3F3	60.01903	-883.677		73.884	280.947	#
H3O+	19.02267	598		35.485	193.139	#
H4F4	80.02537	-1186.932		104.022	350.016	#
H5F5	100.03172	-1490.188		134.161	417.286	#
H6F6	120.03806	-1805.545		163.735	486.619	#
H7F7	140.0444	-2099.699		194.438	548.654	#
He REFERENCE ELEMENT	4.0026	0		20.786	126.154	*
He+	4.00205	2378.453		20.786	131.915	#
I	126.90447	106.76	±0.04	20.786	180.789	#
INO2 NITRO-IODINE	172.91001	60.25		59.366	294.432	#
IO	142.90387	126	±18	33.117	239.835	#
IO2 O-O-I	158.90327	116.5	±40	48.727	296.374	#
IO2 O-I-O	158.90327	159.3	±25	46.697	281.231	#
IO3	174.90267	241.9	±50	61.56	292.975	#
I2	253.8089	62.444		36.889	260.584	*
I2O I-I-O	269.80834	106.7	±40	52.359	330.647	#
I2O I-O-I	269.80834	119.5	±25	51.874	308.111	#
Kr REF ELEMENT	83.8	0		20.786	164.086	*
Kr+	83.79945	1356.963		20.786	175.613	#
MnO (S)	70.93745	-385.221		44.102	59.71	#
MnO2(S)	86.93685	-520.029		54.415	53.049	#
Mn2O3 (S)	157.8743	-959.002		99.034	110.499	#
Mn3O4 Solid-A	228.81175	-1387.799		140.515	155.599	#
Mn5N2(S)	302.70373	-204.2		175.724	187.443	#
MnS Solid	87.00405	-214.2		49.943	78.199	#
MnS2 (S)	119.07005	-223.844		70.075	99.914	#
Mo(cr)	95.94	0		23.933	28.605	*
MoC Solid-C	107.951	-28.451		30.878	36.652	#
MoO2 Solid	127.9388	-588.94		55.982	46.275	#
MoO2	127.9388	-8.314		34.002	252.344	#
Mo2C(S)	203.891	-53.137		60.207	65.814	#
N	14.00674	472.68	±0.4	20.786	153.302	#
ND	16.0208	375.309	±20.9	29.162	187.129	#
NHD Radical	17.02878	187.862	±2	33.997	199.499	#
ND2	18.0349	185.353	±8.4	34.422	204.184	#
ND2H	19.04288	-50.919		36.502	202.358	#
ND3	20.04901	-58.577	±0.4	38.219	203.822	#
NF	33.00514	232.99		30.228	212.908	#
NF2	52.00355	34.421		41.048	249.628	#
NF3	71.00195	-131.7		53.57	260.884	#
NH	15.01468	357.032		29.193	181.224	#
NH+	15.01413	1665.795		32.775	187.651	#
NHF	34.01308	112		35.234	230.806	#
NHF2	53.01149	-103		43.384	252.814	#
NH2 AMIDOGEN RADICAL	16.02262	189.135		33.857	194.996	#
NH2D	18.03672	-44.081		37.375	194.347	#

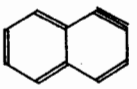
Table 5 (Continued)

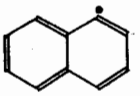
Compound	Mol. Wgt.	$\Delta_f H_{298}$	± kJ/mol	C_{p298} J/mol	S_{298} J/mol	
NH2F	35.02102	-75		36.474	229.534	#
NH3 AMONIA	17.03056	-45.94		35.63	192.77	#
NH2OH	33.02996	-50	±10	46.472	236.181	#
NH4+ AMONIUM ION	18.03795	644.905		34.764	186.095	#
NH4CLO4(l)	117.4888	-295.767		128.072	184.18	#
NO	30.00614	91.269		29.862	210.748	#
NO+	30.00559	990.807		29.123	198.234	#
NOCL	65.45884	64.062		44.619	261.586	#
NOF	49.00454	-65		41.522	248.216	#
NOF3	87.00135	-187		68.067	277.731	#
NO2	46.00554	34.193		37.177	240.171	#
NO2-	46.00609	-200.036		37.215	236.241	#
NO2CL	81.45824	12.5		53.246	272.13	#
NO2F	65.00394	-109		48.987	259.275	#
NO3	62.00494	71.13		46.935	252.623	#
NO3-	62.00549	-310.78		44.724	245.638	#
NO3F	81.00334	15		66.958	293.171	#
N2 REFERENCE ELEMENT	28.01348	0		29.124	191.607	*
N2D2 Cis	32.0416	207.11		39.017	224.332	#
N2F2	66.01029	62.374		56.569	268.216	#
N2F4	104.00709	-22		88.384	317.531	#
N2H	29.02142	249.517	±13.6	34.662	224.505	#
N2H2	30.02936	211.86		35.045	218.333	#
NH2NO2 NITRAMIDE	62.02816	-3		58.678	269.671	#
H3N2 HYDRAZINE RAD	31.0373	225.057	±71	43.267	236.86	#
N2H4(L) Hydrazin	32.04524	50.38		98.839	121.545	#
N2H4 HYDRAZINE	32.04524	95.18	±4.2	48.43	238.466	#
N2O	44.01288	81.6		38.628	220.01	#
N2O+	44.01233	1333.399	±0.63	42.263	233.859	#
N2O3	76.01168	86.631		72.733	314.736	#
N2O4	92.01108	11.111		79.168	304.451	#
N2O5	108.01048	13.3		95.332	355.717	#
N3 AZIDE RADICAL	42.02022	436		36.175	223.072	#
N3H AZIDIC ACID	43.02816	294		44.219	239.33	#
Ne REFERENCE ELEMENT	20.1797	0		20.786	146.33	*
Ne+	20.17915	2086.989		22.115	158.307	#
Ni(cr) REFERENCE ELEMENT	58.6934	0		25.987	29.87	*
NiO Solid-A	74.689	-8.314		44.309	37.991	#
NiS(b) Crystal	90.7594	-87.869		47.121	52.986	*
NiS2(s)	122.8254	-131.381		70.627	71.966	*
Ni3S2(l)	240.2122	-216.325		117.75	133.871	*
Ni3S4(s)	304.3442	-301.121		164.813	186.484	*
O	15.9994	249.175	±0.1	21.912	161.06	#
O-	15.99995	101.664		21.685	157.797	#
O2 REFERENCE ELEMENT	31.9988	0		29.378	205.149	*
O2+	31.99825	1171.828		30.67	205.393	#
O2-	31.99935	-48.028		31.422	209.336	#
O3 OZONE	47.9982	141.8		39.378	239.011	#
P	30.97376	316.39	±1	20.786	163.2	#
PCL3	137.33186	-288.58	±5.4	71.706	311.715	*
PF	49.97217	-52.377	±20.9	31.616	224.968	*
PF2	68.97057	-488.269	±20.9	44.716	262.958	*
PF3	87.96897	-958.457	±3.8	58.801	273.073	*
PF5	125.96578	-1594.433	±2.9	85.05	300.855	*
PH	31.9817	236.097	±33.5	29.158	196.346	*

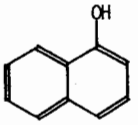
Table 5 (Continued)

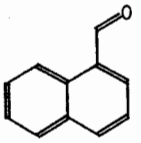
Compound	Mol. Wgt.	$\Delta_f H_{298}$	± kJ/mol	C_{p298} J/mol	S_{298} J/mol	
PH3 PHOSPHINE	33.99758	5.424	±1.7	37.074	210.293	*
PN	44.9805	104.776		29.667	211.126	*
PO	46.97316	-29.597	±4.2	31.725	222.768	*
PO2	62.97256	-314.533		41.397	253.682	*
P2	61.94752	143.651	±2.1	32.057	218.135	*
P4	123.89505	58.917	±2.1	67.326	280.022	*
P4O6	219.89145	-2144.519	±33.5	143.998	345.664	*
P4O10	283.88905	-2904.154	±8.9	188.827	403.974	*
P4O10(s)	283.88905	-3010.022	±8.9	211.82	228.786	*
S(S) REFERENCE ELEMENT	32.066	-0.072		22.801	33.099	*
S	32.066	276.98	±0.25	23.674	167.832	#
SCL	67.5187	156.47	±16.7	37.555	237.334	*
SCL2	102.9714	-17.572	±3.3	50.909	281.641	*
SD	34.0801	138.495	±5	32.528	201.493	*
SF	51.0644	12.971	±6.3	35.157	225.282	*
SF2	70.06281	-296.653	±16.7	44.906	257.708	*
SF3	89.06121	-503.041	±33.5	62.998	286.186	*
SF4	108.05961	-763.18	±20.9	77.62	299.657	*
SF5	127.05802	-908.467	±15.1	89.687	304.774	*
SF5Br	206.96202	-972.8	±59	107.075	333.654	#
SF5CL	162.51072	-1038.9	±10.5	104.344	319.936	#
SF6	146.05642	-1220.502	±0.8	96.994	291.551	*
SN	46.07274	263.583	±105	31.758	222.081	*
SO	48.0654	5.008	±1.3	30.164	221.944	*
SOF2	86.06221	-543.926	±105	57.202	279.156	*
SO2	64.0648	-296.835	±0.21	39.867	248.206	*
SO2CLF	118.5159	-556.476	±21	71.719	302.879	*
SO2CL2	134.9702	-354.802	±2.1	77.218	311.127	*
SO2F2	102.06161	-758.569	±8.4	65.946	283.651	*
SO3	80.0642	-395.753	±0.71	50.692	256.775	*
S2	64.132	128.404	±.0.3	32.481	228.313	*
S2CL	99.5847	78.562	±8.4	50.968	292.162	*
S2CL2	135.0374	-16.736		72.776	327.237	#
S2F2 (SSF2)	102.11681	-401.422	±41.8	63.146	292.729	*
FS2F	102.11681	-336.443	±41.6	66.061	293.985	*
S2F10	254.11603	-2064.386	±29.3	176.702	397.041	#
S2O	80.1314	-56.486	±33.5	44.112	267.029	*
S8	256.528	100.42	±0.63	156.046	430.319	#
Si(cr) REFERENCE ELEMENT	28.0855	0		19.789	18.81	*
SiC(b)	40.0965	-73.22		26.867	16.617	*
SiO2(Lqz)	60.0843	-910.857		44.59	41.463	#
Si2N2O(s)	100.18388	-947.711		67.46	46.06	#
Si3N4(a)	140.28346	-744.77		99.579	112.968	*
SiS2 Solid	92.2175	-213.384		77.482	80.333	#
Xe REFERENCE ELEMENT	131.29	0		20.786	169.686	*
Xe+	131.28945	1176.557		20.786	181.212	#

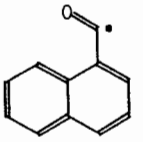
* The polynomials are pinned at 1000 K therefore the property values are not exact at 298 K.
\# The polynomials are pinned at 298 K, therefore the property values are exact.

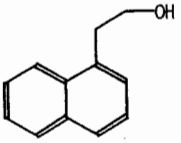

Naphthyne $C_{10}H_6$

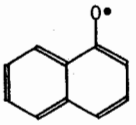

Naphthyl radical $C_{10}H_7$


Naphtol $C_{10}H_7OH$


Naphthaldehyde $C_{10}H_7CHO$

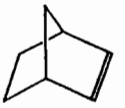

Naphthaldehyde radical $C_{10}H_7C$ =O

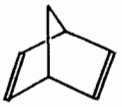

Naphtyl Ethanol $C_{10}H_7C_2H_4OH$


Naphtoxy radical $C_{10}H_7O$ •

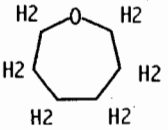
Naphthacene

Norbornane

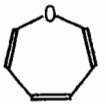

2-Norbornene

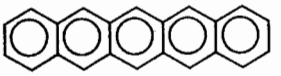

2,5-Norbornene

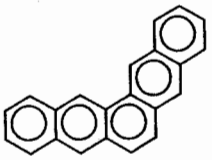
Oxocane

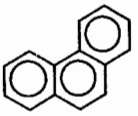


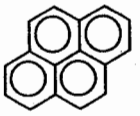
Oxepane


Oxepin


Pentacene


Pentaphene


Phenanthrene


Pyrene

4H-Pyran

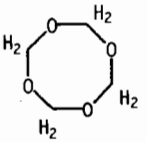
2H-Pyran, tetrahydro

Pyridine

Pyrrole

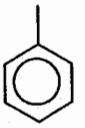
Pyrrolidine

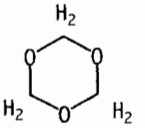
Styrene



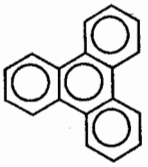
Tetraoxocane

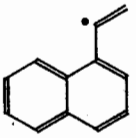
Thiophene

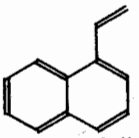

Toluene

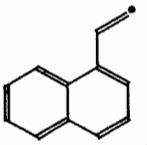


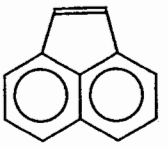
Trioxane

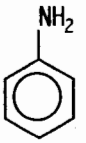

Triphenylene


β-Vinyl, 1-Naphthalene radical $C_{10}H_7C$•=Ch_2

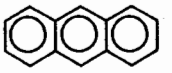

Vinyl Naphthalene $C_{10}H_7C_2H_3$

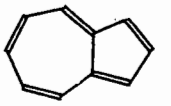

α-Vinyl, 1-Naphthalene radical $C_{10}H_7C$=CH • trans


Acenaphthylene

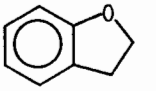


Aniline


Anthracene

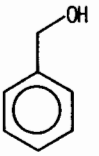

Azulene

Benzene

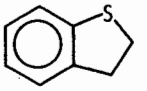


Benzofuran

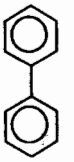
Benzonitrile

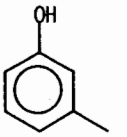


Benzyl alcohol

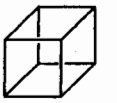


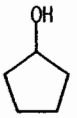
Benzo[b]thiophene


Biphenyl



Cresol


Cubane

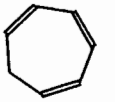


Cyclopentanol

Cyclopentene

1,3-Cyclopentadiene

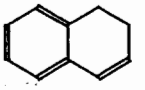
1,3-Cyclopentadiene, 5,5-dimetil-

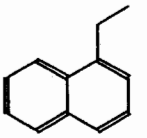

1,3,5-Cycloheptatriene

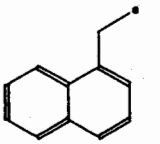
Cyclopropane carbonit rile

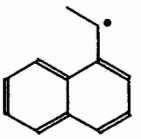
1,4-Dioxane

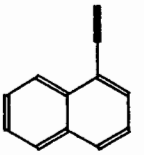
Dioxin

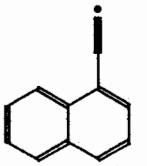

1,2 Dihydro-Naphthalene $C_{10}H_{10}$

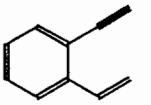

Ethyl 1-Naphthalene $C_{10}H_7C_2H_5$

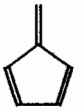

α-Ethyl 1-Naphthalene radical $C_{10}H_7CH_2CH_2\bullet$


β-Ethyl 1-Naphthalene radical $C_{10}H_7CH\bullet CH_3$

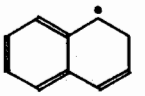

Ethynyl Naphthalene $C_{10}H_7C_2H$

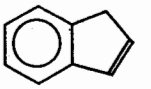

Ethynyl Naphthalene radical $C_{10}H_7C_2\bullet$

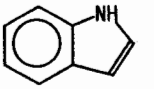

4-Ethynyl-Phenyl-1-Vinyl radical $HC{\equiv}C{-}C_6H_4{-}CH{=}CH\bullet$


Fulvene

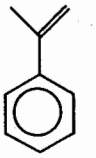
Furan

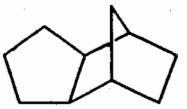

β-Hydro Naphthalene radical $C_{10}H_9\bullet$

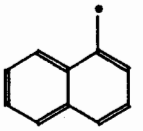

Indene

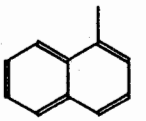


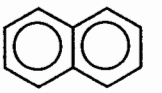
Indole


α-Methylstyrene


4,7-Methano-1H-iden octahydro-


Methyl Naphthyl radical $C_{10}H_7CH_2\bullet$


Methyl Naphthalene $C_{10}H_7CH_3$


Naphthalene