

!VERSION: GENERATED FOR M. SARATHY FROM BUGLER PENTANES C5 (16\_17) AND  
ARAMCO 2.0 (FROM GALWAY WEBSITE)  
!AUTHORS: C3

THERMO

300.000 1000.000 5000.000  
AR G 5/97AR 1 0 0 0G 200.000 6000.00 1000.00  
1  
2.50000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00  
0.00000000E+00 2  
-7.45375000E+02 4.37967491E+00 2.50000000E+00 0.00000000E+00  
0.00000000E+00 3  
0.00000000E+00 0.00000000E+00-7.45375000E+02 4.37967491E+00  
0.00000000E+00 4  
N2 G 8/02N 2 0 0 0G 200.000 6000.00 1000.00  
1  
2.95257637E+00 1.39690040E-03-4.92631603E-07 7.86010195E-11-4.60755204E-  
15 2  
-9.23948688E+02 5.87188762E+00 3.53100528E+00-1.23660988E-04-5.02999433E-  
07 3  
2.43530612E-09-1.40881235E-12-1.04697628E+03 2.96747038E+00  
0.00000000E+00 4  
HE G 5/97HE 1 0 0 0G 200.000 6000.00 1000.00  
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  
H2 TPIS78H 2 0 0 0G 200.000 6000.00 1000.00  
1  
2.93286575E+00 8.26608026E-04-1.46402364E-07 1.54100414E-11-6.88804800E-  
16 2  
-8.13065581E+02-1.02432865E+00 2.34433112E+00 7.98052075E-03-1.94781510E-  
05 3  
2.01572094E-08-7.37611761E-12-9.17935173E+02 6.83010238E-01  
0.00000000E+00 4  
H L 6/94H 1 0 0 0G 200.000 6000.00 1000.00  
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  
O2 RUS 89O 2 0 0 0G 200.000 6000.00 1000.00  
1  
3.66096065E+00 6.56365811E-04-1.41149627E-07 2.05797935E-11-1.29913436E-  
15 2  
-1.21597718E+03 3.41536279E+00 3.78245636E+00-2.99673416E-03 9.84730201E-  
06 3  
-9.68129509E-09 3.24372837E-12-1.06394356E+03 3.65767573E+00  
0.00000000E+00 4  
O L 1/90O 1 0 0 0G 200.000 6000.00 1000.00  
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  
 H2O L 5/89H 2 0 1 0 0G 200.000 6000.00 1000.00  
 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  
 OH IU3/03O 1 H 1 0 0G 200.000 6000.00 1000.00  
 1  
 2.83853033E+00 1.10741289E-03-2.94000209E-07 4.20698729E-11-2.42289890E-  
 15 2  
 3.69780808E+03 5.84494652E+00 3.99198424E+00-2.40106655E-03 4.61664033E-  
 06 3  
 -3.87916306E-09 1.36319502E-12 3.36889836E+03-1.03998477E-01  
 4.48613328E+03 4  
 OHV 1212860 1H 1 G 0300.00 5000.00 1000.00  
 1  
 0.02882730E+02 0.10139743E-02-0.02276877E-05 0.02174683E-09-0.05126305E-  
 14 2  
 5.02650000E+04 0.05595712E+02 0.03637266E+02 0.01850910E-02-0.16761646E-  
 05 3  
 0.02387202E-07-0.08431442E-11 5.00213000E+04 0.13588605E+01  
 4  
 H2O2 T 8/03H 2O 2 0 0G 200.000 6000.00 1000.00  
 1  
 4.57977305E+00 4.05326003E-03-1.29844730E-06 1.98211400E-10-1.13968792E-  
 14 2  
 -1.80071775E+04 6.64970694E-01 4.31515149E+00-8.47390622E-04 1.76404323E-  
 05 3  
 -2.26762944E-08 9.08950158E-12-1.77067437E+04 3.27373319E+00-  
 1.63425145E+04 4  
 HO2 T 1/09H 1O 2 0 0G 200.000 5000.00 1000.00  
 1  
 4.17228741E+00 1.88117627E-03-3.46277286E-07 1.94657549E-11 1.76256905E-  
 16 2  
 3.10206839E+01 2.95767672E+00 4.30179807E+00-4.74912097E-03 2.11582905E-  
 05 3  
 -2.42763914E-08 9.29225225E-12 2.64018485E+02 3.71666220E+00  
 1.47886045E+03 4  
 CO RUS 79C 1O 1 0 0G 200.000 6000.00 1000.00  
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 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  
 CO2 L 7/88C 1O 2 0 0G 200.000 6000.00 1000.00  
 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  
 HOCC T05/06H 1 C 1 O 2 0 G 200.000 6000.00  
 1000.00 1  
 5.39206152E+00 4.11221455E-03-1.48194900E-06 2.39875460E-10-1.43903104E-  
 14 2  
 -2.38606717E+04-2.23529091E+00 2.92207919E+00 7.62453859E-03 3.29884437E-  
 06 3  
 -1.07135205E-08 5.11587057E-12-2.30281524E+04 1.12925886E+01-  
 2.18076591E+04 4  
 CH4 G 8/99C 1 H 4 0 0 G 200.000 6000.00 1000.00  
 1  
 1.65326226E+00 1.00263099E-02-3.31661238E-06 5.36483138E-10-3.14696758E-  
 14 2  
 -1.00095936E+04 9.90506283E+00 5.14911468E+00-1.36622009E-02 4.91453921E-  
 05 3  
 -4.84246767E-08 1.66603441E-11-1.02465983E+04-4.63848842E+00-  
 8.97226656E+03 4  
 CH3 IU0702C 1 H 3 0 0 G 200.000 6000.00 1000.00  
 1  
 0.29781206E+01 0.57978520E-02-0.19755800E-05 0.30729790E-09-0.17917416E-  
 13 2  
 0.16509513E+05 0.47224799E+01 0.36571797E+01 0.21265979E-02 0.54583883E-  
 05 3  
 -0.66181003E-08 0.24657074E-11 0.16422716E+05 0.16735354E+01  
 0.17643935E+05 4  
 CH2 IU3/03C 1 H 2 0 0 G 200.000 6000.00 1000.00  
 1  
 3.14631886E+00 3.03671259E-03-9.96474439E-07 1.50483580E-10-8.57335515E-  
 15 2  
 4.60412605E+04 4.72341711E+00 3.71757846E+00 1.27391260E-03 2.17347251E-  
 06 3  
 -3.48858500E-09 1.65208866E-12 4.58723866E+04 1.75297945E+00  
 4.70504920E+04 4  
 CH2(S) IU6/03C 1 H 2 0 0 G 200.000 6000.00 1000.00  
 1  
 3.13501686E+00 2.89593926E-03-8.16668090E-07 1.13572697E-10-6.36262835E-  
 15 2  
 5.05040504E+04 4.06030621E+00 4.19331325E+00-2.33105184E-03 8.15676451E-  
 06 3  
 -6.62985981E-09 1.93233199E-12 5.03662246E+04-7.46734310E-01  
 5.15727280E+04 4  
 C L 7/88C 1 0 0 0G 200.000 6000.00 1000.00  
 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  
 CH IU3/03C 1 H 1 0 0 G 200.000 6000.00 1000.00  
 1  
 0.25209369E+01 0.17653639E-02-0.46147660E-06 0.59289675E-10-0.33474501E-  
 14 2  
 0.70946769E+05 0.74051829E+01 0.34897583E+01 0.32432160E-03-0.16899751E-  
 05 3  
 0.31628420E-08-0.14061803E-11 0.70612646E+05 0.20842841E+01  
 0.71658188E+05 4

CHV 073003C 1H 1 G 0300.00 5000.00 1000.00  
 1  
 0.02196223E+02 0.02340381E-01-0.07058201E-05 0.09007582E-09-0.03855040E-  
 13 2  
 0.10419559E+06 0.09178373E+02 0.03200202E+02 0.02072875E-01-0.05134431E-  
 04 3  
 0.05733890E-07-0.01955533E-10 0.10393714E+06 0.03331587E+02  
 4  
 CH302H A 7/05C 1 H 4 O 2 0 G 200.000 6000.00 1000.00  
 1  
 7.76538058E+00 8.61499712E-03-2.98006935E-06 4.68638071E-10-2.75339255E-  
 14 2  
 -1.82979984E+04-1.43992663E+01 2.90540897E+00 1.74994735E-02 5.28243630E-  
 06 3  
 -2.52827275E-08 1.34368212E-11-1.68894632E+04 1.13741987E+01-  
 1.52423685E+04 4  
 CH302 H 3C 1O 2 0G 300.000 5000.000  
 1374.000 11  
 6.47970487E+00 7.44401080E-03-2.52348555E-06 3.89577296E-10-2.25182399E-  
 14 2  
 -1.56285441E+03-8.19477074E+00 1.97339205E+00 1.53542340E-02-6.37314891E-  
 06 3  
 3.19930565E-10 2.82193915E-13 2.54278835E+02 1.69194215E+01  
 4  
 CH202H 9/ 1/12 C 1H 3O 2 0G 300.000 5000.000  
 1410.000 21  
 9.24697852E+00 4.60845541E-03-1.53501472E-06 2.34434830E-10-1.34573106E-  
 14 2  
 4.11529953E+03-2.11503248E+01 2.88976454E+00 2.09465776E-02-1.75190772E-  
 05 3  
 7.27819787E-09-1.18912344E-12 6.12390620E+03 1.23802076E+01  
 4  
 CH30H T06/02C 1H 4 O 1 0 G 200.000 6000.00 1000.00  
 1  
 3.52726795E+00 1.03178783E-02-3.62892944E-06 5.77448016E-10-3.42182632E-  
 14 2  
 -2.60028834E+04 5.16758693E+00 5.65851051E+00-1.62983419E-02 6.91938156E-  
 05 3  
 -7.58372926E-08 2.80427550E-11-2.56119736E+04-8.97330508E-01-  
 2.41746056E+04 4  
 CH30 IU1/03C 1 H 3 O 1 0 G 200.000 6000.00 1000.00  
 1  
 4.75779238E+00 7.44142474E-03-2.69705176E-06 4.38090504E-10-2.63537098E-  
 14 2  
 3.78111940E+02-1.96680028E+00 3.71180502E+00-2.80463306E-03 3.76550971E-  
 05 3  
 -4.73072089E-08 1.86588420E-11 1.29569760E+03 6.57240864E+00  
 2.52571660E+03 4  
 CH20H IU2/03C 1 H 3 O 1 0 G 200.000 6000.00  
 1000.00 1  
 5.09314370E+00 5.94761260E-03-2.06497460E-06 3.23008173E-10-1.88125902E-  
 14 2  
 -4.03409640E+03-1.84691493E+00 4.47834367E+00-1.35070310E-03 2.78484980E-  
 05 3  
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 2.04462770E+03 4  
 CH2O T 5/11H 2C 1O 1 0G 200.000 6000.00 1000.00  
 1

3.16952665E+00 6.19320560E-03-2.25056366E-06 3.65975660E-10-2.20149458E-  
 14 2  
 -1.45486831E+04 6.04207898E+00 4.79372312E+00-9.90833322E-03 3.73219990E-  
 05 3  
 -3.79285237E-08 1.31772641E-11-1.43791953E+04 6.02798058E-01-  
 1.31293365E+04 4  
 HCO T 5/03C 1 H 1 O 1 0 G 200.000 6000.00 1000.00  
 1  
 3.92001542E+00 2.52279324E-03-6.71004164E-07 1.05615948E-10-7.43798261E-  
 15 2  
 3.65342928E+03 3.58077056E+00 4.23754610E+00-3.32075257E-03 1.40030264E-  
 05 3  
 -1.34239995E-08 4.37416208E-12 3.87241185E+03 3.30834869E+00  
 5.08749163E+03 4  
 HCOH MAR94 C 1H 20 1 0G 300. 5000. 1398.  
 1  
 9.18749272E+00 1.52011152E-03-6.27603516E-07 1.09727989E-10-6.89655128E-  
 15 2  
 7.81364593E+03-2.73434214E+01-2.82157421E+00 3.57331702E-02-3.80861580E-  
 05 3  
 1.86205951E-08-3.45957838E-12 1.12956672E+04 3.48487757E+01  
 4  
 HO2CHO 6/26/95 THERMC 1H 20 3 0G 300.000 5000.000 1378.00  
 21  
 9.87503878E+00 4.64663708E-03-1.67230522E-06 2.68624413E-10-1.59595232E-  
 14 2  
 -3.80502496E+04-2.24939155E+01 2.42464726E+00 2.19706380E-02-1.68705546E-  
 05 3  
 6.25612194E-09-9.11645843E-13-3.54828006E+04 1.75027796E+01  
 4  
 HOCH2O2H 9/ 1/12 C 1H 40 3 0G 300.000 5000.000  
 1398.000 21  
 1.24531886E+01 7.18221110E-03-2.47029548E-06 3.85611737E-10-2.24774193E-  
 14 2  
 -4.24862928E+04-3.58745197E+01 5.35189713E-01 3.73266553E-02-3.15299511E-  
 05 3  
 1.30352583E-08-2.11473264E-12-3.86609415E+04 2.71776082E+01  
 4  
 HOCH2O2 9/ 1/12 C 1H 30 3 0G 300.000 5000.000  
 1377.000 21  
 1.16406115E+01 5.72826040E-03-2.05362036E-06 3.29070695E-10-1.95188360E-  
 14 2  
 -2.53505769E+04-3.07332064E+01 2.82068616E+00 2.47857094E-02-1.66186399E-  
 05 3  
 4.79633095E-09-4.28087766E-13-2.22077036E+04 1.70599803E+01  
 4  
 OCH2O2H 7/21/14 THERMC 1H 30 3 0G 300.000 5000.000  
 1418.000 31  
 1.29622491E+01 4.21948855E-03-1.54275194E-06 2.50413077E-10-1.49855537E-  
 14 2  
 -1.81326406E+04-3.87016356E+01 4.46349361E-01 3.63049606E-02-3.26130978E-  
 05 3  
 1.37050551E-08-2.20872791E-12-1.41972598E+04 2.72960376E+01  
 4  
 HOCH2O 2/16/99 THERMC 1H 30 2 0G 300.000 5000.000  
 1452.000 11  
 6.39521515E+00 7.43673043E-03-2.50422354E-06 3.84879712E-10-2.21778689E-  
 14 2

-2.41108840E+04-6.63865583E+00 4.11183145E+00 7.53850697E-03 3.77337370E-06 3  
-5.38746005E-09 1.45615887E-12-2.28023001E+04 7.46807254E+00  
4  
O2CHO 6/26/95 THERMC 1H 10 3 0G 300.000 5000.000 1368.00  
11  
7.24075139E+00 4.63312951E-03-1.63693995E-06 2.59706693E-10-1.52964699E-14 2  
-1.87027618E+04-6.49547212E+00 3.96059309E+00 1.06002279E-02-5.25713351E-06 3  
1.01716726E-09-2.87487602E-14-1.73599383E+04 1.17807483E+01  
4  
HOCHO L 8/88H 2C 10 2 0G 200.000 6000.00 1000.00  
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  
OCHO ATCT/AC 1 O 2 H 1 0 G 200.000 6000.000 1000.00  
1  
4.14394211E+00 5.59738818E-03-1.99794019E-06 3.16179193E-10-1.85614483E-14 2  
-1.72459887E+04 5.07778617E+00 4.68825921E+00-4.14871834E-03 2.55066010E-05 3  
-2.84473900E-08 1.04422559E-11-1.69867041E+04 4.28426480E+00-  
1.55992356E+04 4  
C2H6 G 8/88C 2H 6 0 0G 200.000 6000.00 1000.00  
1  
4.04666411E+00 1.53538802E-02-5.47039485E-06 8.77826544E-10-5.23167531E-14 2  
-1.24473499E+04-9.68698313E-01 4.29142572E+00-5.50154901E-03 5.99438458E-05 3  
-7.08466469E-08 2.68685836E-11-1.15222056E+04 2.66678994E+00-  
1.00849652E+04 4  
C2H5 8/ 4/ 4 THERMC 2H 5 0 0G 300.000 5000.000  
1387.000 11  
5.88784390E+00 1.03076793E-02-3.46844396E-06 5.32499257E-10-3.06512651E-14 2  
1.15065499E+04-8.49651771E+00 1.32730217E+00 1.76656753E-02-6.14926558E-06 3  
-3.01143466E-10 4.38617775E-13 1.34284028E+04 1.71789216E+01  
4  
C2H5O2H 9/ 1/12 C 2H 60 2 0G 300.000 5000.000  
1390.000 31  
1.04823538E+01 1.34779879E-02-4.62179078E-06 7.18618519E-10-4.17307436E-14 2  
-2.46578171E+04-2.84294243E+01 1.83755328E+00 3.38053586E-02-2.37548140E-05 3  
9.31974865E-09-1.58003428E-12-2.15814086E+04 1.80977584E+01  
4  
C2H5O2 9/ 1/12 C 2H 50 2 0G 300.000 5000.000  
1389.000 21  
9.50282570E+00 1.20429839E-02-4.09491581E-06 6.33049241E-10-3.66133788E-14 2  
-7.37069391E+03-2.21717130E+01 3.90351912E+00 2.22599212E-02-1.01610079E-05 3

1.71709751E-09 1.88166738E-14-5.09654081E+03 8.98722750E+00  
 4  
 C2H4 8/12/15 C 2H 4 0 0G 300.000 5000.000  
 1392.000 01  
 5.07061289E+00 9.11140768E-03-3.10506692E-06 4.80733851E-10-2.78321396E-  
 14 2  
 3.66391217E+03-6.64501414E+00 4.81118223E-01 1.83778060E-02-9.99633565E-  
 06 3  
 2.73211039E-09-3.01837289E-13 5.44386648E+03 1.85867157E+01  
 4  
 C2H3 8/12/15 C 2H 3 0 0G 300.000 5000.000  
 1400.000 01  
 4.99675415E+00 6.55838271E-03-2.20921909E-06 3.39300272E-10-1.95316926E-  
 14 2  
 3.34604382E+04-3.01451097E+00 1.25545094E+00 1.57481597E-02-1.12218328E-  
 05 3  
 4.50915682E-09-7.74861577E-13 3.47435574E+04 1.69664043E+01  
 4  
 CHOCHO C 2H 2O 2 0G 300.000 5000.000  
 1386.000 11  
 9.75438561E+00 4.97645947E-03-1.74410483E-06 2.75586994E-10-1.61969892E-  
 14 2  
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 C2H2 G 1/91C 2 H 2 0 0 G 200.000 6000.00 1000.00  
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 C2H4O2H 9/ 1/12 C 2H 50 2 0G 300.000 5000.000  
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 C2H4O1-2 L 8/88C 2 H 4 O 1 0 G 200.000 6000.00 1000.00  
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 CH3CHO L 8/88C 2 H 4 O 1 0 G 200.000 6000.00 1000.00  
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 CH3CO IU2/03C 2 H 3 O 1 0 G 200.000 6000.00 1000.00  
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 HCCO T 4/09H 1 C 2 O 1 0 G 200.000 6000.00 1000.00  
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 HCCOH T12/09C 2 H 2 O 1 0 G 200.000 6000.00 1000.00  
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 CH3CO3H 6/26/95 THERMC 2H 40 3 0G 300.000 5000.000  
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 1404.000 31  
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HO2CH2OCHO 2/12/14 THERMC 2H 40 4 0G 300.000 5000.000  
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 4.37330508E+04 4  
 CH3OCO 5/ 8/ 3 THERMC 2H 30 2 0G 300.000 5000.000  
 1601.000 21  
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 CH2OCHO 4/15/ 8 THERMC 2H 30 2 0G 300.000 5000.000  
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 1390.000 21

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 7.55377821E+03-1.03686516E+01-8.97467137E-01 4.15744022E-02-4.94778349E-05 3  
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 1000.0 1  
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 1405.000 41  
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 1.11564001E+04 4

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 C3H6 8/12/15 C 3H 6 0 OG 298.000 6000.000  
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 C3H5-S 8/12/15 C 3H 5 0 OG 300.000 5000.000  
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 C3H5-T 8/12/15 C 3H 5 0 OG 300.000 5000.000  
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 2.95937491E+03-1.36041009E+01 2.83278674E+00-5.21028618E-03 9.29583210E-  
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 6.41047999E+03 4  
 C3H5O KPS12 C 3H 5O 1 OG 300.000 5000.000  
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 CH2CHOCH2 8/ 8/15 C 3H 5O 1 OG 300.000 5000.000  
 1384.000 21



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 C3H6OH1-2 9/ 1/12 C 3H 70 1 0G 300.000 5000.000  
 1395.000 31  
 1.00338281E+01 1.60227373E-02-5.41658448E-06 8.34191172E-10-4.81215988E-  
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 CH3CHCO 03/03/95 THERMC 3H 40 1 0G 300.000 5000.000 1400.00  
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 1392.000 31  
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 HOC3H6O2 9/ 1/12 C 3H 70 3 0G 300.000 5000.000  
 1407.000 41  
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 14 2

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 SC3H5OH 2/ 3/ 9 C 3H 6O 1 OG 300.000 5000.000  
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 C3H5OH T06/10C 3 H 6 O 1 O G 200.000 6000.00 1000.00  
 1  
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 CH2CCH2OH 9/ 8/95 THERMC 3H 5O 1 OG 300.000 5000.000 1372.00  
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 1.71775334E-09 1.42177454E-13 1.17935615E+04 1.52102335E+01  
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 0.60252400E+01 0.11336542E-01-0.40223391E-05 0.64376063E-09-0.38299635E-  
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 C3H4-A L 8/89C 3 H 4 0 0 G 200.000 6000.00 1000.00  
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 C3H3 T 7/11C 3 H 3 0 0 G 200.000 6000.00  
 1000.000 1  
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 CC3H4 T12/81C 3H 4 0 0G 300.000 5000.00 1000.00  
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 E+05 4  
 C3H2 T12/00C 3 H 2 0 0 G 200.000 6000.00 1000.00  
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 7.57571184E+04-9.72894405E+00 2.43417332E+00 1.73013063E-02-1.18294047E-  
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 H2CCC (S) 0C 3H 2 0 0G 200.000 5000.000 1500.00  
 0 1  
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 13 2  
 0.63661864E+05-0.10064283E+02 0.37229726E+01 0.92589854E-02-0.23006191E-  
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 C3H2 (S) 0C 3H 2 0 0G 200.000 5000.000 900.00  
 0 1  
 0.77642570E+01 0.47112774E-02-0.16170637E-05 0.25472406E-09-0.15038572E-  
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 0.66849672E+05-0.15098549E+02 0.52976482E+01 0.16987466E-01-0.24266517E-  
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 0.56514618E+05-0.12000607E+02 0.11295888E+01 0.17287401E-01-0.11366823E-  
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 PC3H4OH-2 4/ 2/13 THERMC 3H 50 1 0G 300.000 5000.000  
 1403.000 21  
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 4.98486803E+03-2.98329329E+01 1.42757363E+00 3.64825569E-02-3.18007132E-  
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 SC3H4OH 3/28/13 C 3H 50 1 0G 300.000 5000.000  
 1407.000 21  
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C3H3O 2/17/14 CZHOUH 3C 30 1 G 298.150 2000.000 1000.00  
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13 2  
3.14931737E+04 5.03216224E+00 8.75023836E-01 3.51184068E-02-3.89901356E-  
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4  
C3H3O2H 1/31/13 C 3H 40 2 OG 300.000 5000.000  
1385.000 31  
1.38152174E+01 8.62174763E-03-3.06710006E-06 4.88874247E-10-2.88888385E-  
14 2  
6.29182941E+03-4.39151257E+01 1.09787313E+00 4.22717882E-02-3.83969355E-  
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1.77405069E-08-3.27674312E-12 1.03592314E+04 2.30651783E+01  
4  
C2HCHO 1/31/13 C 3H 20 1 OG 300.000 5000.000  
2012.000 11  
7.99952054E+00 7.07825497E-03-2.63086819E-06 4.33073185E-10-2.62003284E-  
14 2  
8.71863156E+03-1.57226237E+01 4.20776611E+00 1.34382727E-02-5.15442099E-  
06 3  
-2.24570818E-11 2.74111284E-13 1.02117375E+04 5.43871873E+00  
4  
C2H5CHO 8/12/15 C 3H 60 1 OG 300.000 5000.000  
1449.000 21  
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4  
C2H5CO A10/04C 3 H 5 O 1 0 G 200.000 6000.00 1000.00  
1  
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05 3  
-9.05514997E-08 3.46198215E-11-5.91616484E+03 2.23330599E+00-  
3.94851891E+03 4  
CH2CH2CHO C 3H 50 1 OG 300.000 5000.000  
1437.000 21  
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14 2  
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06 3  
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4  
C2H3CHO KPS12 C 3H 40 1 OG 300.000 5000.000  
1398.000 01  
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4  
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1395.000 01

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 CH3COCH3 8/12/15 C 3H 60 1 0G 300.000 5000.000  
 1394.000 21  
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 CH3COCH2 2/14/13 THERMC 3H 50 1 0G 300.000 5000.000  
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 C4H10 8/12/15 C 4H 10 0 0G 300.000 5000.000  
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 4  
 SC4H9 8/12/15 C 4H 9 0 0G 300.000 5000.000  
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 PC4H90 C 4H 90 1 0G 300.000 5000.000  
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C4H8OOH1-2O2 C 4H 90 4 0G 300.000 5000.000  
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1400.000 61  
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1400.000 61  
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 1400.000 61  
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 C4H7O1-2OOH-4 C 4H 8O 3 OG 300.000 5000.000  
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 2.03028185E+01 1.69331534E-02-5.71128715E-06 8.79005552E-10-5.07088176E-14 2  
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 C4H72-1OOH C 4H 8O 2 OG 300.000 5000.000  
 1381.000 41  
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 -1.74585465E+04-6.55209757E+01 1.29755275E+00 5.59252255E-02-4.08890003E-05 3  
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 9.36512355E-09-1.07548923E-12-4.08644270E+04 1.96071994E+01  
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 C4H71-3OOH C 4H 80 2 OG 300.000 5000.000  
 1392.000 41  
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 2.43179107E-08-4.09788488E-12-1.18018961E+04 3.50420113E+01  
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 C4H71-3,4OOH C 4H 90 4 OG 300.000 5000.000  
 1400.000 71  
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 -2.09468667E+04-7.79984909E+01 2.56890026E+00 6.71962184E-02-5.16999792E-05 3  
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 C4H72-3,4OOH C 4H 90 4 OG 300.000 5000.000  
 1395.000 71  
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HO2CH2CHO 9/ 8/14 C 2H 40 3 0G 300.000 5000.000  
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 2.31272366E-08-4.20787867E-12-2.90608844E+04 3.61860491E+01  
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 IC4H10 8/12/15 C 4H 10 0 0G 300.000 5000.000  
 1397.000 31  
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 4  
 TC4H9 8/12/15 C 4H 9 0 0G 300.000 5000.000  
 1380.000 31  
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 4  
 TC4H9O T08/04C 4 H 9 O 1 0 G 200.000 6000.00 1000.00  
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 7.82602559E+03 4  
 IC4H8O 9/ 1/12 C 4H 80 1 0G 300.000 5000.000  
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 IC3H7CHO 2/22/96 THERMC 4H 80 1 0G 300.000 5000.000  
 1391.000 31

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 8.93548675E-09-1.11327422E-12-9.07755468E+03 2.61991461E+01  
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 05 3  
 1.37243419E-08-2.40573132E-12-1.63939712E+04 1.38187714E+01  
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 05 3  
 1.28844447E-08-2.18165308E-12 2.85270691E+03 1.68774016E+01  
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 IC3H4CHO-A C 4H 50 1 OG 300.000 5000.000  
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 05 3  
 1.48295287E-08-2.43809290E-12 2.44732544E+03 2.08541848E+01  
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 SC4H7OH-I L 2/00C 4H 80 1 OG 300.000 5000.000  
 1395.000 31  
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 05 3  
 9.38191037E-09-1.41171285E-12-2.73561190E+04 1.35316306E+01  
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 05 3  
 1.44634925E-08-2.47536050E-12-6.98183185E+03 1.27623539E+01  
 4  
 CC4H8O 9/ 1/12 C 4H 80 1 OG 300.000 5000.000  
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 05 3  
 3.40602701E-08-6.15674656E-12-2.71582518E+04 3.80875851E+01  
 4  
 IC4H8OOH-IO2 9/ 1/12 C 4H 90 4 OG 300.000 5000.000  
 1367.000 61  
 2.24664901E+01 2.09351287E-02-7.44324128E-06 1.18589255E-09-7.00546897E-  
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 4  
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IC4KETII 7/19/ 0 THERMC 4H 80 3 OG 300.000 5000.000  
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 1402.000 71  
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 TQC4H7OHIQ-I C 4H 90 5 0G 300.000 5000.000  
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 COHQCYC (COC) C 4H 80 4 OG 300.000 5000.000  
 1319.000 51  
 2.44599226E+01 1.64187782E-02-5.74024372E-06 9.05710407E-10-5.31829152E-  
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 4.23694824E-09 8.42033474E-13-5.19694864E+04 1.88941416E+01  
 4  
 QCYC (CCOC) OH C 4H 80 4 OG 300.000 5000.000  
 1411.000 41  
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 2.79282034E-08-4.60981823E-12-5.12529252E+04 4.11897260E+01  
 4  
 HOCOCQ (CH3) 2 C 4H 80 4 OG 300.000 5000.000  
 1380.000 61  
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 1.99184629E-08-3.16007445E-12-7.30943302E+04 2.37255421E+01  
 4  
 IQC4H7OHTO2 C 4H 90 5 OG 300.000 5000.000  
 1389.000 71  
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1.99235553E-08-3.17456897E-12-4.34442789E+04 1.94648622E+01  
 4  
 IQC4H8OTQ-I C 4H 90 5 0G 300.000 5000.000  
 1386.000 71  
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 1391.000 81  
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 2.22754676E-08-3.66067450E-12-3.54133076E+04 2.23024492E+01  
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 CHOC(CH3)OHCH2Q C 4H 80 4 0G 300.000 5000.000  
 1383.000 61  
 2.24480753E+01 1.78753902E-02-6.26904597E-06 9.90084046E-10-5.81417382E-  
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 4  
 CO(CH2OOH)2 C 3H 60 5 0G 300.000 5000.000  
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 CH3COCHO C 3H 40 2 0G 300.000 5000.000  
 1381.000 21  
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 IC3H5OCH2 6/ 2/14 CZHOUH 7C 40 1 G 298.150 2000.000 1000.00  
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 IC4H7OOCH3 C 5H 100 2 0G 300.000 5000.000  
 1386.000 51  
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IC4H700IC4H7 C 8H 140 2 0G 300.000 5000.000  
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 C4H8-1 C 4H 8 0 0G 300.000 5000.000  
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 C4H71-1 C 4H 7 0 0G 300.000 5000.000  
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 C4H71-2 C 4H 7 0 0G 300.000 5000.000  
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 C4H71-3 1/13/16 C 4H 7 0 0G 300.000 5000.000  
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 C4H72-2 8/12/15 C 4H 7 0 0G 300.000 5000.000  
 1378.000 21



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 C4H71-O 4/ 3/ 0 THERMC 4H 70 1 OG 300.000 5000.000  
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 PC4H8OH-2 C 4H 90 1 OG 300.000 5000.000  
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 SC4H8OH-3 C 4H 90 1 OG 300.000 5000.000  
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 C4H71-3OH C 4H 80 1 OG 300.000 5000.000  
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 C4H71-4OH C 4H 80 1 OG 300.000 5000.000  
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 C4H72-1OH C 4H 80 1 0G 300.000 5000.000  
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 NC4KET12OH C 4H 80 2 0G 300.000 5000.000  
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 05 3

1.18022134E-08-1.57485744E-12-4.67781081E+04 2.89999061E+01  
 4  
 SQC4H7OHS-4 C 4H 90 3 OG 300.000 5000.000  
 1414.000 61  
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 SQC4H8OS C 4H 90 3 OG 300.000 5000.000  
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 NC4KET23OH 7/27/15 C 4H 80 2 OG 300.000 5000.000  
 1386.000 41  
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 7.25755846E-09-6.68682869E-13-5.04946247E+04 2.37800424E+01  
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 1417.000 51  
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 4  
 CCY(COCC)OH C 4H 80 2 OG 300.000 5000.000  
 1328.000 21  
 1.03816782E+01 2.53052690E-02-1.00511826E-05 1.68204740E-09-9.58092966E-14 2  
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 C4H7O2-1 9/ 8/14 C 4H 70 1 OG 300.000 5000.000  
 1684.000 21  
 1.12685690E+01 2.01724820E-02-7.41925667E-06 1.21275519E-09-7.30115348E-14 2  
 2.13876442E+03-3.15208064E+01 5.16434924E+00 2.53427725E-02-1.39669041E-06 3  
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 C4H6-1 L10/93C 4.H 6. 0. 0.G 200.000 6000.000 1000.  
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 1.98688798E+04 4

AC3H5OCH2 9/ 8/14 C 4H 70 1 0G 300.000 5000.000  
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 1388.000 41  
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C4H64,2-1OH C 4H 70 1 0G 300.000 5000.000  
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 5.65501810E-10 5.94838384E-13-3.08574102E+03 1.81061546E+01  
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 1401.000 21  
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 C4H5OH-13 9/24/15 C 4H 60 1 0G 300.000 5000.000  
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 SQC4H7OHP-4 C 4H 90 3 0G 300.000 5000.000  
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 2.05238910E-08-3.32050656E-12-2.29059890E+04 2.78546218E+01  
 4  
 CY(CCCO)COH C 4H 80 2 0G 300.000 5000.000  
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 NC4KET21OH C 4H 80 2 0G 300.000 5000.000  
 1507.000 41



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 HOCH2CHO 9/24/15 C 2H 40 2 0G 300.000 5000.000  
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 4  
 C4H71-4OOH C 4H 80 2 0G 300.000 5000.000  
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 1.20405755E-08-1.71650639E-12-1.17754576E+04 2.46384545E+01  
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 C4H71-4O2 9/25/15 C 4H 70 2 0G 300.000 5000.000  
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 4  
 HOCH2COCH2 C 3H 50 2 0G 300.000 5000.000  
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 4  
 HOCHCHO 9/25/15 C 2H 30 2 0G 300.000 5000.000  
 1680.000 21  
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 4  
 PC3H4OH-3 9/25/15 C 3H 50 1 0G 300.000 5000.000  
 1378.000 11  
 1.15297558E+01 1.14381097E-02-4.04415495E-06 6.41949269E-10-3.78242456E-14 2  
 -3.45486444E+03-3.65385497E+01 4.06368169E-01 3.70231405E-02-2.72202689E-05 3  
 1.05783475E-08-1.73632514E-12 5.27160824E+02 2.34781848E+01  
 4  
 PC3H4OH-1 9/25/15 C 3H 50 1 0G 300.000 5000.000  
 1403.000 21  
 1.09468986E+01 1.04014540E-02-3.44082448E-06 5.22105632E-10-2.98049266E-14 2  
 4.11530600E+03-3.11161699E+01 2.07150195E+00 3.50016810E-02-3.01922013E-05 3  
 1.38467853E-08-2.55380109E-12 6.81914209E+03 1.51916605E+01  
 4  
 CH3COCHOH 9/25/15 C 3H 50 2 0G 300.000 5000.000  
 1378.000 31  
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 -2.97609476E+04-3.85682589E+01 2.11183979E+00 3.32521318E-02-1.96834015E-05 3  
 5.40736760E-09-5.32450556E-13-2.58545486E+04 1.77643465E+01  
 4  
 SC2H2OH 9/25/15 C 2H 30 1 0G 300.000 5000.000  
 1410.000 11

7.99235139E+00 5.83109353E-03-1.89242965E-06 2.83129118E-10-1.59933287E-  
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 PC4H8OH-1 C 4H 90 1 OG 300.000 5000.000  
 1392.000 41  
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 PC4H8OH-3 C 4H 90 1 OG 300.000 5000.000  
 1398.000 41  
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 4  
 C4H7O1-4 9/ 8/14 C 4H 70 1 OG 300.000 5000.000  
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 2.64537530E-09 2.43666218E-13 6.16385921E+03 1.73174889E+01  
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 PC4H8OH-4 C 4H 90 1 OG 300.000 5000.000  
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 SC4H8OH-2 C 4H 90 1 OG 300.000 5000.000  
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 1.31285142E+01 6.17948608E-03-1.93387986E-06 2.81892606E-10-1.56244314E-  
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 C4H72-202 9/29/15 C 4H 70 2 OG 300.000 5000.000  
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 C4H71-102 9/29/15 C 4H 70 2 0G 300.000 5000.000  
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 1.13406677E-08-1.57078109E-12 4.04143594E+03 2.06106646E+01  
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 C4H71-202 9/29/15 C 4H 70 2 0G 300.000 5000.000  
 1394.000 31  
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 1.51726193E-08-2.42611664E-12 1.68854104E+03 2.23230947E+01  
 4  
 C3H6OH1-1 10/ 2/15 C 3H 70 1 0G 300.000 5000.000  
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 6.62398992E-09-7.32206246E-13-1.09273174E+04 2.24919343E+01  
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 PC4H8OH-202 C 4H 90 3 0G 300.000 5000.000  
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 SC4H8OH-102 C 4H 90 3 0G 300.000 5000.000  
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 9.96133753E+03-2.97310638E+01 1.01356056E+00 3.35722771E-02-1.96279376E-05 3  
 5.74803850E-09-6.75029065E-13 1.33956759E+04 1.99957382E+01  
 4  
 C4H612 A 8/83C 4H 6 0 0G 300.000 5000.000  
 1374.000 11  
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 5.02139421E-09-3.67977164E-13 1.81439079E+04 2.02191143E+01  
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 C4H6-2 A 8/83C 4H 6 0 0G 300.000 5000.000  
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 1.24831314E+04-2.87129792E+01 1.97152408E+00 2.76790997E-02-1.13396645E-05 3  
 1.02970745E-09 2.75290944E-13 1.57283766E+04 1.42147356E+01  
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 C4H5-I H6W/94C 4H 5 0 0G 300.000 3000.00 1000.00  
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 0.10229092E+02 0.94850138E-02-0.90406445E-07-0.12596100E-08 0.24781468E-12 2  
 0.34642812E+05-0.28564529E+02-0.19932900E-01 0.38005672E-01-0.27559450E-04 3  
 0.77835551E-08 0.40209383E-12 0.37496223E+05 0.24394241E+02  
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 C4H5-N H6W/94C 4H 5 0 0G 300.000 3000.00 1000.00  
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 0.38840301E+05-0.26001846E+02 0.16305321E+00 0.39830137E-01-0.34000128E-04 3  
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 C4H5-2 H6W/94C 4H 5 0 0G 300.000 5000.000  
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 3.25861413E+04-2.88794317E+01 2.31011292E+00 2.83747046E-02-1.63836755E-05 3  
 4.46251967E-09-4.30510879E-13 3.55842945E+04 1.49105965E+01  
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 C4H4 H6W/94C 4H 4 0 0G 300.000 3000.00 1000.00  
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 0.31195992E+05-0.97952118E+01-0.19152479E+01 0.52750878E-01-0.71655944E-04 3  
 0.55072423E-07-0.17286228E-10 0.32978504E+05 0.31419983E+02  
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13 2  
0.56600574E+05-0.19802597E+02 0.20830412E+01 0.40834274E-01-0.62159685E-  
04 3  
0.51679358E-07-0.17029184E-10 0.58005129E+05 0.13617462E+02  
4  
C4H3-N H6W/94C 4H 3 0 OG 300.000 3000.00 1000.00  
1  
0.54328279E+01 0.16860981E-01-0.94313109E-05 0.25703895E-08-0.27456309E-  
12 2  
0.61600680E+05-0.15673981E+01-0.31684113E+00 0.46912100E-01-0.68093810E-  
04 3  
0.53179921E-07-0.16523005E-10 0.62476199E+05 0.24622559E+02  
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C4H2 D11/99C 4H 2 0 OG 300.000 3000.000 1000.  
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0.91576328E+01 0.55430518E-02-0.13591604E-05 0.18780075E-10 0.23189536E-  
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0.52588039E+05-0.23711460E+02 0.10543978E+01 0.41626960E-01-0.65871784E-  
04 3  
0.53257075E-07-0.16683162E-10 0.54185211E+05 0.14866591E+02  
4  
C4H6O25 T 3/97C 4H 60 1 OG 200.000 5000.000 1000.0  
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8.60658242E+00 2.08310051E-02-8.42229481E-06 1.56717640E-09-1.09391202E-  
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05 3  
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1.30831522E+04 4  
C2H3CHOCH2 C 4H 60 1 OG 300.000 5000.000  
1431.000 11  
1.26762790E+01 1.40819509E-02-4.63473868E-06 7.01090838E-10-3.99438277E-  
14 2  
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05 3  
2.15818682E-08-3.69199072E-12 8.58852628E+02 4.28475443E+01  
4  
C4H4O T03/97C 4H 40 1 OG 200.000 6000.0 1000.0  
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9.38935003E+00 1.40291241E-02-5.07755110E-06 8.24137332E-10-4.95319963E-  
14 2  
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05 3  
-9.71562904E-08 4.22733796E-11-5.36785445E+03 2.14945172E+01-  
4.17166616E+03 4  
C4H6O23 T 3/97C 4H 60 1 OG 200.000 5000.000 1000.0  
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1.30831522E+04 4  
CH2CHCHCHO C 4H 50 1 OG 300.000 5000.000  
1385.000 11



1.39299886E+01 1.13228814E-02-3.87393567E-06 6.02378620E-10-3.50120301E-  
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 1.31111496E-08-2.04732021E-12 2.14943141E+03 2.40835867E+01  
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 0.01026888E+03 0.04896164E-01-0.04885081E-05-0.02708566E-08 0.05107013E-  
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 0.02346903E+06-0.02815985E+03 0.04810971E+02 0.01313999E+00 0.09865073E-  
 05 3  
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 1679.000 31  
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 12 2  
 0.85188250E+05-0.92147827E+00 0.11790619E+01 0.55547360E-01-0.73076168E-  
 04 3  
 0.52076736E-07-0.15046964E-10 0.85647312E+05 0.19179199E+02  
 4  
 C6H2 P 1/93C 6H 2 0 0G 300.000 3000.00 1000.00  
 1  
 0.13226281E+02 0.73904302E-02-0.22715381E-05 0.25875217E-09-0.55356741E-  
 14 2  
 0.80565258E+05-0.41201176E+02-0.15932624E+01 0.80530145E-01-0.14800649E-  
 03 3  
 0.13300031E-06-0.45332313E-10 0.83273227E+05 0.27980873E+02  
 4

C6H6                    G 6/01C    6H    6    0    0G    200.000    6000.000  
1000.000            1  
1.10809576E+01 2.07176746E-02-7.52145991E-06 1.22320984E-09-7.36091279E-  
14            2  
4.30641035E+03-4.00413310E+01 5.04818632E-01 1.85020642E-02 7.38345881E-  
05            3  
-1.18135741E-07 5.07210429E-11 8.55247913E+03 2.16412893E+01  
9.96811598E+03            4  
FULVENE                    OC    6H    6    0    0G    200.000    5000.000 1000.00  
0 1  
0.11103525E+02 0.20600685E-01-0.75302224E-05 0.12388695E-08-0.75415976E-  
13            2  
0.20361843E+05-0.36665197E+02-0.71813191E+00 0.37934312E-01 0.11398837E-  
04            3  
-0.41333503E-07 0.18055927E-10 0.24223825E+05 0.27855714E+02  
4  
C6H5                    T04/02C    6H    5    0    0G    200.000    6000.000 1000.  
1  
1.08444762E+01 1.73212473E-02-6.29233249E-06 1.02369961E-09-6.16216828E-  
14            2  
3.55598475E+04-3.53735134E+01 2.10306633E-01 2.04745507E-02 5.89743006E-  
05            3  
-1.01534255E-07 4.47105660E-11 3.95468722E+04 2.52910455E+01  
4.08610970E+04            4  
C6H5OO            3/26/ 9 THERMC    6H    50    2    0G    300.000    5000.000  
1403.000            11  
1.67078262E+01 1.62326229E-02-5.47969630E-06 8.43510060E-10-4.86562431E-  
14            2  
8.14242915E+03-6.08346973E+01-2.99164672E+00 7.03857150E-02-6.34400574E-  
05            3  
2.91548920E-08-5.30706938E-12 1.41320240E+04 4.20142955E+01  
4  
C6H5OOH            3/26/ 9 THERMC    6H    60    2    0G    300.000    5000.000  
1404.000            21  
1.92317474E+01 1.63154699E-02-5.53448904E-06 8.55059974E-10-4.94583790E-  
14            2  
-1.01971012E+04-7.61674471E+01-4.03105975E+00 7.96101888E-02-7.21655013E-  
05            3  
3.27610696E-08-5.85584239E-12-3.10973017E+03 4.54324978E+01  
4  
C6H5OH                    L 4/84C    6H    60    1    0G    300.000    5000.000 1000.  
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  
C6H5O                    T05/02C    6H    50    1    0G    200.000    6000.000 1000.  
1  
1.37221720E+01 1.74688771E-02-6.35504520E-06 1.03492308E-09-6.23410504E-  
14            2  
2.87274751E+02-4.88181680E+01-4.66204455E-01 4.13443975E-02 1.32412991E-  
05            3  
-5.72872769E-08 2.89763707E-11 4.77858391E+03 2.76990274E+01  
6.49467016E+03            4  
C6H4OH            4/ 9/ 9 THERMC    6H    50    1    0G    300.000    5000.000  
1402.000            11



1.73187560E+01 1.36366984E-02-4.68316332E-06 7.29071204E-10-4.23805358E-  
14 2  
1.14990276E+04-6.89986593E+01-5.99875435E+00 8.59063379E-02-9.12525636E-  
05 3  
4.72275890E-08-9.35576749E-12 1.78621926E+04 4.99931427E+01  
4  
OC6H4OH 4/ 9/ 9 THERMC 6H 50 2 OG 300.000 5000.000  
1403.000 11  
2.22718210E+01 1.21038561E-02-4.18429526E-06 6.54475399E-10-3.81746504E-  
14 2  
-2.34827539E+04-9.61035467E+01-8.02205657E+00 1.09403210E-01-1.23489276E-  
04 3  
6.56286805E-08-1.31527870E-11-1.55949156E+04 5.72175202E+01  
4  
O-C6H4O2 AK0405C 6H 40 2 OG 270.000 3000.000 1370.00  
1  
1.23614349E+01 2.40491397E-02-1.16529057E-05 2.71332785E-09-2.47593219E-  
13 2  
-1.67079717E+04-4.00310857E+01-2.36179712E+00 6.86058343E-02-6.39129516E-  
05 3  
3.06903009E-08-5.97357785E-12-1.26704431E+04 3.53724482E+01  
4  
P-C6H4O2 AK0405C 6H 40 2 OG 270.000 3000.000 1370.00  
1  
1.23423732E+01 2.40612690E-02-1.16565184E-05 2.71393504E-09-2.47643065E-  
13 2  
-2.06185312E+04-4.08244024E+01-2.43170113E+00 6.87937608E-02-6.41382837E-  
05 3  
3.08126855E-08-5.99832072E-12-1.65696994E+04 3.48309430E+01  
4  
O-OC6H5OJ WKM C 60 2H 5 OG 300.000 5000.000  
1400.000 01  
1.84625733E+01 1.57607263E-02-5.44671499E-06 8.51765760E-10-4.96759541E-  
14 2  
-1.72770226E+02-7.28742484E+01-2.65459198E+00 7.17179095E-02-6.31552372E-  
05 3  
2.81132946E-08-4.97463333E-12 6.45283150E+03 3.81123139E+01  
4  
P-OC6H5OJ WKM C 60 2H 5 OG 300.000 5000.000  
1400.000 01  
1.82799770E+01 1.59280974E-02-5.50765220E-06 8.61649836E-10-5.02677539E-  
14 2  
-6.25907994E+01-7.25809444E+01-3.29683290E+00 7.27365977E-02-6.36158220E-  
05 3  
2.80683553E-08-4.92279426E-12 6.73402222E+03 4.09349895E+01  
4  
P-C6H3O2 AK0505C 6H 30 2 OG 270.000 3000.000 1290.00  
1  
1.22963699E+01 2.15055142E-02-1.07516136E-05 2.57528163E-09-2.41023652E-  
13 2  
1.15428998E+04-3.72584002E+01-1.57852347E+00 6.55376473E-02-6.50308721E-  
05 3  
3.32026554E-08-6.86665555E-12 1.51750093E+04 3.31518638E+01  
4  
C5H6 T 1/90C 5H 6 0 OG 200.000 6000.000 1000.  
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  
 C5H5 TAK0505C 5H 5 0 0G 298.150 3500.000 969.35  
 1  
 1.33675715E+00 3.24793912E-02-1.67587774E-05 4.03514137E-09-3.70739036E-  
 13 2  
 3.00730524E+04 1.60315806E+01-3.97555452E+00 7.41370991E-02-1.11803345E-  
 04 3  
 9.04628776E-08-2.80999747E-11 3.01769405E+04 3.67153636E+01  
 4  
 C5H6-L 2/ 5/ 9 THERMC 5H 6 0 0G 300.000 5000.000  
 1372.000 21  
 1.29600892E+01 1.48953758E-02-5.23622902E-06 8.27916389E-10-4.86464523E-  
 14 2  
 2.38180800E+04-4.25312093E+01 3.58448213E+00 3.24459626E-02-1.70150991E-  
 05 3  
 4.22715914E-09-4.18452556E-13 2.76514681E+04 9.60644208E+00  
 4  
 C#CCVCCJ GLAR C 5H 5 0 0G 300.000 5000.000  
 1396.000 11  
 1.41230912E+01 1.14233190E-02-3.95851276E-06 6.20128961E-10-3.62097887E-  
 14 2  
 4.25158384E+04-5.02942871E+01-6.16143558E-01 5.06466579E-02-4.48561743E-  
 05 3  
 2.02459419E-08-3.64542145E-12 4.71532377E+04 2.71623299E+01  
 4  
 C5H7 1/22/ 9 WKM C 5H 7 0 0G 300.000 5000.000  
 1377.000 31  
 1.36630213E+01 1.68061358E-02-5.98746539E-06 9.55341072E-10-5.64951981E-  
 14 2  
 1.27238941E+04-5.46331286E+01-6.75118368E+00 6.06461693E-02-4.01260152E-  
 05 3  
 1.22051562E-08-1.33459844E-12 2.01365277E+04 5.62694938E+01  
 4  
 CVCCJCVC 3/1/95 Z&B C 5H 7 0 0G 300.000 5000.000  
 1388.000 21  
 1.40879309E+01 1.62398907E-02-5.64768950E-06 8.86857524E-10-5.18698993E-  
 14 2  
 1.76798698E+04-5.13735038E+01-2.94595603E+00 5.68783623E-02-4.31336497E-  
 05 3  
 1.68169537E-08-2.67926433E-12 2.35156925E+04 3.98188778E+01  
 4  
 CVCCVCCJ Z&B C 5H 7 0 0G 300.000 5000.000  
 1386.000 21  
 1.47302883E+01 1.59030900E-02-5.57729508E-06 8.80604825E-10-5.16963733E-  
 14 2  
 1.74050791E+04-5.42670706E+01-1.60087476E+00 5.38764703E-02-3.96302225E-  
 05 3  
 1.49599474E-08-2.31995284E-12 2.31199746E+04 3.35492960E+01  
 4  
 CVCCJCVCOH 10/6/95 Z&B C 5H 70 1 0G 300.000 5000.000  
 1397.000 31  
 1.67465815E+01 1.58357240E-02-5.44954706E-06 8.49881387E-10-4.94743246E-  
 14 2  
 -4.30972870E+03-6.19378748E+01-2.91175436E+00 6.69362484E-02-5.71603047E-  
 05 3

2.48753749E-08-4.33243894E-12 1.96441523E+03 4.17454344E+01  
 4  
 HOCVCCVO 1/26/ 9 WKM C 3H 40 2 OG 300.000 5000.000  
 1413.000 21  
 1.66505478E+01 6.11745137E-03-2.09080785E-06 3.24985683E-10-1.88875073E-  
 14 2  
 -3.82179939E+04-6.36794754E+01-2.01837189E+00 6.26539783E-02-6.73359280E-  
 05 3  
 3.39430425E-08-6.48917648E-12-3.31367523E+04 3.18162860E+01  
 4  
 CVCCVCCOH 1/23/ 9 WKM C 5H 80 1 OG 300.000 5000.000  
 1396.000 31  
 1.63079670E+01 1.79957763E-02-6.03115896E-06 9.23992259E-10-5.31254053E-  
 14 2  
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 05 3  
 2.00308244E-08-3.38987282E-12-1.03301302E+04 3.07961436E+01  
 4  
 OC5H7O 1/22/ 9 WKM C 5H 70 2 OG 300.000 5000.000  
 1375.000 31  
 1.65416953E+01 1.86677673E-02-6.44836048E-06 1.00787611E-09-5.87521858E-  
 14 2  
 -2.82017168E+04-5.47258181E+01 4.88394767E+00 4.03401300E-02-1.97774150E-  
 05 3  
 3.68903501E-09-3.40202384E-14-2.35295942E+04 9.97070337E+00  
 4  
 OC4H6O 1/23/ 9 WKM C 4H 60 2 OG 300.000 5000.000  
 1382.000 31  
 1.41894774E+01 1.53345510E-02-5.24594862E-06 8.14655154E-10-4.72759368E-  
 14 2  
 -4.10001835E+04-4.43771751E+01 4.21628848E+00 3.57422725E-02-2.04226185E-  
 05 3  
 5.63821367E-09-5.88888993E-13-3.72055911E+04 1.02814620E+01  
 4  
 OC4H5O 1/23/ 9 WKM C 4H 50 2 OG 300.000 5000.000  
 1388.000 21  
 1.32138775E+01 1.37339051E-02-4.62639517E-06 7.10941370E-10-4.09538499E-  
 14 2  
 -2.16535271E+04-3.64185255E+01 4.60550978E+00 3.30498712E-02-2.13102363E-  
 05 3  
 7.37021089E-09-1.08289438E-12-1.85460831E+04 1.01599453E+01  
 4  
 O2CCHOOJ Z&B C 2H 10 4 OG 300.000 5000.000  
 1682.000 01  
 1.09910849E+01 7.46985861E-03-2.75568271E-06 4.51353051E-10-2.72108652E-  
 14 2  
 -3.51335323E+04-2.11652231E+01 8.91497688E+00 8.60571847E-03 5.24416766E-  
 07 3  
 -2.79301331E-09 7.62963051E-13-3.40867754E+04-8.72978273E+00  
 4  
 HOCVCCJVO 1/26/ 9 WKM C 3H 30 2 OG 300.000 5000.000  
 1414.000 11  
 1.52720985E+01 5.02586331E-03-1.68408578E-06 2.58390706E-10-1.48849424E-  
 14 2  
 -1.98506828E+04-5.54641734E+01 6.07270082E-01 4.96011303E-02-5.32300885E-  
 05 3  
 2.68392951E-08-5.13094510E-12-1.58814562E+04 1.94817133E+01  
 4

C5H5OH 5/ 2/91 THE.MC 5H 60 1 0G 300.000 5000.000  
 1398.000 11  
 1.53433477E+01 1.50754059E-02-5.13553582E-06 7.95807816E-10-4.61311517E-  
 14 2  
 -1.19645453E+04-5.85204430E+01-4.26822012E+00 6.62446749E-02-5.68494038E-  
 05 3  
 2.46858526E-08-4.26820696E-12-5.75581338E+03 4.47962850E+01  
 4  
 C5H5O 5/16/90 THERMC 5H 50 1 0G 300.000 5000.000  
 1392.000 01  
 1.48322894E+01 1.40483376E-02-4.92302051E-06 7.77041219E-10-4.56103939E-  
 14 2  
 1.45523665E+04-5.73228191E+01-2.83112840E+00 5.67277287E-02-4.44757303E-  
 05 3  
 1.74924447E-08-2.76004847E-12 2.04992154E+04 3.69634411E+01  
 4  
 C5H4OH T 8/99C 5H 50 1 0G 200.000 6000.000 1000.  
 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  
 C5H4O T 8/99C 5H 40 1 0G 200.000 6000.000 1000.  
 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  
 C5H3O TAK0905C 5H 30 1 0G 300.000 3500.000 1500.00  
 1  
 1.19961781E+01 1.34287065E-02-5.90045309E-06 1.22553862E-09-9.86114716E-  
 14 2  
 2.89592010E+04-4.07548249E+01-3.03242604E+00 5.43937201E-02-4.95018348E-  
 05 3  
 2.25523751E-08-4.10727920E-12 3.35644081E+04 3.78374823E+01  
 4  
 CJVCCVCCVO 2/ 5/ 9 THERMC 5H 50 1 0G 300.000 5000.000  
 1396.000 21  
 1.62360823E+01 1.18297101E-02-4.11454219E-06 6.46026823E-10-3.77767639E-  
 14 2  
 1.93499885E+04-5.83498817E+01-5.06628841E-01 6.04671965E-02-5.97396749E-  
 05 3  
 2.96804228E-08-5.76240010E-12 2.42765544E+04 2.82994148E+01  
 4  
 CVCCVCCJVO 2/ 5/ 9 THERMC 5H 50 1 0G 300.000 5000.000  
 1399.000 11  
 1.53178248E+01 1.27352911E-02-4.35882964E-06 6.76912763E-10-3.92771371E-  
 14 2  
 7.60582726E+03-5.43599625E+01-2.18492198E-01 5.92100223E-02-5.89241174E-  
 05 3  
 2.97411920E-08-5.85244770E-12 1.20600764E+04 2.55968530E+01  
 4  
 CJVCCVO 4/ 8/94 THERMC 3H 30 1 0G 300.000 5000.000  
 1402.000 11

1.07482537E+01 6.19822688E-03-2.06130981E-06 3.14418872E-10-1.80309517E-  
14 2  
1.51410162E+04-3.01266033E+01 1.46654466E+00 3.23390476E-02-3.05588208E-  
05 3  
1.44081861E-08-2.65600505E-12 1.78850058E+04 1.80850321E+01  
4  
NC5H12 9/ 8/14 C 5H 12 0 OG 300.000 5000.000  
1393.000 41  
+1.58289132E+01+2.59344752E-02-8.83016276E-06+1.36654986E-09-7.91029283E-  
14 2  
-2.59397429E+04-6.05558457E+01-2.99551806E-01+5.94963054E-02-3.41764359E-  
05 3  
+9.47896058E-09-9.73675086E-13-  
1.98959978E+04+2.75742132E+01+0.00000000E+00 4  
C5H11-1 9/ 8/14 C 5H 11 0 OG 300.000 5000.000  
1394.000 41  
+1.51918481E+01+2.40339049E-02-8.19717624E-06+1.27002751E-09-7.35727956E-  
14 2  
-8.02148517E+02-5.36479311E+01+9.83190194E-02+5.58653605E-02-3.28855625E-  
05 3  
+9.58366873E-09-1.08641370E-  
12+4.82065818E+03+2.86921367E+01+0.00000000E+00 4  
C5H11-2 9/ 8/14 C 5H 11 0 OG 300.000 5000.000  
1395.000 41  
+1.47177050E+01+2.41667557E-02-8.18647646E-06+1.26271867E-09-7.29267957E-  
14 2  
-2.26027771E+03-5.06071115E+01+8.17689455E-01+4.92653514E-02-2.13785619E-  
05 3  
+1.85532454E-09+7.06259101E-  
13+3.26221492E+03+2.65876082E+01+0.00000000E+00 4  
C5H11-3 9/ 8/14 C 5H 11 0 OG 300.000 5000.000  
1395.000 41  
+1.47177050E+01+2.41667557E-02-8.18647646E-06+1.26271867E-09-7.29267957E-  
14 2  
-2.26027771E+03-5.12965931E+01+8.17689455E-01+4.92653514E-02-2.13785619E-  
05 3  
+1.85532454E-09+7.06259101E-  
13+3.26221492E+03+2.58981266E+01+0.00000000E+00 4  
C5H11O2H-1 9/ 8/14 C 5H 12O 2 OG 300.000 5000.000  
1393.000 61  
+2.08826791E+01+2.61587380E-02-8.96860003E-06+1.39463023E-09-8.10033260E-  
14 2  
-3.71864314E+04-8.01917306E+01+7.56966700E-01+7.13994143E-02-4.75006334E-  
05 3  
+1.62337006E-08-2.26834390E-12-  
3.00009521E+04+2.85558826E+01+0.00000000E+00 4  
C5H11O2H-2 9/ 8/14 C 5H 12O 2 OG 300.000 5000.000  
1400.000 61  
+2.11347974E+01+2.56494323E-02-8.72650240E-06+1.34983451E-09-7.81086942E-  
14 2  
-3.90416300E+04-8.21964012E+01+1.06841342E+00+7.36472213E-02-5.31234084E-  
05 3  
+2.02380955E-08-3.18671855E-12-  
3.21746715E+04+2.51901593E+01+0.00000000E+00 4  
C5H11O2H-3 9/ 8/14 C 5H 12O 2 OG 300.000 5000.000  
1400.000 61  
+2.11347974E+01+2.56494323E-02-8.72650240E-06+1.34983451E-09-7.81086942E-  
14 2

-3.90416300E+04-8.35753644E+01+1.06841342E+00+7.36472213E-02-5.31234084E-05 3  
+2.02380955E-08-3.18671855E-12-  
3.21746715E+04+2.38111961E+01+0.00000000E+00 4  
C5H11O2-1 9/ 8/14 C 5H 11O 2 OG 300.000 5000.000  
1392.000 51  
+1.99508904E+01+2.48182054E-02-8.50415197E-06+1.32191009E-09-7.67596518E-14 2  
-1.99782879E+04-7.43587406E+01+1.47849612E+00+6.56222617E-02-4.24002295E-05 3  
+1.39455731E-08-1.86035665E-12-  
1.33065245E+04+2.57184992E+01+0.00000000E+00 4  
C5H11O2-2 9/ 8/14 C 5H 11O 2 OG 300.000 5000.000  
1401.000 51  
+2.01379084E+01+2.43048677E-02-8.24744582E-06+1.27344965E-09-7.35953601E-14 2  
-2.17777897E+04-7.59194124E+01+1.95945265E+00+6.73012650E-02-4.74261817E-05 3  
+1.76453313E-08-2.71599328E-12-  
1.55102022E+04+2.15326067E+01+0.00000000E+00 4  
C5H11O2-3 9/ 8/14 C 5H 11O 2 OG 300.000 5000.000  
1401.000 51  
+2.01379084E+01+2.43048677E-02-8.24744582E-06+1.27344965E-09-7.35953601E-14 2  
-2.17777897E+04-7.72983757E+01+1.95945265E+00+6.73012650E-02-4.74261817E-05 3  
+1.76453313E-08-2.71599328E-12-  
1.55102022E+04+2.01536434E+01+0.00000000E+00 4  
C5H11O-1 9/ 8/14 C 5H 11O 1 OG 300.000 5000.000  
1396.000 41  
+1.87118024E+01+2.36054696E-02-8.05610528E-06+1.24900841E-09-7.23989034E-14 2  
-1.84133036E+04-7.11769229E+01+1.61443159E+00+5.84449099E-02-3.26027513E-05 3  
+7.76525028E-09-4.48739932E-13-  
1.20210227E+04+2.23620687E+01+0.00000000E+00 4  
C5H11O-2 9/ 8/14 C 5H 11O 1 OG 300.000 5000.000  
1407.000 41  
+1.85178187E+01+2.33560329E-02-7.87896503E-06+1.21190761E-09-6.98572825E-14 2  
-2.01488741E+04-7.05224357E+01+1.80797841E+00+5.95687062E-02-3.62936785E-05 3  
+1.05785660E-08-1.11086649E-12-  
1.41294991E+04+2.01085450E+01+0.00000000E+00 4  
C5H11O-3 9/ 8/14 C 5H 11O 1 OG 300.000 5000.000  
1407.000 41  
+1.85178187E+01+2.33560329E-02-7.87896503E-06+1.21190761E-09-6.98572825E-14 2  
-2.01488741E+04-7.19013990E+01+1.80797841E+00+5.95687062E-02-3.62936785E-05 3  
+1.05785660E-08-1.11086649E-12-  
1.41294991E+04+1.87295817E+01+0.00000000E+00 4  
C5H10OOH1-2 9/8/14 C 5H 11O 2 OG 300.000 5000.000  
1396.000 61  
+2.00795991E+01+2.43589475E-02-8.36202795E-06+1.30140406E-09-7.56329790E-14 2  
-1.33166011E+04-7.30604965E+01+2.65531081E+00+6.13777489E-02-3.72526890E-05 3

+1.10683497E-08-1.26575773E-12-  
6.87569412E+03+2.18610512E+01+0.00000000E+00 4  
C5H10OOH1-3 9/8/14 C 5H 110 2 0G 300.000 5000.000  
1396.000 61  
+1.94584083E+01+2.46031733E-02-8.38534822E-06+1.29883762E-09-7.52367289E-  
14 2  
-1.33548974E+04-6.90616123E+01+2.21641946E+00+5.96426514E-02-3.30151174E-  
05 3  
+7.82801873E-09-4.53626906E-13-  
6.89038067E+03+2.53165655E+01+0.00000000E+00 4  
C5H10OOH1-4 9/8/14 C 5H 110 2 0G 300.000 5000.000  
1396.000 61  
+1.94584083E+01+2.46031733E-02-8.38534822E-06+1.29883762E-09-7.52367289E-  
14 2  
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05 3  
+7.82801873E-09-4.53626906E-13-  
6.89038067E+03+2.53165655E+01+0.00000000E+00 4  
C5H10OOH1-5 9/8/14 C 5H 110 2 0G 300.000 5000.000  
1393.000 61  
+2.02627427E+01+2.43041392E-02-8.36491479E-06+1.30408546E-09-7.58781596E-  
14 2  
-1.20792388E+04-7.41332935E+01+9.60306204E-01+6.85338215E-02-4.72580697E-  
05 3  
+1.69913164E-08-2.53055987E-12-  
5.25227210E+03+2.99005842E+01+0.00000000E+00 4  
C5H10OOH2-1 9/8/14 C 5H 110 2 0G 300.000 5000.000  
1401.000 61  
+2.11683533E+01+2.30995637E-02-7.85421525E-06+1.21454488E-09-7.02697376E-  
14 2  
-1.41652579E+04-7.96524097E+01+1.97482622E+00+6.85026751E-02-4.88793184E-  
05 3  
+1.80505063E-08-2.71515676E-12-  
7.58936343E+03+2.31709703E+01+0.00000000E+00 4  
C5H10OOH2-3 9/8/14 C 5H 110 2 0G 300.000 5000.000  
1410.000 61  
+2.03599510E+01+2.36444020E-02-8.00996599E-06+1.23543694E-09-7.13457143E-  
14 2  
-1.51264004E+04-7.50912668E+01+3.03844851E+00+6.35523371E-02-4.29455468E-  
05 3  
+1.50665567E-08-2.16139351E-12-  
9.06691319E+03+1.81118164E+01+0.00000000E+00 4  
C5H10OOH2-4 9/8/14 C 5H 110 2 0G 300.000 5000.000  
1410.000 61  
+1.98843630E+01+2.37470675E-02-7.98273943E-06+1.22497373E-09-7.04946509E-  
14 2  
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05 3  
+1.11809673E-08-1.20043769E-12-  
9.09500363E+03+2.11388648E+01+0.00000000E+00 4  
C5H10OOH2-5 9/8/14 C 5H 110 2 0G 300.000 5000.000  
1401.000 61  
+2.05595155E+01+2.35923560E-02-8.01736916E-06+1.23918525E-09-7.16674070E-  
14 2  
-1.39059417E+04-7.62751847E+01+1.46239008E+00+7.00773603E-02-5.18935110E-  
05 3  
+2.03023923E-08-3.27212476E-12-  
7.45896384E+03+2.56255897E+01+0.00000000E+00 4

C5H100OH3-1 9/8/14 C 5H 110 2 OG 300.000 5000.000  
1401.000 61  
+2.05595155E+01+2.35923560E-02-8.01736916E-06+1.23918525E-09-7.16674070E-  
14 2  
-1.39059417E+04-7.69646663E+01+1.46239008E+00+7.00773603E-02-5.18935110E-  
05 3  
+2.03023923E-08-3.27212476E-12-  
7.45896384E+03+2.49361080E+01+0.00000000E+00 4  
C5H100OH3-2 9/8/14 C 5H 110 2 OG 300.000 5000.000  
1410.000 61  
+2.03599510E+01+2.36444020E-02-8.00996599E-06+1.23543694E-09-7.13457143E-  
14 2  
-1.51264004E+04-7.57807484E+01+3.03844851E+00+6.35523371E-02-4.29455468E-  
05 3  
+1.50665567E-08-2.16139351E-12-  
9.06691319E+03+1.74223348E+01+0.00000000E+00 4  
C5H100I-2 9/ 8/14 C 5H 100 1 OG 300.000 5000.000  
1424.000 31  
+1.76453140E+01+2.17647043E-02-7.28831391E-06+1.11571673E-09-6.41056178E-  
14 2  
-2.49627812E+04-6.94780751E+01-5.22384549E+00+7.95280569E-02-6.27918049E-  
05 3  
+2.51187341E-08-3.99106436E-12-  
1.76152192E+04+5.15328120E+01+0.00000000E+00 4  
C5H100I-3 9/ 8/14 C 5H 100 1 OG 300.000 5000.000  
1445.000 21  
+1.61536944E+01+2.22699220E-02-7.20967982E-06+1.07781327E-09-6.08828236E-  
14 2  
-2.51216994E+04-6.18744318E+01-7.38770073E+00+8.62948016E-02-7.34565945E-  
05 3  
+3.18221366E-08-5.43057938E-12-  
1.80648633E+04+6.09884425E+01+0.00000000E+00 4  
C5H100I-4 9/ 8/14 C 5H 100 1 OG 300.000 5000.000  
1470.000 11  
+1.56838302E+01+2.28597182E-02-7.36869093E-06+1.09855828E-09-6.19425653E-  
14 2  
-3.52365120E+04-6.06986511E+01-7.99511075E+00+8.48027993E-02-6.84820969E-  
05 3  
+2.79646707E-08-4.48601572E-12-  
2.79347448E+04+6.36835324E+01+0.00000000E+00 4  
C5H100I-5 9/ 8/14 C 5H 100 1 OG 300.000 5000.000  
1447.000 01  
+1.58722584E+01+2.41484940E-02-8.02830905E-06+1.22306406E-09-7.00384536E-  
14 2  
-3.58667196E+04-6.73548909E+01-8.45066821E+00+8.36041573E-02-6.24375031E-  
05 3  
+2.32498119E-08-3.38258239E-12-  
2.79060038E+04+6.19634163E+01+0.00000000E+00 4  
C5H1002-3 9/ 8/14 C 5H 100 1 OG 300.000 5000.000  
1415.000 31  
+1.76695497E+01+2.16741351E-02-7.23760886E-06+1.10546424E-09-6.34044008E-  
14 2  
-2.67999740E+04-7.01762004E+01-6.83688134E+00+9.00167224E-02-8.09486382E-  
05 3  
+3.71523167E-08-6.73312332E-12-  
1.94907358E+04+5.73459463E+01+0.00000000E+00 4  
C5H1002-4 9/ 8/14 C 5H 100 1 OG 300.000 5000.000  
1396.000 21



+1.58873476E+01+2.48573824E-02-1.03962573E-05+1.95192708E-09-1.29464891E-13 2  
-2.72224431E+04-6.26943208E+01-6.91381150E+00+8.65695113E-02-7.51445092E-05 3  
+3.29307332E-08-5.77631101E-12-  
2.02336617E+04+5.66267224E+01+0.00000000E+00 4  
C5H10OOH1-2O2 9/14 C 5H 11O 4 OG 300.000 5000.000  
1394.000 71  
+2.71105703E+01+2.34082367E-02-8.11719657E-06+1.27230537E-09-7.43221831E-14 2  
-3.41406290E+04-1.08093476E+02+2.92123878E+00+7.67601721E-02-5.10111840E-05 3  
+1.59643052E-08-1.82979631E-12-  
2.55486792E+04+2.27306226E+01+0.00000000E+00 4  
C5H10OOH1-3O2 9/14 C 5H 11O 4 OG 300.000 5000.000  
1394.000 71  
+2.71105703E+01+2.34082367E-02-8.11719657E-06+1.27230537E-09-7.43221831E-14 2  
-3.41406290E+04-1.08093476E+02+2.92123878E+00+7.67601721E-02-5.10111840E-05 3  
+1.59643052E-08-1.82979631E-12-  
2.55486792E+04+2.27306226E+01+0.00000000E+00 4  
C5H10OOH1-4O2 9/14 C 5H 11O 4 OG 300.000 5000.000  
1394.000 71  
+2.71105703E+01+2.34082367E-02-8.11719657E-06+1.27230537E-09-7.43221831E-14 2  
-3.41406290E+04-1.08093476E+02+2.92123878E+00+7.67601721E-02-5.10111840E-05 3  
+1.59643052E-08-1.82979631E-12-  
2.55486792E+04+2.27306226E+01+0.00000000E+00 4  
C5H10OOH1-5O2 9/14 C 5H 11O 4 OG 300.000 5000.000  
1390.000 71  
+2.58212210E+01+2.46140917E-02-8.55565938E-06+1.34293065E-09-7.85178268E-14 2  
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+1.63241251E-08-2.04839461E-12-  
2.33970141E+04+2.58821117E+01+0.00000000E+00 4  
C5H10OOH2-1O2 9/14 C 5H 11O 4 OG 300.000 5000.000  
1394.000 71  
+2.71105703E+01+2.34082367E-02-8.11719657E-06+1.27230537E-09-7.43221831E-14 2  
-3.41406290E+04-1.08093476E+02+2.92123878E+00+7.67601721E-02-5.10111840E-05 3  
+1.59643052E-08-1.82979631E-12-  
2.55486792E+04+2.27306226E+01+0.00000000E+00 4  
C5H10OOH2-3O2 9/14 C 5H 11O 4 OG 300.000 5000.000  
1405.000 71  
+2.51554088E+01+2.42476887E-02-8.22109032E-06+1.26886123E-09-7.33157779E-14 2  
-3.49522107E+04-9.69775586E+01+2.94958658E+00+7.94696642E-02-6.12300085E-05 3  
+2.45360891E-08-3.99243941E-12-  
2.76263457E+04+2.10066180E+01+0.00000000E+00 4  
C5H10OOH2-4O2 9/14 C 5H 11O 4 OG 300.000 5000.000  
1405.000 71  
+2.51554088E+01+2.42476887E-02-8.22109032E-06+1.26886123E-09-7.33157779E-14 2

-3.49522107E+04-9.69775586E+01+2.94958658E+00+7.94696642E-02-6.12300085E-05 3  
+2.45360891E-08-3.99243941E-12-  
2.76263457E+04+2.10066180E+01+0.00000000E+00 4  
C5H10OOH2-5O2 9/14 C 5H 11O 4 OG 300.000 5000.000  
1394.000 71  
+2.71105703E+01+2.34082367E-02-8.11719657E-06+1.27230537E-09-7.43221831E-14 2  
-3.41406290E+04-1.08093476E+02+2.92123878E+00+7.67601721E-02-5.10111840E-05 3  
+1.59643052E-08-1.82979631E-12-  
2.55486792E+04+2.27306226E+01+0.00000000E+00 4  
C5H10OOH3-1O2 9/14 C 5H 11O 4 OG 300.000 5000.000  
1394.000 71  
+2.71105703E+01+2.34082367E-02-8.11719657E-06+1.27230537E-09-7.43221831E-14 2  
-3.41406290E+04-1.08093476E+02+2.92123878E+00+7.67601721E-02-5.10111840E-05 3  
+1.59643052E-08-1.82979631E-12-  
2.55486792E+04+2.27306226E+01+0.00000000E+00 4  
C5H10OOH3-2O2 9/14 C 5H 11O 4 OG 300.000 5000.000  
1405.000 71  
+2.51554088E+01+2.42476887E-02-8.22109032E-06+1.26886123E-09-7.33157779E-14 2  
-3.49522107E+04-9.69775586E+01+2.94958658E+00+7.94696642E-02-6.12300085E-05 3  
+2.45360891E-08-3.99243941E-12-  
2.76263457E+04+2.10066180E+01+0.00000000E+00 4  
C5H91-2,3OOH 9/14 C 5H 11O 4 OG 300.000 5000.000  
1405.000 81  
+2.55056147E+01+2.36990320E-02-8.07032909E-06+1.24934920E-09-7.23427367E-14 2  
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+2.44460527E-08-3.95034020E-12-  
1.96516956E+04+2.32188202E+01+0.00000000E+00 4  
C5H91-2,4OOH 9/14 C 5H 11O 4 OG 300.000 5000.000  
1405.000 81  
+2.55056147E+01+2.36990320E-02-8.07032909E-06+1.24934920E-09-7.23427367E-14 2  
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+2.44460527E-08-3.95034020E-12-  
1.96516956E+04+2.32188202E+01+0.00000000E+00 4  
C5H91-2,5OOH 9/14 C 5H 11O 4 OG 300.000 5000.000  
1397.000 81  
+2.50741397E+01+2.44380043E-02-8.40704928E-06+1.31038422E-09-7.62381905E-14 2  
-2.51871158E+04-9.38667514E+01+2.56086129E+00+7.80408775E-02-5.74863330E-05 3  
+2.18761227E-08-3.39924240E-12-  
1.74851061E+04+2.66588551E+01+0.00000000E+00 4  
C5H91-3,4OOH 9/14 C 5H 11O 4 OG 300.000 5000.000  
1405.000 81  
+2.54680852E+01+2.36307420E-02-8.02474436E-06+1.23994908E-09-7.17032304E-14 2  
-2.70635665E+04-9.67605580E+01+2.48775154E+00+8.15271831E-02-6.44013124E-05 3

+2.63443736E-08-4.35804025E-12-  
1.95635349E+04+2.50626503E+01+0.00000000E+00 4  
C5H91-3,50OH 9/14 C 5H 110 4 OG 300.000 5000.000  
1397.000 81  
+2.75716451E+01+2.26282394E-02-7.85651555E-06+1.23251566E-09-7.20426920E-  
14 2  
-2.62702922E+04-1.08648340E+02+2.50132978E+00+7.93141150E-02-5.51608762E-  
05 3  
+1.83963651E-08-2.32880956E-12-  
1.75129588E+04+2.64329747E+01+0.00000000E+00 4  
C5H91-4,50OH 9/14 C 5H 110 4 OG 300.000 5000.000  
1397.000 81  
+2.75716451E+01+2.26282394E-02-7.85651555E-06+1.23251566E-09-7.20426920E-  
14 2  
-2.62702922E+04-1.08648340E+02+2.50132978E+00+7.93141150E-02-5.51608762E-  
05 3  
+1.83963651E-08-2.32880956E-12-  
1.75129588E+04+2.64329747E+01+0.00000000E+00 4  
C5H92-1,30OH 9/14 C 5H 110 4 OG 300.000 5000.000  
1413.000 81  
+2.46778451E+01+2.47896676E-02-8.53168232E-06+1.33018418E-09-7.74050315E-  
14 2  
-2.64008851E+04-9.18794025E+01+3.42922915E+00+7.33174178E-02-5.05533009E-  
05 3  
+1.77709491E-08-2.53421378E-12-  
1.89212844E+04+2.26144479E+01+0.00000000E+00 4  
C5H92-1,40OH 9/14 C 5H 110 4 OG 300.000 5000.000  
1413.000 81  
+2.46778451E+01+2.47896676E-02-8.53168232E-06+1.33018418E-09-7.74050315E-  
14 2  
-2.64008851E+04-9.18794025E+01+3.42922915E+00+7.33174178E-02-5.05533009E-  
05 3  
+1.77709491E-08-2.53421378E-12-  
1.89212844E+04+2.26144479E+01+0.00000000E+00 4  
C5H92-1,50OH 9/14 C 5H 110 4 OG 300.000 5000.000  
1399.000 81  
+2.63836136E+01+2.38373273E-02-8.31679219E-06+1.30877666E-09-7.66591074E-  
14 2  
-2.52930801E+04-1.01118754E+02+3.43107332E+00+7.25133538E-02-4.53395240E-  
05 3  
+1.29499313E-08-1.26534785E-12-  
1.69000809E+04+2.37843821E+01+0.00000000E+00 4  
C5H92-3,40OH 9/14 C 5H 110 4 OG 300.000 5000.000  
1418.000 81  
+2.51070211E+01+2.40686276E-02-8.20467040E-06+1.27103065E-09-7.36339262E-  
14 2  
-2.83591157E+04-9.49637963E+01+3.76788328E+00+7.47668469E-02-5.41780015E-  
05 3  
+2.01841133E-08-3.04867679E-12-  
2.10823293E+04+1.92561961E+01+0.00000000E+00 4  
C5H92-3,50OH 9/14 C 5H 110 4 OG 300.000 5000.000  
1413.000 81  
+2.46778451E+01+2.47896676E-02-8.53168232E-06+1.33018418E-09-7.74050315E-  
14 2  
-2.64008851E+04-9.18794025E+01+3.42922915E+00+7.33174178E-02-5.05533009E-  
05 3  
+1.77709491E-08-2.53421378E-12-  
1.89212844E+04+2.26144479E+01+0.00000000E+00 4

C5H92-4,500H 9/14 C 5H 110 4 OG 300.000 5000.000  
1413.000 81  
+2.47514622E+01+2.41459993E-02-8.18238994E-06+1.26250806E-09-7.29352454E-14 2  
-2.63782993E+04-9.11444444E+01+4.06621416E+00+7.20273834E-02-4.95956461E-05 3  
+1.70908613E-08-2.31584179E-12-  
1.92523266E+04+1.99316930E+01+0.00000000E+00 4  
C5H93-1,200H 9/14 C 5H 110 4 OG 300.000 5000.000  
1413.000 81  
+2.46778451E+01+2.47896676E-02-8.53168232E-06+1.33018418E-09-7.74050315E-14 2  
-2.64008851E+04-9.18794025E+01+3.42922915E+00+7.33174178E-02-5.05533009E-05 3  
+1.77709491E-08-2.53421378E-12-  
1.89212844E+04+2.26144479E+01+0.00000000E+00 4  
C5H93-1,400H 9/14 C 5H 110 4 OG 300.000 5000.000  
1413.000 81  
+2.46778451E+01+2.47896676E-02-8.53168232E-06+1.33018418E-09-7.74050315E-14 2  
-2.64008851E+04-9.18794025E+01+3.42922915E+00+7.33174178E-02-5.05533009E-05 3  
+1.77709491E-08-2.53421378E-12-  
1.89212844E+04+2.26144479E+01+0.00000000E+00 4  
C5H93-1,500H 9/14 C 5H 110 4 OG 300.000 5000.000  
1399.000 81  
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+1.31290152E-08-1.43358803E-12-  
1.70587842E+04+2.30262907E+01+0.00000000E+00 4  
C5H93-2,400H 9/14 C 5H 110 4 OG 300.000 5000.000  
1418.000 81  
+2.51070211E+01+2.40686276E-02-8.20467040E-06+1.27103065E-09-7.36339262E-14 2  
-2.83591157E+04-9.56532779E+01+3.76788328E+00+7.47668469E-02-5.41780015E-05 3  
+2.01841133E-08-3.04867679E-12-  
2.10823293E+04+1.85667144E+01+0.00000000E+00 4  
C5H91-300H 9/8/14 C 5H 100 2 OG 300.000 5000.000  
1394.000 51  
+2.24660467E+01+2.00408413E-02-6.84550040E-06+1.06266050E-09-6.16741604E-14 2  
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+2.83331852E-08-4.76826956E-12-  
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C5H91-400H 9/8/14 C 5H 100 2 OG 300.000 5000.000  
1402.000 51  
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+1.94278468E-08-3.12175781E-12-  
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C5H91-500H 9/8/14 C 5H 100 2 OG 300.000 5000.000  
1392.000 51

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 C5H92-10OH 9/8/14 C 5H 100 2 OG 300.000 5000.000  
 1382.000 51  
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 C5H92-40OH 9/8/14 C 5H 100 2 OG 300.000 5000.000  
 1389.000 51  
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 05 3  
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 C5H92-50OH 9/8/14 C 5H 100 2 OG 300.000 5000.000  
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 C5H901-20OH-3 9/14 C 5H 100 3 OG 300.000 5000.000  
 1422.000 51  
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 14 2  
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 05 3  
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 C5H901-20OH-4 9/14 C 5H 100 3 OG 300.000 5000.000  
 1422.000 51  
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 05 3  
 +2.45435115E-08-3.63637746E-12-  
 3.02443795E+04+3.81009801E+01+0.00000000E+00 4  
 C5H901-20OH-5 9/14 C 5H 100 3 OG 300.000 5000.000  
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 14 2  
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 +2.66150873E-08-4.08265327E-12-  
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 C5H901-30OH-2 9/14 C 5H 100 3 OG 300.000 5000.000  
 1421.000 41  
 +2.29238871E+01+2.22244781E-02-7.50929996E-06+1.15689292E-09-6.67794310E-  
 14 2

-3.93149495E+04-9.38426660E+01-4.67708778E+00+9.25191737E-02-7.56245586E-05 3  
+3.08655754E-08-4.96974700E-12-  
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C5H9O1-3OOH-4 9/14 C 5H 100 3 0G 300.000 5000.000  
1421.000 41  
+2.29238871E+01+2.22244781E-02-7.50929996E-06+1.15689292E-09-6.67794310E-14 2  
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+3.08655754E-08-4.96974700E-12-  
3.05178886E+04+5.19807893E+01+0.00000000E+00 4  
C5H9O1-3OOH-5 9/14 C 5H 100 3 0G 300.000 5000.000  
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+2.21702811E+01+2.28760461E-02-7.73630997E-06+1.19254044E-09-6.88630410E-14 2  
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+3.02210571E-08-4.80852681E-12-  
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C5H9O1-4OOH-2 9/14 C 5H 100 3 0G 300.000 5000.000  
1417.000 31  
+2.17260410E+01+2.34146274E-02-7.86187868E-06+1.20571561E-09-6.93653621E-14 2  
-4.90509096E+04-8.83590566E+01-9.18084516E+00+1.08786371E-01-9.86756121E-05 3  
+4.49207522E-08-8.03087742E-12-  
3.98013189E+04+7.26760969E+01+0.00000000E+00 4  
C5H9O1-4OOH-3 9/14 C 5H 100 3 0G 300.000 5000.000  
1417.000 31  
+2.17260410E+01+2.34146274E-02-7.86187868E-06+1.20571561E-09-6.93653621E-14 2  
-4.90509096E+04-8.83590566E+01-9.18084516E+00+1.08786371E-01-9.86756121E-05 3  
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C5H9O1-4OOH-5 9/14 C 5H 100 3 0G 300.000 5000.000  
1411.000 31  
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-4.72411464E+04-8.60552096E+01-9.29661331E+00+1.04958911E-01-9.00892767E-05 3  
+3.89843596E-08-6.68819849E-12-  
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C5H9O1-5OOH-2 9/14 C 5H 100 3 0G 300.000 5000.000  
1407.000 21  
+2.24618796E+01+2.42252273E-02-8.36381388E-06+1.30712783E-09-7.62010208E-14 2  
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+3.77712411E-08-6.32248900E-12-  
3.97499469E+04+7.18166046E+01+0.00000000E+00 4  
C5H9O1-5OOH-3 9/14 C 5H 100 3 0G 300.000 5000.000  
1407.000 21  
+2.24618796E+01+2.42252273E-02-8.36381388E-06+1.30712783E-09-7.62010208E-14 2  
-5.00102121E+04-9.83780898E+01-9.63082131E+00+1.06539535E-01-8.95953916E-05 3

+3.77712411E-08-6.32248900E-12-  
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 C5H9O2-3OOH-1 9/14 C 5H 100 3 0G 300.000 5000.000  
 1436.000 51  
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 14 2  
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 05 3  
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 C5H9O2-3OOH-4 9/14 C 5H 100 3 0G 300.000 5000.000  
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 C5H9O2-3OOH-5 9/14 C 5H 100 3 0G 300.000 5000.000  
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 C5H9O2-4OOH-1 9/14 C 5H 100 3 0G 300.000 5000.000  
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 C5H9O2-4OOH-3 9/14 C 5H 100 3 0G 300.000 5000.000  
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 C5H9O1-2O-5 9/8/14 C 5H 90 2 0G 300.000 5000.000  
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 CH2CH2OCH2CH2CHO 4 C 5H 90 2 0G 300.000 5000.000  
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NC5KET12 9/ 8/14 C 5H 100 3 OG 300.000 5000.000  
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 14 2  
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 NC5KET13 9/ 8/14 C 5H 100 3 OG 300.000 5000.000  
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 NC5KET14 9/ 8/14 C 5H 100 3 OG 300.000 5000.000  
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 NC5KET23 9/ 8/14 C 5H 100 3 OG 300.000 5000.000  
 1390.000 61  
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 NC5KET24 9/ 8/14 C 5H 100 3 OG 300.000 5000.000  
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 NC5KET25 9/ 8/14 C 5H 100 3 OG 300.000 5000.000  
 1395.000 61



+2.09051806E+01+2.29956432E-02-7.75343394E-06+1.19262969E-09-6.87612656E-14 2  
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 4.40485734E+04+1.96186974E+01+0.00000000E+00 4  
 NC5KET31 9/ 8/14 C 5H 100 3 OG 300.000 5000.000  
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 -5.08471346E+04-8.02429953E+01+4.06393861E+00+5.46274576E-02-2.50666165E-05 3  
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 NC5KET32 9/ 8/14 C 5H 100 3 OG 300.000 5000.000  
 1388.000 61  
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 -5.22889844E+04-9.61325613E+01+3.80342038E-01+7.67072849E-02-5.67635185E-05 3  
 +2.07068449E-08-2.96497951E-12-  
 4.41579478E+04+3.21097700E+01+0.00000000E+00 4  
 NC5KET120 9/ 8/14 C 5H 90 2 OG 300.000 5000.000  
 1377.000 41  
 +2.09367959E+01+2.00874425E-02-7.04829670E-06+1.11330293E-09-6.53771464E-14 2  
 -3.04314417E+04-8.04081881E+01+2.82328315E+00+5.56013887E-02-3.02956498E-05 3  
 +6.22735484E-09-8.25379616E-14-  
 2.35055878E+04+1.92120018E+01+0.00000000E+00 4  
 NC5KET130 9/ 8/14 C 5H 90 2 OG 300.000 5000.000  
 1323.000 41  
 +2.11225120E+01+1.90830240E-02-6.52403075E-06+1.01368310E-09-5.88793478E-14 2  
 -3.11151636E+04-8.21812017E+01+3.92095399E+00+4.94038774E-02-1.99599619E-05 3  
 -1.05666833E-09+1.70331197E-12-  
 2.43649054E+04+1.33502699E+01+0.00000000E+00 4  
 NC5KET140 9/ 8/14 C 5H 90 2 OG 300.000 5000.000  
 1323.000 41  
 +2.11225120E+01+1.90830240E-02-6.52403075E-06+1.01368310E-09-5.88793478E-14 2  
 -3.11151636E+04-8.21812017E+01+3.92095399E+00+4.94038774E-02-1.99599619E-05 3  
 -1.05666833E-09+1.70331197E-12-  
 2.43649054E+04+1.33502699E+01+0.00000000E+00 4  
 NC5KET150 9/ 8/14 C 5H 90 2 OG 300.000 5000.000  
 1489.000 41  
 +1.92273388E+01+2.11348590E-02-7.32088660E-06+1.14667396E-09-6.69507752E-14 2  
 -2.85866827E+04-7.08964819E+01+3.41522476E+00+4.72023685E-02-1.66453220E-05 3  
 -2.39548810E-09+1.83814508E-12-  
 2.21147912E+04+1.77035103E+01+0.00000000E+00 4  
 NC5KET210 9/ 8/14 C 5H 90 2 OG 300.000 5000.000  
 1669.000 41  
 +1.55374345E+01+2.65967153E-02-9.82520086E-06+1.61087197E-09-9.71864472E-14 2

-2.96220202E+04-4.97983106E+01+7.57725086E+00+3.09672386E-02+2.94905694E-06 3  
 -1.10969895E-08+3.01674992E-12-2.56340563E+04-2.16720088E+00+0.00000000E+00 4  
 NC5KET230 9/ 8/14 C 5H 90 2 OG 300.000 5000.000  
 1383.000 41  
 +1.95245872E+01+2.08858647E-02-7.23257140E-06+1.13238277E-09-6.60902126E-14 2  
 -3.34926354E+04-7.21145428E+01+3.56460361E+00+5.18213432E-02-2.70330790E-05 3  
 +5.19426451E-09+1.69499746E-14-2.73448675E+04+1.58030522E+01+0.00000000E+00 4  
 NC5KET240 9/ 8/14 C 5H 90 2 OG 300.000 5000.000  
 1382.000 41  
 +1.87900628E+01+2.10010240E-02-7.16188369E-06+1.11001257E-09-6.43339326E-14 2  
 -3.32898658E+04-6.78862933E+01+4.40946289E+00+4.75586902E-02-2.19238261E-05 3  
 +2.43250490E-09+5.88504938E-13-2.76535939E+04+1.17394140E+01+0.00000000E+00 4  
 NC5KET250 9/ 8/14 C 5H 90 2 OG 300.000 5000.000  
 1433.000 41  
 +1.81303967E+01+2.13611121E-02-7.24506108E-06+1.11897303E-09-6.47006005E-14 2  
 -3.16682816E+04-6.41505194E+01+4.40785464E+00+4.34772079E-02-1.40284695E-05 3  
 -3.02310104E-09+1.86768676E-12-2.60265017E+04+1.28766258E+01+0.00000000E+00 4  
 NC5KET310 9/ 8/14 C 5H 90 2 OG 300.000 5000.000  
 1426.000 41  
 +1.92416140E+01+2.07624762E-02-7.12773261E-06+1.11092657E-09-6.46775655E-14 2  
 -3.25710561E+04-7.19638232E+01+5.37524822E+00+3.49659305E-02+3.67920037E-06 3  
 -1.56750631E-08+4.84743343E-12-2.61248405E+04+8.64755527E+00+0.00000000E+00 4  
 NC5KET320 9/ 8/14 C 5H 90 2 OG 300.000 5000.000  
 1539.000 41  
 +1.90206162E+01+2.10022758E-02-7.20628551E-06+1.12155484E-09-6.51936687E-14 2  
 -3.33553472E+04-6.97524186E+01+4.55782533E+00+4.55546283E-02-1.73485031E-05 3  
 -9.24152417E-10+1.38889438E-12-2.74919397E+04+1.10596626E+01+0.00000000E+00 4  
 NC5DIONE13 10/15 THERMC 5H 80 2 OG 300.000 5000.000  
 1380.000 41  
 +1.81672199E+01+1.95477748E-02-6.78556722E-06+1.06428037E-09-6.21973311E-14 2  
 -5.11134997E+04-6.80388452E+01+1.16337913E+00+5.32067868E-02-2.90297512E-05 3  
 +5.99807535E-09-7.60467747E-14-4.46714058E+04+2.53180917E+01+0.00000000E+00 4  
 NC5DIONE24 10/15 THERMC 5H 80 2 OG 300.000 5000.000  
 1393.000 41  
 +1.63259547E+01+2.07678096E-02-7.12494176E-06+1.10833798E-09-6.43882952E-14 2  
 -5.38361320E+04-5.71667682E+01+1.23573850E+00+5.44884679E-02-3.57895292E-05 3

+1.21944125E-08-1.71810392E-12-  
4.84057706E+04+2.44807388E+01+0.00000000E+00 4  
C5H10OH23 9/ 8/14 C 5H 110 1 0G 300.000 5000.000  
1447.000 51  
+1.70150141E+01+2.35005444E-02-7.77847758E-06+1.18102788E-09-6.74584591E-  
14 2  
-2.30013982E+04-5.87178603E+01+9.23102001E-01+5.84732430E-02-3.47946675E-  
05 3  
+9.61256846E-09-8.64039220E-13-  
1.72758426E+04+2.84227761E+01+0.00000000E+00 4  
O2C5H10OH23 9/8/14 C 5H 110 3 0G 300.000 5000.000  
1413.000 61  
+2.25663309E+01+2.36960784E-02-7.89320309E-06+1.20343029E-09-6.89316529E-  
14 2  
-4.25964462E+04-8.48729630E+01+1.48292990E+00+7.92100619E-02-6.45238925E-  
05 3  
+2.75597603E-08-4.74651399E-12-  
3.59663215E+04+2.60236189E+01+0.00000000E+00 4  
OCH2CHO 9/ 8/14 C 2H 30 2 0G 300.000 5000.000  
1468.000 11  
+9.83472746E+00+7.77895515E-03-2.78174926E-06+4.44911597E-10-2.63530280E-  
14 2  
-1.50740413E+04-2.41644767E+01+6.12784775E+00+6.67998271E-03+1.00125301E-  
05 3  
-1.06887671E-08+2.76652784E-12-1.28216539E+04-8.09763223E-  
01+0.00000000E+00 4  
CH2OCH2CHO 9/ 8/14 C 3H 50 2 0G 300.000 5000.000  
1386.000 31  
+1.11192754E+01+1.27912900E-02-4.35464414E-06+6.73922275E-10-3.90118722E-  
14 2  
-1.79694096E+04-2.74688068E+01+4.09796526E+00+2.50971166E-02-1.04380487E-  
05 3  
+6.95156168E-10+3.93228907E-13-  
1.51203149E+04+1.16942054E+01+0.00000000E+00 4  
C2H4OCHO 9/ 8/14 C 3H 50 2 0G 300.000 5000.000  
1684.000 21  
+1.22682078E+01+1.37336751E-02-5.06732537E-06+8.30265992E-10-5.00728023E-  
14 2  
-2.09125606E+04-3.56985038E+01+3.11985293E+00+3.19514120E-02-1.67508873E-  
05 3  
+3.25914973E-09-4.96818754E-14-  
1.76239471E+04+1.42845094E+01+0.00000000E+00 4  
C5H10OOH1-3OH 10/14/15 C 5H 120 3 0G 300.000 5000.000  
1403.000 71  
+2.31192753E+01+2.59986683E-02-8.82860426E-06+1.36395720E-09-7.88606733E-  
14 2  
-5.79892376E+04-8.81999105E+01+3.54670341E-01+8.27825400E-02-6.38327513E-  
05 3  
+2.58589986E-08-4.28053334E-12-  
5.04620388E+04+3.27492018E+01+0.00000000E+00 4  
C5H10OOH2-4OH 10/14/15 C 5H 120 3 0G 300.000 5000.000  
1411.000 71  
+2.35162773E+01+2.51435990E-02-8.42079438E-06+1.28867610E-09-7.40107760E-  
14 2  
-5.98557610E+04-9.09142876E+01+7.69420941E-01+8.47002755E-02-6.89331076E-  
05 3  
+2.93938563E-08-5.06044347E-12-  
5.26556407E+04+2.88739602E+01+0.00000000E+00 4

C5H10OOH3-1OH 10/14/15 C 5H 120 3 OG 300.000 5000.000  
1406.000 71  
+2.38716811E+01+2.53396515E-02-8.59895412E-06+1.32803347E-09-7.67709894E-  
14 2  
-5.82703781E+04-9.26845624E+01+7.53538721E-01+8.16716738E-02-6.11918401E-  
05 3  
+2.36490302E-08-3.69940856E-12-  
5.05457936E+04+3.05276339E+01+0.00000000E+00 4  
NC5CYCPER13 11/15 THERMC 5H 100 3 OG 300.000 5000.000  
1407.000 31  
+2.41561308E+01+2.24095731E-02-7.74873939E-06+1.21233645E-09-7.07323367E-  
14 2  
-5.55344567E+04-1.03522127E+02-4.99453890E+00+9.45988114E-02-7.58465481E-  
05 3  
+3.02152876E-08-4.76416624E-12-  
4.59881161E+04+5.13024248E+01+0.00000000E+00 4  
NC5CYCPER24 11/15 THERMC 5H 100 3 OG 300.000 5000.000  
1408.000 31  
+2.22820691E+01+2.33310062E-02-7.91636135E-06+1.22269476E-09-7.06906786E-  
14 2  
-5.60698326E+04-9.35418515E+01-4.25869873E+00+9.26924392E-02-7.79864322E-  
05 3  
+3.34971276E-08-5.74390775E-12-  
4.76901635E+04+4.62163973E+01+0.00000000E+00 4  
NC5CYCPER31 11/15 THERMC 5H 100 3 OG 300.000 5000.000  
1400.000 31  
+2.20861156E+01+2.39837041E-02-8.24798762E-06+1.28546679E-09-7.47886437E-  
14 2  
-5.42162418E+04-9.20233359E+01-4.01647605E+00+8.90855731E-02-7.09557408E-  
05 3  
+2.89246712E-08-4.75384108E-12-  
4.56274320E+04+4.65938612E+01+0.00000000E+00 4  
IC5H12 17/8/15 C 5H 12 0 OG 300.000 5000.000  
1397.000 41  
+1.58024165E+01+2.58962455E-02-8.80211277E-06+1.36051024E-09-7.86804753E-  
14 2  
-2.64876700E+04-6.08691324E+01-1.61700908E+00+6.68962508E-02-4.65394790E-  
05 3  
+1.75637406E-08-2.80513304E-12-  
2.03922408E+04+3.27016966E+01+0.00000000E+00 4  
AC5H11 17/8/15 C 5H 11 0 OG 300.000 5000.000  
1397.000 41  
+1.52292407E+01+2.38482717E-02-8.09849455E-06+1.25096662E-09-7.23133933E-  
14 2  
-1.35828406E+03-5.42832371E+01-1.22777654E+00+6.32926027E-02-4.52076107E-  
05 3  
+1.75515079E-08-2.87257258E-  
12+4.32562497E+03+3.38598206E+01+0.00000000E+00 4  
BC5H11 17/8/15 C 5H 11 0 OG 300.000 5000.000  
1385.000 41  
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14 2  
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05 3  
+8.82319315E-10+7.56537666E-  
13+1.29054584E+03+2.12275239E+01+0.00000000E+00 4  
CC5H11 17/8/15 C 5H 11 0 OG 300.000 5000.000  
1402.000 41

+1.43628831E+01+2.43459715E-02-8.21904266E-06+1.26457869E-09-7.28991288E-  
 14 2  
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 05 3  
 +7.61177489E-09-6.45328560E-  
 13+2.66542853E+03+2.78232188E+01+0.00000000E+00 4  
 DC5H11 17/8/15 C 5H 11 0 0G 300.000 5000.000  
 1397.000 41  
 +1.52292407E+01+2.38482717E-02-8.09849455E-06+1.25096662E-09-7.23133933E-  
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 12+4.32562497E+03+3.31703389E+01+0.00000000E+00 4  
 AC5H90-A2 9/ 8/14 C 5H 90 1 0G 300.000 5000.000  
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 14 2  
 -3.95848360E+03-6.08201916E+01+4.66263417E+00+3.89775126E-02-1.12815501E-  
 05 3  
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 12+1.47086581E+03+8.21346271E+00+0.00000000E+00 4  
 AC5H1102H 17/8/15 C 5H 120 2 0G 300.000 5000.000  
 1397.000 61  
 +2.08513274E+01+2.60811030E-02-8.91735578E-06+1.38397232E-09-8.02716539E-  
 14 2  
 -3.77194279E+04-8.04522304E+01-4.76374815E-01+7.83789321E-02-5.91712555E-  
 05 3  
 +2.38263919E-08-3.97732270E-12-  
 3.05087904E+04+3.32977557E+01+0.00000000E+00 4  
 BC5H1102H 17/8/15 C 5H 120 2 0G 300.000 5000.000  
 1389.000 61  
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 14 2  
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 3.49638594E+04+2.35201019E+01+0.00000000E+00 4  
 CC5H1102H 17/8/15 C 5H 120 2 0G 300.000 5000.000  
 1406.000 61  
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 DC5H1102H 17/8/15 C 5H 120 2 0G 300.000 5000.000  
 1397.000 61  
 +2.08513274E+01+2.60811030E-02-8.91735578E-06+1.38397232E-09-8.02716539E-  
 14 2  
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 AC5H1102 17/8/15 C 5H 110 2 0G 300.000 5000.000  
 1396.000 51  
 +1.98700905E+01+2.47772405E-02-8.46413614E-06+1.31283774E-09-7.61129402E-  
 14 2

-2.04831687E+04-7.43156588E+01+3.54375282E-01+7.21758552E-02-5.35556462E-05 3  
 +2.12668171E-08-3.51577739E-12-  
 1.38320365E+04+2.99444593E+01+0.00000000E+00 4  
 BC5H1102 17/8/15 C 5H 110 2 OG 300.000 5000.000  
 1386.000 51  
 +1.97546009E+01+2.47324523E-02-8.41611775E-06+1.30187335E-09-7.53316999E-14 2  
 -2.44671820E+04-7.68414190E+01+1.53424363E+00+6.94504944E-02-5.16917529E-05 3  
 +2.08690207E-08-3.52552510E-12-  
 1.82806722E+04+2.03720098E+01+0.00000000E+00 4  
 CC5H1102 17/8/15 C 5H 110 2 OG 300.000 5000.000  
 1405.000 51  
 +2.02075561E+01+2.39554458E-02-8.06286681E-06+1.23797865E-09-7.12608001E-14 2  
 -2.23074093E+04-7.73358025E+01+7.15981794E-01+7.44249188E-02-5.92758872E-05 3  
 +2.52115515E-08-4.38572885E-12-  
 1.60198108E+04+2.56128856E+01+0.00000000E+00 4  
 DC5H1102 17/8/15 C 5H 110 2 OG 300.000 5000.000  
 1396.000 51  
 +1.98700905E+01+2.47772405E-02-8.46413614E-06+1.31283774E-09-7.61129402E-14 2  
 -2.04831687E+04-7.50051405E+01+3.54375282E-01+7.21758552E-02-5.35556462E-05 3  
 +2.12668171E-08-3.51577739E-12-  
 1.38320365E+04+2.92549776E+01+0.00000000E+00 4  
 AC5H110 17/8/15 C 5H 110 1 OG 300.000 5000.000  
 1400.000 41  
 +1.82339413E+01+2.37923987E-02-8.07056384E-06+1.24592855E-09-7.19996103E-14 2  
 -1.87450473E+04-6.87958505E+01+8.43924842E-01+6.29723769E-02-4.12079336E-05 3  
 +1.37396229E-08-1.84097585E-12-  
 1.25819035E+04+2.50753974E+01+0.00000000E+00 4  
 BC5H110 17/8/15 C 5H 110 1 OG 300.000 5000.000  
 1378.000 41  
 +1.85549393E+01+2.44786662E-02-8.51926880E-06+1.33803108E-09-7.82547188E-14 2  
 -2.23664355E+04-7.33946136E+01+3.67366095E+00+5.17139422E-02-2.49457898E-05 3  
 +4.54084943E-09-3.31184982E-14-  
 1.63228000E+04+9.40461313E+00+0.00000000E+00 4  
 CC5H110 17/8/15 C 5H 110 1 OG 300.000 5000.000  
 1409.000 41  
 +1.83213656E+01+2.35429297E-02-7.94470460E-06+1.22205357E-09-7.04356618E-14 2  
 -2.06340316E+04-7.05656058E+01+6.91613929E-01+6.60697133E-02-4.75285795E-05 3  
 +1.81072449E-08-2.84499699E-12-  
 1.46546569E+04+2.36233979E+01+0.00000000E+00 4  
 DC5H110 17/8/15 C 5H 110 1 OG 300.000 5000.000  
 1400.000 41  
 +1.82339413E+01+2.37923987E-02-8.07056384E-06+1.24592855E-09-7.19996103E-14 2  
 -1.87450473E+04-6.94853322E+01+8.43924842E-01+6.29723769E-02-4.12079336E-05 3

+1.37396229E-08-1.84097585E-12-  
1.25819035E+04+2.43859158E+01+0.00000000E+00 4  
AC5H100OH-A 17/8/15 C 5H 110 2 0G 300.000 5000.000  
1398.000 61  
+2.02759160E+01+2.40402125E-02-8.21726177E-06+1.27508622E-09-7.39470430E-  
14 2  
-1.25890306E+04-7.45432540E+01-8.93967860E-02+7.48083410E-02-5.79088207E-  
05 3  
+2.38676428E-08-4.05836117E-12-  
5.79120759E+03+3.37720278E+01+0.00000000E+00 4  
AC5H100OH-B 17/8/15 C 5H 110 2 0G 300.000 5000.000  
1390.000 61  
+1.90362050E+01+2.51437855E-02-8.60836129E-06+1.33715660E-09-7.76005723E-  
14 2  
-1.49721354E+04-6.67702235E+01+3.65133886E+00+5.70948447E-02-3.30634881E-  
05 3  
+9.52430167E-09-1.08604128E-12-  
9.15524576E+03+1.73958096E+01+0.00000000E+00 4  
AC5H100OH-C 17/8/15 C 5H 110 2 0G 300.000 5000.000  
1402.000 61  
+1.94269993E+01+2.45167400E-02-8.32902433E-06+1.28716724E-09-7.44370182E-  
14 2  
-1.38808710E+04-6.93043169E+01+1.24166589E+00+6.55076365E-02-4.30153204E-  
05 3  
+1.43717235E-08-1.92812556E-12-  
7.43857517E+03+2.88519661E+01+0.00000000E+00 4  
AC5H100OH-D 17/8/15 C 5H 110 2 0G 300.000 5000.000  
1398.000 61  
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14 2  
-1.25890306E+04-7.45432540E+01-8.93967860E-02+7.48083410E-02-5.79088207E-  
05 3  
+2.38676428E-08-4.05836117E-12-  
5.79120759E+03+3.37720278E+01+0.00000000E+00 4  
BC5H100OH-A 17/8/15 C 5H 110 2 0G 300.000 5000.000  
1389.000 61  
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14 2  
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05 3  
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14 2  
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14 2  
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CC5H10OOH-A 17/8/15 C 5H 110 2 OG 300.000 5000.000  
 1407.000 61  
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 +2.76118292E-08-4.88689574E-12-  
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 +1.37408612E-08-2.01545549E-12-  
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 1398.000 61  
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 A-BC5H100 17/8/15 C 5H 100 1 OG 300.000 5000.000  
 1424.000 31



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+1.99929340E-08-3.05569594E-12-  
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B-CC5H100 9/ 8/14 C 5H 100 1 OG 300.000 5000.000  
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AC5H100OH-AO2 8/15 C 5H 110 4 OG 300.000 5000.000  
1397.000 71  
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AC5H100OH-BO2 8/15 C 5H 110 4 OG 300.000 5000.000  
1389.000 71  
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AC5H10OOH-DO2 8/15 C 5H 110 4 OG 300.000 5000.000  
1397.000 71  
+2.49284926E+01+2.49502228E-02-8.57455029E-06+1.33547829E-09-7.76537998E-14 2  
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BC5H10OOH-AO2 8/15 C 5H 110 4 OG 300.000 5000.000  
1389.000 71  
+2.48032671E+01+2.49329192E-02-8.54000436E-06+1.32701219E-09-7.70333881E-14 2  
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BC5H10OOH-CO2 8/15 C 5H 110 4 OG 300.000 5000.000  
1396.000 71  
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BC5H10OOH-DO2 8/15 C 5H 110 4 OG 300.000 5000.000  
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 DC5H10OOH-CO2 8/15 C 5H 110 4 OG 300.000 5000.000  
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 C5H9A-C,DOOH 8/15 C 5H 110 4 OG 300.000 5000.000  
 1406.000 81  
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 1681.000 81

+2.63011187E+01+2.38231644E-02-8.29527214E-06+1.30384489E-09-7.63133641E-14 2  
-2.62801782E+04-1.01764259E+02+2.40737385E+00+7.31844750E-02-4.34551328E-05 3  
+1.06843813E-08-6.06073375E-13-  
1.74826725E+04+2.86070302E+01+0.00000000E+00 4  
C5H9C-A,BOOH 8/15 C 5H 110 4 OG 300.000 5000.000  
1393.000 81  
+2.49289305E+01+2.44398284E-02-8.37848298E-06+1.30269965E-09-7.56543783E-14 2  
-2.90312299E+04-9.50950095E+01+3.83902707E+00+7.67534526E-02-5.93019661E-05 3  
+2.43350243E-08-4.12011052E-12-  
2.19645331E+04+1.71683879E+01+0.00000000E+00 4  
C5H9C-A,DOOH 8/15 C 5H 110 4 OG 300.000 5000.000  
1681.000 81  
+2.63011187E+01+2.38231644E-02-8.29527214E-06+1.30384489E-09-7.63133641E-14 2  
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C5H9C-B,DOOH 8/15 C 5H 110 4 OG 300.000 5000.000  
1393.000 81  
+2.49289305E+01+2.44398284E-02-8.37848298E-06+1.30269965E-09-7.56543783E-14 2  
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C5H9D-A,BOOH 8/15 C 5H 110 4 OG 300.000 5000.000  
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C5H9A-COOH 9/ 8/14 C 5H 100 2 OG 300.000 5000.000  
1396.000 51  
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C5H9A-DOOH 9/ 8/14 C 5H 100 2 OG 300.000 5000.000  
1393.000 51  
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+2.06470792E-08-3.33664189E-12-  
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C5H9B-DOOH 9/ 8/14 C 5H 100 2 OG 300.000 5000.000  
1385.000 51  
+2.11330268E+01+2.15086873E-02-7.42113144E-06+1.15934717E-09-6.75687044E-14 2  
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C5H9C-AOOH 9/ 8/14 C 5H 100 2 OG 300.000 5000.000  
1396.000 51  
+1.95116301E+01+2.27723060E-02-7.82629606E-06+1.21895173E-09-7.08783753E-14 2  
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C5H9OA-AOOH-B 8/15 C 5H 100 3 0G 300.000 5000.000  
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+3.42124943E-08-5.80022917E-12-  
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C5H9OA-BOOH-A 8/15 C 5H 100 3 0G 300.000 5000.000  
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C5H9OA-BOOH-C 8/15 C 5H 100 3 0G 300.000 5000.000  
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C5H9OA-COOH-A 8/15 C 5H 100 3 0G 300.000 5000.000  
1416.000 41  
+2.19787258E+01+2.27762232E-02-7.64127053E-06+1.17119291E-09-6.73502124E-  
14 2  
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05 3  
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+4.41170689E-08-8.01854503E-12-  
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C5H9OA-COOH-D 8/15 C 5H 100 3 OG 300.000 5000.000  
1416.000 41  
+2.19787258E+01+2.27762232E-02-7.64127053E-06+1.17119291E-09-6.73502124E-14 2  
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C5H9OA-DOOH-A 8/15 C 5H 100 3 OG 300.000 5000.000  
1412.000 31  
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C5H9OA-DOOH-B 8/15 C 5H 100 3 OG 300.000 5000.000  
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C5H9OB-COOH-A 8/15 C 5H 100 3 OG 300.000 5000.000  
1427.000 51  
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C5H9OB-COOH-D 8/15 C 5H 100 3 OG 300.000 5000.000  
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+2.33660026E+01+2.12967547E-02-7.16311642E-06+1.10028483E-09-6.33839052E-14 2  
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C5H9OB-DOOH-A 9/14 C 5H 100 3 OG 300.000 5000.000  
1420.000 41



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 C5H9OB-DOOH-C 9/14 C 5H 100 3 OG 300.000 5000.000  
 1416.000 41  
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 C5H9OC-DOOH-A 8/15 C 5H 100 3 OG 300.000 5000.000  
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4.31638560E+04+1.74830999E+01+0.00000000E+00 4  
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1396.000 61  
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4.09936393E+04+2.25509833E+01+0.00000000E+00 4  
IC5KETCA 17/8/15 C 5H 100 3 OG 300.000 5000.000  
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4.52388966E+04+1.90774795E+01+0.00000000E+00 4  
IC5KETCB 17/8/15 C 5H 100 3 OG 300.000 5000.000  
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IC5KETDB 17/8/15 C 5H 100 3 OG 300.000 5000.000  
1381.000 61  
+2.22545164E+01+2.21858094E-02-7.54539826E-06+1.16735178E-09-6.75734913E-14 2  
-5.19970461E+04-8.78431657E+01+2.45036196E+00+6.83213847E-02-4.82822981E-05 3  
+1.73840001E-08-2.52418883E-12-  
4.51554184E+04+1.84815016E+01+0.00000000E+00 4  
IC5KETDC 17/8/15 C 5H 100 3 OG 300.000 5000.000  
1391.000 61  
+2.57459735E+01+1.95157132E-02-6.70259887E-06+1.04493380E-09-6.08454008E-14 2  
-4.96555982E+04-1.04885682E+02-2.47013912E+00+9.30872396E-02-8.13203099E-05 3

+3.57768012E-08-6.26400503E-12-  
4.06868372E+04+4.38329357E+01+0.00000000E+00 4  
IC5KETAAO 17/8/15 C 5H 90 2 0G 300.000 5000.000  
1670.000 41  
+1.54491093E+01+2.58830088E-02-9.38194545E-06+1.51919963E-09-9.08764412E-  
14 2  
-2.73128942E+04-4.89349130E+01+6.20340512E+00+3.78488938E-02-8.21632367E-  
06 3  
-4.45998794E-09+1.69104440E-12-  
2.33706795E+04+3.88282175E+00+0.00000000E+00 4  
IC5KETABO 17/8/15 C 5H 90 2 0G 300.000 5000.000  
1680.000 41  
+1.74003757E+01+2.43634015E-02-8.89217693E-06+1.44672950E-09-8.68336325E-  
14 2  
-2.96359315E+04-6.26150618E+01+2.44492593E+00+5.39988220E-02-2.76353434E-  
05 3  
+5.14986988E-09-2.28548561E-14-  
2.42538749E+04+1.91347808E+01+0.00000000E+00 4  
IC5KETACO 17/8/15 C 5H 90 2 0G 300.000 5000.000  
1405.000 41  
+1.87759820E+01+2.09363794E-02-7.11851372E-06+1.10072541E-09-6.36812526E-  
14 2  
-3.10560920E+04-6.84256552E+01+3.17102493E+00+5.52252992E-02-3.48045866E-  
05 3  
+1.07470812E-08-1.26264879E-12-  
2.54634549E+04+1.60763592E+01+0.00000000E+00 4  
IC5KETADO 17/8/15 C 5H 90 2 0G 300.000 5000.000  
1670.000 41  
+1.54491093E+01+2.58830088E-02-9.38194545E-06+1.51919963E-09-9.08764412E-  
14 2  
-2.73128942E+04-4.89349130E+01+6.20340512E+00+3.78488938E-02-8.21632367E-  
06 3  
-4.45998794E-09+1.69104440E-12-  
2.33706795E+04+3.88282175E+00+0.00000000E+00 4  
IC5KETCAO 17/8/15 C 5H 90 2 0G 300.000 5000.000  
1514.000 41  
+1.72485932E+01+2.16326796E-02-7.22890702E-06+1.10467817E-09-6.33813429E-  
14 2  
-3.21371394E+04-5.86643290E+01+4.75737279E+00+4.52905574E-02-2.09520730E-  
05 3  
+2.65371883E-09+4.60703138E-13-  
2.73333149E+04+1.02325004E+01+0.00000000E+00 4  
IC5KETCBO 17/8/15 C 5H 90 2 0G 300.000 5000.000  
1510.000 41  
+1.93742496E+01+2.06425485E-02-7.06983683E-06+1.09902869E-09-6.38342204E-  
14 2  
-3.47003768E+04-7.43848166E+01+4.60922258E+00+4.63105317E-02-1.85546802E-  
05 3  
-2.86158793E-10+1.27532426E-12-  
2.87895902E+04+7.87701574E+00+0.00000000E+00 4  
IC5KETCDO 17/8/15 C 5H 90 2 0G 300.000 5000.000  
1489.000 41  
+1.78986194E+01+2.13374499E-02-7.19313241E-06+1.10668165E-09-6.38266549E-  
14 2  
-3.16063716E+04-6.33320448E+01+7.66113508E+00+3.31212888E-02-2.76253288E-  
06 3  
-8.32131128E-09+2.78275744E-12-2.68823428E+04-  
4.11946991E+00+0.00000000E+00 4

IC5KETDAO 17/8/15 C 5H 90 2 OG 300.000 5000.000  
 1485.000 41  
 +1.95835650E+01+2.02788959E-02-6.90312559E-06+1.06869517E-09-6.18931202E-  
 14 2  
 -2.89934666E+04-7.27514739E+01+2.77854914E+00+5.49042648E-02-3.12957279E-  
 05 3  
 +7.33340136E-09-3.35699979E-13-  
 2.28103088E+04+1.89499650E+01+0.00000000E+00 4  
 IC5KETDBO 17/8/15 C 5H 90 2 OG 300.000 5000.000  
 1519.000 41  
 +2.00669200E+01+2.02402238E-02-6.97500713E-06+1.08902290E-09-6.34524956E-  
 14 2  
 -3.25858999E+04-7.80517736E+01+5.21028340E+00+4.44018385E-02-1.51327339E-  
 05 3  
 -2.59536762E-09+1.79445594E-12-  
 2.64639770E+04+5.32661738E+00+0.00000000E+00 4  
 IC5KETDCO 17/8/15 C 5H 90 2 OG 300.000 5000.000  
 1385.000 41  
 +2.06749614E+01+2.01791491E-02-7.04935407E-06+1.11015087E-09-6.50552099E-  
 14 2  
 -3.08738095E+04-8.00272702E+01+1.74667514E+00+6.15641942E-02-4.06488995E-  
 05 3  
 +1.31250854E-08-1.65755406E-12-  
 2.40252952E+04+2.26218438E+01+0.00000000E+00 4  
 AC5H10OH 17/8/15 C 5H 110 1 OG 300.000 5000.000  
 1396.000 51  
 +1.64350382E+01+2.48732260E-02-8.43959366E-06+1.30322470E-09-7.53261177E-  
 14 2  
 -2.28956938E+04-5.51681478E+01+1.23496772E+00+5.48298602E-02-2.85379159E-  
 05 3  
 +6.14801654E-09-2.41162327E-13-  
 1.70643706E+04+2.84296007E+01+0.00000000E+00 4  
 BC5H10OH 17/8/15 C 5H 110 1 OG 300.000 5000.000  
 1384.000 51  
 +1.69551854E+01+2.50397308E-02-8.62897621E-06+1.34632322E-09-7.83770200E-  
 14 2  
 -2.52556374E+04-6.12549178E+01+2.16094248E+00+5.26897228E-02-2.56800949E-  
 05 3  
 +4.72180512E-09-1.32098054E-14-  
 1.93564411E+04+2.07680728E+01+0.00000000E+00 4  
 CC5H10OH 17/8/15 C 5H 110 1 OG 300.000 5000.000  
 1408.000 51  
 +1.76376123E+01+2.33184854E-02-7.78464125E-06+1.18857749E-09-6.81463457E-  
 14 2  
 -2.21964329E+04-6.38737345E+01-1.66278849E+00+7.47656913E-02-6.14804272E-  
 05 3  
 +2.69357912E-08-4.78920793E-12-  
 1.61297989E+04+3.75225406E+01+0.00000000E+00 4  
 AO2C5H10OH 17/8/15 C 5H 110 3 OG 300.000 5000.000  
 1391.000 61  
 +2.19522107E+01+2.48781991E-02-8.44297007E-06+1.30371698E-09-7.53469325E-  
 14 2  
 -4.34404184E+04-8.34515565E+01+1.20882689E+00+7.78602587E-02-6.16377315E-  
 05 3  
 +2.60506873E-08-4.52025263E-12-  
 3.66524607E+04+2.64078764E+01+0.00000000E+00 4  
 BO2C5H10OH 17/8/15 C 5H 110 3 OG 300.000 5000.000  
 1395.000 61

+2.28865971E+01+2.40778073E-02-8.16957904E-06+1.26165301E-09-7.29326115E-  
14 2  
-4.48764864E+04-8.92415513E+01+2.71004906E+00+7.28069687E-02-5.37414655E-  
05 3  
+2.08815586E-08-3.34176454E-12-  
3.80276500E+04+1.85552934E+01+0.00000000E+00 4  
CO2C5H10OH 17/8/15 C 5H 110 3 OG 300.000 5000.000  
1406.000 61  
+2.22413769E+01+2.43138793E-02-8.17987283E-06+1.25568258E-09-7.22730962E-  
14 2  
-4.13059915E+04-8.36980772E+01-1.39598520E-01+8.39732940E-02-7.03813054E-  
05 3  
+3.10327500E-08-5.52297544E-12-  
3.42801244E+04+3.38677944E+01+0.00000000E+00 4  
IC3H5COCH3 9/ 8/14 C 5H 80 1 OG 300.000 5000.000  
1392.000 31  
+1.49935813E+01+1.97788403E-02-6.78313207E-06+1.05481230E-09-6.12614698E-  
14 2  
-2.60877929E+04-5.26202086E+01+1.54292407E+00+5.05432300E-02-3.42434122E-  
05 3  
+1.25252368E-08-1.95302231E-12-  
2.12702785E+04+1.99855884E+01+0.00000000E+00 4  
IC3H5COCH2 9/ 8/14 C 5H 70 1 OG 300.000 5000.000  
1394.000 31  
+1.62814836E+01+1.63492954E-02-5.64820836E-06+8.82756224E-10-5.14522209E-  
14 2  
-4.28650692E+03-5.91075528E+01+1.42097745E+00+5.34336638E-02-4.21903633E-  
05 3  
+1.76937615E-08-3.06075290E-  
12+6.91082980E+02+1.99522060E+01+0.00000000E+00 4  
AC3H4COCH3 9/ 8/14 C 5H 70 1 OG 300.000 5000.000  
1384.000 21  
+1.60405803E+01+1.62938876E-02-5.49275040E-06+8.45442040E-10-4.87866397E-  
14 2  
-8.30972832E+03-5.83003416E+01+9.48806278E-01+5.17869173E-02-3.74867620E-  
05 3  
+1.40294881E-08-2.14698694E-12-  
3.10553556E+03+2.26479362E+01+0.00000000E+00 4  
NEOC5H12 9/ 8/14 C 5H 12 0 OG 300.000 5000.000  
1459.000 41  
+2.13410465E+01+2.32500105E-02-8.36387815E-06+1.34306692E-09-7.97752777E-  
14 2  
-3.18056043E+04-1.00649903E+02+8.60482114E-01+4.63444251E-02+2.26557531E-  
06 3  
-1.91739545E-08+6.07291520E-12-  
2.24020628E+04+1.78235950E+01+0.00000000E+00 4  
NEOC5H11 9/ 8/14 C 5H 11 0 OG 300.000 5000.000  
1375.000 41  
+1.17983312E+01+3.59579648E-02-1.44108662E-05+2.46307665E-09-1.52118262E-  
13 2  
-3.86101387E+03-4.41297337E+01+9.68072098E+00+7.07718151E-03+4.53301778E-  
05 3  
-3.61952123E-08+8.06654396E-12+1.05116941E+03-  
1.94358274E+01+0.00000000E+00 4  
NEOC5H11O2H 9/8/14 C 5H 120 2 OG 300.000 5000.000  
2019.000 61  
+2.01975284E+01+2.97380281E-02-1.09930813E-05+1.80338361E-09-1.08851734E-  
13 2

-3.95165952E+04-8.23753662E+01+3.55225748E-01+6.91131421E-02-3.61242956E-05 3  
+6.97537323E-09-9.54855674E-14-  
3.23388889E+04+2.61109340E+01+0.00000000E+00 4  
NEOC5H11O2 9/8/14 C 5H 11O 2 OG 300.000 5000.000  
1682.000 51  
+1.93713105E+01+2.82612571E-02-1.04670110E-05+1.71917414E-09-1.03854375E-13 2  
-2.23544131E+04-7.71662358E+01+1.08144664E+00+6.33534647E-02-3.11938784E-05 3  
+4.88883786E-09+2.48584189E-13-  
1.56455031E+04+2.32475108E+01+0.00000000E+00 4  
NEOC5H11O 9/ 8/14 C 5H 11O 1 OG 300.000 5000.000  
1374.000 41  
+1.47920426E+01+3.60239861E-02-1.44548775E-05+2.47285304E-09-1.52828569E-13 2  
-2.12880602E+04-5.86605592E+01+1.11399567E+01+9.95551445E-03+4.37547263E-05 3  
-3.60663886E-08+8.13722634E-12-1.57739963E+04-  
2.54644054E+01+0.00000000E+00 4  
NEOC5H10OOH 9/8/14 C 5H 11O 2 OG 300.000 5000.000  
1686.000 61  
+1.98216577E+01+2.74351153E-02-1.01763800E-05+1.67311287E-09-1.01142157E-13 2  
-1.44846637E+04-7.65499851E+01+7.26388728E-01+6.54763558E-02-3.46433563E-05 3  
+6.82220142E-09-1.22217205E-13-  
7.61522056E+03+2.77840799E+01+0.00000000E+00 4  
NEO-C5H10O 9/ 8/14 C 5H 10O 1 OG 300.000 5000.000  
1465.000 21  
+1.88696363E+01+2.18446364E-02-7.48656898E-06+1.16574180E-09-6.78305009E-14 2  
-2.76538327E+04-8.33848438E+01-5.80125483E+00+7.19986445E-02-4.12060995E-05 3  
+8.52947622E-09+2.15532151E-14-  
1.85918283E+04+5.13449073E+01+0.00000000E+00 4  
NEOC5H10OOH-O2 914 C 5H 11O 4 OG 300.000 5000.000  
2038.000 71  
+2.43460937E+01+2.84840536E-02-1.05961421E-05+1.74545495E-09-1.05654571E-13 2  
-3.35348323E+04-9.58566184E+01+2.12490773E+00+7.51548100E-02-4.39349794E-05 3  
+1.09212325E-08-8.06703541E-13-  
2.57458785E+04+2.47165260E+01+0.00000000E+00 4  
NEOC5H9Q2 9/ 8/14 C 5H 11O 4 OG 300.000 5000.000  
2050.000 81  
+2.48112747E+01+2.76461534E-02-1.03017544E-05+1.69884890E-09-1.02912689E-13 2  
-2.56663214E+04-9.64118626E+01+1.90419491E+00+7.68023849E-02-4.67666506E-05 3  
+1.25175307E-08-1.11211508E-12-  
1.77393477E+04+2.75076242E+01+0.00000000E+00 4  
NEOC5KET 9/ 8/14 C 5H 10O 3 OG 300.000 5000.000  
1396.000 61  
+2.11457411E+01+2.34263362E-02-8.03514708E-06+1.24990645E-09-7.26173329E-14 2  
-4.99812693E+04-8.04502172E+01+1.99299705E+00+6.63799852E-02-4.41434233E-05 3

+1.47656228E-08-1.97164356E-12-  
4.31727732E+04+2.30090729E+01+0.00000000E+00 4  
NEOC5KETOX 9/ 8/14 C 5H 90 2 0G 300.000 5000.000  
1677.000 41  
+1.62834087E+01+2.47667618E-02-8.89982283E-06+1.43325482E-09-8.54232652E-  
14 2  
-2.99100005E+04-5.60198008E+01+3.76958673E+00+4.84037082E-02-2.22215659E-  
05 3  
+2.98251470E-09+2.98064950E-13-  
2.52993970E+04+1.27918996E+01+0.00000000E+00 4  
NEOC5KEJOL 9/ 8/14 C 5H 90 2 0G 300.000 5000.000  
1402.000 51  
+1.78858167E+01+2.12423369E-02-7.21947714E-06+1.11609095E-09-6.45625691E-  
14 2  
-3.87680922E+04-6.36233643E+01+1.30298806E+00+5.84132694E-02-3.81961088E-  
05 3  
+1.24622441E-08-1.59437417E-12-  
3.28976593E+04+2.59154966E+01+0.00000000E+00 4  
NEOC5H9O-OOH 9/14 C 5H 100 3 0G 300.000 5000.000  
1429.000 41  
+2.34301312E+01+2.26473800E-02-7.84730788E-06+1.22994662E-09-7.18633905E-  
14 2  
-3.86378493E+04-1.00093171E+02-4.33879286E+00+8.23095013E-02-5.24634537E-  
05 3  
+1.40859094E-08-1.00626405E-12-  
2.87630624E+04+5.04065995E+01+0.00000000E+00 4  
PC4H8CHO-1O2 10/8/15 C 5H 90 3 0G 300.000 5000.000  
1385.000 51  
+2.46719452E+01+1.85504127E-02-6.42209840E-06+1.00647312E-09-5.88171032E-  
14 2  
-3.18555321E+04-9.71440808E+01-4.63291072E-01+8.02504798E-02-6.47236563E-  
05 3  
+2.62037194E-08-4.25127975E-12-  
2.34955268E+04+3.66761324E+01+0.00000000E+00 4  
PC4H8CHO-2O2 10/8/15 C 5H 90 3 0G 300.000 5000.000  
1404.000 51  
+2.16725120E+01+2.03883823E-02-6.89025420E-06+1.06159257E-09-6.12789415E-  
14 2  
-3.20581874E+04-8.08233009E+01+3.75698588E+00+5.99220385E-02-3.84711370E-  
05 3  
+1.16653123E-08-1.26664695E-12-  
2.57207120E+04+1.60217605E+01+0.00000000E+00 4  
PC4H8CHO-3O2 10/8/15 C 5H 90 3 0G 300.000 5000.000  
1404.000 51  
+2.16725120E+01+2.03883823E-02-6.89025420E-06+1.06159257E-09-6.12789415E-  
14 2  
-3.20581874E+04-8.08233009E+01+3.75698588E+00+5.99220385E-02-3.84711370E-  
05 3  
+1.16653123E-08-1.26664695E-12-  
2.57207120E+04+1.60217605E+01+0.00000000E+00 4  
PC4H8CHO-4O2 10/8/15 C 5H 90 3 0G 300.000 5000.000  
1385.000 51  
+2.12856144E+01+2.12771293E-02-7.31814716E-06+1.14082494E-09-6.63900040E-  
14 2  
-3.02079416E+04-7.82029614E+01+3.37850952E+00+5.77659231E-02-3.28975023E-  
05 3  
+7.80995858E-09-4.14571925E-13-  
2.35309122E+04+1.97380195E+01+0.00000000E+00 4

C4H7CHO-2 10/8/15 THERMC 5H 80 1 0G 300.000 5000.000  
1390.000 31  
+1.62588601E+01+1.87787531E-02-6.45805165E-06+1.00641261E-09-5.85466414E-  
14 2  
-2.44023233E+04-5.96450353E+01+3.69688874E-04+5.71382743E-02-4.15287925E-  
05 3  
+1.58289787E-08-2.49867087E-12-  
1.87655817E+04+2.75869712E+01+0.00000000E+00 4  
C4H7CHO-3 10/8/15 THERMC 5H 80 1 0G 300.000 5000.000  
1385.000 31  
+1.55930799E+01+1.96344789E-02-6.81722246E-06+1.06912344E-09-6.24665079E-  
14 2  
-2.08408048E+04-5.47830431E+01+4.14190085E-01+5.12150376E-02-3.06682310E-  
05 3  
+8.72168876E-09-9.15725235E-13-  
1.51552520E+04+2.81574532E+01+0.00000000E+00 4  
C4H7CHO-4 10/8/15 THERMC 5H 80 1 0G 300.000 5000.000  
2020.000 31  
+1.37156197E+01+2.16425024E-02-7.67112142E-06+1.22483309E-09-7.25906717E-  
14 2  
-1.91110565E+04-4.33806662E+01+1.15814338E+00+4.81746752E-02-2.67363172E-  
05 3  
+6.50396537E-09-4.78416928E-13-  
1.47390215E+04+2.46792248E+01+0.00000000E+00 4  
NC3H7COCH3 10/6/15 THERMC 5H 100 1 0G 300.000 5000.000  
1387.000 41  
+1.59632618E+01+2.26394805E-02-7.56430418E-06+1.15632032E-09-6.63757297E-  
14 2  
-3.92822369E+04-5.65033421E+01+2.22465879E+00+4.82791863E-02-2.21019858E-  
05 3  
+2.64029906E-09+5.23720489E-13-  
3.39379060E+04+1.94495002E+01+0.00000000E+00 4  
C2H5COC2H5 10/6/15 THERMC 5H 100 1 0G 300.000 5000.000  
1421.000 41  
+1.65155931E+01+2.18966306E-02-7.26184066E-06+1.10537530E-09-6.32910022E-  
14 2  
-3.96722497E+04-6.11243728E+01+3.04335984E+00+4.24811577E-02-1.12087588E-  
05 3  
-5.05051822E-09+2.35367193E-12-  
3.40615638E+04+1.48305047E+01+0.00000000E+00 4  
NC3H7COCH2 10/6/15 THERMC 5H 90 1 0G 300.000 5000.000  
1393.000 41  
+1.72611127E+01+1.91828746E-02-6.41680319E-06+9.82027213E-10-5.64270287E-  
14 2  
-1.74829806E+04-6.30397964E+01+2.14964962E+00+5.09715972E-02-2.97744827E-  
05 3  
+7.64275255E-09-5.47753503E-13-  
1.19838512E+04+1.91969246E+01+0.00000000E+00 4  
CH3CH2CHCOCH3 10/6/15 C 5H 90 1 0G 300.000 5000.000  
1428.000 41  
+1.53040392E+01+2.03924168E-02-6.74389287E-06+1.02444156E-09-5.85693457E-  
14 2  
-1.95765010E+04-4.96835091E+01+3.62180151E+00+3.78869197E-02-9.52099354E-  
06 3  
-4.70140858E-09+2.11456934E-12-  
1.46643385E+04+1.63246571E+01+0.00000000E+00 4  
CH3CHCH2COCH3 10/6/15 C 5H 90 1 0G 300.000 5000.000  
1313.000 41



+1.45647685E+01+2.10276788E-02-6.95711397E-06+1.05654321E-09-6.03737583E-14 2  
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CH2CH2CH2COCH3 10/6/15 C 5H 90 1 OG 300.000 5000.000  
2010.000 41  
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+6.44110554E-09-5.11322699E-13-  
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CH2CH2COC2H5 10/6/15 C 5H 90 1 OG 300.000 5000.000  
1418.000 41  
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CH3CHCOC2H5 10/6/15 C 5H 90 1 OG 300.000 5000.000  
1426.000 41  
+1.52590939E+01+2.06874083E-02-6.90185396E-06+1.05491074E-09-6.05775562E-14 2  
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-1.01813061E-08+3.34232716E-12-  
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NC52ONEO2-3 10/8/15 C 5H 90 3 OG 300.000 5000.000  
1389.000 51  
+2.32384890E+01+1.91383699E-02-6.48795686E-06+1.00265179E-09-5.80286197E-14 2  
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+2.51922695E-08-4.15673555E-12-  
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NC52ONEO2-4 10/8/15 C 5H 90 3 OG 300.000 5000.000  
1419.000 51  
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+1.07130185E-08-1.15039744E-12-  
2.95536320E+04+1.27650471E+01+0.00000000E+00 4  
NC52ONEO2-5 10/8/15 C 5H 90 3 OG 300.000 5000.000  
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+6.76825508E-09-2.84375003E-13-  
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NC53ONEO2-1 10/8/15 C 5H 90 3 OG 300.000 5000.000  
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 -5.62683827E-09+2.63012314E-12-  
 2.73321757E+04+1.51181731E+01+0.00000000E+00 4  
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 1386.000 51  
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 NC52ONE-3 10/ 8/15 THERMC 5H 80 1 OG 300.000 5000.000  
 1388.000 31  
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 +1.26179448E-08-1.96289033E-12-  
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 NC52ONE-4 10/ 8/15 THERMC 5H 80 1 OG 300.000 5000.000  
 1395.000 31  
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 NC53ONE-1 10/ 8/15 THERMC 5H 80 1 OG 300.000 5000.000  
 1388.000 31  
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 C5H10OH11 10/ 7/15 THERMC 5H 110 1 OG 300.000 5000.000  
 1394.000 51  
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C5H9OH1-3 10/ 8/15 C 5H 100 1 0G 300.000 5000.000  
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PC4H8CHO-1 C 5H 90 1 0G 300.000 5000.000  
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PC4H8CHO-2 C 5H 90 1 0G 300.000 5000.000  
1426.000 41

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 PC4H8CHO-3 C 5H 9O 1 OG 300.000 5000.000  
 1426.000 41  
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 C5H9O12-5 C 5H 9O 1 OG 300.000 5000.000  
 1428.000 31  
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 14 2

```

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+2.46895048E-08-3.96232760E-
12+7.08653513E+03+5.15668737E+01+0.00000000E+00      4
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1458.000      21
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05      3
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12+6.54668516E+03+5.80476602E+01+0.00000000E+00      4
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05      3
+2.72423613E-08-4.41750289E-12-
3.23749643E+03+6.36020351E+01+0.00000000E+00      4
C5H9O23-1      C      5H      9O      1      OG      300.000      5000.000
1424.000      31
+1.77401551E+01+1.92298085E-02-6.43473125E-06+9.84654362E-10-5.65624830E-
14      2
-2.05448135E+03-6.82408862E+01-4.67636252E+00+7.74809264E-02-6.42244373E-
05      3
+2.68440080E-08-4.43868315E-
12+4.97926865E+03+4.97877901E+01+0.00000000E+00      4
C5H9O23-5      C      5H      9O      1      OG      300.000      5000.000
1424.000      31
+1.77401551E+01+1.92298085E-02-6.43473125E-06+9.84654362E-10-5.65624830E-
14      2
-2.05448135E+03-6.82408862E+01-4.67636252E+00+7.74809264E-02-6.42244373E-
05      3
+2.68440080E-08-4.43868315E-
12+4.97926865E+03+4.97877901E+01+0.00000000E+00      4
C5H9O24-1      C      5H      9O      1      OG      300.000      5000.000
1398.000      21
+1.40157807E+01+2.51554423E-02-1.11149003E-05+2.14885206E-09-1.44559627E-
13      2
-1.54769089E+03-4.88521063E+01-6.45048964E+00+8.25684509E-02-7.30635550E-
05      3
+3.23767886E-08-5.72480023E-
12+4.47417427E+03+5.74524602E+01+0.00000000E+00      4
!-----
!-----
!----- AJOUT DAGAUT -----
!-----
NO      N      1O      1O      0O      OG      300.00      5000.00      1000.00
1
0.32454400E+01 0.12691400E-02-0.50159000E-06 0.91690000E-10-0.62800000E-
14      2
0.98008000E+04 0.64170000E+01 0.33765400E+01 0.12530600E-02-0.33027500E-
05      3
0.52178100E-08-0.24462600E-11 0.98180000E+04 0.58300000E+01
4
NO2      N      1O      2O      0O      OG      300.00      5000.00      1000.00
1

```

0.46828600E+01 0.24624300E-02-0.10422600E-05 0.19769000E-09-0.13920000E-  
 13 2  
 0.22613000E+04 0.98900000E+00 0.26706000E+01 0.78385000E-02-0.80638600E-  
 05 3  
 0.61617100E-08-0.23201500E-11 0.28963000E+04 0.11612000E+02  
 4  
 CH3NO Nitrosomethyl2/09C 1.H 3.N 1.O 1.G 200.000 6000.000 1000.00  
 1  
 5.04711802E+00 9.21544305E-03-3.29034831E-06 5.28940397E-10-3.15689858E-  
 14 2  
 6.23718102E+03-7.74395570E-01 5.18534727E+00-6.34085575E-03 4.57171139E-  
 05 3  
 -5.30421813E-08 1.99501601E-11 6.93771506E+03 2.18492659E+00  
 8.51040025E+03 4  
 CH3NO2 T01/00C 1.H 3.N 1.O 2.G 200.000 6000.000 1000.00  
 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 T05/98C 1.H 3.N 1.O 3.G 200.000 6000.000 1000.00  
 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  
 CH3ONO A 5/05C 1.H 3.O 2.N 1.G 200.000 6000.000 1000.00  
 1  
 6.93605239E+00 9.97319424E-03-3.60642537E-06 5.83462161E-10-3.50058729E-  
 14 2  
 -1.08381899E+04-6.98144573E+00 6.15261387E+00-2.91937431E-03 4.14526828E-  
 05 3  
 -4.93954776E-08 1.85608328E-11-9.85260262E+03 8.04057190E-01-  
 7.87057806E+03 4  
 HONO H 1N 1O 2O 3O 300.00 5000.00 1000.00  
 1  
 0.54868900E+01 0.42180600E-02-0.16491400E-05 0.29719000E-09-0.20210000E-  
 13 2  
 -0.11268600E+05-0.29970000E+01 0.22904100E+01 0.14099220E-01-0.13678720E-  
 04 3  
 0.74987800E-08-0.18769100E-11-0.10431900E+05 0.13281000E+02  
 4  
 H2CNO2 RADICAL T08/07C 1.H 2.N 1.O 2.G 200.000 6000.000 1000.00  
 1  
 7.57504807E+00 7.01471036E-03-2.51481162E-06 4.05670550E-10-2.42796598E-  
 14 2  
 1.23880080E+04-1.15985589E+01 2.42742248E+00 1.60496442E-02 2.84727836E-  
 06 3  
 -1.82218429E-08 9.35383557E-12 1.40120587E+04 1.61086425E+01  
 1.54427130E+04 4  
 HNO H 1N 1O 1O 300.00 5000.00 1000.00  
 1  
 0.36151400E+01 0.32124900E-02-0.12603400E-05 0.22673000E-09-0.15360000E-  
 13 2

0.10661900E+05 0.48100000E+01 0.27844000E+01 0.66096500E-02-0.93002200E-  
 05 3  
 0.94379800E-08-0.37531500E-11 0.10918800E+05 0.90360000E+01  
 4  
 H2NO H 2N 10 10 OG 300.00 4000.00 1500.00  
 1  
 0.05673346E+02 0.02298837E-01-0.01774446E-05-0.01103482E-08 0.01859762E-  
 12 2  
 0.05569325E+05-0.06153540E+02 0.02530590E+02 0.08596035E-01-0.05471030E-  
 04 3  
 0.02276249E-07-0.04648073E-11 0.06868030E+05 0.01126651E+03  
 4  
 N2O N 2O 10 00 OG 300.00 5000.00 1000.00  
 1  
 0.47189800E+01 0.28737100E-02-0.11975000E-05 0.22506000E-09-0.15750000E-  
 13 2  
 0.81658000E+04-0.16570000E+01 0.25430600E+01 0.94921900E-02-0.97927800E-  
 05 3  
 0.62638400E-08-0.19018300E-11 0.87651000E+04 0.95110000E+01  
 4  
 C2O 121286C 2O 1 G 0300.00 5000.00 1000.00  
 1  
 0.04849809E+02 0.02947585E-01-0.01090729E-04 0.01792562E-08-0.01115758E-  
 12 2  
 0.03282055E+06-0.06453226E+01 0.03368851E+02 0.08241803E-01-0.08765145E-  
 04 3  
 0.05569262E-07-0.01540009E-10 0.03317081E+06 0.06713314E+02  
 4  
 C5H2 160387C 5H 2 0 OG 300.000 5000.000  
 1403.000 01  
 1.31045263E+01 5.58350349E-03-1.96405048E-06 3.10895694E-10-1.82888034E-  
 14 2  
 7.78647483E+04-4.66963542E+01 2.29340217E+00 3.41864672E-02-3.10646796E-  
 05 3  
 1.37481623E-08-2.37886387E-12 8.12207913E+04 1.00728332E+01  
 4  
 HCCCHCCH 160387C 5H 3 0 OG 300.000 5000.000  
 1399.000 01  
 1.20901052E+01 7.97135686E-03-2.65858204E-06 4.06070219E-10-2.33012143E-  
 14 2  
 6.32468663E+04-3.77214660E+01 3.49152197E+00 3.03630920E-02-2.52539718E-  
 05 3  
 1.08322022E-08-1.86417704E-12 6.59751096E+04 7.59522209E+00  
 4  
 C4H5C2H 0C 6H 6 0 OG 200.000 5000.000 1000.00  
 0 1  
 0.11103525E+02 0.20600685E-01-0.75302224E-05 0.12388695E-08-0.75415976E-  
 13 2  
 0.20361843E+05-0.36665197E+02-0.71813191E+00 0.37934312E-01 0.11398837E-  
 04 3  
 -0.41333503E-07 0.18055927E-10 0.24223825E+05 0.27855714E+02  
 4  
 C4H 121686C 4H 1 G 0300.00 5000.00 1000.00  
 1  
 6.24288178E+00 6.19368255E-03-2.08593156E-06 3.08220338E-10-1.63648256E-  
 14 2  
 7.56801875E+04-7.21080589E+00 5.02324677E+00 7.09237531E-03-6.07376194E-  
 09 3



-2.27575225E-09 8.08699407E-13 7.62381250E+04-6.94259405E-02  
 4  
 H2CCCCCH 160387C 5H 3 0 0G 300.000 5000.000  
 1399.000 01  
 1.20901052E+01 7.97135686E-03-2.65858204E-06 4.06070219E-10-2.33012143E-  
 14 2  
 6.32468663E+04-3.77214660E+01 3.49152197E+00 3.03630920E-02-2.52539718E-  
 05 3  
 1.08322022E-08-1.86417704E-12 6.59751096E+04 7.59522209E+00  
 4  
 O3 L 5/900 3 0 0 0G 200.000 6000.000 1000.  
 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  
 N L 6/88N 1 0 0 0G 200.000 6000.000 1000.  
 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  
 NH ATcT/AN 1.H 1. 0. 0.G 200.000 6000.000 1000.  
 1  
 2.78372644E+00 1.32985888E-03-4.24785573E-07 7.83494442E-11-5.50451310E-  
 15 2  
 4.23461945E+04 5.74084863E+00 3.49295037E+00 3.11795720E-04-1.48906628E-  
 06 3  
 2.48167402E-09-1.03570916E-12 4.21059722E+04 1.84834973E+00  
 4.31525130E+04 4  
 NH2 AMIDOGEN RAD IU3/03N 1.H 2. 0. 0.G 200.000 3000.000 1000.  
 1  
 2.59263049E+00 3.47683597E-03-1.08271624E-06 1.49342558E-10-5.75241187E-  
 15 2  
 2.18865421E+04 7.90565351E+00 4.19198016E+00-2.04602827E-03 6.67756134E-  
 06 3  
 -5.24907235E-09 1.55589948E-12 2.14991387E+04-9.04785244E-02  
 2.27072912E+04 4  
 NH3 Anharmonic RUS 89N 1.H 3. 0. 0.G 200.000 6000.000 1000.  
 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  
 NO3 ATcT/AN 1.O 3. 0. 0.G 200.000 6000.000 1000.  
 1  
 7.48347702E+00 2.57772064E-03-1.00945831E-06 1.72314063E-10-1.07154008E-  
 14 2  
 6.12990474E+03-1.41618136E+01 2.17359330E+00 1.04902685E-02 1.10472669E-  
 05 3  
 -2.81561867E-08 1.36583960E-11 7.81290905E+03 1.46022090E+01  
 8.97563416E+03 4

HNO3 T 8/03H 1.N 1.0 3. 0.G 200.000 6000.000 1000.  
 1  
 8.03098942E+00 4.46958589E-03-1.72459491E-06 2.91556153E-10-1.80102702E-  
 14 2  
 -1.93138183E+04-1.62616537E+01 1.69329154E+00 1.90167702E-02-8.25176697E-  
 06 3  
 -6.06113827E-09 4.65236978E-12-1.74198909E+04 1.71839838E+01-  
 1.61524852E+04 4  
 NNH T 8/11N 2.H 1. 0. 0.G 200.000 6000.000 1000.  
 1  
 3.42744423E+00 3.23295234E-03-1.17296299E-06 1.90508356E-10-1.14491506E-  
 14 2  
 2.87676026E+04 6.39209233E+00 4.25474632E+00-3.45098298E-03 1.37788699E-  
 05 3  
 -1.33263744E-08 4.41023397E-12 2.87932080E+04 3.28551762E+00  
 3.00058572E+04 4  
 N2H2 equil & transT 9/11N 2.H 2. 0. 0.G 200.000 6000.000 1000.  
 1  
 1.31115117E+00 9.00187208E-03-3.14911824E-06 4.81449581E-10-2.71897891E-  
 14 2  
 2.33863341E+04 1.64091067E+01 4.91066031E+00-1.07791880E-02 3.86516489E-  
 05 3  
 -3.86501698E-08 1.34852134E-11 2.28241901E+04 9.10273396E-02  
 2.40806734E+04 4  
 N2H3 Rad. T 7/11N 2.H 3. 0. 0.G 200.000 6000.000 1000.  
 1  
 4.04483566E+00 7.31130186E-03-2.47625799E-06 3.83733021E-10-2.23107573E-  
 14 2  
 2.53241420E+04 2.88423392E+00 3.42125505E+00 1.34901590E-03 2.23459071E-  
 05 3  
 -2.99727732E-08 1.20978970E-11 2.58198956E+04 7.83176309E+00  
 2.70438066E+04 4  
 N2H4 HYDRAZINE L 5/90N 2H 4 0 0G 200.000 6000.000 1000.  
 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  
 C5H11ONO-1 H 11C 50 3N 1G 100.000 5000.000 1173.05  
 1  
 1.44934646E+01 4.49786965E-02-2.00914268E-05 3.93354739E-09-2.84091383E-  
 13 2  
 -1.86443283E+04-3.91359975E+01 1.05024560E+00 9.08188264E-02-7.87078982E-  
 05 3  
 3.72463357E-08-7.38368626E-12-1.54904081E+04 2.78654258E+01  
 4  
 C5H11ONO-2 H 11C 50 3N 1G 100.000 5000.000 1288.39  
 1  
 1.70504920E+01 4.06920770E-02-1.76433639E-05 3.39619401E-09-2.42510695E-  
 13 2  
 -2.11748940E+04-5.47166710E+01 8.36171304E-01 9.10323526E-02-7.62522795E-  
 05 3  
 3.37231810E-08-6.12723488E-12-1.69968605E+04 2.76164989E+01  
 4  
 C5H11ONO-3 H 11C 50 3N 1G 100.000 5000.000 1288.39  
 1

1.70504920E+01 4.06920770E-02-1.76433639E-05 3.39619401E-09-2.42510695E-  
13 2  
-2.11748940E+04-5.47166710E+01 8.36171304E-01 9.10323526E-02-7.62522795E-  
05 3  
3.37231810E-08-6.12723488E-12-1.69968605E+04 2.76164989E+01  
4  
NC3H7NO2 C 3H 7N 1O 2G 0300.00 4000.00 1500.00  
1!Burcat 2000  
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  
IC3H7NO2 C 3H 7N 1O 2G 0300.00 4000.00 1500.00  
1!la misma que para NC3H7NO2  
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  
C2H5NO2 C 2H 5N 1O 2G 0300.00 4000.00 1500.00  
1!Burcat 2000  
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  
PC4H9NO2 C 4H 9N 1O 2G 0300.00 4000.00 1500.00  
1!Burcat 2000  
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  
SC4H9NO2 C 4H 9N 1O 2G 0300.00 4000.00 1500.00  
1!la misma que para PC4H9NO2  
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  
C5H11-1NO2 C 5H 11N 1O 2G 0300.00 4000.00 1500.00  
1!Burcat 2000 (sacados de PFR\_Tol\_NOx, ahí sólo especifica C5H11NO2)  
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  
C5H11-2NO2 C 5H 11N 1O 2G 0300.00 4000.00 1500.00  
1!pongo los mismos que para C5H11-1NO2  
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

C5H11-3NO2 C 5H 11N 1O 2G 0300.00 4000.00 1500.00

!pongo los mismos que para C5H11-1NO2

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

HNO2 equil ATcT T 9/11H 1.N 1.O 2. 0.G 200.000 6000.000 1000.

1

5.79182717E+00 3.65162554E-03-1.29293390E-06 2.06892796E-10-1.23154749E-14 2

-1.15953895E+04-4.05538852E+00 3.21415915E+00 8.12778066E-03 1.65998916E-06 3

-9.52814708E-09 4.87131424E-12-1.07830727E+04 9.82200056E+00-9.46538040E+03 4

END